

SIX-CHARACTER REFERENCE-DATE CODES

Letters	Reference	Numbers
g	Glenn Research Center	Month/year calculated
j	Chase:NIST-JANAF Thermochemical Tables. Chase,1998	Month/year of table
tpis	Gurvich,:Thermodynamic Properties of Individual Substances	Year of volume
n	TRC Thermodynamic Tables, NIST	Month/year of table
bar	Barin:Thermochemical Data of Pure Substances. Barin,1989	Year of volume
coda	CODATA Key Values for Thermodynamics. Cox,1989	Year of volume
srd	Standard Reference Data	Year of JPCRD journal

ORDER OF SPECIES

- 1) Gaseous products/reactants
- 2) Condensed products/reactants
- 3) Gaseous/condensed reactants only (starts with "Air")

thermo

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200.00 1000.00 6000.00 20000. 11/06/01
e- Ref-Species. Chase,1998 3/82.
3 g12/98 E 1.00 0.00 0.00 0.00 0.00 0.000548579903
0.000
298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
6197.428
0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00
0.000000000D+00
0.000000000D+00 0.000000000D+00 -7.453750000D+02-
1.172081224D+01
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
6197.428
0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00
0.000000000D+00
0.000000000D+00 0.000000000D+00 -7.453750000D+02-
1.172081224D+01
6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
6197.428
0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00
0.000000000D+00
0.000000000D+00 0.000000000D+00 -7.453750000D+02-
1.172081224D+01

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Ag                Hf:Cox,1989. Moore,1971. Gordon,1999.
3 g10/97 AG  1.00    0.00    0.00    0.00    0.00 0    107.86820
284900.000
  200.000    1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0
6197.428
  0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00
0.000000000D+00
  0.000000000D+00 0.000000000D+00                                3.352002370D+04
6.562819350D+00
  1000.000    6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0
6197.428
-3.309926370D+05 9.820086420D+02 1.381179917D+00 6.170899990D-04-
1.688114600D-07
  2.008826848D-11-5.627285655D-16                                2.726719171D+04
1.456862733D+01
  6000.000    20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0
6197.428
-3.717441500D+08 2.758069172D+05-7.385982610D+01 9.606158720D-03-
5.393935740D-07
  1.358856730D-11-1.272610104D-16                                -2.107724971D+06
6.628374570D+02
Ag+                Moore,1971. Gordon,1999.
3 g10/97 AG  1.00E  -1.00    0.00    0.00    0.00 0    107.86765
1022093.730
  298.150    1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0
6197.530
  3.691132750D+06-4.316983000D+04 2.028445385D+02-4.658413740D-01
5.586200510D-04
-3.154880975D-07 6.578702060D-11                                3.371574470D+05-
1.142924427D+03
  1000.000    6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0
6197.530
-5.327432350D+07 1.310710631D+05-1.098820208D+02 4.826002760D-02-
1.093661557D-05
  1.263835910D-09-5.852542535D-14                                -7.439122510D+05
8.446266190D+02
  6000.000    20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0
6197.530
-2.119469170D+08 1.159621936D+05-2.220792532D+01 2.938747589D-03-
1.822389545D-07
  5.823925360D-12-7.455184012D-17                                -8.068014150D+05
2.271702823D+02
Ag-                Hotop,1985. Gordon,1999.
3 g10/97 AG  1.00E  1.00    0.00    0.00    0.00 0    107.86875
153078.728
  298.150    1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0
6197.428
  0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00
0.000000000D+00
  0.000000000D+00 0.000000000D+00                                1.766565919D+04
5.869679800D+00
  1000.000    6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0
6197.428
  0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00
0.000000000D+00
  0.000000000D+00 0.000000000D+00                                1.766565919D+04
5.869679800D+00
  6000.000    20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0
6197.428
  0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00
0.000000000D+00

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0.000000000D+00 0.000000000D+00 1.766565919D+04  
 5.869679800D+00  
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 3 g12/97 AL 1.00 0.00 0.00 0.00 0.00 0 26.98154  
 330000.000  
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 2.432362152D-07  
 1.538281506D-10-3.944375734D-14 3.887412680D+04  
 6.086585765D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6918.671  
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 1.529455262D-08  
 -9.971670260D-13 5.053278264D-16 3.823288650D+04  
 6.600920155D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6918.671  
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 1.070103856D-06  
 3.592110900D-11-4.696039394D-16 -2.901050501D+06  
 9.491883160D+02  
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 3 g 1/98 AL 1.00E -1.00 0.00 0.00 0.00 0 26.98099  
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 6197.428  
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 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 1.090644788D+05  
 3.791005780D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 -4.181183250D+03-9.948557270D+00 2.548615878D+00-5.878760040D-05  
 3.132291294D-08  
 -7.748894630D-12 7.274447690D-16 1.091011485D+05  
 3.488667290D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
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 8.932051950D-07  
 2.719381070D-11-3.367986284D-16 -4.268693020D+06  
 1.141245444D+03  
 AL- Chase,1998 p65 6/83. EA:Hotop,1985. Gordon,1999.  
 3 g 3/97 AL 1.00E 1.00 0.00 0.00 0.00 0 26.98209  
 281090.113  
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 6756.213  
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 8.577259640D-06  
 -5.476260000D-09 1.322714061D-12 3.490616980D+04-  
 5.957097700D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
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 2.888305470D-07  
 -3.253240510D-11 1.472436088D-15 4.780306540D+04-  
 1.536906816D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6756.213

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 4.413313240D-09  
 -1.445353715D-13 1.905752608D-18 5.241871250D+04  
 1.451781383D+00  
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 2 tpris96 AL 1.00BR 1.00 0.00 0.00 0.00 0 106.88554  
 14325.015  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
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 2.077304770D-06  
 -1.261267579D-09 3.166335970D-13 1.635024429D+03-  
 2.323594886D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9571.115  
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 1.172854627D-10-7.178742760D-15 -1.217812867D+04  
 2.204450764D+01  
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 140662.125  
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 13397.875  
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 5.516512990D-06  
 -3.340053040D-09 8.368476840D-13 -1.540591306D+04-  
 1.742171366D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13397.875  
 -3.523782900D+05 4.671544170D+02 7.111908190D+00-5.551709200D-04  
 3.166301130D-07  
 -5.521028330D-11 3.176725950D-15 -2.265004078D+04-  
 2.695610360D+00  
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 2 tpris96 AL 1.00BR 3.00 0.00 0.00 0.00 0 266.69354 -  
 410476.664  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17943.336  
 4.718948840D+04-1.053853163D+03 1.350747168D+01-6.639869930D-03  
 7.269276830D-06  
 -4.278049490D-09 1.045573281D-12 -4.699440330D+04-  
 3.667936780D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17943.336  
 -8.935527440D+04-2.678035134D+01 1.002063997D+01-8.458764400D-06  
 1.904243317D-09  
 -2.215195785D-13 1.038219389D-17 -5.249247640D+04-  
 1.579666403D+01  
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 2 tpris96 AL 1.00C 1.00 0.00 0.00 0.00 0 38.99224  
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 1.665566136D-06  
 -7.121649210D-10 1.271188744D-13 8.383436110D+04-  
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 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9058.109

1.937001487D+06-6.749117790D+03 1.347525643D+01-5.850802650D-03  
 1.926461091D-06  
 -2.585922351D-10 1.222659806D-14 1.225363649D+05-  
 6.152244872D+01  
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 2 tps96 AL 1.00C 2.00 0.00 0.00 0.00 0 51.00294  
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 1.524087465D+04-2.649987059D+02 6.280414900D+00-1.786037647D-04  
 3.791907740D-06  
 -3.999450070D-09 1.299752388D-12 8.092763280D+04-  
 6.247291862D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12262.776  
 1.466017895D+05-1.362764489D+03 8.457759150D+00-3.678901680D-04  
 7.903174500D-08  
 -8.880023720D-12 4.053633950D-16 8.705924230D+04-  
 2.127956728D+01  
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 2 tps96 AL 1.00CL 1.00 0.00 0.00 0.00 0 62.43424 -  
 51007.443  
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 9323.112  
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 3.101582418D-06  
 -1.815268376D-09 4.414662340D-13 -5.202736030D+03-  
 7.383305224D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9323.112  
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 7.280541600D-07  
 1.182380673D-10-6.660498130D-15 -2.496164448D+04  
 2.616924759D+01  
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 2 j 6/76 AL 1.00CL 1.00E -1.00 0.00 0.00 0 62.43369  
 861849.307  
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 7.816593580D+00  
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 6.347511330D-07  
 -1.158320344D-10 6.870022460D-15 9.318332700D+04  
 4.047513900D+00  
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 2 tps96 AL 1.00CL 2.00 0.00 0.00 0.00 0 97.88694 -  
 240874.252  
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 12846.859  
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 5.823420560D-06  
 -3.306542450D-09 7.831562100D-13 -2.607627110D+04-  
 2.393365135D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12846.859

4.303453060D+05-1.552370585D+03 8.760657420D+00-9.467450060D-04  
 2.401844880D-07  
 -2.427836709D-11 8.390123470D-16 -2.145884709D+04-  
 1.803642587D+01  
 ALCL3 Gurvich,1996a pt1 p173 pt2 p134.  
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 584678.863  
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 16400.803  
 7.750600970D+04-1.440779717D+03 1.401744141D+01-6.381631240D-03  
 5.871674720D-06  
 -2.908872278D-09 5.994050890D-13 -6.579343180D+04-  
 4.494018811D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16400.803  
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 3.724664660D-09  
 -4.275526780D-13 1.982341329D-17 -7.343407470D+04-  
 2.045131441D+01  
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 264060.446  
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 5.858471280D-06  
 4.388109920D-09-1.256906273D-12 -3.117572862D+04  
 2.032567172D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8892.107  
 -7.111229050D+05 1.903013316D+03 2.191607179D+00 1.421471467D-03-  
 4.179634770D-07  
 6.153804400D-11-2.945403999D-15 -4.540728960D+04  
 1.613163743D+01  
 ALF+ Chase,1998 p92.  
 2 j 6/76 AL 1.00F 1.00E -1.00 0.00 0.00 0 45.97939  
 692233.561  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
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 8.839786990D-06  
 6.343579590D-09-1.645011685D-12 8.370237450D+04  
 6.764015580D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
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 6.041232579D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12133.195

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2.382317949D-08  
4.443785760D-12-5.486977850D-16 -5.100943200D+04-  
1.091165058D+01  
ALFCL2 Gurvich,1996a pt1 p183 pt2 p146.  
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791395.404  
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15738.260  
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3.356822540D-09-1.085329228D-12 -9.162049260D+04-  
3.206065851D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
15738.260  
-1.720360526D+05-1.193340759D+02 1.008894431D+01-3.550993810D-05  
7.830952610D-09  
-8.961734230D-13 4.145330260D-17 -9.804185470D+04-  
2.127047629D+01  
ALF2 Gurvich,1996a pt1 p153 pt2 p117.  
2 tpris96 AL 1.00F 2.00 0.00 0.00 0.00 0 64.97834 -  
631764.175  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
11600.932  
2.994951991D+04-2.194199915D+02 3.416748760D+00 1.272953936D-02-  
1.883312206D-05  
1.330702256D-08-3.680118630D-12 -7.607537650D+04  
8.759626916D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
11600.932  
-2.146896245D+05 3.096840150D+01 6.816399620D+00 1.820129379D-04-  
7.793677440D-08  
1.472534201D-11-8.803695300D-16 -7.884002680D+04-  
7.915370474D+00  
ALF2- Gurvich,1996a pt1 p154 pt2 p118.  
2 tpris96 AL 1.00F 2.00E 1.00 0.00 0.00 0 64.97889 -  
853230.685  
298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
11331.815  
1.233369037D+05-1.348195504D+03 8.611178050D+00 2.245141297D-04-  
2.424673201D-06  
2.214132430D-09-6.602713960D-13 -9.708437460D+04-  
2.192617549D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
11331.815  
-1.590076965D+05-2.060486516D+02 7.155289380D+00-6.260167690D-05  
1.391935746D-08  
-1.603901265D-12 7.461508520D-17 -1.040479429D+05-  
1.122696648D+01  
ALF2CL Gurvich,1996a pt1 p182 pt2 p145.  
2 tpris96 AL 1.00F 2.00CL 1.00 0.00 0.00 0 100.43104 -  
999128.145  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
14827.517  
5.677412090D+04-8.869829470D+02 8.752746550D+00 8.195791200D-03-  
1.380480934D-05  
1.032703706D-08-2.948968416D-12 -1.177936778D+05-  
1.858347808D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
14827.517

-2.115422988D+05-1.959188681D+02 1.014576850D+01-5.813219350D-05  
 1.281071982D-08  
 -1.465366277D-12 6.776002450D-17 -1.227153110D+05-  
 2.359853846D+01  
 ALF3 Gurvich,1996a pt1 p157 pt2 p120.  
 2 tpris96 AL 1.00F 3.00 0.00 0.00 0.00 0 83.97675 -  
 1209276.938  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14043.722  
 4.410263520D+04-5.667495740D+02 5.833072850D+00 1.603535069D-02-  
 2.413263602D-05  
 1.714106160D-08-4.747543200D-12 -1.443349991D+05-  
 5.461613658D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14043.722  
 -2.493972160D+05-2.911202519D+02 1.021662932D+01-8.642985970D-05  
 1.905713108D-08  
 -2.181058411D-12 1.009055287D-16 -1.475694276D+05-  
 2.703983244D+01  
 ALF4- Gurvich,1996a pt1 p159 pt2 p121.  
 2 tpris96 AL 1.00F 4.00E 1.00 0.00 0.00 0 102.97570 -  
 1951600.806  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16786.835  
 2.312010037D+05-3.235376780D+03 2.017865547D+01-9.108193500D-03  
 6.679552630D-06  
 -2.606075106D-09 4.110060510D-13 -2.211784563D+05-  
 8.677268282D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16786.835  
 -3.217411610D+05-2.612097043D+02 1.319792654D+01-8.010135410D-05  
 1.786204421D-08  
 -2.062751964D-12 9.612581770D-17 -2.381577915D+05-  
 4.231634322D+01  
 ALH Gurvich,1996a pt1 p139 pt2 p106.  
 2 tpris96 AL 1.00H 1.00 0.00 0.00 0.00 0 27.98948  
 249250.804  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8668.104  
 -3.759114030D+04 5.089002230D+02 1.128086896D+00 3.988660910D-03-  
 2.150790303D-07  
 -2.176790819D-09 1.020805902D-12 2.644431827D+04  
 1.650021856D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8668.104  
 6.802018430D+06-2.178416933D+04 3.032713047D+01-1.503343597D-02  
 4.492142360D-06  
 -6.178450370D-10 3.115205260D-14 1.658301221D+05-  
 1.876766425D+02  
 ALHCL Gurvich,1996a pt1 p178 pt2 p138.  
 2 tpris96 AL 1.00H 1.00CL 1.00 0.00 0.00 0 63.44218  
 10521.966  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10886.572  
 3.587169760D+04-5.916249990D+02 6.944542380D+00-2.511543148D-03  
 6.471332550D-06  
 -5.642277140D-09 1.715950436D-12 2.750930479D+03-  
 9.903752973D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10886.572



-1.683915330D+05-8.862301790D+02 8.062379400D+00-9.200551470D-04  
 3.949817220D-07  
 -6.401086760D-11 3.578354100D-15 3.641504850D+03-  
 1.800687603D+01  
 ALHCL2 Gurvich,1996a pt1 p179 pt2 p140.  
 2 tpis96 AL 1.00H 1.00CL 2.00 0.00 0.00 0 98.89488 -  
 351278.965  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13676.196  
 1.184828615D+05-2.054157118D+03 1.574696513D+01-1.476257296D-02  
 2.065336978D-05  
 -1.420198850D-08 3.826279860D-12 -3.434277460D+04-  
 5.761184971D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13676.196  
 9.608063940D+04-1.485540161D+03 1.103592709D+01-3.956955200D-04  
 8.465843730D-08  
 -9.483336520D-12 4.319033530D-16 -3.669216390D+04-  
 3.236863081D+01  
 ALHF Gurvich,1996a pt1 p164 pt2 p125.  
 2 tpis96 AL 1.00H 1.00F 1.00 0.00 0.00 0 46.98788 -  
 182614.484  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10572.121  
 -9.289545100D+03 1.335515868D+02 2.772448680D+00 6.751415030D-03-  
 4.133846140D-06  
 5.865704070D-10 2.276158011D-13 -2.384685845D+04  
 1.228752581D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10572.121  
 7.342169250D+05-3.462164130D+03 1.039714588D+01-1.750737965D-03  
 4.615687860D-07  
 -5.390414740D-11 2.340478515D-15 -2.965279722D+03-  
 3.713172313D+01  
 ALHFCL Gurvich,1996a pt1 p184 pt2 p147.  
 2 tpis96 AL 1.00H 1.00F 1.00CL 1.00 0.00 0 82.44058 -  
 555244.524  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12532.636  
 1.290373237D+05-2.142099873D+03 1.485434420D+01-1.140326930D-02  
 1.564521768D-05  
 -1.067574855D-08 2.857255247D-12 -5.818303070D+04-  
 5.483425532D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12532.636  
 4.068987130D+04-1.502129854D+03 1.105214126D+01-4.031587730D-04  
 8.645252220D-08  
 -9.700659520D-12 4.423629510D-16 -6.129888110D+04-  
 3.403564562D+01  
 ALHF2 Gurvich,1996a pt1 p166 pt2 p127.  
 2 tpis96 AL 1.00H 1.00F 2.00 0.00 0.00 0 65.98628 -  
 765299.182  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12299.975  
 1.050181431D+05-1.398654202D+03 9.166334840D+00 3.867286870D-03-  
 4.830841090D-06  
 3.099287181D-09-8.440702990D-13 -8.659048800D+04-  
 2.557299683D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12299.975

-4.419947300D+03-1.612826324D+03 1.113336052D+01-4.351812660D-04  
9.344396160D-08  
-1.049431425D-11 4.788333980D-16 -8.606916190D+04-  
3.676383785D+01  
ALH2 Gurvich,1996a pt1 p142 pt2 p107.  
2 tpris96 AL 1.00H 2.00 0.00 0.00 0.00 0 28.99742  
276774.934  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
10090.834  
1.455182996D+04-2.153768996D+02 5.144370230D+00-3.965222030D-03  
1.340900203D-05  
-1.216744854D-08 3.743107130D-12 3.311037940D+04-  
3.608799711D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
10090.834  
1.432910601D+05-2.365907684D+03 9.085667190D+00-1.308536612D-03  
4.777191360D-07  
-7.324721890D-11 3.997900940D-15 4.485951850D+04-  
3.220814285D+01  
ALH2CL Gurvich,1996a pt1 p179 pt2 p139.  
2 tpris96 AL 1.00H 2.00CL 1.00 0.00 0.00 0 64.45012 -  
106345.406  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
11253.251  
9.303828980D+04-1.328188016D+03 9.424763590D+00-3.277660590D-03  
1.004231609D-05  
-8.948123090D-09 2.708031665D-12 -7.647437930D+03-  
2.682512913D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
11253.251  
3.166929930D+05-3.094037914D+03 1.215872020D+01-8.248269590D-04  
1.765027123D-07  
-1.977372723D-11 9.006176280D-16 2.411845642D+03-  
4.718391553D+01  
ALH2F Gurvich,1996a pt1 p165 pt2 p126.  
2 tpris96 AL 1.00H 2.00F 1.00 0.00 0.00 0 47.99582 -  
316655.854  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
10764.801  
8.906039290D+04-9.750803930D+02 5.870772320D+00 6.896663690D-03-  
4.045817280D-06  
7.219318660D-10 7.329846740D-14 -3.425302600D+04-  
9.387539141D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
10764.801  
2.711514962D+05-3.169623480D+03 1.221401118D+01-8.465600260D-04  
1.812341995D-07  
-2.030947985D-11 9.251825820D-16 -2.259217746D+04-  
4.941337333D+01  
ALH3 Gurvich,1996a pt1 p145 pt2 p109.  
2 tpris96 AL 1.00H 3.00 0.00 0.00 0.00 0 30.00536  
128896.080  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
10410.580  
1.481207909D+04-2.836495340D+01 2.507597126D+00 7.315920510D-03  
2.331766687D-06  
-6.389209890D-09 2.456885069D-12 1.463189428D+04  
8.313187700D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
10410.580

5.885458550D+05-4.595785660D+03 1.320893344D+01-1.226849004D-03  
2.626580824D-07  
-2.943725869D-11 1.341177648D-15 3.991716950D+04-  
6.181829295D+01

ALI Gurvich,1996a pt1 p191 pt2 p153.

2 tpris96 AL 1.00I 1.00 0.00 0.00 0.00 0 153.88601  
67395.017

200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
9751.117

1.870854131D+03-1.543184003D+02 5.074391880D+00-1.120584830D-03  
1.386302156D-06

-8.540782280D-10 2.180358492D-13 7.517443690D+03  
6.688267622D-01

1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
9751.117

4.752817920D+05-1.198028588D+03 5.433685360D+00-1.004479306D-04-  
1.005928846D-07

4.568173190D-11-3.960201360D-15 1.464627816D+04-  
3.141199746D+00

ALI2 Gurvich,1996a pt1 p193 pt2 p154.

2 tpris96 AL 1.00I 2.00 0.00 0.00 0.00 0 280.79048 -  
33812.954

200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
13923.046

1.423413595D+04-4.646575690D+02 8.722674910D+00-3.560519290D-03  
4.188682290D-06

-2.616026962D-09 6.720195510D-13 -3.846133330D+03-  
1.073076578D+01

1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
13923.046

-3.35599020D+05 4.743347940D+02 7.106501390D+00-5.529965340D-04  
3.161480314D-07

-5.515489160D-11 3.174155820D-15 -9.785488850D+03-  
5.602275944D-01

ALI3 Gurvich,1996a pt1 p195 pt2 p156.

2 tpris96 AL 1.00I 3.00 0.00 0.00 0.00 0 407.69495 -  
191330.433

200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
19003.567

2.706032439D+04-7.559936810D+02 1.271396349D+01-5.466884090D-03  
6.297618920D-06

-3.864209610D-09 9.774132440D-13 -2.220966921D+04-  
2.847883861D+01

1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
19003.567

-6.357427470D+04-1.578772280D+01 1.001249733D+01-5.228673120D-06  
1.196173520D-09

-1.409194490D-13 6.671276390D-18 -2.611455525D+04-  
1.247999813D+01

ALN Gurvich,1996a pt1 p204 pt2 p164.

2 tpris96 AL 1.00N 1.00 0.00 0.00 0.00 0 40.98828  
438829.011

200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
9265.111

2.716645079D+04-2.543491110D+02 3.538987720D+00 5.296256160D-03-  
9.845700610D-06

8.452209040D-09-2.592304568D-12 5.309994910D+04  
5.399436684D+00

1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
9265.111

3.821214220D+06-1.067776595D+04 1.449174222D+01-3.727227130D-03  
7.922770960D-07  
-8.086892210D-11 2.893539736D-15 1.205236340D+05-  
7.288584973D+01

ALO Gurvich,1996a pt1 p122 pt2 p96.

3 tpi96 AL 1.000 1.00 0.00 0.00 0.00 0 42.98094  
67319.006

200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
8788.106

-7.683391100D+03 2.957969549D+02 4.808108440D-01 1.169224855D-02-  
1.595428871D-05

1.060766814D-08-2.647888708D-12 5.843672170D+03  
2.160997839D+01

1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
8788.106

1.565721161D+04 3.855741010D+03-5.926079780D+00 9.050960420D-03-  
2.930661549D-06

4.238529070D-10-2.280655341D-14 -1.331694655D+04  
6.830663436D+01

6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
8788.106

4.165661210D+07-3.768608760D+04 1.547867956D+01-9.568730340D-04  
2.493109541D-08

6.688940290D-14-8.998673700D-18 2.957786517D+05-  
9.427715804D+01

ALO+ Chase,1998 p133.

2 j12/79 AL 1.000 1.00E -1.00 0.00 0.00 0 42.98039  
992993.000

298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
9089.716

2.829178513D+04-4.179087100D+02 5.313299870D+00-1.410883046D-03  
2.526524021D-06

-2.005474816D-09 5.762553550D-13 1.203648109D+05-  
3.410565930D+00

1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
9089.716

2.710846446D+04-6.998653420D+02 5.787815840D+00-6.871895460D-04  
2.075047303D-07

-2.655281004D-11 1.283129660D-15 1.218682226D+05-  
7.051035880D+00

ALO- Gurvich,1996a pt1 p125 pt2 p98.

2 g11/97 AL 1.000 1.00E 1.00 0.00 0.00 0 42.98149 -  
272921.782

298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
8744.718

2.078075267D+04 2.859351226D+00 1.901912370D+00 7.301045660D-03-  
9.139769870D-06

5.652983190D-09-1.396787103D-12 -3.359267730D+04  
1.296339858D+01

1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
8744.718

-6.971948290D+04-2.320553036D+02 4.672784330D+00-4.266447040D-05  
1.632506336D-08

-1.727134051D-12 8.136840640D-17 -3.307718930D+04-  
2.155922595D+00

ALOCL Gurvich,1996a pt1 p176 pt2 p136.

2 tpi96 AL 1.000 1.00CL 1.00 0.00 0.00 0 78.43364 -  
301564.570

200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
11906.037

-5.144627790D+03-5.886297070D+01 4.452316930D+00 9.288235090D-03-  
 1.246894823D-05  
 8.178073540D-09-2.130739934D-12 -3.759683650D+04  
 2.476857081D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11906.037  
 -1.258027706D+05-2.420565961D+02 7.681130020D+00-7.268741700D-05  
 1.611337534D-08  
 1.852889749D-12 8.607278220D-17 -3.754326050D+04-  
 1.475818894D+01  
 ALOCL2 Gurvich,1996a pt1 p178 pt2 p137.  
 2 tps96 AL 1.000 1.00CL 2.00 0.00 0.00 0 113.88634 -  
 402308.669  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15752.494  
 6.902637130D+04-1.189297500D+03 1.161842739D+01 2.818279805D-04-  
 3.145010615D-06  
 3.168380650D-09-1.032375462D-12 -4.483323070D+04-  
 3.165475922D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15752.494  
 -1.707713922D+05-1.180013804D+02 1.008798517D+01-3.513858040D-05  
 7.751187030D-09  
 -8.872470600D-13 4.104815440D-17 -5.124944140D+04-  
 2.059253750D+01  
 ALOF Gurvich,1996a pt1 p163 pt2 p123.  
 2 tps96 AL 1.000 1.00F 1.00 0.00 0.00 0 61.97934 -  
 572289.603  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11003.003  
 7.030578360D+03-1.154575430D+02 3.378823590D+00 1.283929158D-02-  
 1.749748388D-05  
 1.162605473D-08-3.064218613D-12 -6.959381700D+04  
 5.994804586D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11003.003  
 -1.641020297D+05-3.277770290D+02 7.744519740D+00-9.788649440D-05  
 2.165743208D-08  
 -2.486541919D-12 1.153633944D-16 -6.974085090D+04-  
 1.717253748D+01  
 ALOF2 Gurvich,1996a pt1 p164 pt2 p124.  
 2 tps96 AL 1.000 1.00F 2.00 0.00 0.00 0 80.97774 -  
 773649.771  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14055.387  
 4.756085290D+04-6.124318360D+02 6.050223660D+00 1.559291479D-02-  
 2.366136797D-05  
 1.688366194D-08-4.690583100D-12 -9.171827490D+04-  
 4.956258224D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14055.387  
 -2.496681413D+05-2.837821503D+02 1.021108125D+01-8.418303430D-05  
 1.855520828D-08  
 -2.122974022D-12 9.819319100D-17 -9.521804190D+04-  
 2.522534812D+01  
 ALOF2- Chase,1998 p98 6/76.  
 2 g 2/01 AL 1.000 1.00F 2.00E 1.00 0.00 0 80.97829 -  
 972289.619  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14076.981

1.540605112D+05-1.928054597D+03 1.255806423D+01-4.904035370D-04-  
 2.341783347D-06  
 2.415138600D-09-7.471809250D-13 -1.091430174D+05-  
 4.265821750D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14076.981  
 -2.389881459D+05-2.880143725D+02 1.021700240D+01-8.747062000D-05  
 1.944846334D-08  
 -2.241045051D-12 1.042591053D-16 -1.190576566D+05-  
 2.600779629D+01  
 ALOH Gurvich,1996a pt1 p145 pt2 p110.  
 2 tpris96 AL 1.000 1.00H 1.00 0.00 0.00 0 43.98888 -  
 192762.171  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10351.931  
 5.876493180D+04-9.449422690D+02 7.820599180D+00 5.858888470D-04-  
 4.083666810D-06  
 4.587229340D-09-1.563936726D-12 -1.993283011D+04-  
 2.065043885D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10351.931  
 7.882068110D+05-2.263671626D+03 7.823954880D+00 1.821171456D-04-  
 8.263729320D-08  
 1.265414876D-11-6.875972530D-16 -1.039808093D+04-  
 2.209032458D+01  
 ALOHCL Gurvich,1996a pt1 p180 pt2 p141.  
 2 tpris96 AL 1.000 1.00H 1.00CL 1.00 0.00 0 79.44158 -  
 373785.740  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13918.918  
 1.636360341D+04-1.915959416D+02 4.711170470D+00 1.388068475D-02-  
 1.999018454D-05  
 1.439647350D-08-4.033330450D-12 -4.568083720D+04  
 4.644201841D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13918.918  
 7.967115510D+05-2.843470502D+03 1.095559970D+01-1.099328162D-04-  
 1.344506283D-08  
 4.415893770D-12-2.973546112D-16 -2.969861461D+04-  
 3.296114562D+01  
 ALOHCL2 Gurvich,1996a pt1 p181 pt2 p143.  
 2 tpris96 AL 1.000 1.00H 1.00CL 2.00 0.00 0 114.89428 -  
 725145.408  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17149.806  
 3.971929860D+04-7.751554960D+02 9.494051530D+00 1.074401359D-02-  
 1.676464791D-05  
 1.259706368D-08-3.613177980D-12 -8.584796930D+04-  
 1.993482425D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17149.806  
 7.385929760D+05-2.863204228D+03 1.397062327D+01-1.160311527D-04-  
 1.208248796D-08  
 4.258327630D-12-2.900049181D-16 -7.293048000D+04-  
 4.681835640D+01  
 ALOHF Gurvich,1996a pt1 p166 pt2 p128.  
 2 tpris96 AL 1.000 1.00H 1.00F 1.00 0.00 0 62.98728 -  
 574211.575  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13315.081

-1.556003336D+03 2.886581999D+02 7.703793290D-01 2.450406329D-02-  
 3.417811010D-05  
 2.388932902D-08-6.570480510D-12 -7.177222560D+04  
 2.453071801D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13315.081  
 7.557113130D+05-2.936702803D+03 1.102455104D+01-1.373078030D-04-  
 7.432816160D-09  
 3.729981220D-12-2.657027781D-16 -5.340130900D+04-  
 3.527397302D+01  
 ALOHF2 Gurvich,1996a pt1 p168 pt2 p130.  
 2 tpris96 AL 1.000 1.00H 1.00F 2.00 0.00 0 81.98568 -  
 1141510.711  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15428.498  
 1.738263538D+04-1.307687299D+02 3.312381920D+00 2.784734099D-02-  
 3.982363210D-05  
 2.809344456D-08-7.764574200D-12 -1.384133568D+05  
 1.004739945D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15428.498  
 6.530119920D+05-3.034017232D+03 1.409719788D+01-1.663681799D-04-  
 1.011564183D-09  
 2.993805003D-12-2.315956955D-16 -1.223052213D+05-  
 5.151210690D+01  
 ALO2 Gurvich,1996a pt1 p126 pt2 p99.  
 2 tpris96 AL 1.000 2.00 0.00 0.00 0.00 0 58.98034 -  
 38657.871  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13361.629  
 4.338480450D+04-4.735292260D+02 6.001717670D+00 7.094420880D-03-  
 1.129107996D-05  
 8.252691680D-09-2.327652976D-12 -3.826145800D+03-  
 4.830022480D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13361.629  
 1.187216642D+05-8.335625400D+02 8.309301190D+00-3.538667220D-04  
 5.967069460D-08  
 4.014897700D-14-3.515702520D-16 -2.033107586D+03-  
 1.715063884D+01  
 ALO2- Gurvich,1996a pt1 p128 pt2 p100.  
 2 tpris96 AL 1.000 2.00E 1.00 0.00 0.00 0 58.98089 -  
 452572.223  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10644.677  
 1.178678641D+05-1.507186304D+03 9.524749750D+00-5.207989020D-04-  
 1.586902345D-06  
 1.700455028D-09-5.301419770D-13 -4.825469270D+04-  
 3.081215859D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10644.677  
 -1.872410758D+05-2.338853263D+02 7.676070020D+00-7.093570300D-05  
 1.576717569D-08  
 -1.816494162D-12 8.449707960D-17 -5.594640560D+04-  
 1.773751567D+01  
 AL(OH)2 Gurvich,1996a pt1 p149 pt2 p113.  
 2 tpris96 AL 1.000 2.00H 2.00 0.00 0.00 0 60.99622 -  
 507660.670  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14027.535

4.397316910D+03 1.327680339D+02 1.093947024D+00 3.054059173D-02-  
 4.375943350D-05  
 3.174617430D-08-9.004259400D-12 -6.315437390D+04  
 2.101977655D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14027.535  
 1.669643735D+06-5.924738280D+03 1.549480264D+01-5.383488080D-04  
 5.413044530D-08  
 -1.196022328D-12-1.082001733D-16 -2.697525061D+04-  
 6.617911543D+01  
 AL(OH)2CL Gurvich,1996a pt1 p181 pt2 p142.  
 2 tpis96 AL 1.000 2.00H 2.00CL 1.00 0.00 0 96.44892 -  
 859056.724  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17222.037  
 2.477879709D+04-4.454577210D+02 5.928470200D+00 2.730162734D-02-  
 4.041405370D-05  
 2.974210410D-08-8.477150600D-12 -1.033778030D+05-  
 3.679945445D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17222.037  
 1.603911487D+06-5.767232240D+03 1.817772266D+01-3.691816150D-04  
 1.137918702D-08  
 4.083079400D-12-3.641323430D-16 -7.118699850D+04-  
 7.757542241D+01  
 AL(OH)2F Gurvich,1996a pt1 p167 pt2 p129.  
 2 tpis96 AL 1.000 2.00H 2.00F 1.00 0.00 0 79.99462 -  
 1069628.708  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16472.051  
 2.132812662D+04-1.932900224D+02 3.069174664D+00 3.555017330D-02-  
 5.181158330D-05  
 3.753520280D-08-1.059220701D-11 -1.295797992D+05  
 1.001897011D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16472.051  
 1.559238236D+06-5.841273030D+03 1.823229919D+01-3.907805420D-04  
 1.610928938D-08  
 3.544784060D-12-3.393453880D-16 -9.623100890D+04-  
 7.971351802D+01  
 AL(OH)3 Gurvich,1996a pt1 p150 pt2 p115.  
 2 tpis96 AL 1.000 3.00H 3.00 0.00 0.00 0 78.00356 -  
 1012667.542  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17594.767  
 -1.402475452D+04 3.696073460D+02-2.979600650D-01 4.929859350D-02-  
 6.981572280D-05  
 5.014801700D-08-1.412480165D-11 -1.255260760D+05  
 2.711490074D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17594.767  
 2.477063616D+06-8.968617250D+03 2.280320998D+01-8.320292250D-04  
 8.663494430D-08  
 -2.420287082D-12-1.331746442D-16 -7.015278640D+04-  
 1.121899198D+02  
 ALS Gurvich,1996a pt1 p197 pt2 p158.  
 2 tpis96 AL 1.00S 1.00 0.00 0.00 0.00 0 59.04754  
 232682.009  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9088.109



2.611742801D+04-3.470673890D+02 4.436204590D+00 3.340168210D-03-  
 8.410199670D-06  
 8.508185110D-09-2.780868507D-12 2.863779062D+04  
 7.522959526D-01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9088.109  
 8.909844290D+06-2.507677454D+04 2.893456134D+01-9.839766820D-03  
 2.045319809D-06  
 -2.087970890D-10 8.152792520D-15 1.885761615D+05-  
 1.786036203D+02  
 ALS2 Gurvich,1996a pt1 p198 pt2 p159.  
 2 tpris96 AL 1.00S 2.00 0.00 0.00 0.00 0 91.11354  
 248535.279  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14428.779  
 4.252335410D+04-7.764603300D+02 9.801068960D+00-3.910680090D-03  
 3.875695970D-06  
 -2.082025593D-09 4.682935890D-13 3.167961540D+04-  
 2.178094603D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14428.779  
 -6.852563540D+04-2.671667739D+01 7.520193860D+00-8.148565100D-06  
 1.811865152D-09  
 -2.086958125D-13 9.703246380D-18 2.758362737D+04-  
 7.873457337D+00  
 AL2 Gurvich,1996a pt1 p118 pt2 p95.  
 2 tpris96 AL 2.00 0.00 0.00 0.00 0.00 0 53.96308  
 501301.722  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10139.122  
 -5.281509650D+03-1.727374523D+01 4.604077010D+00-2.616467770D-04  
 6.302319970D-07  
 -3.290938590D-10 8.888365140D-14 5.900706390D+04  
 3.060188921D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10139.122  
 -2.320724102D+06 9.218707890D+03-9.446951870D+00 9.999920010D-03-  
 3.154798085D-06  
 4.361544810D-10-2.241157240D-14 2.904589544D+03  
 9.960320745D+01  
 AL2Br6 Gurvich,1996a pt1 p190 pt2 p152.  
 2 tpris96 AL 2.00BR 6.00 0.00 0.00 0.00 0 533.38708 -  
 942422.811  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 38217.189  
 6.483319700D+04-1.947687811D+03 2.886989822D+01-1.365825785D-02  
 1.557883731D-05  
 -9.486942000D-09 2.385519396D-12 -1.101526833D+05-  
 1.025934782D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 38217.189  
 -1.731829490D+05-4.342299780D+01 2.203414210D+01-1.421187503D-05  
 3.238631340D-09  
 -3.803879760D-13 1.796525455D-17 -1.202338355D+05-  
 6.201054950D+01  
 AL2C2 Gurvich,1996a pt1 p206 pt2 p167.  
 2 tpris96 AL 2.00C 2.00 0.00 0.00 0.00 0 77.98448  
 544978.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16165.001

1.110987147D+04-3.502434230D+02 8.598856000D+00 1.832528671D-03  
 1.035743392D-06  
 -2.091649890D-09 7.716068700D-13 6.492764190D+04-  
 1.645080239D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16165.001  
 1.597651967D+05-1.644007203D+03 1.164643675D+01-4.379215430D-04  
 9.369640110D-08  
 -1.049615854D-11 4.780468930D-16 7.204889810D+04-  
 3.648164252D+01  
 AL2CL6 Gurvich,1996a pt1 p175 pt2 p135.  
 2 tpris96 AL 2.00CL 6.00 0.00 0.00 0.00 0 266.67928 -  
 1296876.242  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 34147.090  
 1.340935279D+05-3.001037953D+03 3.143000879D+01-1.700408496D-02  
 1.786540089D-05  
 -1.015419943D-08 2.409630451D-12 -1.471830046D+05-  
 1.274445425D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 34147.090  
 -2.752975554D+05-9.248235970D+01 2.207058224D+01-2.870537915D-05  
 6.423325690D-09  
 -7.436585200D-13 3.472064670D-17 -1.629157014D+05-  
 7.091603141D+01  
 AL2F6 Gurvich,1996a pt1 p160 pt2 p122.  
 2 tpris96 AL 2.00F 6.00 0.00 0.00 0.00 0 167.95350 -  
 2632491.231  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 26064.089  
 1.915061289D+05-3.168240250D+03 2.245374802D+01 1.271532036D-02-  
 2.488697302D-05  
 1.955252096D-08-5.712084890D-12 -3.049962550D+05-  
 9.396473101D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 26064.089  
 -5.852982610D+05-5.450571990D+02 2.240686320D+01-1.627323704D-04  
 3.595225040D-08  
 -4.121201440D-12 1.909095384D-16 -3.219683910D+05-  
 8.589867941D+01  
 AL2I6 Gurvich,1996a pt1 p196 pt2 p157.  
 2 tpris96 AL 2.00I 6.00 0.00 0.00 0.00 0 815.38990 -  
 487747.035  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 40920.966  
 2.587571514D+04-1.280719742D+03 2.677715820D+01-9.913018470D-03  
 1.168760413D-05  
 -7.303918530D-09 1.874532749D-12 -5.891105550D+04-  
 8.330209321D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 40920.966  
 -1.210112399D+05-2.467542774D+01 2.201992650D+01-8.462022590D-06  
 1.957831901D-09  
 -2.326573151D-13 1.108910373D-17 -6.548523750D+04-  
 5.528536481D+01  
 AL2O Gurvich,1996a pt1 p129 pt2 p101.  
 2 tpris96 AL 2.00O 1.00 0.00 0.00 0.00 0 69.96248 -  
 148611.286  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12776.514

7.776530700D+03-1.294235361D+02 4.912509520D+00 8.604223450D-03-  
 1.217703648D-05  
 8.314634870D-09-2.237722201D-12 -1.886512879D+04-  
 2.806368311D-02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12776.514  
 -1.171074351D+05-1.783009166D+02 7.633215360D+00-5.335931770D-05  
 1.180702791D-08  
 -1.355444579D-12 6.287323890D-17 -1.947580149D+04-  
 1.415764167D+01  
 AL20+ Chase,1998 p151 12/79.  
 2 g 1/01 AL 2.000 1.00E -1.00 0.00 0.00 0 69.96193  
 648970.248  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12981.148  
 6.828925720D+04-9.098504170D+02 8.896563010D+00-7.772554380D-04-  
 4.034655620D-07  
 6.977315050D-10-2.417262484D-13 8.085007550D+04-  
 2.176216731D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12981.148  
 -1.102225105D+05-1.214571732D+02 7.591595950D+00-3.694539160D-05  
 8.218520320D-09  
 -9.473649720D-13 4.408621350D-17 7.614943580D+04-  
 1.282233856D+01  
 AL202 Gurvich,1996a pt1 p131 pt2 p102.  
 2 tpi96 AL 2.000 2.00 0.00 0.00 0.00 0 85.96188 -  
 403095.587  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15842.613  
 -1.940560042D+04 2.508489836D+02 3.621403790D+00 1.951385302D-02-  
 2.560329071D-05  
 1.662721576D-08-4.312396200D-12 -5.172697280D+04  
 9.923995945D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15842.613  
 -1.940611656D+05-4.609752430D+02 1.084375637D+01-1.376042893D-04  
 3.044733119D-08  
 -3.496193920D-12 1.622305079D-16 -4.963055780D+04-  
 2.946538090D+01  
 AL202+ Chase,1998 p153 12/79.  
 2 g 2/01 AL 2.000 2.00E -1.00 0.00 0.00 0 85.96133  
 557438.835  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14975.135  
 8.292034990D+04-1.757427015D+03 1.525328567D+01-8.983131330D-03  
 8.953954500D-06  
 -4.840586200D-09 1.096696856D-12 7.311677140D+04-  
 5.517092550D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14975.135  
 -1.652005184D+05-6.021606970D+01 1.004626917D+01-1.892194088D-05  
 4.253301200D-09  
 -4.942390420D-13 2.314507373D-17 6.386219000D+04-  
 2.345753361D+01  
 AL203 Gurvich,1996a pt1 p137 pt2 p105.  
 2 tpi96 AL 2.000 3.00 0.00 0.00 0.00 0 101.96128 -  
 546890.530  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19598.070

-7.443374320D+03 8.829004210D+01 5.264662640D+00 2.507678848D-02-  
 3.434541650D-05  
 2.302516980D-08-6.122529280D-12 -6.872685950D+04  
 2.202324298D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19598.070  
 -2.777784969D+05-4.917465930D+02 1.386703888D+01-1.469381940D-04  
 3.250406490D-08  
 -3.730867350D-12 1.730444284D-16 -6.790757850D+04-  
 4.375559873D+01  
 AL2S Gurvich,1996a pt1 p199 pt2 p160.  
 2 tpris96 AL 2.00S 1.00 0.00 0.00 0.00 0 86.02908  
 220679.131  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14003.931  
 4.094624370D+04-7.797172470D+02 9.814423100D+00-3.940339820D-03  
 3.912465430D-06  
 -2.105891677D-09 4.746001080D-13 2.833963305D+04-  
 2.465065808D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14003.931  
 -7.043437370D+04-2.676376869D+01 7.520233820D+00-8.166123060D-06  
 1.816026040D-09  
 -2.091989298D-13 9.727537700D-18 2.422718377D+04-  
 1.066579238D+01  
 AL2S2 Gurvich,1996a pt1 p200 pt2 p161.  
 2 tpris96 AL 2.00S 2.00 0.00 0.00 0.00 0 118.09508  
 135287.321  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18099.521  
 6.614587320D+04-1.111319537D+03 1.257007304D+01-1.456053256D-03-  
 5.851627110D-07  
 1.390055053D-09-5.496468200D-13 1.914456895D+04-  
 3.600274552D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18099.521  
 -1.377806456D+05-7.705032500D+01 1.055723566D+01-2.277554487D-05  
 5.007682850D-09  
 -5.715862120D-13 2.637999240D-17 1.313336091D+04-  
 2.256849054D+01  
 Ar Ref-Elm. Moore,1971. Gordon,1999.  
 3 g 3/98 AR 1.00 0.00 0.00 0.00 0.00 0 39.94800  
 0.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -7.453750000D+02  
 4.379674910D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 2.010538475D+01-5.992661070D-02 2.500069401D+00-3.992141160D-08  
 1.205272140D-11  
 -1.819015576D-15 1.078576636D-19 -7.449939610D+02  
 4.379180110D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 -9.951265080D+08 6.458887260D+05-1.675894697D+02 2.319933363D-02-  
 1.721080911D-06  
 6.531938460D-11-9.740147729D-16 -5.078300340D+06  
 1.465298484D+03

Ar+ Moore,1971. IP:Moore,1970a. Gordon,1999.

3 g 1/99 AR 1.00E -1.00 0.00 0.00 0.00 0 39.94745  
1526778.407  
298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6205.988  
-5.731209170D+04 7.930791470D+02-1.717121217D+00 1.044184018D-02-  
1.180207501D-05  
6.528134780D-09-1.447558130D-12 1.790572230D+05  
2.949150950D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6205.988  
-3.835965400D+05 8.162019700D+02 2.301342628D+00-4.952983770D-06  
1.205108477D-08  
-2.185050286D-12 1.265493898D-16 1.771811455D+05  
7.947507480D+00  
6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6205.988  
1.006884827D+07-6.624361280D+03 4.446908200D+00-3.017567664D-04  
2.612882069D-08  
-1.201637769D-12 2.299206903D-17 2.349504137D+05-  
1.032262257D+01

B Martin,1998. Odintzova,1979. Gordon,1999.

3 g 9/98 B 1.00 0.00 0.00 0.00 0.00 0 10.81100  
575598.760  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6316.060  
1.182394638D+02-7.009916910D-02 2.500236159D+00-4.584213700D-07  
5.123185830D-10  
-3.057217674D-13 7.533815325D-17 6.848359080D+04  
4.209501920D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6316.060  
-1.072659610D+05 3.225307160D+02 2.126407232D+00 2.106579339D-04-  
5.937129160D-08  
7.377427990D-12-2.282443381D-16 6.643413100D+04  
6.877069670D+00  
6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6316.060  
-4.150001310D+08 2.329576796D+05-4.720913710D+01 4.877655960D-03-  
2.069413791D-07  
3.233519090D-12-1.824076527D-18 -1.802904743D+06  
4.439617640D+02

B+ Moore,1971. IP:Moore,1970a. Gordon,1999.

3 g 9/98 B 1.00E -1.00 0.00 0.00 0.00 0 10.81045  
1382315.528  
298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428  
7.849791190D-02-8.947480950D-04 2.500004085D+00-9.577271230D-09  
1.218136411D-11  
-7.986752520D-15 2.113769829D-18 1.655080260D+05  
2.419053631D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428  
-8.911548030D+03 4.587790090D+00 2.531500086D+00-4.903949100D-05  
2.853326582D-08  
-7.382175910D-12 7.120721560D-16 1.654526303D+05  
2.238669780D+00  
6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428  
-7.977322890D+08 4.734044940D+05-1.055286044D+02 1.170310076D-02-  
6.075531110D-07

1.484174716D-11-1.328323987D-16 -3.609116960D+06  
9.497399750D+02  
B- Hotop,1985. Gordon,1999.  
3 g 9/98 B 1.00E 1.00 0.00 0.00 0.00 0 10.81155  
542631.498  
298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6272.598  
2.201568105D+01-4.740468880D-03 2.500014238D+00-2.497056599D-08  
2.556360708D-11  
-1.415274780D-14 3.271770710D-18 6.451791880D+04  
4.616367290D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6272.598  
2.118018248D+01 2.070697496D-04 2.499999729D+00 1.456693631D-10-  
3.888571760D-14  
5.090598630D-18-2.601566168D-22 6.451789140D+04  
4.616455830D+00  
6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6272.598  
-1.311386485D+02 9.028908800D-02 2.499978572D+00 2.606391052D-09-  
1.716068068D-13  
5.810865540D-18-7.925029090D-23 6.451717400D+04  
4.616640300D+00  
BBr Gurvich,1996a pt1 p91 pt2 p70.  
2 g 9/98 B 1.00BR 1.00 0.00 0.00 0.00 0 90.71500  
240952.358  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
8997.058  
3.796093500D+04-4.976096020D+02 5.267008200D+00-3.742840190D-05-  
1.131544370D-06  
1.261945702D-09-4.288811880D-13 3.038125367D+04-  
4.353407330D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
8997.058  
2.536858027D+05-6.405909500D+02 4.666823470D+00 4.175486390D-04-  
2.963714868D-07  
7.519119540D-11-4.835368320D-15 3.189084340D+04-  
8.255870910D-01  
BBr2 Gurvich,1996a pt1 p92 pt2 p71.  
2 g 9/98 B 1.00BR 2.00 0.00 0.00 0.00 0 170.61900  
97828.617  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
12200.717  
6.516550710D+04-9.029590760D+02 8.063817800D+00 1.129849010D-03-  
4.195482390D-06  
3.965658770D-09-1.283029835D-12 1.470466408D+04-  
1.336453164D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
12200.717  
-4.191633370D+05 4.157688470D+02 7.148169830D+00-5.689590750D-04  
3.195441770D-07  
-5.553176990D-11 3.191136760D-15 6.118982050D+03-  
5.502759620D+00  
BBr3 Gurvich,1996a pt1 p93 pt2 p72.  
2 tpis96 B 1.00BR 3.00 0.00 0.00 0.00 0 250.52300 -  
205300.000  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
15702.797  
3.968073690D+04-6.331087160D+02 8.054551570D+00 9.777571300D-03-  
1.614866025D-05

1.216119883D-08-3.516539610D-12 -2.366723308D+04-  
 1.106099390D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15702.797  
 -1.901046795D+05-1.503627687D+02 1.010999896D+01-4.323095110D-05  
 9.409696190D-09  
 -1.065218470D-12 4.883048770D-17 -2.742553062D+04-  
 1.997496003D+01  
 BC Gurvich,1996a pt1 p108 pt2 p86.  
 2 g 9/98 B 1.00C 1.00 0.00 0.00 0.00 0 22.82170  
 838161.905  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8735.105  
 -3.915758000D+04 7.284538060D+02-1.552743361D+00 1.552898673D-02-  
 1.976857863D-05  
 1.272066405D-08-3.229982780D-12 9.644913680D+04  
 3.248204466D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8735.105  
 -2.346280674D+06 6.450751300D+03-2.619532384D+00 3.339160500D-03-  
 4.508022140D-07  
 1.351919576D-11 8.265104270D-16 5.786685070D+04  
 5.037884876D+01  
 BC2 Gurvich,1996a pt1 p109 pt2 p87.  
 2 g 9/98 B 1.00C 2.00 0.00 0.00 0.00 0 34.83240  
 801258.725  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11687.825  
 -2.987422175D+04 3.643126580D+02 2.963469415D+00 6.561750150D-03-  
 3.539767240D-06  
 1.927356029D-10 3.118724866D-13 9.304835730D+04  
 1.083424193D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11687.825  
 1.525485889D+06-5.987862380D+03 1.408384855D+01-3.747499800D-03  
 1.081927223D-06  
 -1.378744645D-10 6.473822000D-15 1.311204013D+05-  
 6.337215498D+01  
 BCL Gurvich,1996a pt1 p73 pt2 p51.  
 2 g 9/98 B 1.00CL 1.00 0.00 0.00 0.00 0 46.26370  
 183173.437  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8861.337  
 2.202458989D+04-1.700511155D+02 3.066075869D+00 5.595070180D-03-  
 8.460870410D-06  
 6.084733410D-09-1.702889433D-12 2.197402537D+04  
 6.388969190D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8861.337  
 -7.421262540D+04 2.638090127D+02 3.600227650D+00 1.018866266D-03-  
 4.666184120D-07  
 9.849002030D-11-6.468818170D-15 1.912726480D+04  
 5.235308150D+00  
 BCL+ Chase,1998 p198.  
 2 j 6/68 B 1.00CL 1.00E -1.00 0.00 0.00 0 46.26315  
 1234280.000  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8860.318  
 6.514405420D+04-6.845541010D+02 5.527276820D+00-4.458357450D-04-  
 4.557728840D-07

6.370858160D-10-2.134366120D-13 1.509424507D+05-  
 6.918256120D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8860.318  
 -2.169423542D+05 3.589975160D+02 4.035208370D+00 3.274452430D-04-  
 8.634578450D-08  
 1.207061044D-11-5.262253270D-16 1.445477224D+05  
 3.488212290D+00  
 BCL0H Gurvich,1996a pt1 p83 pt2 p61.  
 2 g 9/98 B 1.00CL 1.000 1.00H 1.00 0.00 0 63.27104 -  
 234005.381  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12431.519  
 -2.898427288D+04 6.894046580D+02-2.288138069D+00 3.349428620D-02-  
 4.725225980D-05  
 3.326981310D-08-9.224238860D-12 -3.261981100D+04  
 3.976885940D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12431.519  
 7.027738440D+05-2.857391274D+03 1.091175840D+01-8.107709340D-05-  
 2.124440337D-08  
 5.409912440D-12-3.464153840D-16 -1.307221888D+04-  
 3.585169510D+01  
 BCL(OH)2 Gurvich,1996a pt1 p85 pt2 p62.  
 2 tpis96 B 1.00CL 1.000 2.00H 2.00 0.00 0 80.27838 -  
 805387.658  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13565.103  
 8.072623010D+04-8.594619820D+02 2.705039614D+00 3.878799620D-02-  
 5.721734350D-05  
 4.145850330D-08-1.168536754D-11 -9.379910740D+04  
 7.134977090D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13565.103  
 1.423878191D+06-5.849704070D+03 1.792165219D+01-2.009909087D-04-  
 3.393435780D-08  
 9.838560760D-12-6.472678820D-16 -6.474261760D+04-  
 8.100400080D+01  
 BCL2 Gurvich,1996a pt1 p74 pt2 p52.  
 2 tpis96 B 1.00CL 2.00 0.00 0.00 0.00 0 81.71640 -  
 60881.490  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11513.621  
 3.598879420D+04-3.602826500D+02 4.157685450D+00 1.152877450D-02-  
 1.816567395D-05  
 1.341714418D-08-3.840822860D-12 -6.765107050D+03  
 5.182300860D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11513.621  
 3.501403130D+05-1.662203590D+03 8.839534720D+00-9.772544110D-04  
 2.467356248D-07  
 -2.501151018D-11 8.722954560D-16 5.682909440D+02-  
 2.148349445D+01  
 BCL2+ Chase,1998 p203 12/79.  
 2 g 1/01 B 1.00CL 2.00E -1.00 0.00 0.00 0 81.71585  
 672315.402  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12848.802  
 8.065956240D+04-1.149602601D+03 1.016765297D+01-3.586494910D-03  
 2.837145924D-06



-1.225075731D-09 2.224794198D-13 8.478617410D+04-  
 2.937258095D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12848.802  
 3.029293331D+05-1.305533159D+03 8.920390060D+00-7.289919640D-04  
 1.727833266D-07  
 -1.523567337D-11 4.226911440D-16 8.653415770D+04-  
 2.267467717D+01  
 BCL2OH Gurvich,1996a pt1 p86 pt2 p63.  
 2 tpi96 B 1.00CL 2.000 1.00H 1.00 0.00 0 98.72374 -  
 604917.444  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14051.769  
 2.099755170D+04-2.470699169D+02 2.578761742D+00 3.120362393D-02-  
 4.545314050D-05  
 3.242011770D-08-9.039822660D-12 -7.309028620D+04  
 1.273657699D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14051.769  
 5.878113790D+05-2.982969317D+03 1.400662004D+01-1.194189832D-04-  
 1.269775742D-08  
 4.422892190D-12-3.004089365D-16 -5.824168070D+04-  
 5.150859140D+01  
 BCL3 Gurvich,1996a pt1 p76 pt2 p53.  
 2 tpi96 B 1.00CL 3.00 0.00 0.00 0.00 0 117.16910 -  
 404500.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13970.666  
 2.392970339D+04-4.140378860D+02 5.488035260D+00 1.648395682D-02-  
 2.456196216D-05  
 1.743876340D-08-4.845222140D-12 -4.839469840D+04-  
 1.675366720D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13970.666  
 -2.417408819D+05-2.921539509D+02 1.021668480D+01-8.623637100D-05  
 1.897792088D-08  
 -2.168726841D-12 1.002154013D-16 -5.074834440D+04-  
 2.546863529D+01  
 BF Gurvich,1996a pt1 p56 pt2 p36.  
 2 g10/97 B 1.00F 1.00 0.00 0.00 0.00 0 29.80940 -  
 106931.884  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8694.670  
 -5.238954730D+04 8.118476640D+02-1.141614903D+00 1.161249417D-02-  
 1.175212617D-05  
 6.019232780D-09-1.238293129D-12 -1.774541998D+04  
 3.005086287D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8694.670  
 -3.746389780D+05 5.604493910D+02 3.609186110D+00 6.187216930D-04-  
 1.778938770D-07  
 2.426601527D-11-9.394651580D-16 -1.819179292D+04  
 3.716609290D+00  
 BFCL Gurvich,1996a pt1 p86 pt2 p64.  
 2 tpi96 B 1.00F 1.00CL 1.00 0.00 0.00 0 65.26210 -  
 279184.068  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11033.040  
 -2.363512735D+04 4.383168980D+02 3.918095720D-01 1.719990692D-02-  
 2.139592424D-05

1.337389186D-08-3.371164690D-12 -3.687166590D+04  
 2.668102062D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11033.040  
 -1.086309561D+05-5.233438480D+02 7.297504740D+00-3.054410701D-05-  
 3.154598306D-08  
 1.052290533D-11-7.615432260D-16 -3.305891210D+04-  
 1.186587285D+01  
**BFCL2** Gurvich,1996a pt1 p88 pt2 p66.  
 2 tpi96 B 1.00F 1.00CL 2.00 0.00 0.00 0 100.71480 -  
 643000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13230.913  
 4.402551240D+03-1.571398929D+02 4.016322310D+00 1.743396078D-02-  
 2.252789060D-05  
 1.433673443D-08-3.648755580D-12 -7.822452620D+04  
 6.886085810D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13230.913  
 -2.233613309D+05-6.440602960D+02 1.047861848D+01-1.911892367D-04  
 4.224887790D-08  
 -4.847266920D-12 2.247974725D-16 -7.740626480D+04-  
 2.814631458D+01  
**BFOH** Gurvich,1996a pt1 p71 pt2 p48.  
 2 g 9/98 B 1.00F 1.00O 1.00H 1.00 0.00 0 46.81674 -  
 451631.678  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11973.122  
 -7.563953670D+04 1.354838128D+03-5.648210110D+00 3.870274660D-02-  
 5.037659180D-05  
 3.339592640D-08-8.847822950D-12 -6.194446110D+04  
 5.800362820D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11973.122  
 7.251318090D+05-3.215620850D+03 1.117909777D+01-1.883881929D-04  
 2.579708080D-09  
 2.665158100D-12-2.186647438D-16 -3.716808080D+04-  
 3.978463490D+01  
**BF(OH)2** Gurvich,1996a pt1 p71 pt2 p49.  
 2 tpi96 B 1.00F 1.00O 2.00H 2.00 0.00 0 63.82408 -  
 1049889.539  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12885.220  
 1.381800676D+04 2.529637004D+02-3.844552040D+00 5.255140850D-02-  
 7.193117730D-05  
 4.948309910D-08-1.345922496D-11 -1.283123258D+05  
 4.293659370D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12885.220  
 1.422037640D+06-6.257297570D+03 1.822460686D+01-3.221396450D-04-  
 7.126739900D-09  
 6.758699770D-12-5.042554540D-16 -9.186254190D+04-  
 8.527895050D+01  
**BF2** Gurvich,1996a pt1 p58 pt2 p37.  
 2 tpi96 B 1.00F 2.00 0.00 0.00 0.00 0 48.80781 -  
 499426.904  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10612.202  
 -6.787651760D+04 1.085903536D+03-3.023320961D+00 2.326503687D-02-  
 2.641444147D-05

1.515620683D-08-3.518559180D-12 -6.640918250D+04  
4.431968310D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
10612.202  
-1.153091296D+05-8.109800120D+02 7.602709230D+00-2.409209242D-04  
5.328471860D-08  
-6.118797940D-12 2.839984178D-16 -5.796222170D+04-  
1.655644047D+01  
BF2+ Chase,1998 p211.  
2 j12/70 B 1.00F 2.00E -1.00 0.00 0.00 0 48.80726  
322586.400  
298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
10612.483  
-2.938356477D+04 2.955698598D+02 1.894274526D+00 1.280508319D-02-  
1.388757254D-05  
7.624366750D-09-1.706339371D-12 3.598992440D+04  
1.384803311D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
10612.483  
-1.769409966D+05-5.343685180D+02 7.728052910D+00-1.958622052D-06-  
2.419680893D-08  
5.732533810D-12-3.216354230D-16 3.908745050D+04-  
1.936560315D+01  
BF2- Gurvich,1996a pt1 p60 pt2 p38.  
2 tpi96 B 1.00F 2.00E 1.00 0.00 0.00 0 48.80835 -  
733802.963  
298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
10433.571  
2.109765318D+04 1.439564600D+02 2.604646296D-01 1.817373751D-02-  
2.241565287D-05  
1.369712886D-08-3.355952680D-12 -8.971801780D+04  
2.351692604D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
10433.571  
-1.709920627D+05-6.156219790D+02 7.458871370D+00-1.836703248D-04  
4.064363960D-08  
-4.667700950D-12 2.166264840D-16 -8.741404530D+04-  
1.620604664D+01  
BF2CL Gurvich,1996a pt1 p87 pt2 p65.  
2 tpi96 B 1.00F 2.00CL 1.00 0.00 0.00 0 84.26051 -  
888000.000  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
12323.693  
4.500101250D+03-1.196284966D+02 3.198635140D+00 1.743426933D-02-  
1.994070287D-05  
1.125136430D-08-2.544020371D-12 -1.076779851D+05  
1.008194481D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
12323.693  
-2.066817398D+05-1.024447292D+03 1.075843981D+01-3.023235319D-04  
6.672521470D-08  
-7.649941900D-12 3.546224500D-16 -1.046936725D+05-  
3.229995570D+01  
BF2OH Gurvich,1996a pt1 p72 pt2 p50.  
2 tpi96 B 1.00F 2.00O 1.00H 1.00 0.00 0 65.81515 -  
1092217.322  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
12395.887  
-7.522521650D+03 4.367121690D+02-3.128973474D+00 4.323957680D-02-  
5.785494040D-05

3.885858130D-08-1.038574523D-11 -1.344259458D+05  
 4.139170550D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12395.887  
 5.760759250D+05-3.611900190D+03 1.446897640D+01-3.028293733D-04  
 2.764337508D-08  
 -1.905493170D-13-8.694971940D-17 -1.133589041D+05-  
 5.896981510D+01  
**BF3** Gurvich,1996a pt1 p62 pt2 p39.  
 2 tpi96 B 1.00F 3.00 0.00 0.00 0.00 0 67.80621 -  
 1136000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11651.226  
 3.465584000D+03 2.133198651D+01 1.641245191D+00 1.993755064D-02-  
 2.150119930D-05  
 1.145669081D-08-2.442285789D-12 -1.379455591D+05  
 1.625533544D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11651.226  
 -1.819767014D+05-1.405347931D+03 1.103412258D+01-4.104591050D-04  
 9.031277570D-08  
 -1.033057360D-11 4.780551830D-16 -1.323136863D+05-  
 3.738386080D+01  
**BF4-** Gurvich,1996a pt1 p63 pt2 p40.  
 2 tpi96 B 1.00F 4.00E 1.00 0.00 0.00 0 86.80516 -  
 1761265.998  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13795.643  
 2.068485200D+05-2.463190805D+03 1.206414196D+01 1.102766923D-02-  
 1.751720760D-05  
 1.201346256D-08-3.150588626D-12 -2.010569206D+05-  
 4.610826940D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13795.643  
 -4.373241710D+05-7.759289410D+02 1.358222575D+01-2.341024178D-04  
 5.196915940D-08  
 -5.982245780D-12 2.781163206D-16 -2.127251877D+05-  
 4.953369700D+01  
**BH** Bauschlicher,1990. Gurvich,1996a pt1 p28 pt2 p19.  
 2 g12/99 B 1.00H 1.00 0.00 0.00 0.00 0 11.81894  
 448727.204  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8639.104  
 2.063082550D+04-3.682502520D+02 6.071337870D+00-8.728321070D-03  
 1.458566459D-05  
 -1.036840401D-08 2.779462579D-12 5.460459920D+04-  
 1.300392582D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8639.104  
 -1.098531663D+06-1.745890126D+02 8.442426810D+00-5.440196670D-03  
 2.718307052D-06  
 -4.839812210D-10 2.868523222D-14 5.016735670D+04-  
 2.971030686D+01  
**BHCL** Gurvich,1996a pt1 p81 pt2 p58.  
 2 g 9/98 B 1.00H 1.00CL 1.00 0.00 0.00 0 47.27164  
 141418.307  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10304.807  
 4.763274910D+04-4.420016520D+02 3.975645880D+00 8.541698760D-03-  
 1.377785182D-05

1.131521587D-08-3.569659180D-12 1.822278428D+04  
 3.028442880D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10304.807  
 3.499991720D+05-2.238404757D+03 8.711106050D+00-1.088882906D-03  
 4.189301090D-07  
 -6.568711260D-11 3.620067600D-15 2.841240364D+04-  
 2.589567177D+01  
 BHCL2 Gurvich,1996a pt1 p82 pt2 p60.  
 2 tpris96 B 1.00H 1.00CL 2.00 0.00 0.00 0 82.72434 -  
 251883.529  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11745.632  
 4.419914810D+04-2.384739577D+02 1.356682235D+00 2.517866897D-02-  
 3.632910400D-05  
 2.644335581D-08-7.625044110D-12 -3.003877914D+04  
 1.787023528D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11745.632  
 4.110996060D+05-2.858027441D+03 1.179547506D+01-6.322817970D-04  
 1.269551549D-07  
 -1.352862344D-11 5.921653510D-16 -1.617288760D+04-  
 4.217902060D+01  
 BHF Gurvich,1996a pt1 p68 pt2 p45.  
 2 g 9/98 B 1.00H 1.00F 1.00 0.00 0.00 0 30.81734 -  
 76012.343  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10042.057  
 -4.908362260D+04 9.610760210D+02-2.919850316D+00 2.149156633D-02-  
 2.595677863D-05  
 1.693492714D-08-4.553648840D-12 -1.466925195D+04  
 4.160709310D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10042.057  
 1.184821300D+06-4.677435180D+03 1.067328148D+01-1.606366598D-03  
 3.704534700D-07  
 -3.797882750D-11 1.432441145D-15 1.802640937D+04-  
 4.285931170D+01  
 BHFCL Gurvich,1996a pt1 p90 pt2 p69.  
 2 tpris96 B 1.00H 1.00F 1.00CL 1.00 0.00 0 66.27004 -  
 483036.620  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11414.539  
 5.761169720D+02 3.042156250D+02-9.808900360D-01 2.803843648D-02-  
 3.676734020D-05  
 2.499824138D-08-6.873421640D-12 -6.050207390D+04  
 3.132841413D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11414.539  
 4.390778920D+05-3.137181709D+03 1.200286161D+01-7.153669340D-04  
 1.453878608D-07  
 -1.565197070D-11 6.910075060D-16 -4.232368340D+04-  
 4.466543560D+01  
 BHF2 Gurvich,1996a pt1 p69 pt2 p47.  
 2 tpris96 B 1.00H 1.00F 2.00 0.00 0.00 0 49.81575 -  
 739613.811  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10659.347  
 -8.353540280D+04 1.616659766D+03-8.161405670D+00 4.153786790D-02-  
 4.921063280D-05

3.054165306D-08-7.786813980D-12 -9.748065460D+04  
 7.038630750D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10659.347  
 4.660876960D+05-3.728100490D+03 1.244152658D+01-8.906843190D-04  
 1.841732568D-07  
 -2.010774349D-11 8.979196590D-16 -6.978142930D+04-  
 5.103218040D+01  
 BH2 Jacox,1994. Kolbuszewski,1996. Gurvich,1996a p32.  
 2 g 2/00 B 1.00H 2.00 0.00 0.00 0.00 0 12.82688  
 328909.059  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10023.559  
 2.812557296D+04-3.000083489D+02 4.824221000D+00-2.186429819D-04  
 1.485457398D-06  
 3.893739680D-10-6.331629390D-13 3.991988420D+04-  
 5.042682850D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10023.559  
 1.360117365D+06-4.917704490D+03 9.758971030D+00-7.415870640D-04  
 1.269760019D-07  
 -1.187742442D-11 4.682552510D-16 6.890292660D+04-  
 4.190490120D+01  
 BH2CL Gurvich,1996a pt1 p82 pt2 p59.  
 2 tpis96 B 1.00H 2.00CL 1.00 0.00 0.00 0 48.27958 -  
 80845.754  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10426.902  
 1.646638117D+04 1.277320942D+02 1.300268921D-01 1.938143193D-02-  
 2.316389616D-05  
 1.607896164D-08-4.668337650D-12 -1.112112215D+04  
 2.308499180D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10426.902  
 1.427215437D+06-6.265564340D+03 1.382183005D+01-1.313843556D-03  
 2.587131606D-07  
 -2.713845270D-11 1.172827257D-15 2.639387516D+04-  
 6.399726240D+01  
 BH2F Gurvich,1996a pt1 p69 pt2 p46.  
 2 tpis96 B 1.00H 2.00F 1.00 0.00 0.00 0 31.82528 -  
 323956.732  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10137.922  
 -8.837920440D+04 1.705285929D+03-8.061246130D+00 3.643188680D-02-  
 4.152482550D-05  
 2.620135756D-08-6.930886410D-12 -4.787273410D+04  
 6.862087670D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10137.922  
 1.435082111D+06-6.625320170D+03 1.409165008D+01-1.422469060D-03  
 2.828724718D-07  
 -2.992498948D-11 1.302618926D-15 -7.937192670D+02-  
 6.801356400D+01  
 BH3 Allendorf,1997. Jacox,1998 p212. Martin,1992.  
 2 g 1/00 B 1.00H 3.00 0.00 0.00 0.00 0 13.83482  
 104746.599  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10059.699  
 -6.619635070D+04 1.262658391D+03-4.654355900D+00 2.461795131D-02-  
 2.501537437D-05

1.562330756D-08-4.323949480D-12 5.667587980D+03  
 4.666504620D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10059.699  
 1.855778950D+06-8.002492370D+03 1.505692199D+01-1.790456689D-03  
 3.612511100D-07  
 -3.866035910D-11 1.698508879D-15 5.967537070D+04-  
 7.994046160D+01  
 BH3NH3 Gurvich,1996a pt1 p106 pt2 p84.  
 2 tpi96 B 1.00H 6.00N 1.00 0.00 0.00 0 30.86538 -  
 115000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12681.530  
 -1.811063598D+05 3.010341543D+03-1.524271135D+01 6.215637750D-02-  
 5.959881850D-05  
 3.267429360D-08-7.751243090D-12 -2.934278877D+04  
 1.087399627D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12681.530  
 4.354925960D+06-1.824235232D+04 3.162999830D+01-3.208243610D-03  
 5.885075450D-07  
 -5.808535530D-11 2.382578600D-15 9.438118030D+04-  
 1.897865780D+02  
 BH4 Radical. Saxon,1993. Yu,1998.  
 2 g 5/00 B 1.00H 4.00 0.00 0.00 0.00 0 14.84276  
 255210.477  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10770.877  
 2.734274578D+04-8.473619380D+01 1.551871695D+00 1.439765491D-02-  
 6.111152360D-06  
 -1.324417559D-10 5.133008150D-13 3.022048074D+04  
 1.250358328D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10770.877  
 1.354714146D+06-7.870762750D+03 1.826170610D+01-1.948275329D-03  
 4.072706890D-07  
 -4.482710900D-11 2.014115885D-15 7.470249490D+04-  
 9.686086890D+01  
 BH5 Schreiner,1994.  
 2 g 8/00 B 1.00H 5.00 0.00 0.00 0.00 0 15.85070  
 92933.658  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12572.458  
 -5.603075360D+04 1.457641959D+03-8.245037630D+00 4.817478230D-02-  
 5.535104700D-05  
 3.578299590D-08-9.717757500D-12 3.424238930D+03  
 6.695881520D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12572.458  
 2.472199159D+06-1.110339842D+04 2.243395706D+01-2.121632568D-03  
 4.038994240D-07  
 -4.121910490D-11 1.741706383D-15 7.561744630D+04-  
 1.243306259D+02  
 BI Gurvich,1996a pt1 p94 pt2 p73.  
 2 g 9/98 B 1.00I 1.00 0.00 0.00 0.00 0 137.71547  
 325987.502  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9142.202  
 3.517449530D+04-5.445819300D+02 6.027511010D+00-2.387237926D-03  
 2.244796277D-06

-1.110001347D-09 2.280204403D-13 4.071910130D+04-  
 7.288049840D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9142.202  
 2.132872626D+06-6.283684960D+03 1.123964343D+01-3.258856750D-03  
 7.064282150D-07  
 -4.230068930D-11-4.208078470D-16 7.797634810D+04-  
 4.664042610D+01  
 BI2 Gurvich,1996a pt1 p95 pt2 p74.  
 2 g 9/98 B 1.00I 2.00 0.00 0.00 0.00 0 264.61994  
 238096.324  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12688.424  
 6.640975900D+04-1.044411994D+03 9.734197240D+00-3.952557540D-03  
 3.165567780D-06  
 -1.273764644D-09 1.879968132D-13 3.205750890D+04-  
 2.012407058D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12688.424  
 -3.924022230D+05 4.422902350D+02 7.129623580D+00-5.619634060D-04  
 3.180760520D-07  
 -5.537079720D-11 3.183959700D-15 2.291972638D+04-  
 3.201793240D+00  
 BI3 Gurvich,1996a pt1 p96 pt2 p75.  
 2 tpis96 B 1.00I 3.00 0.00 0.00 0.00 0 391.52441  
 21400.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16933.072  
 6.243114890D+04-1.002408628D+03 1.106650075D+01 1.609588058D-03-  
 5.147250250D-06  
 4.732514020D-09-1.512999796D-12 5.160348150D+03-  
 2.420687643D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16933.072  
 -1.506176506D+05-8.167210610D+01 1.005937867D+01-2.319396215D-05  
 5.019966730D-09  
 -5.654349630D-13 2.580651348D-17 -4.261687910D+02-  
 1.617962779D+01  
 BN Gurvich,1996a pt1 p104 pt2 p83.  
 2 g 9/98 B 1.00N 1.00 0.00 0.00 0.00 0 24.81774  
 574726.408  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8961.108  
 -4.569707580D+04 6.704286070D+02 3.615089080D-02 7.339487510D-03-  
 4.969033490D-06  
 1.229031380D-09 6.340281520D-14 6.485465080D+04  
 2.539870138D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8961.108  
 -2.276932705D+05-1.025649298D+02 4.414586810D+00 2.561670989D-04-  
 1.612994942D-08  
 -6.526052930D-13 5.749466120D-17 6.784465130D+04-  
 6.778544480D-01  
 BO Gurvich,1996a pt1 p10 pt2 p8.  
 3 g 9/98 B 1.00O 1.00 0.00 0.00 0.00 0 26.81040  
 20406.404  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8674.104  
 -1.166216822D+04 9.217579390D+01 3.655498490D+00-3.118542920D-03  
 9.008329830D-06



-8.017789990D-09 2.472952292D-12 8.738284780D+02  
 4.482847390D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8674.104  
 1.788600589D+04-6.309019630D+02 4.574528400D+00 1.988001643D-04-  
 9.702963480D-08  
 1.870854291D-11-1.030218131D-15 4.841311090D+03-  
 3.398890580D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8674.104  
 -1.592699514D+08 1.210955629D+05-3.136823502D+01 5.110037760D-03-  
 3.461020740D-07  
 1.148046833D-11-1.504899225D-16 -9.345065760D+05  
 3.026123907D+02  
 BO- Gurvich,1996a pt1 p13 pt2 p10.  
 2 g 9/98 B 1.000 1.00E 1.00 0.00 0.00 0 26.81095 -  
 277791.076  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8674.024  
 -8.242023210D+04 9.203636900D+02-2.302659981D-01 6.229904120D-03-  
 3.157624391D-06  
 1.184578107D-10 2.819228693D-13 -3.911141220D+04  
 2.599226838D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8674.024  
 2.122804369D+05-1.262124688D+03 5.383167310D+00-3.181049100D-04  
 7.288988250D-08  
 -8.141708920D-12 3.715364390D-16 -2.706892261D+04-  
 9.773753670D+00  
 BOCL Gurvich,1996a pt1 p79 pt2 p55.  
 2 tpis96 B 1.000 1.00CL 1.00 0.00 0.00 0 62.26310 -  
 318536.695  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10607.913  
 7.052380640D+04-1.315301429D+03 1.130087727D+01-1.207112050D-02  
 1.880516131D-05  
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 3.698463240D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10607.913  
 1.557148487D+05-1.446254968D+03 8.509448050D+00-3.859007380D-04  
 8.262268820D-08  
 -9.261027460D-12 4.219998010D-16 -3.203589040D+04-  
 2.372714015D+01  
 BOCL2 Gurvich,1996a pt1 p79 pt2 p56.  
 2 tpis96 B 1.000 1.00CL 2.00 0.00 0.00 0 97.71580 -  
 361565.512  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13169.650  
 7.322667360D+03-2.027726965D+02 4.161924090D+00 1.733309456D-02-  
 2.263908718D-05  
 1.452275190D-08-3.719593120D-12 -4.414441880D+04  
 6.520414900D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13169.650  
 -2.297527041D+05-6.194567930D+02 1.046075518D+01-1.841620739D-04  
 4.071215430D-08  
 -4.672246550D-12 2.167237536D-16 -4.371538420D+04-  
 2.743571136D+01  
 BOF Gurvich,1996a pt1 p65 pt2 p42.

2 tpis96 B 1.000 1.00F 1.00 0.00 0.00 0 45.80880 -  
 592978.311  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9988.295  
 7.226802650D+04-1.131386630D+03 8.816054520D+00-4.627694570D-03  
 7.801299580D-06  
 -5.681205840D-09 1.534732094D-12 -6.711116010D+04-  
 2.547957229D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9988.295  
 1.937020297D+05-1.739112297D+03 8.695650860D+00-4.518895570D-04  
 9.591019080D-08  
 -1.067806769D-11 4.840007660D-16 -6.330152390D+04-  
 2.702458617D+01  
 BOF2 Gurvich,1996a pt1 p66 pt2 p43.  
 2 tpis96 B 1.000 1.00F 2.00 0.00 0.00 0 64.80721 -  
 832767.700  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11611.458  
 7.227794130D+03 2.148783624D+01 1.157840301D+00 2.250585296D-02-  
 2.610731536D-05  
 1.508824929D-08-3.518364850D-12 -1.013995733D+05  
 2.010127136D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11611.458  
 -2.205028861D+05-1.254238690D+03 1.092551380D+01-3.680144000D-04  
 8.107164940D-08  
 -9.281275060D-12 4.297549300D-16 -9.680447580D+04-  
 3.482853330D+01  
 BOH Gurvich,1996a pt1 p41 pt2 p24.  
 2 tpis96 B 1.000 1.00H 1.00 0.00 0.00 0 27.81834 -  
 6756.578  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10031.524  
 -7.521410270D+04 1.391444703D+03-5.630330180D+00 2.966358811D-02-  
 3.830835180D-05  
 2.550606424D-08-6.795857210D-12 -8.341300280D+03  
 5.517690040D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10031.524  
 8.447498570D+05-3.016982887D+03 8.083864700D+00-1.609855388D-04-  
 2.191830959D-09  
 3.127133119D-12-2.376665451D-16 1.647698495D+04-  
 2.603227947D+01  
 BO2 Gurvich,1996a pt1 p14 pt2 p11.  
 2 g10/97 B 1.000 2.00 0.00 0.00 0.00 0 42.80980 -  
 309121.947  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10772.157  
 -4.141090640D+04 7.198854610D+02-1.477629435D+00 2.277415194D-02-  
 2.786326934D-05  
 1.718462069D-08-4.278991440D-12 -4.177657690D+04  
 3.258458010D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10772.157  
 -3.834452340D+04-9.563261140D+02 8.200962780D+00-2.062130802D-04  
 9.872288990D-09  
 8.158366760D-12-7.527519660D-16 -3.423564020D+04-  
 2.224772278D+01  
 BO2- Gurvich,1996a pt1 p16 pt2 p13.

2 tpi96 B 1.000 2.00E 1.00 0.00 0.00 0 42.81035 -  
 714493.991  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9597.541  
 5.324279690D+04-7.326313030D+02 5.902470000D+00 2.437465200D-03-  
 4.878803950D-07  
 -8.475724760D-10 4.080781180D-13 -8.344293680D+04-  
 1.053931911D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9597.541  
 1.199226372D+05-1.715766982D+03 8.701038220D+00-4.601242120D-04  
 9.867011870D-08  
 -1.107288516D-11 5.050183240D-16 -7.825789690D+04-  
 2.839356505D+01  
 B(OH)2 Gurvich,1996a pt1 p46 pt2 p28.  
 2 g 9/98 B 1.000 2.00H 2.00 0.00 0.00 0 44.82568 -  
 425243.642  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11971.658  
 1.491659222D+03 3.648184840D+02-2.906006389D+00 4.136834460D-02-  
 5.782584220D-05  
 4.069783560D-08-1.126499791D-11 -5.375483660D+04  
 3.888535180D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11971.658  
 1.557023406D+06-5.784710760D+03 1.487391235D+01-1.821804765D-04-  
 3.803541640D-08  
 1.030332746D-11-6.685889830D-16 -1.806810301D+04-  
 6.590268900D+01  
 BS Gurvich,1996a pt1 p97 pt2 p76.  
 2 g10/98 B 1.00S 1.00 0.00 0.00 0.00 0 42.87700  
 273519.405  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8724.105  
 -3.839490100D+04 6.989417490D+02-1.213980460D+00 1.396391264D-02-  
 1.689881284D-05  
 1.038889985D-08-2.582063989D-12 2.865685472D+04  
 3.154823443D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8724.105  
 1.358760165D+06-4.364035960D+03 9.034307590D+00-2.114548699D-03  
 4.189275310D-07  
 -1.354787322D-11-1.360684605D-15 5.913065450D+04-  
 3.336693370D+01  
 BS2 Gurvich,1996a pt1 p99 pt2 p77.  
 2 g 9/98 B 1.00S 2.00 0.00 0.00 0.00 0 74.94300  
 63867.460  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13559.560  
 1.820264374D+04-5.150671890D+02 8.547515000D+00-1.626155268D-03  
 1.866387194D-06  
 -1.277165468D-09 3.681980690D-13 8.186839750D+03-  
 1.778380851D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13559.560  
 5.120402510D+05-1.938581076D+03 9.814873460D+00-1.339731606D-03  
 3.754301160D-07  
 -4.400383780D-11 1.887662968D-15 1.736535000D+04-  
 2.757542709D+01  
 B2 Gurvich,1996a pt1 p8 pt2 p7.

2 g 9/98 B 2.00 0.00 0.00 0.00 0.00 0 21.62200  
857370.506  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
8805.106  
-1.516418096D+05 2.630168946D+03-1.381358321D+01 5.216225190D-02-  
6.930494740D-05  
4.469410390D-08-1.128496456D-11 8.995251050D+04  
9.813118490D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
8805.106  
1.094594495D+06-2.602735739D+03 6.909456210D+00-6.405949890D-04  
1.951732355D-07  
-2.555902119D-11 1.053557323D-15 1.187807611D+05-  
1.949045025D+01

B2C Gurvich,1996a pt1 p110 pt2 p88.  
2 g 9/98 B 2.00C 1.00 0.00 0.00 0.00 0 33.63270  
800432.614  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
11723.114  
-4.166519870D+04 5.797779520D+02 1.411017091D+00 1.174705713D-02-  
1.066474425D-05  
4.717232620D-09-7.970013260D-13 9.196874200D+04  
1.769254387D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
11723.114  
1.159241019D+06-4.567798810D+03 1.228672097D+01-2.500830701D-03  
6.409979850D-07  
-6.932935770D-11 2.672933741D-15 1.222442137D+05-  
5.199066186D+01

B2CL4 Gurvich,1996a pt1 p77 pt2 p54.  
2 g10/97 B 2.00CL 4.00 0.00 0.00 0.00 0 163.43280 -  
490000.000  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
21588.132  
4.285555130D+04-7.280748810D+02 9.315763670D+00 2.331629623D-02-  
3.511247610D-05  
2.464057658D-08-6.735479960D-12 -5.819023240D+04-  
1.622084979D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
21588.132  
-6.427987030D+05 5.078562990D+02 1.486725022D+01 2.026983515D-06  
6.272718810D-09  
-1.218822573D-12 7.241208410D-17 -6.820066000D+04-  
4.139111770D+01

B2F4 Gurvich,1996a pt1 p64 pt2 p41.  
2 g10/97 B 2.00F 4.00 0.00 0.00 0.00 0 97.61561 -  
1438000.000  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
17680.793  
-5.971695640D+04 8.189425440D+02-6.437671290D-01 3.858966070D-02-  
4.313053190D-05  
2.404463223D-08-5.393559350D-12 -1.790041225D+05  
3.552179970D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
17680.793  
3.855865890D+04-2.928842655D+03 1.792063736D+01-9.523998270D-04  
1.614708845D-07  
-1.428613504D-11 5.218739670D-16 -1.613051924D+05-  
7.184803250D+01

B2H Adams,1989. Yu,1998.

2 g 7/00 B 2.00H 1.00 0.00 0.00 0.00 0 22.62994  
 796262.497  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10115.597  
 8.775579740D+04-1.343931564D+03 9.832099150D+00-5.607137750D-03  
 5.730651050D-06  
 -2.266436197D-09 1.972352080D-13 1.009908698D+05-  
 3.282461480D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10115.597  
 6.175545750D+05-2.627897466D+03 9.084905070D+00-5.389418330D-04  
 1.050714700D-07  
 -1.092459556D-11 4.684854660D-16 1.099537555D+05-  
 3.164029910D+01  
 B2H2 Curtiss,1989a. Yu,1998.  
 2 g 7/00 B 2.00H 2.00 0.00 0.00 0.00 0 23.63788  
 454677.939  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10573.239  
 1.421617322D+05-2.138011262D+03 1.317732399D+01-8.942658070D-03  
 1.127804935D-05  
 -5.787886200D-09 1.000813871D-12 6.372319250D+04-  
 5.346982740D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10573.239  
 1.240614592D+06-5.368965020D+03 1.379292454D+01-1.136749748D-03  
 2.245617156D-07  
 -2.361530467D-11 1.022604572D-15 8.506511490D+04-  
 6.435461300D+01  
 B2H3 Adams,1989. Yu,1998.  
 2 g 6/00 B 2.00H 3.00 0.00 0.00 0.00 0 24.64582  
 351072.721  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11938.621  
 9.425147160D+04-1.075866284D+03 6.383999390D+00 1.167858327D-02-  
 1.429661252D-05  
 1.128776882D-08-3.681325060D-12 4.635335080D+04-  
 1.400002845D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11938.621  
 1.771506902D+06-7.872260930D+03 1.789447015D+01-1.709304785D-03  
 3.409575430D-07  
 -3.614543680D-11 1.575671409D-15 8.737711890D+04-  
 9.054629460D+01  
 B2H3,db 2-Bridges. Adams,1989. Yu,1998.  
 2 g 7/00 B 2.00H 3.00 0.00 0.00 0.00 0 24.64582  
 353408.227  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11911.227  
 6.064014840D+04-7.524466330D+02 5.584483840D+00 1.080468494D-02-  
 8.649032810D-06  
 4.748333310D-09-1.309096028D-12 4.491792300D+04-  
 8.873686820D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11911.227  
 1.497731017D+06-7.219314140D+03 1.750463766D+01-1.579698800D-03  
 3.164103470D-07  
 -3.367225150D-11 1.472919654D-15 8.324349670D+04-  
 8.779549260D+01  
 B2H4 1-Bridge. Ruscic,1989b. Curtiss,1989b.

2 g 8/00 B 2.00H 4.00 0.00 0.00 0.00 0 25.65376  
 211162.059  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12339.859  
 4.000132300D+04-3.071548876D+02 1.763071673D+00 2.646361882D-02-  
 3.066168202D-05  
 2.163781936D-08-6.491835410D-12 2.581033714D+04  
 1.015267130D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12339.859  
 2.292078842D+06-1.059832517D+04 2.268612155D+01-2.363586598D-03  
 4.762173070D-07  
 -5.090100400D-11 2.233911590D-15 8.638591980D+04-  
 1.246794566D+02  
 B2H4,db 2-Bridges.Ruscic,1989b. Curtiss,1989b.  
 2 g 7/00 B 2.00H 4.00 0.00 0.00 0.00 0 25.65376  
 209932.448  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11528.648  
 -1.781496923D+04 5.716048040D+02-2.763085348D+00 3.125348696D-02-  
 2.709524346D-05  
 1.341728634D-08-3.004352798D-12 2.158138307D+04  
 3.675872940D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11528.648  
 1.886854256D+06-1.010045614D+04 2.247110812D+01-2.319968667D-03  
 4.731879960D-07  
 -5.110673030D-11 2.262693782D-15 8.233487000D+04-  
 1.237455797D+02  
 B2H5 1-Bridge. Ruscic,1989a. Trachtman,1989.  
 2 g 5/00 B 2.00H 5.00 0.00 0.00 0.00 0 26.66170  
 254783.889  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12220.789  
 3.830965450D+04-4.066148050D+01-1.422523787D+00 3.674595270D-02-  
 3.851989710D-05  
 2.444494440D-08-6.821722940D-12 3.008956452D+04  
 2.802425895D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12220.789  
 2.696691012D+06-1.320019835D+04 2.735260413D+01-2.961879012D-03  
 5.984999430D-07  
 -6.413748550D-11 2.821187823D-15 1.064524901D+05-  
 1.559654379D+02  
 B2H5,db 2-Bridges. Ruscic,1989a. Trachtman,1989.  
 2 g 5/00 B 2.00H 5.00 0.00 0.00 0.00 0 26.66170  
 275150.616  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11667.516  
 1.424446027D+04 4.204558200D+02-3.700451250D+00 3.672053100D-02-  
 3.193503730D-05  
 1.695013434D-08-4.257038140D-12 3.046684683D+04  
 4.245495820D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11667.516  
 2.571729448D+06-1.356829858D+04 2.781376038D+01-3.192365030D-03  
 6.561165260D-07  
 -7.127333940D-11 3.169492650D-15 1.106370527D+05-  
 1.597214457D+02  
 B2H6 Hf:Gurvich,1996a pt1 p37. Yu,1998. Duncan,1985.

2 g 5/00 B 2.00H 6.00 0.00 0.00 0.00 0 27.66964  
 36600.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11932.313  
 -1.052844558D+04 1.041795556D+03-8.960518860D+00 5.492480880D-02-  
 5.305197050D-05  
 3.011904756D-08-7.688768300D-12 -9.259374350D+02  
 6.812592430D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11932.313  
 2.835765414D+06-1.567600163D+04 3.226122330D+01-3.738609730D-03  
 7.718806460D-07  
 -8.414454540D-11 3.752223380D-15 9.358378550D+04-  
 1.920223395D+02  
 B20 Gurvich,1996a pt1 p19 pt2 p14.  
 2 g 9/98 B 2.000 1.00 0.00 0.00 0.00 0 37.62140  
 192798.018  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11783.018  
 -5.699546760D+04 1.018000465D+03-2.636481947D+00 2.746009279D-02-  
 3.632432720D-05  
 2.406890217D-08-6.384129720D-12 1.703874394D+04  
 3.855346110D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11783.018  
 -1.628723220D+05-3.876289810D+02 7.787723520D+00-1.146822108D-04  
 2.528097612D-08  
 -2.893783941D-12 1.339210475D-16 2.263035354D+04-  
 1.908513011D+01  
 B202 Gurvich,1996a pt1 p19 pt2 p15.  
 2 tpi96 B 2.000 2.00 0.00 0.00 0.00 0 53.62080 -  
 457711.486  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13396.618  
 8.174391690D+04-1.732702797D+03 1.605560926D+01-2.160057288D-02  
 3.566854570D-05  
 -2.660198794D-08 7.531833240D-12 -4.899632900D+04-  
 6.172702390D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13396.618  
 4.605789660D+05-2.990079203D+03 1.256764079D+01-7.850974950D-04  
 1.672537624D-07  
 -1.867694780D-11 8.486190670D-16 -4.015748150D+04-  
 4.874413710D+01  
 B203 Gurvich,1996a pt1 p25 pt2 p18.  
 2 tpi96 B 2.000 3.00 0.00 0.00 0.00 0 69.62020 -  
 835382.271  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14418.729  
 7.379611910D+04-1.263620592D+03 1.072681512D+01 3.841383720D-04  
 5.976058380D-06  
 -6.552891350D-09 2.123951064D-12 -9.628183140D+04-  
 3.088078011D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14418.729  
 3.905035300D+05-3.691348210D+03 1.555502598D+01-9.707645510D-04  
 2.068887872D-07  
 -2.310858356D-11 1.050136734D-15 -8.263054410D+04-  
 6.390863440D+01  
 B2(OH)4 Gurvich,1996a pt1 p52 pt2 p33.

2 g 9/98 B 2.000 4.00H 4.00 0.00 0.00 0 89.65136 -  
 1254987.531  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19443.069  
 -1.728717249D+04 8.495913480D+02-8.715959570D+00 9.362362610D-02-  
 1.278784165D-04  
 8.813671160D-08-2.400605571D-11 -1.564337133D+05  
 7.120169310D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19443.069  
 2.983925656D+06-1.207469577D+04 3.162610570D+01-5.163682440D-04-  
 4.232093970D-08  
 1.671977280D-11-1.156366726D-15 -8.280976970D+04-  
 1.653010498D+02  
 B2S Gurvich,1996a pt1 p100, pt2 p78.  
 2 g 9/98 B 2.00S 1.00 0.00 0.00 0.00 0 53.68800  
 622260.705  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13182.705  
 6.638609300D+04-9.201185690D+02 8.699831340D+00 7.645589010D-04-  
 3.709026030D-06  
 3.642373980D-09-1.197766071D-12 7.770375800D+04-  
 2.251709650D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13182.705  
 -1.211501483D+05-6.473398450D+01 7.546825610D+00-1.820541450D-05  
 3.923951170D-09  
 -4.403862380D-13 2.003651718D-17 7.258531870D+04-  
 1.394968435D+01  
 B2S2 Gurvich,1996a pt1 p100 pt2 p79.  
 2 tpi96 B 2.00S 2.00 0.00 0.00 0.00 0 85.75400  
 138317.112  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14569.112  
 -7.061549970D+04 7.182944780D+02 1.919797788D+00 2.036407461D-02-  
 2.309813846D-05  
 1.311616725D-08-2.996394781D-12 1.100829019D+04  
 1.855406084D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14569.112  
 -1.641535014D+05-7.742865640D+02 1.107731737D+01-2.313278554D-04  
 5.125614290D-08  
 -5.894081230D-12 2.738673834D-16 1.733003515D+04-  
 3.359763500D+01  
 B2S3 Gurvich,1996a pt1 p102 pt2 p81.  
 2 tpi96 B 2.00S 3.00 0.00 0.00 0.00 0 117.82000  
 17754.057  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19938.057  
 -3.431268500D+04 5.587615370D+02 3.414077410D+00 2.398333891D-02-  
 2.841617637D-05  
 1.690005199D-08-4.060070710D-12 -3.027690575D+03  
 1.846771683D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19938.057  
 -1.905855086D+05-9.348342480D+02 1.369333613D+01-2.766647250D-04  
 6.110155800D-08  
 -7.008048570D-12 3.249524620D-16 2.906433760D+03-  
 3.946866660D+01  
 B3H7,C2v C2v symmetry. Stanton,1989b.



2 g 8/00 B 3.00H 7.00 0.00 0.00 0.00 0 39.48858  
 176019.139  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14818.439  
 1.086009469D+05-7.921536800D+02-9.577368040D-01 5.656119290D-02-  
 6.405034500D-05  
 4.281322960D-08-1.227580455D-11 2.430638819D+04  
 2.102582666D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14818.439  
 3.598592140D+06-1.863701968D+04 3.993998830D+01-4.275410160D-03  
 8.705358820D-07  
 -9.385105020D-11 4.147865310D-15 1.272154092D+05-  
 2.379769856D+02  
 B3H7,Cs Cs symmetry. Stanton,1989b.  
 2 g 8/00 B 3.00H 7.00 0.00 0.00 0.00 0 39.48858  
 159318.322  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14083.322  
 5.298169330D+04 4.071745370D+02-9.635730530D+00 7.944312000D-02-  
 9.306456820D-05  
 6.105147350D-08-1.685927691D-11 1.707069083D+04  
 6.873966560D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14083.322  
 3.281576450D+06-1.811096595D+04 3.963832460D+01-4.178424110D-03  
 8.526829060D-07  
 -9.209600240D-11 4.076496770D-15 1.213622564D+05-  
 2.357090217D+02  
 B3H9 Hf:McKee,1990. Stanton,1989a.  
 2 g 7/00 B 3.00H 9.00 0.00 0.00 0.00 0 41.50446  
 138908.800  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17329.935  
 8.483214900D+04-5.206163040D+02-4.665701210D-01 5.346983860D-02-  
 4.155796820D-05  
 1.944135439D-08-4.541227350D-12 1.805101100D+04  
 2.110804198D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17329.935  
 3.863999500D+06-2.229433407D+04 4.875046150D+01-5.418449260D-03  
 1.125767651D-06  
 -1.233226406D-10 5.520348180D-15 1.422187123D+05-  
 2.958240102D+02  
 B3N3H6 Borazole. Gurvich,1996a pt1 p107 pt2 p85.  
 2 tpris96 B 3.00N 3.00H 6.00 0.00 0.00 0 80.50086 -  
 512000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16221.348  
 -1.552621082D+05 4.010211270D+03-3.382491300D+01 1.624575582D-01-  
 2.065528647D-04  
 1.368862991D-07-3.673470900D-11 -8.051253400D+04  
 1.995000773D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16221.348  
 3.739245170D+06-1.941238951D+04 4.445070030D+01-3.210308050D-03  
 5.717465420D-07  
 -5.486692140D-11 2.191943197D-15 4.758426160D+04-  
 2.641156603D+02  
 B3O3CL3 Gurvich,1996a pt1 p80 pt2 p57.

2 tpis96 B 3.000 3.00CL 3.00 0.00 0.00 0 186.78930 -  
 1635982.041  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 24451.781  
 -4.284452800D+04 1.005623966D+03-4.556519630D+00 8.117967140D-02-  
 1.038385803D-04  
 6.621422330D-08-1.695748504D-11 -2.040907277D+05  
 5.466113080D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 24451.781  
 -7.414059810D+05-2.527447455D+03 2.687263667D+01-7.463389360D-04  
 1.646334110D-07  
 -1.886231553D-11 8.737926310D-16 -1.923509858D+05-  
 1.185636327D+02  
 B303FCL2 Gurvich,1996a pt1 p89 pt2 p68.  
 2 tpis96 B 3.000 3.00F 1.00CL 2.00 0.00 0 170.33500 -  
 1883807.681  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 23448.139  
 -3.719120070D+04 8.673745890D+02-4.095778460D+00 7.815563970D-02-  
 9.767035170D-05  
 6.097610090D-08-1.532880319D-11 -2.331383552D+05  
 5.198087630D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 23448.139  
 -7.162360830D+05-2.851210308D+03 2.710953133D+01-8.400919640D-04  
 1.852318684D-07  
 -2.121694694D-11 9.827291560D-16 -2.202729252D+05-  
 1.210679418D+02  
 B303F2CL Gurvich,1996a pt1 p89 pt2 p67.  
 2 tpis96 B 3.000 3.00F 2.00CL 1.00 0.00 0 153.88071 -  
 2132816.827  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22260.991  
 -5.277015540D+04 1.104904696D+03-5.854181050D+00 7.953943100D-02-  
 9.592660770D-05  
 5.799856310D-08-1.416698348D-11 -2.640400115D+05  
 6.071246930D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22260.991  
 -6.810787490D+05-3.370009020D+03 2.748953579D+01-9.905442560D-04  
 2.182908440D-07  
 -2.499573480D-11 1.157532106D-15 -2.472114785D+05-  
 1.261501577D+02  
 B303F3 Gurvich,1996a pt1 p67 pt2 p44.  
 2 tpis96 B 3.000 3.00F 3.00 0.00 0.00 0 137.42641 -  
 2382699.078  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 21200.738  
 -7.251549780D+04 1.400996228D+03-7.906716200D+00 8.217161850D-02-  
 9.633152660D-05  
 5.668194260D-08-1.349024305D-11 -2.953461728D+05  
 7.001536830D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 21200.738  
 -6.629822910D+05-3.784946870D+03 2.779526578D+01-1.112096232D-03  
 2.450806704D-07  
 -2.806484980D-11 1.299750466D-15 -2.748865475D+05-  
 1.315605015D+02  
 B4H4 Yu,1998. Mach,1994.

2 g 8/00 B 4.00H 4.00 0.00 0.00 0.00 0 47.27576  
 326190.400  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14936.602  
 2.171791579D+05-2.598282557D+03 9.845440610D+00 3.026309140D-02-  
 4.128334160D-05  
 3.089368344D-08-9.353384260D-12 5.079143480D+04-  
 3.770757210D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14936.602  
 1.937200886D+06-1.078185932D+04 2.879625241D+01-2.401547707D-03  
 4.837756780D-07  
 -5.170490230D-11 2.269138182D-15 9.836595390D+04-  
 1.561814117D+02

B4H10 Wagman,1982 p123. McKee,1990. Dain,1981.  
 2 g 5/00 B 4.00H 10.00 0.00 0.00 0.00 0 53.32340  
 66100.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15485.574  
 -3.296604820D+04 2.440532922D+03-2.685332563D+01 1.406499347D-01-  
 1.586710574D-04  
 9.874594130D-08-2.601426018D-11 -3.091924018D+03  
 1.589905532D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15485.574  
 4.030474130D+06-2.560629762D+04 5.687233660D+01-6.178567860D-03  
 1.280621032D-06  
 -1.400254585D-10 6.258866560D-15 1.506009087D+05-  
 3.520714200D+02

B4H12 Shen,1993. Yu,1998.  
 2 g 5/00 B 4.00H 12.00 0.00 0.00 0.00 0 55.33928  
 188236.114  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 21748.714  
 7.152170300D+04-1.590351575D+02-4.719771660D+00 8.811228900D-02-  
 8.604946880D-05  
 5.123535510D-08-1.379865250D-11 2.194186547D+04  
 4.187897400D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 21748.714  
 6.158360800D+06-3.202086730D+04 6.660443600D+01-7.406369280D-03  
 1.512993908D-06  
 -1.635619071D-10 7.245385140D-15 2.054586275D+05-  
 4.142106860D+02

B5H9 Hf:Chase,1998 p303  
 3/65.McKee,1990.Beaudet,1988.Yu,1998.  
 2 g 6/00 B 5.00H 9.00 0.00 0.00 0.00 0 63.12646  
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 9.866680210D-05  
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 7.663090480D+01  
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 3.371060460D+02

Ba Gurvich,1996. Moore,1971. Moore,1970a. Gordon,1999.

3 g10/97 BA 1.00 0.00 0.00 0.00 0.00 0 137.32700  
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 7.807601830D-06  
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 2.607063698D+01  
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 1.295568595D-07  
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 4.370610780D+01  
 BaBr Gurvich,1996a pt1 p576 pt2 p437.  
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 75324.677  
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 -1.936413749D-10 4.124048530D-14 -1.736328141D+04  
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 3.574187820D+00  
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 348697.630  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
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 8.355724000D-07  
 -4.685258510D-10 1.095343103D-13 4.125155990D+04  
 1.896275774D+00  
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 9668.230  
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 2.396147871D-09  
 5.479458600D-14 1.174342316D-18 4.055100150D+04  
 4.503762960D+00  
 BaCL2 Gurvich,1996a pt1 p575 pt2 p436.  
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 -4.386759060D-14 2.125803293D-18 -6.219095270D+04-  
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 BaF Gurvich,1996a pt1 p562 pt2 p429.  
 2 tpi96 BA 1.00F 1.00 0.00 0.00 0.00 0 156.32540 -  
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 9342.112

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 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
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 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9201.714  
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 2.612088236D-09  
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 2.783167711D+00  
 BaF2 Gurvich,1996a pt1 p569 pt2 p432.  
 2 tpis96 BA 1.00F 2.00 0.00 0.00 0.00 0 175.32381 -  
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 13437.017  
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 8731.105  
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 1.802974829D-05  
 1.133031115D-08-2.865589059D-12 2.097478889D+04  
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 8731.105  
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 -1.052342502D-10 1.111101879D-14 -8.954070380D+04  
 1.182377538D+02  
 BaI Gurvich,1996a pt1 p581 pt2 p440.  
 2 tpis96 BA 1.00I 1.00 0.00 0.00 0.00 0 264.23147 -  
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 10397.125

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1.741605400D-10-3.370062760D-14 -2.636169733D+03  
8.201924680D+00  
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10397.125  
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2 tpi96 BA 1.00I 2.00 0.00 0.00 0.00 0 391.13594 -  
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15790.435  
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BaO Gurvich,1996a pt1 p550 pt2 p419.  
3 tpi96 BA 1.00O 1.00 0.00 0.00 0.00 0 153.32640 -  
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6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
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 Be Hf:Cox,1989. Kramida,1997. Gordon,1999.  
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 -2.273387650D-12 1.196838345D-17 1.866686325D+06-  
 3.752337400D+02  
 Be+ Moore,1971. Moore,1970a. Gordon,1999.  
 3 g 1/98 BE 1.00E -1.00 0.00 0.00 0.00 0 9.01163  
 1229701.328  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 1.471528569D+05  
 2.839228698D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 -9.478135980D+04 2.768325398D+02 2.191388413D+00 1.648824289D-04-  
 4.280166820D-08  
 4.542350470D-12-6.270417825D-17 1.453850986D+05  
 5.055503840D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 -2.321269508D+08 1.525464518D+05-3.651092580D+01 4.812692090D-03-  
 2.928878120D-07

8.899649840D-12-1.055676610D-16 -1.052744318D+06  
 3.402173130D+02  
 Be++ Moore,1970a. Gordon,1999.  
 3 g 3/97 BE 1.00E -2.00 0.00 0.00 0.00 0 9.01108  
 2993001.528  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 3.592279160D+05  
 2.145990203D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 3.592279160D+05  
 2.145990203D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 3.592279160D+05  
 2.145990203D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 3.592279160D+05  
 2.145990203D+00  
 BeBr Gurvich,1996a pt1 p374 pt2 p300.  
 2 tpi96 BE 1.00BR 1.00 0.00 0.00 0.00 0 88.91618  
 132446.308  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8971.108  
 3.746288060D+04-4.722339070D+02 5.039409040D+00 5.798853220D-04-  
 1.937634343D-06  
 1.793372625D-09-5.672295580D-13 1.723135679D+04-  
 2.573912886D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8971.108  
 8.217238140D+05-2.850509348D+03 8.017266020D+00-2.105663212D-03  
 6.849136340D-07  
 -9.989129320D-11 5.192456840D-15 3.229372870D+04-  
 2.326810811D+01  
 BeBr2 Gurvich,1996a pt1 p377 pt2 p302.  
 2 tpi96 BE 1.00BR 2.00 0.00 0.00 0.00 0 168.82018 -  
 234062.499  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12837.501  
 -2.118698678D+04 2.090382611D+02 3.731171310D+00 1.115501549D-02-  
 1.542821761D-05  
 1.052354444D-08-2.850006057D-12 -3.090456277D+04  
 9.458917720D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12837.501  
 -1.041331811D+05-1.543443092D+02 7.614465410D+00-4.556700630D-05  
 1.003180548D-08  
 -1.146879501D-12 5.301795380D-17 -2.984527608D+04-  
 1.149360980D+01  
 BeCL Gurvich,1996a pt1 p369, pt2 p295.  
 2 tpi96 BE 1.00CL 1.00 0.00 0.00 0.00 0 44.46488  
 56693.107  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8861.107  
 2.016138947D+04-1.413988978D+02 2.898223773D+00 6.069925510D-03-  
 9.162038470D-06

6.612620660D-09-1.859126853D-12 6.626691440D+03  
 7.900170930D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8861.107  
 2.808845146D+05-1.103100122D+03 5.671189830D+00-5.443000450D-04  
 1.459036606D-07  
 -1.230971735D-11 9.900804760D-17 1.224649804D+04-  
 8.382381490D+00  
 BeCL2 Gurvich,1996a pt1 p373 pt2 p298.  
 2 tpris96 BE 1.00CL 2.00 0.00 0.00 0.00 0 79.91758 -  
 361539.140  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12080.860  
 -2.229957657D+04 1.528781667D+02 3.714994710D+00 1.067776550D-02-  
 1.397766942D-05  
 9.066693560D-09-2.350292311D-12 -4.590428230D+04  
 6.682544310D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12080.860  
 -1.154087460D+05-2.484300053D+02 7.685672140D+00-7.444960370D-05  
 1.649479787D-08  
 -1.895997075D-12 8.804973950D-17 -4.468747280D+04-  
 1.500338533D+01  
 BeF Gurvich,1996a pt1 p363, pt2 p291.  
 2 tpris96 BE 1.00F 1.00 0.00 0.00 0.00 0 28.01059 -  
 170624.795  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8711.105  
 -4.664497230D+04 7.887178850D+02-1.463363201D+00 1.381790494D-02-  
 1.591299964D-05  
 9.352931520D-09-2.229211181D-12 -2.522627476D+04  
 3.197634300D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8711.105  
 -1.857941543D+05 4.776082770D+01 4.269986020D+00 2.310668473D-04-  
 6.657214920D-08  
 1.152149888D-11-6.335586440D-16 -2.257950960D+04-  
 2.184787270D-01  
 BeF2 Gurvich,1996a pt1 p366 pt2 p293.  
 2 tpris96 BE 1.00F 2.00 0.00 0.00 0.00 0 47.00899 -  
 796588.236  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10879.764  
 7.490270240D+03-2.878053102D+02 5.434712820D+00 3.903233460D-03-  
 2.214865601D-06  
 -1.965806119D-10 4.042362270D-13 -9.591615640D+04-  
 5.616616920D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10879.764  
 -6.482018070D+04-7.684556060D+02 8.062860840D+00-2.227502549D-04  
 4.891598660D-08  
 -5.587886720D-12 2.583409761D-16 -9.395495490D+04-  
 2.125660266D+01  
 BeH Gurvich,1996a pt1 p356, pt2 p286.  
 2 tpris96 BE 1.00H 1.00 0.00 0.00 0.00 0 10.02012  
 342252.104  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8648.104  
 -1.615149125D+03-5.935286080D+01 4.507269100D+00-5.264189610D-03  
 1.145319967D-05

-9.247883590D-09 2.700364753D-12 4.030193040D+04-  
 3.485117050D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8648.104  
 -2.424081636D+06 6.597398460D+03-3.626316480D+00 4.579634350D-03-  
 1.163329056D-06  
 1.297785691D-10-5.291885810D-15 -2.489846221D+03  
 5.216018690D+01  
 BeH+ Chase,1998 p391 9/66.  
 3 g 1/01 BE 1.00H 1.00E -1.00 0.00 0.00 0 10.01957  
 1178218.951  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8643.951  
 -3.220611020D+04 2.520229596D+02 3.207719570D+00-2.191287290D-03  
 6.902534490D-06  
 -5.769522630D-09 1.656414969D-12 1.392530660D+05  
 3.307044770D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8643.951  
 4.622341590D+05-1.760169629D+03 5.379905550D+00 2.742462444D-05-  
 1.167208170D-07  
 3.557177910D-11-2.569695765D-15 1.515859734D+05-  
 1.369222641D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8643.951  
 2.282300776D+08-1.214880850D+05 2.642762928D+01-1.410369386D-03  
 3.776812140D-08  
 6.975949060D-14-1.287263021D-17 1.127119075D+06-  
 2.060147218D+02  
 BeH2 Martin,1992. Martin,1997.  
 2 g 4/01 BE 1.00H 2.00 0.00 0.00 0.00 0 11.02806  
 161098.903  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9219.103  
 9.065314900D+04-1.320657220D+03 9.901308060D+00-1.255772231D-02  
 2.205704068D-05  
 -1.633609388D-08 4.505103240D-12 2.464561869D+04-  
 3.635826750D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9219.103  
 6.074262010D+05-3.407534250D+03 9.792370360D+00-8.254614820D-04  
 1.915656246D-07  
 -1.962774813D-11 8.929908660D-16 3.793105200D+04-  
 4.254653580D+01  
 BeI Gurvich,1996a pt1 p378, pt2 p303.  
 2 tpi96 BE 1.00I 1.00 0.00 0.00 0.00 0 135.91665  
 207454.309  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9089.109  
 3.530054810D+04-5.190950260D+02 5.714505240D+00-1.409073640D-03  
 7.664772120D-07  
 -2.601945105D-11-8.230960640D-14 2.637903657D+04-  
 5.140997840D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9089.109  
 -5.328206620D+05 1.139497861D+03 3.629171660D+00 1.704033769D-04  
 1.067048688D-07  
 -3.589457880D-11 2.722769560D-15 1.585474307D+04  
 9.370951270D+00  
 BeI2 Gurvich,1996a pt1 p380 pt2 p305.

2 tpis96 BE 1.00I 2.00 0.00 0.00 0.00 0 262.82112 -  
 64759.451  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13440.549  
 3.592726180D+02-4.866059010D+01 5.241571180D+00 7.830305060D-03-  
 1.169525374D-05  
 8.389583910D-09-2.356636003D-12 -9.333220920D+03  
 2.896318281D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13440.549  
 -9.392372840D+04-8.959214380D+01 7.565554790D+00-2.577727326D-05  
 5.614265330D-09  
 -6.359663850D-13 2.917080336D-17 -9.814768620D+03-  
 9.032042810D+00  
 BeN Chase,1998 p403.  
 2 j 6/63 BE 1.00N 1.00 0.00 0.00 0.00 0 23.01892  
 42700.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8725.221  
 -4.247783630D+04 7.590188900D+02-1.561469235D+00 1.496945721D-02-  
 1.835608880D-05  
 1.146861461D-08-2.897470581D-12 4.683003320D+04  
 3.256974020D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8725.221  
 -5.909696160D+04-3.078649431D+02 4.727959150D+00-3.928158830D-05  
 2.006201069D-08  
 -2.300018068D-12 1.066101831D-16 5.156095710D+04-  
 3.031378018D+00  
 BeO Gurvich,1996a pt1 p351, pt2 p280.  
 3 tpis96 BE 1.00O 1.00 0.00 0.00 0.00 0 25.01158  
 128940.304  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8688.104  
 -4.869458320D+04 7.213473620D+02-3.784157320D-01 8.792203850D-03-  
 7.070151260D-06  
 2.250175620D-09-2.799117872D-14 1.101466639D+04  
 2.574081184D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8688.104  
 -3.503472450D+07 1.055859473D+05-1.165011722D+02 6.477369480D-02-  
 1.649656058D-05  
 2.005558400D-09-9.426891790D-14 -6.570018000D+05  
 8.640898030D+02  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8688.104  
 -7.440106320D+07 4.309665300D+04-1.019586064D-01 2.617209088D-04-  
 2.461810861D-08  
 1.124733698D-12-1.832802285D-17 -3.402379380D+05  
 4.487040230D+01  
 BeOH Gurvich,1996a pt1 p358 pt2 p288.  
 2 tpis96 BE 1.00O 1.00H 1.00 0.00 0.00 0 26.01952 -  
 99717.721  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10798.450  
 -3.853024520D+04 4.498059290D+02 1.532096459D+00 1.299912603D-02-  
 1.708979996D-05  
 1.169968182D-08-3.163183710D-12 -1.559046567D+04  
 1.545542930D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10798.450

8.550330310D+05-2.646537838D+03 8.204784630D+00 1.110814513D-05-  
 4.265364000D-08  
 7.926511920D-12-4.645419520D-16 3.121216271D+03-  
 2.571641308D+01  
 BeOH+ Chase,1998 p393.  
 3 j12/75 BE 1.000 1.00H 1.00E -1.00 0.00 0 26.01897  
 759983.920  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9550.904  
 7.106119160D+04-8.068981600D+02 5.603107810D+00 4.932070860D-03-  
 7.722847160D-06  
 5.910889810D-09-1.695201901D-12 9.440782420D+04-  
 1.088099852D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9550.904  
 8.134874390D+05-2.814653683D+03 8.381145010D+00-6.942073280D-05-  
 2.369535806D-08  
 5.678106380D-12-3.583253560D-16 1.073129932D+05-  
 2.901093335D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9550.904  
 -6.279111750D+06 2.090044240D+03 7.025559910D+00 5.492111300D-05-  
 3.446137200D-09  
 1.115947764D-13-1.461494242D-18 6.914837000D+04-  
 1.732443156D+01  
 Be(OH)2 Gurvich,1996a pt1 p360 pt2 p290.  
 2 tpis96 BE 1.000 2.00H 2.00 0.00 0.00 0 43.02686 -  
 638864.416  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15225.858  
 7.863089830D+03-7.397142250D+02 1.043303334D+01 4.514249530D-03-  
 6.950601530D-06  
 5.777030040D-09-1.727199382D-12 -7.585676960D+04-  
 3.301466610D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15225.858  
 1.722889403D+06-5.242477190D+03 1.486877785D+01 3.931498360D-05-  
 8.920276310D-08  
 1.630912925D-11-9.505371140D-16 -4.642823840D+04-  
 6.476804020D+01  
 BeS Gurvich,1996a pt1 p381 pt2 p307.  
 2 tpis96 BE 1.00S 1.00 0.00 0.00 0.00 0 41.07818  
 247095.306  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8780.106  
 -7.390579080D+03 2.828134792D+02 6.552019400D-01 1.076012495D-02-  
 1.398380157D-05  
 8.818418890D-09-2.110588578D-12 2.751593294D+04  
 1.980497213D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8780.106  
 -1.655708361D+07 5.431466120D+04-6.351859250D+01 3.964091990D-02-  
 1.078978696D-05  
 1.394030343D-09-6.936955040D-14 -3.121559628D+05  
 4.803455300D+02  
 Be2 Gurvich,1996a pt1 p346 pt2 p277.  
 2 tpis96 BE 2.00 0.00 0.00 0.00 0.00 0 18.02436  
 637543.318  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9838.118

-1.580873810D+05 2.035567774D+03-3.691580630D+00 1.028818435D-02-  
 9.603854510D-06  
 4.707519420D-09-9.374688790D-13 6.526968370D+04  
 4.879324990D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9838.118  
 1.010034484D+05 1.414207488D+02 2.292070182D+00 1.543331824D-04-  
 5.801043000D-08  
 1.003129697D-11-5.682818340D-16 7.550139730D+04  
 1.238758616D+01  
 Be2CL4 Gurvich,1996a pt1 p374 pt2 p299.  
 2 tpi96 BE 2.00CL 4.00 0.00 0.00 0.00 0 159.83516 -  
 819604.973  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22641.384  
 1.216152589D+05-2.000824823D+03 1.723384275D+01 5.810448280D-03-  
 1.362970089D-05  
 1.156602362D-08-3.552255800D-12 -9.206475470D+04-  
 6.137960900D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22641.384  
 -3.354920080D+05-2.316199283D+02 1.617047912D+01-6.734405950D-05  
 1.472073032D-08  
 -1.672352806D-12 7.688773970D-17 -1.031075197D+05-  
 5.047010500D+01  
 Be2F4 Gurvich,1996a pt1 p368 pt2 p294.  
 2 tpi96 BE 2.00F 4.00 0.00 0.00 0.00 0 94.01798 -  
 1731699.842  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19834.508  
 -6.327701870D+03-6.902533720D+01 5.470937230D+00 3.097341347D-02-  
 4.094310060D-05  
 2.668113685D-08-6.942909560D-12 -2.105979269D+05-  
 2.073546195D-01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19834.508  
 -3.681834950D+05-9.439191480D+02 1.670099855D+01-2.797974015D-04  
 6.178061720D-08  
 -7.083080190D-12 3.282791040D-16 -2.089045725D+05-  
 6.092665760D+01  
 Be2O Gurvich,1996a pt1 p353 pt2 p282.  
 2 tpi96 BE 2.00O 1.00 0.00 0.00 0.00 0 34.02376 -  
 37033.803  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11190.386  
 -4.263673570D+02-1.159556261D+02 4.082677770D+00 1.015885064D-02-  
 1.326015538D-05  
 8.488955360D-09-2.168039077D-12 -5.362258120D+03  
 1.253737886D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11190.386  
 -1.412646378D+05-3.498644590D+02 7.760932680D+00-1.044953518D-04  
 2.313342334D-08  
 -2.657722263D-12 1.233820439D-16 -5.172385490D+03-  
 1.854887619D+01  
 Be2OF2 Chase,1998 p417.  
 2 j 6/66 BE 2.00O 1.00F 2.00 0.00 0.00 0 72.02057 -  
 1204574.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16584.874

-2.783491921D+04 1.782881461D+02 4.094251360D+00 2.270142496D-02-  
 2.672688189D-05  
 1.572575618D-08-3.736070580D-12 -1.480081903D+05  
 7.353494770D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16584.874  
 -2.281826506D+05-1.130355396D+03 1.383400563D+01-3.316080640D-04  
 7.304921010D-08  
 -8.362704380D-12 3.872184980D-16 -1.431390587D+05-  
 4.739150230D+01  
 Be202 Gurvich,1996a pt1 p354 pt2 p283.  
 2 tpris96 BE 2.000 2.00 0.00 0.00 0.00 0 50.02316 -  
 411635.309  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10928.932  
 -3.031719530D+04 1.163353177D+03-8.733155950D+00 5.372002930D-02-  
 7.279439190D-05  
 4.894928250D-08-1.312147056D-11 -5.546936880D+04  
 6.953282640D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10928.932  
 -3.960576640D+05-9.074948830D+02 1.067160422D+01-2.670905218D-04  
 5.877629990D-08  
 -6.718664090D-12 3.105949075D-16 -4.861114330D+04-  
 3.616546890D+01  
 Be303 Gurvich,1996a pt1 p355 pt2 p284.  
 2 tpris96 BE 3.000 3.00 0.00 0.00 0.00 0 75.03475 -  
 1023720.628  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15125.733  
 -2.738072346D+04 8.743832600D+02-6.599606120D+00 6.533021140D-02-  
 8.762305740D-05  
 5.817244790D-08-1.540600500D-11 -1.284679012D+05  
 5.837203120D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15125.733  
 -5.890809360D+05-1.392823588D+03 1.703450699D+01-4.127330740D-04  
 9.107529150D-08  
 -1.043465231D-11 4.833053770D-16 -1.219045534D+05-  
 7.000614510D+01  
 Be404 Gurvich,1996a pt1 p356 pt2 p285.  
 2 tpris96 BE 4.000 4.00 0.00 0.00 0.00 0 100.04633 -  
 1649294.582  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15833.899  
 -6.893255640D+04 1.687565069D+03-1.479616594D+01 1.007319774D-01-  
 1.291057622D-04  
 8.243136760D-08-2.111283987D-11 -2.072877151D+05  
 1.002507262D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15833.899  
 -8.841338460D+05-2.726394165D+03 2.402941774D+01-8.114675460D-04  
 1.794255972D-07  
 -2.059359498D-11 9.552905330D-16 -1.923710587D+05-  
 1.136620750D+02  
 Br Hf:Cox,1989. Moore,1971. Moore,1970a. Gordon,1999.  
 3 g 3/97 BR 1.00 0.00 0.00 0.00 0.00 0 79.90400  
 111870.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428



-3.700293910D+03 6.145215420D+01 2.092120721D+00 1.376818870D-03-  
 2.445566658D-06  
 2.050975161D-09-5.144249091D-13 1.242508647D+04  
 8.996166200D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 -4.789717400D+06 1.692051999D+04-2.024085357D+01 1.395620355D-02-  
 3.656230560D-06  
 4.489781000D-10-2.122507526D-14 -9.207054960D+04  
 1.661695929D+02  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 -1.240248003D+08 7.034034730D+04-1.023087313D+01 1.373755814D-03-  
 7.476473480D-08  
 2.160883187D-12-2.659054603D-17 -5.563101070D+05  
 1.226657143D+02  
 Br+ Moore,1971. Moore,1970a. Gordon,1999.  
 3 g10/97 BR 1.00E -1.00 0.00 0.00 0.00 0 79.90345  
 1257927.034  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.434  
 3.981187420D+04-4.751581470D+02 4.734578980D+00-5.169324790D-03  
 5.905857520D-06  
 -2.885129283D-09 5.054894290D-13 1.529052046D+05-  
 5.769283220D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.434  
 1.741149829D+06-5.455465670D+03 8.470663350D+00-2.683465574D-03  
 6.590454560D-07  
 -7.953770300D-11 3.735898818D-15 1.851781643D+05-  
 3.637909030D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.434  
 -6.174903280D+07 3.641704160D+04-5.739744680D+00 1.067497350D-03-  
 7.127689890D-08  
 2.155618820D-12-1.769476126D-17 -1.399767498D+05  
 7.931577700D+01  
 Br- Hotop,1985. Gordon,1999.  
 3 g10/97 BR 1.00E 1.00 0.00 0.00 0.00 0 79.90455 -  
 219000.472  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.708492743D+04  
 5.419556170D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.708492743D+04  
 5.419556170D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.708492743D+04  
 5.419556170D+00  
 BrCL Gurvich,1989 pt1 p213 pt2 p112.  
 2 tpi89 BR 1.00CL 1.00 0.00 0.00 0.00 0 115.35670  
 14789.113

200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9407.113  
 1.653291583D+04-3.578769280D+02 5.700622160D+00-2.201257188D-03  
 2.415146969D-06  
 -1.371032976D-09 3.227803420D-13 2.252619279D+03-  
 4.155663570D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9407.113  
 -1.284863067D+05-1.138379626D+03 7.964040800D+00-3.438056670D-03  
 1.524999514D-06  
 -2.761469114D-10 1.694450407D-14 5.938264260D+03-  
 1.925044779D+01  
 BrF Gurvich,1989 pt1 p208 pt2 p109.  
 2 tpis89 BR 1.00F 1.00 0.00 0.00 0.00 0 98.90240 -  
 58851.445  
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 9021.108  
 3.836143190D+04-5.184611970D+02 5.458327050D+00-5.656843100D-04-  
 4.121311970D-07  
 7.859913480D-10-3.036161520D-13 -5.595539910D+03-  
 4.901129500D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9021.108  
 3.771388470D+06-1.267493430D+04 2.080555930D+01-1.026359360D-02  
 3.308203590D-06  
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 1.130253600D+02  
 BrF3 Gurvich,1989 pt1 p211 pt2 p110.  
 2 tpis89 BR 1.00F 3.00 0.00 0.00 0.00 0 136.89921 -  
 255600.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14711.620  
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 6.982030260D-06  
 -3.242757960D-09 6.164751460D-13 -2.345341551D+04-  
 5.522633600D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14711.620  
 -1.886532240D+05-8.245232970D+01 1.006180694D+01-2.477319092D-05  
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 2.298937369D+01  
 BrF5 Gurvich,1989 pt1 p212 pt2 p111.  
 2 tpis89 BR 1.00F 5.00 0.00 0.00 0.00 0 174.89602 -  
 428800.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19174.543  
 2.211366805D+05-4.024809220D+03 2.734900212D+01-1.832254979D-02  
 1.721754649D-05  
 -8.753508630D-09 1.860196959D-12 -3.537447670D+04-  
 1.244296466D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19174.543  
 -3.757647640D+05-1.575896472D+02 1.611869838D+01-4.776497800D-05  
 1.059755365D-08  
 -1.218527723D-12 5.657535450D-17 -5.667266800D+04-  
 5.540839310D+01  
 BrO Chase,1996a.  
 2 j 3/96 BR 1.00O 1.00 0.00 0.00 0.00 0 95.90340  
 125800.000

200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9061.000  
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 2.527867438D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9061.000  
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 7.569536840D-07  
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 5.361048360D+01  
 OBrO Chase,1996a.  
 2 j 3/96 BR 1.000 2.00 0.00 0.00 0.00 0 111.90280  
 151954.526  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11394.630  
 3.470213230D+04-3.401341820D+02 3.932251620D+00 1.215938586D-02-  
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 6.361235180D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11394.630  
 -1.624504660D+05-1.453689372D+02 7.105822130D+00-4.141362070D-05  
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 9.111817920D+00  
 BrOO Chase,1996a.  
 2 j 3/96 BR 1.000 2.00 0.00 0.00 0.00 0 111.90280  
 108000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12850.660  
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 1.607446878D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12850.660  
 6.172483480D+03-6.585049660D+02 7.483955330D+00-1.920530746D-04  
 4.226946170D-08  
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 9.850380240D+00  
 BrO3 Chase,1996a.  
 2 j 3/96 BR 1.000 3.00 0.00 0.00 0.00 0 127.90220  
 220820.685  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13100.841  
 1.063901881D+05-1.501928813D+03 9.703657430D+00 8.133000760D-03-  
 1.531857845D-05  
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 2.735125430D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13100.841  
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 2 tpis89 BR 2.00 0.00 0.00 0.00 0.00 0 159.80800  
 30910.000

200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9725.117  
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 2.932401703D-06  
 -1.954889514D-09 5.312307890D-13 3.521475050D+03-  
 1.964151570D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9725.117  
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 2.754164226D-07  
 -6.217506760D-11 7.375341620D-15 -7.036584160D+04  
 7.878478020D+01  
 BrBrO Chase,1996a.  
 2 j 3/96 BR 2.000 1.00 0.00 0.00 0.00 0 175.80740  
 168000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13137.498  
 1.617498037D+04-2.464406776D+02 5.912858450D+00 4.980354280D-03-  
 8.099958250D-06  
 6.072776260D-09-1.753715313D-12 1.974012093D+04  
 2.009704963D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13137.498  
 -8.537101750D+04-6.487046070D+01 7.047159350D+00-1.843088186D-05  
 3.992267860D-09  
 -4.500687950D-13 2.055867395D-17 1.821566655D+04-  
 3.162186125D+00  
 BrOBr Chase,1996a.  
 2 j 3/96 BR 2.000 1.00 0.00 0.00 0.00 0 175.80740  
 107639.006  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12399.058  
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 3.913701070D-06  
 -1.805444867D-09 3.366132550D-13 1.642921537D+04-  
 2.350319399D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12399.058  
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 2.576958549D-09  
 -2.941186078D-13 1.357198784D-17 1.076942321D+04-  
 5.697779380D+00  
 C Hf:Douglas,1955. Moore,1970b. Gordon,1999.  
 3 g 7/97 C 1.00 0.00 0.00 0.00 0.00 0 12.01070  
 716680.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6535.895  
 6.495031470D+02-9.649010860D-01 2.504675479D+00-1.281448025D-05  
 1.980133654D-08  
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 4.747924288D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6535.895  
 -1.289136472D+05 1.719528572D+02 2.646044387D+00-3.353068950D-04  
 1.742092740D-07  
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 4.130047418D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6535.895  
 4.432528010D+08-2.886018412D+05 7.737108320D+01-9.715281890D-03  
 6.649595330D-07

-2.230078776D-11 2.899388702D-16 2.355273444D+06-  
 6.405123160D+02  
 C+ Moore,1970b. Gordon,1999.  
 3 g 6/98 C 1.00E -1.00 0.00 0.00 0.00 0 12.01015  
 1809444.482  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6649.282  
 2.258535929D+03-1.574575687D+00 2.503637730D+00-5.202878370D-06  
 4.516908390D-09  
 -2.181431053D-12 4.495047033D-16 2.168951913D+05  
 4.345699505D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6649.282  
 1.255112551D+04-3.411874670D+01 2.543383218D+00-2.805120849D-05  
 9.751641970D-09  
 -1.736855394D-12 1.246191931D-16 2.171001786D+05  
 4.063913515D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6649.282  
 5.618135320D+05-6.047058900D+03 5.884541470D+00-7.211894530D-04  
 6.823484110D-08  
 -2.599878590D-12 3.633868358D-17 2.581370458D+05-  
 2.280019759D+01  
 C- Hotop,1985. Gordon,1999.  
 3 g 3/98 C 1.00E 1.00 0.00 0.00 0.00 0 12.01125  
 588314.236  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6218.836  
 4.671291530D+00-1.986169369D-03 2.500008638D+00-1.976750928D-08  
 2.478947477D-11  
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 4.879570141D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6218.836  
 4.253175720D+00 5.778186480D-04 2.499999424D+00 2.836136231D-10-  
 7.327253420D-14  
 9.478507810D-18-4.830487320D-22 7.001217170D+04  
 4.879624211D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
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 1.223289007D+01-5.196185830D-03 2.500001344D+00-1.743497251D-10  
 1.206609009D-14  
 -4.252419790D-19 5.992333270D-24 7.001221630D+04  
 4.879608421D+00  
 CBr Gurvich,1991 pt1 p157 pt2 p137.  
 2 tpris91 C 1.00BR 1.00 0.00 0.00 0.00 0 91.91470  
 490431.816  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9615.116  
 4.324446880D+03-1.596366559D+02 4.857856590D+00-4.389439160D-04  
 4.408863630D-07  
 -2.281330618D-10 5.445618220D-14 5.847677250D+04  
 1.351169646D-01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9615.116  
 1.021862102D+06-3.243484360D+03 8.388226560D+00-2.242155508D-03  
 6.988355370D-07  
 -9.719134370D-11 4.716976240D-15 7.805924060D+04-  
 2.518386915D+01  
 CBr2 Gurvich,1991 pt1 p159 pt2 p138.

2 tpis91 C 1.00BR 2.00 0.00 0.00 0.00 0 171.81870  
 336623.319  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12196.819  
 7.248197840D+04-1.128261230D+03 9.822303380D+00-3.872748100D-03  
 2.904819596D-06  
 -1.061380159D-09 1.297474642D-13 4.437771600D+04-  
 2.361121795D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12196.819  
 -7.441431410D+05 4.215427830D+02 8.796797740D+00-2.726562507D-03  
 1.336438546D-06  
 -2.304854483D-10 1.337493953D-14 3.364618140D+04-  
 1.599565135D+01  
 CBr3 Gurvich,1991 pt1 p160 pt2 p139.  
 2 tpis91 C 1.00BR 3.00 0.00 0.00 0.00 0 251.72270  
 235000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15582.455  
 8.563516260D+04-1.275764123D+03 1.117190031D+01 2.341705749D-03-  
 6.540671410D-06  
 5.736717140D-09-1.777823046D-12 3.243215890D+04-  
 2.766468801D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15582.455  
 -1.926498949D+05-1.324072178D+02 1.009808665D+01-3.895040820D-05  
 8.550445010D-09  
 -9.747493680D-13 4.494245590D-17 2.541576129D+04-  
 1.866868947D+01  
 CBr4 Kudchadker,1975.  
 2 g 8/99 C 1.00BR 4.00 0.00 0.00 0.00 0 331.62670  
 79500.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 20373.314  
 1.023083739D+05-1.735600709D+03 1.651317914D+01-3.147664747D-03  
 2.924135486D-07  
 1.360605681D-09-6.431758650D-13 1.500502543D+04-  
 5.536476760D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 20373.314  
 -2.059785072D+05-1.048517002D+02 1.307772550D+01-3.086857556D-05  
 6.775309810D-09  
 -7.721837540D-13 3.559218240D-17 5.615893940D+03-  
 3.283787630D+01  
 CCL Hf:Kumaran,1997. Gurvich,1991 pt1 p106 pt2 p81.  
 2 g 8/99 C 1.00CL 1.00 0.00 0.00 0.00 0 47.46340  
 432611.058  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9395.113  
 1.707070049D+04-1.463803497D+01 2.334108251D+00 7.202099130D-03-  
 1.034120045D-05  
 7.228106700D-09-1.985123755D-12 5.123350300D+04  
 1.200819438D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9395.113  
 5.900507630D+05-2.075311460D+03 6.880017230D+00-1.294796228D-03  
 3.883137980D-07  
 -5.006981630D-11 2.218229619D-15 6.358922050D+04-  
 1.610665420D+01  
 CCLBr3 Gurvich,1991 pt1 p171 pt2 p152.

2 tpi91 C 1.00CL 1.00BR 3.00 0.00 0.00 0 287.17540  
 65000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19568.242  
 1.021596752D+05-1.746281176D+03 1.598215634D+01-1.350975234D-03-  
 2.330039129D-06  
 3.201856270D-09-1.150412393D-12 1.341967771D+04-  
 5.285079200D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19568.242  
 -2.282709343D+05-1.277037936D+02 1.309470658D+01-3.763326710D-05  
 8.264715600D-09  
 -9.424237560D-13 4.345940760D-17 3.930463310D+03-  
 3.315414190D+01  
 CCL2 Hf:Kumaran,1997. Jacox,1994. Shin,1990.  
 2 g 8/99 C 1.00CL 2.00 0.00 0.00 0.00 0 82.91610  
 222940.147  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11422.758  
 7.509623150D+04-1.034728559D+03 8.061704540D+00 1.487134213D-03-  
 4.564817110D-06  
 3.954885810D-09-1.166197091D-12 3.052409293D+04-  
 1.739692777D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11422.758  
 -6.437455170D+06 1.958413353D+04-1.604038625D+01 1.238833906D-02-  
 3.013367274D-06  
 3.473468920D-10-1.553272793D-14 -9.961242160D+04  
 1.556949206D+02  
 CCL2Br2 Gurvich,1991 pt1 p170 pt2 p151.  
 2 tpi91 C 1.00CL 2.00BR 2.00 0.00 0.00 0 242.72410  
 10000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18691.912  
 1.018495619D+05-1.740854039D+03 1.521338304D+01 1.128256510D-03-  
 5.875405490D-06  
 5.659886970D-09-1.821576512D-12 6.918572190D+03-  
 5.015386190D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18691.912  
 -2.553347012D+05-1.598005477D+02 1.311860930D+01-4.717443870D-05  
 1.036912808D-08  
 -1.183321687D-12 5.460612690D-17 -2.588636980D+03-  
 3.461705690D+01  
 CCL3 Hf:Hudgens,1991. TRC(12/93) tuv7270.  
 2 n12/93 C 1.00CL 3.00 0.00 0.00 0.00 0 118.36880  
 71128.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14400.000  
 3.414471650D+04-5.547969730D+02 6.845544390D+00 1.242006495D-02-  
 2.036896881D-05  
 1.554979993D-08-4.568940110D-12 9.388568820D+03-  
 7.143609870D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14400.000  
 -5.427572540D+05 6.809020620D+02 9.047723620D+00 1.324277766D-04  
 6.301263040D-08  
 -2.656639200D-11 2.105668053D-15 3.866216150D+02-  
 1.528746989D+01  
 CCL3Br Gurvich,1991 pt1 p169 pt2 p150.

2 tpi91 C 1.00CL 3.00BR 1.00 0.00 0.00 0 198.27280 -  
 43000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17984.549  
 1.049668463D+05-1.793828482D+03 1.489250892D+01 2.397128310D-03-  
 7.789615470D-06  
 7.016617110D-09-2.196069746D-12 9.101349310D+02-  
 5.058348820D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17984.549  
 -2.772324186D+05-1.840310333D+02 1.313673812D+01-5.443910010D-05  
 1.197658923D-08  
 -1.367818632D-12 6.316164790D-17 -8.895857690D+03-  
 3.669528890D+01  
 CCL4 Gurvich,1991 pt1 p111 pt2 p84.  
 2 tpi91 C 1.00CL 4.00 0.00 0.00 0.00 0 153.82150 -  
 95600.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17158.512  
 1.093385626D+05-1.861731846D+03 1.449632467D+01 3.949485160D-03-  
 1.010805379D-05  
 8.645514170D-09-2.642368852D-12 -4.948006230D+03-  
 5.180285920D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17158.512  
 -3.043078255D+05-2.168170491D+02 1.316132386D+01-6.431124890D-05  
 1.416482497D-08  
 -1.619343320D-12 7.483974350D-17 -1.512320070D+04-  
 3.996845470D+01  
 CF Hf:TRC(6/88) w6950. Gurvich,1991 pt1 p74 pt2 p55.  
 2 tpi91 C 1.00F 1.00 0.00 0.00 0.00 0 31.00910  
 242300.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9065.109  
 -4.582786680D+04 7.972635890D+02-1.364936319D+00 1.312359375D-02-  
 1.457012892D-05  
 8.253276680D-09-1.896351845D-12 2.438259620D+04  
 3.248065280D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9065.109  
 -1.329807100D+05-1.214340891D+02 4.452413620D+00 1.293786948D-04-  
 3.670550590D-08  
 6.590212390D-12-3.731261610D-16 2.815934108D+04-  
 6.640468730D-01  
 CF+ Chase,1998 p579 12/70.  
 2 g12/99 C 1.00F 1.00E -1.00 0.00 0.00 0 31.00855  
 1145564.099  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8697.499  
 -5.975213200D+04 9.276863650D+02-1.866581982D+00 1.384340912D-02-  
 1.513428860D-05  
 8.518556340D-09-1.959577655D-12 1.323519410D+05  
 3.412013190D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8697.499  
 -8.053762780D+04-3.390275090D+02 4.708373500D+00-3.963148310D-05  
 2.497996218D-08  
 -5.236790430D-12 5.313949130D-16 1.381337068D+05-  
 3.920514730D+00  
 CFBr3 Gurvich,1991 pt1 p166 pt2 p146.



2 tpis91 C 1.00F 1.00BR 3.00 0.00 0.00 0 270.72110 -  
 120000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18243.104  
 5.149244280D+04-9.364796640D+02 1.044260886D+01 1.205370047D-02-  
 1.876290291D-05  
 1.344488618D-08-3.730545760D-12 -1.243246293D+04-  
 2.363948551D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18243.104  
 -2.729158956D+05-3.328164650D+02 1.324822519D+01-9.927077540D-05  
 2.193640054D-08  
 -2.515424945D-12 1.165680878D-16 -1.730185479D+04-  
 3.626818430D+01  
 CFCL Hf:Gurvich,1991 pt1 p135 pt2 p107. Jacox,1994.  
 2 g 9/99 C 1.00F 1.00CL 1.00 0.00 0.00 0 66.46180  
 25845.774  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10902.382  
 1.541997945D+04-8.274039810D+01 2.501701822D+00 1.390738086D-02-  
 1.895734700D-05  
 1.261934581D-08-3.333453820D-12 2.411755114D+03  
 1.331516417D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10902.382  
 -2.681630077D+05-2.328091539D+00 6.834633830D+00 1.565270633D-04-  
 5.967755160D-08  
 9.820924460D-12-5.058897210D-16 3.017669604D+02-  
 9.005091900D+00  
 CFCLBr2 Gurvich,1991 pt1 p175 pt2 p158.  
 2 tpis91 C 1.00F 1.00CL 1.00BR 2.00 0.00 0 226.26980 -  
 175000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17498.023  
 5.898799740D+04-1.050714861D+03 1.039349401D+01 1.273690622D-02-  
 1.999097478D-05  
 1.438204230D-08-4.000130350D-12 -1.837799602D+04-  
 2.417479330D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17498.023  
 -2.960811596D+05-3.531276200D+02 1.326346169D+01-1.053860298D-04  
 2.329085080D-08  
 -2.670979639D-12 1.237844667D-16 -2.387594306D+04-  
 3.684977470D+01  
 CFCL2 Gurvich,1991 pt1 p138 pt2 p110.  
 2 tpis91 C 1.00F 1.00CL 2.00 0.00 0.00 0 101.91450 -  
 105000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13216.954  
 2.611398792D+04-3.353565900D+02 4.094673080D+00 1.960244711D-02-  
 2.762775193D-05  
 1.880124302D-08-5.047410300D-12 -1.251298871D+04  
 6.870873730D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13216.954  
 -2.653118323D+05-4.469724170D+02 1.033334881D+01-1.333673368D-04  
 2.948755634D-08  
 -3.383306200D-12 1.568746348D-16 -1.393160489D+04-  
 2.556818855D+01  
 CFCL2Br Gurvich,1991 pt1 p175 pt2 p157.

2 tpi91 C 1.00F 1.00CL 2.00BR 1.00 0.00 0 181.81850 -  
 235000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16730.573  
 6.529959220D+04-1.135235485D+03 1.009526872D+01 1.401380147D-02-  
 2.191705096D-05  
 1.573404132D-08-4.369340340D-12 -2.504488145D+04-  
 2.451093598D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16730.573  
 -3.215455050D+05-3.884129620D+02 1.328990796D+01-1.160048581D-04  
 2.564498787D-08  
 -2.941639768D-12 1.363542881D-16 -3.097421144D+04-  
 3.871357190D+01  
 CFCL3 Hf:TRC(6/89) w7350. Gurvich,1991 pt1 p140 pt2 p112.  
 2 g 7/99 C 1.00F 1.00CL 3.00 0.00 0.00 0 137.36720 -  
 283700.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16063.584  
 7.400174000D+04-1.252282466D+03 1.001327229D+01 1.475107601D-02-  
 2.315635251D-05  
 1.664207025D-08-4.622929960D-12 -3.020508601D+04-  
 2.708388070D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16063.584  
 -3.450464780D+05-4.177821450D+02 1.331196736D+01-1.248759531D-04  
 2.761391353D-08  
 -3.168207640D-12 1.468834601D-16 -3.674067190D+04-  
 4.156887040D+01  
 CF2 Hf:TRC(6/88) w6950. Jacox,1998.  
 2 g 9/99 C 1.00F 2.00 0.00 0.00 0 50.00751 -  
 186600.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10350.912  
 -3.797026270D+04 8.731800030D+02-3.460191570D+00 2.746253741D-02-  
 3.474621900D-05  
 2.204470693D-08-5.621750850D-12 -2.746797157D+04  
 4.456778070D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10350.912  
 -1.086428547D+05-5.854989140D+02 7.018648950D+00 3.929186150D-04-  
 2.603822675D-07  
 6.142196390D-11-4.172833260D-15 -2.152945157D+04-  
 1.356143285D+01  
 CF2+ Chase,1998 p583 12/70. Jacox,1994.  
 2 g 9/99 C 1.00F 2.00E -1.00 0.00 0.00 0 50.00696  
 949341.299  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10341.999  
 -2.892373827D+04 6.049354610D+02-9.721866660D-01 1.808478341D-02-  
 1.980065782D-05  
 1.101640055D-08-2.500457119D-12 1.102755670D+05  
 3.247591470D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10341.999  
 -6.488966070D+04-1.064283593D+03 7.785702100D+00-3.158347626D-04  
 7.130804080D-08  
 -8.533183590D-12 4.251638820D-16 1.178446465D+05-  
 1.819424707D+01  
 CF2Br2 Gurvich,1991 pt1 p166 pt2 p145.

2 tpis91 C 1.00F 2.00BR 2.00 0.00 0.00 0 209.81551 -  
 380000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16279.997  
 1.261404028D+04-2.815725114D+02 5.098032130D+00 2.502548939D-02-  
 3.438853190D-05  
 2.297615553D-08-6.080161430D-12 -4.642763750D+04  
 3.094167118D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16279.997  
 -3.327669300D+05-6.184352490D+02 1.346170049D+01-1.849172548D-04  
 4.092591340D-08  
 -4.699810430D-12 2.180811799D-16 -4.715186610D+04-  
 4.105369240D+01  
 CF2CL Gurvich,1991 pt1 p136 pt2 p108.  
 2 tpis91 C 1.00F 2.00CL 1.00 0.00 0.00 0 85.46021 -  
 275000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12432.273  
 8.914558350D+03-1.768816959D+01 1.607015025D+00 2.473626554D-02-  
 3.270738940D-05  
 2.126351830D-08-5.509831110D-12 -3.427306250D+04  
 1.929680163D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12432.273  
 -2.802346654D+05-6.860314850D+02 1.051143635D+01-2.046954963D-04  
 4.528897180D-08  
 -5.200229030D-12 2.412971450D-16 -3.308179480D+04-  
 2.874900312D+01  
 CF2CLBr Gurvich,1991 pt1 p173 pt2 p156.  
 2 tpis91 C 1.00F 2.00CL 1.00BR 1.00 0.00 0 165.36421 -  
 435000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15528.243  
 2.696699365D+04-4.678832270D+02 5.244809420D+00 2.530121349D-02-  
 3.508443520D-05  
 2.354353958D-08-6.246161130D-12 -5.198382730D+04  
 8.532860590D-01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15528.243  
 -3.592828840D+05-6.539283590D+02 1.348831524D+01-1.956099469D-04  
 4.329775970D-08  
 -4.972644370D-12 2.307575050D-16 -5.365141170D+04-  
 4.224914180D+01  
 CF2CL2 Hf:TRC(6/89) w7350.Gurvich,1991 pt1 p139 pt2 p111.  
 2 g 7/99 C 1.00F 2.00CL 2.00 0.00 0.00 0 120.91291 -  
 490800.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14881.094  
 3.841258750D+04-6.139499820D+02 5.269667190D+00 2.574105783D-02-  
 3.587376480D-05  
 2.411600130D-08-6.402236900D-12 -5.784541330D+04-  
 1.957462299D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14881.094  
 -3.827448550D+05-6.933774800D+02 1.351791274D+01-2.075114435D-04  
 4.594021610D-08  
 -5.276874600D-12 2.449037044D-16 -6.021527770D+04-  
 4.479580790D+01  
 CF3 Hf:TRC(6/88) w6950. Jacox,1998.

2 g 8/99 C 1.00F 3.00 0.00 0.00 0.00 0 69.00591 -  
 467400.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11491.470  
 -2.978307106D+04 7.153678830D+02-3.498185380D+00 3.595457990D-02-  
 4.507974430D-05  
 2.821808450D-08-7.098047020D-12 -6.059997030D+04  
 4.502592640D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11491.470  
 -2.997305557D+05-1.046989457D+03 1.077923191D+01-3.116087076D-04  
 6.891351430D-08  
 -7.911225640D-12 3.670593020D-16 -5.425304400D+04-  
 3.417038790D+01  
 CF3+ Chase,1998 p583 12/71. Jacox,1998.  
 2 g 9/99 C 1.00F 3.00E -1.00 0.00 0.00 0 69.00536  
 423617.480  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11541.280  
 -3.587463540D+04 3.743506700D+02 7.787413930D-01 1.929435768D-02-  
 1.892815770D-05  
 9.363908760D-09-1.885759656D-12 4.775581720D+04  
 2.224044005D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11541.280  
 -2.910919531D+04-1.996658183D+03 1.144279678D+01-5.653393040D-04  
 1.232297113D-07  
 -1.399758046D-11 6.443017950D-16 5.902345800D+04-  
 4.080349990D+01  
 CF3Br Gurvich,1991 pt1 p165 pt2 p144.  
 2 tpi91 C 1.00F 3.00BR 1.00 0.00 0.00 0 148.90991 -  
 648800.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14444.028  
 -5.439489010D+03 1.243615190D+02 9.231941950D-01 3.481044380D-02-  
 4.549645490D-05  
 2.932836552D-08-7.548000360D-12 -8.023396760D+04  
 2.232999096D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14444.028  
 -3.834088510D+05-9.719093300D+02 1.372477396D+01-2.901710612D-04  
 6.421892200D-08  
 -7.375688770D-12 3.423154250D-16 -7.765306310D+04-  
 4.717367210D+01  
 CF3CL Hf:TRC(6/89) w7350. Gurvich,1991 pt1 p137 pt2 p109.  
 2 g 7/99 C 1.00F 3.00CL 1.00 0.00 0.00 0 104.45861 -  
 704200.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13790.751  
 1.499409978D+04-1.365768572D+02 1.452912370D+00 3.404765070D-02-  
 4.473777640D-05  
 2.888115112D-08-7.434171330D-12 -8.547166640D+04  
 1.727326664D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13790.751  
 -4.066042120D+05-1.022626507D+03 1.376252628D+01-3.052722979D-04  
 6.755966040D-08  
 -7.759315250D-12 3.601192290D-16 -8.410559370D+04-  
 4.913412370D+01  
 CF4 Hf:TRC(12/94) w6520. Gurvich,1991 pt1 p79 pt2 p58.

2 g 7/99 C 1.00F 4.00 0.00 0.00 0.00 0 88.00431 -  
 933120.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12730.313  
 9.817458500D+03 1.163343483D+02-1.288338636D+00 3.959566910D-02-  
 4.996244210D-05  
 3.125339346D-08-7.841700320D-12 -1.138502297D+05  
 2.938656548D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12730.313  
 -4.164456780D+05-1.414797167D+03 1.405124837D+01-4.199093860D-04  
 9.278921610D-08  
 -1.064575830D-11 4.937099680D-16 -1.094691149D+05-  
 5.487105000D+01  
 CH Gurvich,1979 pt1 p37 pt2 p39.  
 3 tpis79 C 1.00H 1.00 0.00 0.00 0.00 0 13.01864  
 597370.604  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8625.104  
 2.220590133D+04-3.405411530D+02 5.531452290D+00-5.794964260D-03  
 7.969554880D-06  
 -4.465911590D-09 9.596338320D-13 7.240783270D+04-  
 9.107673050D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8625.104  
 2.060763440D+06-5.396206660D+03 7.856293850D+00-7.965907450D-04  
 1.764308305D-07  
 -1.976386267D-11 5.030429510D-16 1.062236592D+05-  
 3.154757439D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8625.104  
 -8.068368690D+08 4.575450540D+05-9.843975080D+01 1.235244098D-02-  
 8.485608570D-07  
 3.040410624D-11-4.400315170D-16 -3.595851590D+06  
 8.953477440D+02  
 CH+ Gurvich,1991 pt1 p38 pt2 p32.  
 3 tpis91 C 1.00H 1.00E -1.00 0.00 0.00 0 13.01809  
 1630571.004  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8628.104  
 3.019607105D+04-4.618141310D+02 6.225641190D+00-7.775711800D-03  
 1.094489485D-05  
 -6.675487910D-09 1.565232409D-12 1.972491928D+05-  
 1.431512811D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8628.104  
 -7.102094670D+06 1.828354883D+04-1.312691402D+01 6.191717360D-03-  
 2.909421253D-07  
 -1.134243575D-10 1.105962085D-14 7.541296040D+04  
 1.243984829D+02  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8628.104  
 -3.160070489D+08 1.436699396D+05-1.108443407D+01 1.562285754D-04  
 4.928498470D-08  
 -2.896872362D-12 4.982255990D-17 -1.013672855D+06  
 1.489353241D+02  
 CHBr3 Kudchadker,1975.  
 2 g 8/99 C 1.00H 1.00BR 3.00 0.00 0.00 0 252.73064  
 16740.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15906.601

4.346576860D+04-4.999634420D+02 5.620222110D+00 2.079346321D-02-  
 2.921336328D-05  
 2.066942448D-08-5.781220910D-12 2.627830062D+03  
 1.247904015D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15906.601  
 6.274234950D+05-3.378711100D+03 1.487852612D+01-5.932745270D-04  
 1.082421577D-07  
 -1.061012665D-11 4.319152450D-16 1.877234659D+04-  
 5.311909650D+01  
 CHCL Hf:TRC(12/93) w7270.Gurvich,1991. Jacox,1998.  
 2 g 9/99 C 1.00H 1.00CL 1.00 0.00 0.00 0 48.47134  
 297100.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10200.443  
 -2.699912334D+05 4.351199730D+03-2.275911813D+01 7.550621760D-02-  
 9.071997970D-05  
 5.256971860D-08-1.189769182D-11 1.416862680D+04  
 1.520980719D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10200.443  
 -9.548061900D+05 2.174413794D+03 4.867645370D+00 8.321641860D-04-  
 1.536948638D-07  
 1.529236537D-11-6.596159360D-16 1.880121810D+04  
 2.674752101D+00  
 CHCLBr2 Gurvich,1991 pt1 p173 pt2 p155.  
 2 tpis91 C 1.00H 1.00CL 1.00BR 2.00 0.00 0 208.27934  
 10000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15291.236  
 3.815380250D+04-4.084175110D+02 4.639244020D+00 2.325990646D-02-  
 3.222988860D-05  
 2.254671151D-08-6.256507740D-12 1.483809044D+03  
 6.175233120D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15291.236  
 6.042865300D+05-3.438241010D+03 1.494162631D+01-6.228427970D-04  
 1.153724426D-07  
 -1.147291377D-11 4.733482860D-16 1.822460958D+04-  
 5.407259140D+01  
 CHCL2 TRC(12/93) tuv7270.  
 2 n12/93 C 1.00H 1.00CL 2.00 0.00 0.00 0 83.92404  
 95800.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12800.000  
 5.638556130D+04-6.562455420D+02 6.068818020D+00 9.744122600D-03-  
 1.275310131D-05  
 8.552386720D-09-2.231582700D-12 1.330447798D+04-  
 4.533546180D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12800.000  
 8.849393710D+05-3.526969730D+03 1.186372153D+01-5.002376120D-04  
 6.133860400D-08  
 -1.885433405D-12-1.234221421D-16 3.071136475D+04-  
 4.088906930D+01  
 CHCL2Br Gurvich,1991 pt1 p172 pt2 p154.  
 2 tpis91 C 1.00H 1.00CL 2.00BR 1.00 0.00 0 163.82804  
 45000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14729.895

3.294022650D+04-3.275301170D+02 3.773235240D+00 2.536466143D-02-  
 3.472666990D-05  
 2.404666618D-08-6.621730930D-12 -5.425565080D+03  
 9.433406510D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14729.895  
 5.924876440D+05-3.509475610D+03 1.499349593D+01-6.433062570D-04  
 1.198581809D-07  
 -1.198476716D-11 4.969948070D-16 1.197251405D+04-  
 5.602688330D+01  
 CHCL3 Gurvich,1991 pt1 p127 pt2 p98.  
 2 g 7/99 C 1.00H 1.00CL 3.00 0.00 0.00 0 119.37674 -  
 102700.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14305.494  
 3.395333290D+04-3.047428785D+02 2.923672263D+00 2.830547858D-02-  
 3.712424690D-05  
 2.551365915D-08-6.987659550D-12 -1.235063157D+04  
 1.115555277D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14305.494  
 6.136052740D+05-3.715087170D+03 1.510777247D+01 2.362584336D-04  
 1.297140438D-07  
 -1.267494791D-11 5.259022310D-16 6.203313450D+03-  
 5.992577670D+01  
 CHF Hf:TRC(6/88) w695. Jacox,1998.  
 2 g 8/99 C 1.00H 1.00F 1.00 0.00 0.00 0 32.01704  
 108800.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9981.216  
 -7.868585830D+04 1.300218466D+03-3.947685250D+00 2.114995848D-02-  
 2.239962738D-05  
 1.283155181D-08-2.904778136D-12 5.824389720D+03  
 4.785453770D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9981.216  
 3.994085420D+06-7.962756200D+03 6.755595090D+00 4.949836570D-03-  
 2.101763812D-06  
 3.348232950D-10-1.886825050D-14 6.706134940D+04-  
 2.381240379D+01  
 CHFBr2 Gurvich,1991 pt1 p168 pt2 p149.  
 2 tpis91 C 1.00H 1.00F 1.00BR 2.00 0.00 0 191.82504 -  
 175000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14359.556  
 -1.820197980D+04 4.362249670D+02-3.733854170D-01 3.388631400D-02-  
 4.371298530D-05  
 2.889569295D-08-7.683915110D-12 -2.465611586D+04  
 3.320478790D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14359.556  
 5.935751630D+05-3.742656580D+03 1.517184031D+01-7.158039030D-04  
 1.360636972D-07  
 -1.385897355D-11 5.844209110D-16 -2.347676027D+03-  
 5.765783430D+01  
 CHFCL Gurvich,1991 pt1 p147 pt2 p121.  
 2 tpis91 C 1.00H 1.00F 1.00CL 1.00 0.00 0 67.46974 -  
 83144.704  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11145.955

-7.113008510D+04 1.377872745D+03-6.484617240D+00 3.890972490D-02-  
 4.800735220D-05  
 3.073300019D-08-7.982853410D-12 -1.751793745D+04  
 6.373895200D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11145.955  
 6.622163580D+05-3.809007980D+03 1.223880469D+01-7.467182750D-04  
 1.434767850D-07  
 -1.475406631D-11 6.273780680D-16 1.018987746D+04-  
 4.658366230D+01  
 CHFCLBr Gurvich,1991 pt1 p176 pt2 p159.  
 2 tps91 C 1.00H 1.00F 1.00CL 1.00BR 1.00 0 147.37374 -  
 230000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13787.186  
 -1.959240614D+04 4.901723270D+02-1.259408503D+00 3.617708470D-02-  
 4.654244960D-05  
 3.065240659D-08-8.123903600D-12 -3.139900705D+04  
 3.710450640D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13787.186  
 5.800117510D+05-3.823337850D+03 1.522809062D+01-7.373906310D-04  
 1.407097155D-07  
 -1.438245319D-11 6.083867150D-16 -8.552249900D+03-  
 5.903678010D+01  
 CHFCL2 Hf:TRC(6/89) w7350. Gurvich,1991 pt1 p149 pt2 p124.  
 2 g 7/99 C 1.00H 1.00F 1.00CL 2.00 0.00 0 102.92244 -  
 284900.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13294.362  
 -1.734959015D+04 4.924913200D+02-1.854635884D+00 3.782786280D-02-  
 4.863343040D-05  
 3.197197630D-08-8.459057990D-12 -3.788749270D+04  
 3.801529670D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13294.362  
 5.640113020D+05-3.887083300D+03 1.527760246D+01-7.576487420D-04  
 1.452498792D-07  
 -1.490796515D-11 6.328998500D-16 -1.484736185D+04-  
 6.167536390D+01  
 CHF2 TRC(6/88) tuv6950.  
 2 n 6/88 C 1.00H 1.00F 2.00 0.00 0.00 0 51.01545 -  
 238900.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10920.000  
 -1.469690117D+05 2.553397313D+03-1.302627630D+01 5.438128460D-02-  
 6.713418790D-05  
 4.287651730D-08-1.110824216D-11 -4.179372160D+04  
 9.939930250D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10920.000  
 5.526806550D+05-3.696009170D+03 1.208610573D+01-6.498588100D-04  
 1.120846220D-07  
 -9.814147010D-12 3.349192390D-16 -9.437068420D+03-  
 4.704416200D+01  
 CHF2Br Gurvich,1991 pt1 p168 pt2 p148.  
 2 tps91 C 1.00H 1.00F 2.00BR 1.00 0.00 0 130.91945 -  
 422000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13169.504



-7.714510160D+04 1.422544046D+03-6.684393650D+00 4.738389150D-02-  
 5.830588750D-05  
 3.695720470D-08-9.495485280D-12 -5.878500930D+04  
 6.608639090D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13169.504  
 5.767706840D+05-4.177716080D+03 1.550150581D+01-8.490147290D-04  
 1.657177491D-07  
 -1.727828054D-11 7.435627230D-16 -2.966147348D+04-  
 6.349380140D+01  
 CHF2CL Hf:TRC(6/89) w7350. Gurvich,1991 pt1 p148 pt2 p123.  
 2 g 7/99 C 1.00H 1.00F 2.00CL 1.00 0.00 0 86.46815 -  
 482800.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12367.496  
 -7.240579410D+04 1.365510973D+03-7.153222080D+00 4.854987970D-02-  
 5.948781670D-05  
 3.750966190D-08-9.589524420D-12 -6.565932800D+04  
 6.657211710D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12367.496  
 5.629493730D+05-4.298673050D+03 1.558191398D+01-8.789278480D-04  
 1.720248689D-07  
 -1.797910869D-11 7.753391700D-16 -3.634067160D+04-  
 6.611262000D+01  
 CHF3 Hf:TRC(12/89) w6880. Gurvich,1991 pt1 p97 pt2 p72.  
 2 g 8/99 C 1.00H 1.00F 3.00 0.00 0.00 0 70.01385 -  
 693300.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11566.886  
 -1.095132260D+05 2.042273879D+03-1.166213079D+01 5.785807770D-02-  
 6.857135060D-05  
 4.212118380D-08-1.053196888D-11 -9.395470050D+04  
 8.935920650D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11566.886  
 5.685232020D+05-4.728361700D+03 1.586728516D+01-7.382348650D-04  
 1.970841706D-07  
 -2.062115571D-11 8.970599640D-16 -5.923196370D+04-  
 7.161273220D+01  
 CHI3 Kudchadker,1975.  
 2 g 8/99 C 1.00H 1.00I 3.00 0.00 0.00 0 393.73205  
 210873.600  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17156.587  
 5.252923590D+04-7.242166470D+02 8.018623340D+00 1.470995487D-02-  
 2.163843469D-05  
 1.594571452D-08-4.601437960D-12 2.678186915D+04-  
 8.605054840D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17156.587  
 6.294205430D+05-3.184061570D+03 1.479622178D+01-5.749555500D-04  
 1.062025541D-07  
 -1.052804696D-11 4.329720020D-16 4.103609800D+04-  
 4.901357390D+01  
 CH2 Hf:TRC(4/89) w1928. Jacox,1998. Bunker,1983.  
 2 g 8/99 C 1.00H 2.00 0.00 0.00 0.00 0 14.02658  
 388800.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10027.417

3.218921730D+04-2.877601815D+02 4.203583820D+00 3.455405960D-03-  
 6.746193340D-06  
 7.654571640D-09-2.870328419D-12 4.714808010D+04-  
 2.143628603D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10027.417  
 2.550418031D+06-7.971625390D+03 1.228924487D+01-1.699122922D-03  
 2.991728605D-07  
 -2.767007492D-11 1.051341740D-15 9.623400180D+04-  
 6.094739910D+01  
 CH2Br2 Kudchadker, 1975.  
 2 g 8/99 C 1.00H 2.00BR 2.00 0.00 0.00 0 173.83458 -  
 14770.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12614.407  
 4.797308010D+03 3.613859240D+02-1.819592338D+00 3.477048340D-02-  
 4.498546180D-05  
 3.068623685D-08-8.434846340D-12 -4.481497060D+03  
 3.827123590D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12614.407  
 1.528284441D+06-6.673414950D+03 1.670213316D+01-1.166351237D-03  
 2.122634493D-07  
 -2.075472240D-11 8.428577700D-16 3.600706640D+04-  
 7.448065490D+01  
 CH2CL Hf:TRC(12/93) w7270. Gurvich,1991 pt1 p122. Jacox,1998.  
 2 g12/99 C 1.00H 2.00CL 1.00 0.00 0.00 0 49.47928  
 119200.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10979.920  
 -3.188585630D+04 6.333163210D+02-1.164065495D+00 2.160586080D-02-  
 2.545462163D-05  
 1.693887757D-08-4.660078600D-12 1.020142540D+04  
 3.230834380D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10979.920  
 1.662438334D+06-6.441125720D+03 1.359753722D+01-1.140536810D-03  
 2.087760159D-07  
 -2.052347186D-11 8.375772270D-16 5.212906120D+04-  
 6.148587180D+01  
 CH2CLBr Gurvich,1991 pt1 p171 pt2 p153.  
 2 tpis91 C 1.00H 2.00CL 1.00BR 1.00 0.00 0 129.38328 -  
 45000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12190.747  
 -1.307948755D+04 6.455860380D+02-3.577349910D+00 3.833687230D-02-  
 4.864252050D-05  
 3.261622330D-08-8.852877390D-12 -9.402272530D+03  
 4.748806410D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12190.747  
 1.525016309D+06-6.823334160D+03 1.682769102D+01-1.219735119D-03  
 2.244964495D-07  
 -2.219063248D-11 9.104705130D-16 3.320239920D+04-  
 7.637571410D+01  
 CH2CL2 Gurvich,1991 pt1 p125 pt2 p97.  
 2 tpis91 C 1.00H 2.00CL 2.00 0.00 0.00 0 84.93198 -  
 95000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11854.077

-2.509841179D+04 8.687667380D+02-5.094669210D+00 4.150049990D-02-  
 5.199772150D-05  
 3.445944260D-08-9.270292520D-12 -1.638978840D+04  
 5.396889260D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11854.077  
 1.529279337D+06-6.976954760D+03 1.694154931D+01-1.265053995D-03  
 2.344766734D-07  
 -2.333227421D-11 9.632834730D-16 2.806318171D+04-  
 7.949454570D+01  
 CH2F TRC(6/88) tuv6950.  
 2 n 6/88 C 1.00H 2.00F 1.00 0.00 0.00 0 33.02498 -  
 31800.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11129.000  
 -8.569712530D+04 1.392226749D+03-4.382052590D+00 2.645916948D-02-  
 2.848145663D-05  
 1.732706028D-08-4.442061440D-12 -1.169444586D+04  
 5.049499200D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11129.000  
 2.535399502D+06-9.358439020D+03 1.700366206D+01-3.062919929D-03  
 7.612869080D-07  
 -9.664554980D-11 4.844768100D-15 5.228391310D+04-  
 8.707551570D+01  
 CH2FBr Gurvich,1991 pt1 p167 pt2 p147.  
 2 tpi91 C 1.00H 2.00F 1.00BR 1.00 0.00 0 112.92898 -  
 215000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11622.586  
 -9.256109530D+04 1.811985865D+03-9.698346870D+00 5.035848670D-02-  
 6.070272680D-05  
 3.878250800D-08-1.012615992D-11 -3.537509620D+04  
 8.140396050D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11622.586  
 1.539975462D+06-7.231551360D+03 1.714566439D+01-1.350184394D-03  
 2.538022824D-07  
 -2.558977386D-11 1.069310946D-15 1.509604224D+04-  
 8.062053710D+01  
 CH2FCL Hf:TRC(6/89) w7350. Gurvich,1991 pt1 p147 pt2 p122.  
 2 g 7/99 C 1.00H 2.00F 1.00CL 1.00 0.00 0 68.47768 -  
 265700.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11252.357  
 -1.071340332D+05 2.081328396D+03-1.155723697D+01 5.441482110D-02-  
 6.518622740D-05  
 4.133159880D-08-1.071935103D-11 -4.264756210D+04  
 9.035922890D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11252.357  
 1.536120418D+06-7.378939730D+03 1.725797178D+01-1.395645457D-03  
 2.639247747D-07  
 -2.675653563D-11 1.123582778D-15 9.813710460D+03-  
 8.313643210D+01  
 CH2F2 Hf:TRC(12/89) w6880. Gurvich,1991 pt1 p96 pt2 p71.  
 2 g 8/99 C 1.00H 2.00F 2.00 0.00 0.00 0 52.02339 -  
 452300.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10693.327

-1.819917500D+05 3.174427890D+03-1.714256906D+01 6.411353830D-02-  
 7.313592120D-05  
 4.426384160D-08-1.103877216D-11 -7.027058950D+04  
 1.207331926D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10693.327  
 1.546609496D+06-7.876883330D+03 1.768770469D+01-1.581298721D-03  
 3.068917255D-07  
 -3.183405460D-11 1.363827177D-15 -9.800135960D+03-  
 8.907420360D+01  
 CH2I2 Kudchadker, 1975. Kudchadker, 1976.  
 2 g 8/99 C 1.00H 2.00I 2.00 0.00 0.00 0 267.83552  
 117570.400  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13250.428  
 2.738133757D+04-8.972568040D+01 1.387869408D+00 2.733482611D-02-  
 3.619408770D-05  
 2.539187610D-08-7.145585160D-12 1.338767276D+04  
 2.241870165D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13250.428  
 1.512892716D+06-6.442912400D+03 1.659026137D+01-1.135551520D-03  
 2.073750250D-07  
 -2.033902231D-11 8.282283700D-16 5.058219030D+04-  
 7.125235140D+01  
 CH3 Hf:TRC(4/89) w1928. Jacox, 1998.  
 2 g 8/99 C 1.00H 3.00 0.00 0.00 0.00 0 15.03452  
 146900.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10366.340  
 -2.876188806D+04 5.093268660D+02 2.002143949D-01 1.363605829D-02-  
 1.433989346D-05  
 1.013556725D-08-3.027331936D-12 1.411181918D+04  
 2.022772791D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10366.340  
 2.760802663D+06-9.336531170D+03 1.487729606D+01-1.439429774D-03  
 2.444477951D-07  
 -2.224555778D-11 8.395065760D-16 7.484719570D+04-  
 7.919682400D+01  
 CH3Br Kudchadker, 1975.  
 2 g 8/99 C 1.00H 3.00BR 1.00 0.00 0.00 0 94.93852 -  
 37740.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10612.655  
 -7.115585770D+04 1.524705928D+03-8.230445210D+00 4.239973210D-02-  
 4.946979890D-05  
 3.194433340D-08-8.531237080D-12 -1.251753591D+04  
 7.048127770D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10612.655  
 2.524874348D+06-1.011876098D+04 1.865902163D+01-1.797673690D-03  
 3.298520110D-07  
 -3.250912030D-11 1.330179925D-15 5.540576390D+04-  
 9.778664460D+01  
 CH3CL Gurvich, 1991 pt1 p122 pt2 p95.  
 2 tpis91 C 1.00H 3.00CL 1.00 0.00 0.00 0 50.48722 -  
 81870.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10416.144

-9.841971100D+04 1.983700841D+03-1.084512305D+01 4.777980050D-02-  
 5.515516260D-05  
 3.506176140D-08-9.236103960D-12 -1.994689506D+04  
 8.399657440D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10416.144  
 2.522463305D+06-1.030115447D+04 1.882725852D+01-1.872291294D-03  
 3.473372860D-07  
 -3.458887220D-11 1.428941079D-15 5.111417410D+04-  
 1.006571478D+02  
 CH3F Hf:TRC(12/89) w6880. Gurvich,1991 pt1 p93 pt2 p69.  
 2 g 8/99 C 1.00H 3.00F 1.00 0.00 0.00 0 34.03292 -  
 237700.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10135.229  
 -2.029821878D+05 3.447331130D+03-1.768994275D+01 5.945275800D-02-  
 6.469528250D-05  
 3.859418040D-08-9.626541530D-12 -4.577926220D+04  
 1.228382176D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10135.229  
 2.561903188D+06-1.086052758D+04 1.929446920D+01-2.070973131D-03  
 3.929124530D-07  
 -3.994503420D-11 1.681447081D-15 3.563508510D+04-  
 1.061158456D+02  
 CH3I Kudchadker,1975.  
 2 g 8/99 C 1.00H 3.00I 1.00 0.00 0.00 0 141.93899  
 13765.360  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10815.834  
 -4.516462740D+04 1.086208429D+03-5.663176270D+00 3.683171710D-02-  
 4.321393500D-05  
 2.833483666D-08-7.684383690D-12 -4.303830650D+03  
 5.688562690D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10815.834  
 2.511915982D+06-9.960289990D+03 1.856907132D+01-1.768191331D-03  
 3.242206260D-07  
 -3.192942010D-11 1.305407821D-15 6.066929950D+04-  
 9.590777040D+01  
 CH2OH Hydroxymethyl Radical. Johnson,1996.  
 2 g11/00 C 1.00H 3.00O 1.00 0.00 0.00 0 31.03392 -  
 17800.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11781.000  
 -1.560076238D+05 2.685446279D+03-1.342022420D+01 5.757139470D-02-  
 7.284449990D-05  
 4.836648860D-08-1.293492601D-11 -1.596820410D+04  
 9.963033700D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11781.000  
 2.250349506D+06-8.173186060D+03 1.599639179D+01-8.704133720D-04  
 6.069183950D-08  
 4.408349460D-12-5.702309500D-16 4.645313430D+04-  
 7.835158450D+01  
 CH2OH+ Hydroxymethyl Cation. Johnson,1996.  
 2 g11/00 C 1.00H 3.00O 1.00E -1.00 0.00 0 31.03337  
 716400.000  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10149.000

-1.077080841D+05 2.252082711D+03-1.188167865D+01 4.602316960D-02-  
 4.879736880D-05  
 2.876413471D-08-7.100226500D-12 7.484447770D+04  
 9.027928570D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10149.000  
 2.603333487D+06-1.009953810D+04 1.730843898D+01-6.946390320D-04  
 3.009715083D-08  
 5.221485980D-12-5.090183790D-16 1.465402426D+05-  
 9.223955280D+01  
 CH3O Hf:Gurvich,1991 pt1 p67. Jacox,1998 p271.  
 2 g 7/00 C 1.00H 3.000 1.00 0.00 0.00 0 31.03392  
 13000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11302.050  
 8.657117660D+04-6.631685250D+02 2.257455672D+00 2.266283789D-02-  
 2.970566403D-05  
 2.199341353D-08-6.588043380D-12 4.174102130D+03  
 8.174777900D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11302.050  
 2.101188243D+06-8.841968800D+03 1.822645731D+01-1.743485034D-03  
 3.340434270D-07  
 -3.430673160D-11 1.473897771D-15 5.309582060D+04-  
 9.422500590D+01  
 CH4 Gurvich,1991 pt1 p44 pt2 p36.  
 2 g 8/99 C 1.00H 4.00 0.00 0.00 0.00 0 16.04246 -  
 74600.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10016.202  
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 3.619054430D-05  
 2.026853043D-08-4.976705490D-12 -2.331314360D+04  
 8.904322750D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10016.202  
 3.730042760D+06-1.383501485D+04 2.049107091D+01-1.961974759D-03  
 4.727313040D-07  
 -3.728814690D-11 1.623737207D-15 7.532066910D+04-  
 1.219124889D+02  
 CH3OH Hf:TRC(6/87) w5030. Chen,1977.  
 2 g 7/00 C 1.00H 4.000 1.00 0.00 0.00 0 32.04186 -  
 200940.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11435.277  
 -2.416642886D+05 4.032147190D+03-2.046415436D+01 6.903698070D-02-  
 7.598932690D-05  
 4.598208360D-08-1.158706744D-11 -4.433261170D+04  
 1.400142190D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11435.277  
 3.411570760D+06-1.345500201D+04 2.261407623D+01-2.141029179D-03  
 3.730050540D-07  
 -3.498846390D-11 1.366073444D-15 5.636081560D+04-  
 1.277814279D+02  
 CI Gurvich,1991 pt1 p176 pt2 p160.  
 2 tpis91 C 1.00I 1.00 0.00 0.00 0.00 0 138.91517  
 570200.814  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9494.114

1.043011064D+05-1.715427168D+03 1.288874952D+01-1.828504834D-02  
 2.135468356D-05  
 -1.286980869D-08 3.167047660D-12 7.550784700D+04-  
 4.496811320D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9494.114  
 -2.408229894D+05 3.447387040D+02 4.976968700D+00-8.444815390D-04  
 5.061239720D-07  
 -1.047700525D-10 6.740843140D-15 6.451342020D+04  
 1.090913159D+00  
 CI2 Gurvich,1991 pt1 p178 pt2 p161.  
 2 tpi91 C 1.00I 2.00 0.00 0.00 0.00 0 265.81964  
 468393.633  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12643.133  
 6.028289810D+04-1.043205435D+03 1.017465942D+01-5.535671710D-03  
 5.630319010D-06  
 -3.108249657D-09 7.202469560D-13 5.964896550D+04-  
 2.310319208D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12643.133  
 -7.028655530D+05 3.082750393D+02 9.046427050D+00-2.946736644D-03  
 1.424347233D-06  
 -2.453183410D-10 1.425270291D-14 5.021134210D+04-  
 1.560349377D+01  
 CI3 Gurvich,1991 pt1 p178 pt2 p162.  
 2 g 9/99 C 1.00I 3.00 0.00 0.00 0.00 0 392.72411  
 405983.951  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16831.451  
 8.596784250D+04-1.347703793D+03 1.272103659D+01-2.442876357D-03  
 2.511609978D-07  
 1.024658583D-09-4.872692960D-13 5.310716510D+04-  
 3.238492900D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16831.451  
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 -6.181417000D-13 2.851262022D-17 4.582589530D+04-  
 1.494825345D+01  
 CI4 Kudchadker,1975. Kudchadker,1976.  
 2 g 8/99 C 1.00I 4.00 0.00 0.00 0.00 0 519.62858  
 267943.360  
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 CN Hf: Huang,1992. Gurvich,1979 pt1 p212 pt2 p210.  
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 8672.104

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 -9.878300500D-09 2.843137221D-12 5.228455380D+04-  
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 8672.104  
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 1.325929798D-07  
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 9.318692990D-13 6.358139930D-18 -7.962594120D+05  
 1.913139662D+02  
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 3 tpris91 C 1.00N 1.00E -1.00 0.00 0.00 0 26.01689  
 1798890.904  
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 8682.104  
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 2.039918841D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
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 1.191208566D-06  
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 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
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 2.964625010D+02  
 CN- Gurvich,1991 pt1 p218 pt2 p205.  
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 4.478462770D-06  
 -4.403151290D-09 1.349001191D-12 4.362078340D+03  
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 8671.104  
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 8.856147080D-08  
 -9.722872320D-12 4.434205690D-16 1.647976581D+04-  
 1.175502468D+01  
 CNN Gurvich,1991 pt1 p220 pt2 p208. Jacox,1994.  
 2 g12/99 C 1.00N 2.00 0.00 0.00 0.00 0 40.02418  
 633484.056  
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 10377.660  
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 2.183423906D-05  
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 3.528151210D+01



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 1.088178985D-08  
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 1.966012024D+01  
 CO Gurvich,1979 pt1 p25 pt2 p29.  
 3 tpris79 C 1.000 1.00 0.00 0.00 0.00 0 28.01010 -  
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 7.859241350D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
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 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8671.104  
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 3.297772080D-06  
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 2.060704786D+03  
 CO+ Gurvich,1991 pt1 p26 pt2 p22.  
 3 tpris91 C 1.000 1.00E -1.00 0.00 0.00 0 28.00955  
 1247789.204  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8671.104  
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 8.193945750D-06  
 -6.463814690D-09 1.803727574D-12 1.482345898D+05  
 3.990547070D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8671.104  
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 2.489507047D-07  
 5.267566420D-11-3.289510270D-15 1.555050724D+05-  
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 8671.104  
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 1.580717484D+01  
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 9.113555710D-08

-3.111441728D-12-2.040435218D-16 6.914470150D+03-  
 1.998919813D+01  
 COCL2 Gurvich,1991 pt1 p119 pt2 p92.  
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 219500.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
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 7.688477320D-06  
 -5.858841200D-09 1.687786559D-12 -2.054252334D+04-  
 3.834768230D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12878.622  
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 3.233304360D+01  
 COFCL Gurvich,1991 pt1 p146 pt2 p120.  
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 11903.798  
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 7.902548080D-06  
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 1.316924217D+01  
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 11903.798  
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 -1.069291346D-11 4.901756640D-16 -4.599667230D+04-  
 3.525880370D+01  
 COF2 Gurvich,1991 pt1 p89 pt2 p66.  
 2 tpris91 C 1.000 1.00F 2.00 0.00 0.00 0 66.00691 -  
 640000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11133.929  
 5.263393150D+04-4.618603390D+02 2.774114516D+00 1.831931082D-02-  
 2.130172554D-05  
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 9.467181460D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11133.929  
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 1.175232744D-07  
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 4.009695000D+01  
 COHCL Gurvich,1991 pt1 p134 pt2 p106.  
 2 tpris91 C 1.000 1.00H 1.00CL 1.00 0.00 0 64.47074 -  
 164211.876  
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 11006.282  
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 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
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-1.958378539D-11 8.512046830D-16 4.330496440D+03-  
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 COHF Gurvich,1991 pt1 p106 pt2 p80.  
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 374590.361  
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 COS Gurvich,1991 pt1 p211 pt2 p200.  
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 141700.000  
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 393510.000  
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 2.254177493D+03  
 CO2+ Gurvich,1991 pt1 p30 pt2 p26.  
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2.133567772D+01  
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COOH Gurvich,1991 pt1 p60 pt2 p46.  
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21300.000  
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10813.349  
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2.425918417D-05  
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1.332996131D-07  
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5.068065510D+01  
CP Gurvich,1991 pt1 p231 pt2 p219.  
2 tpi91 C 1.00P 1.00 0.00 0.00 0.00 0 42.98446  
520161.805  
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8715.105  
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9.514083880D-09-2.210281109D-12 5.792634670D+04  
3.311647920D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
8715.105  
-5.449937150D+06 1.688345926D+04-1.595692200D+01 1.136028761D-02-  
2.846541330D-06  
3.379364040D-10-1.554457397D-14 -4.554517740D+04  
1.451324059D+02  
CS Hf:Prinslow,1991. Gurvich,1991 pt1 p206 pt2 p198.  
2 g11/01 C 1.00S 1.00 0.00 0.00 0.00 0 44.07670  
278550.078  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
8708.378  
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1.574407905D-05  
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3.308544730D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
8708.378  
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4.146335910D-07  
4.504757080D-11-5.945457730D-16 1.681020727D+04  
1.874051623D+01  
CS2 Gurvich,1991 pt1 p209 pt2 p199.

2 g 6/95 C 1.00S 2.00 0.00 0.00 0.00 0 76.14270  
 116700.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
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 3.031927747D-07  
 -1.737645373D-09 7.793989390D-13 1.477761119D+04-  
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 10664.223  
 -1.390419724D+06 3.354975500D+03 3.019247723D+00 2.876437543D-03-  
 9.076812720D-07  
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 1.565117643D+01  
 C2 Gurvich,1991 pt1 p9 pt2 p8.  
 3 tpis91 C 2.00 0.00 0.00 0.00 0.00 0 24.02140  
 830457.322  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10169.122  
 5.559634510D+05-9.980126440D+03 6.681620370D+01-1.743432724D-01  
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 -1.703467580D-07 4.684527730D-11 1.445869634D+05-  
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 10169.122  
 6.315145920D+06 1.365420661D+04-3.996903670D+00 1.937561376D-03-  
 1.584446580D-07  
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 6.614329920D+01  
 C2+ Gurvich,1991 pt1 p14 pt2 p10.  
 3 tpis91 C 2.00E -1.00 0.00 0.00 0.00 0 24.02085  
 2004775.532  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8685.104  
 -9.913423840D+04 1.347170609D+03-3.476753160D+00 1.676429424D-02-  
 1.865908025D-05  
 1.091134647D-08-2.434913818D-12 2.335454800D+05  
 4.406644620D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8685.104  
 3.836292810D+06-6.242062450D+03 2.779245639D+00 6.065865860D-03-  
 2.452799858D-06  
 3.882942500D-10-2.190639912D-14 2.857447553D+05  
 7.297383490D-01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8685.104  
 4.992689800D+07-2.017309121D+04 6.342227540D+00 6.369922600D-04-  
 1.036760828D-07  
 4.943272920D-12-7.988804260D-17 4.120857610D+05-  
 2.112967169D+01  
 C2- Gurvich,1991 pt1 p15 pt2 p12.  
 2 tpis91 C 2.00E 1.00 0.00 0.00 0.00 0 24.02195  
 480766.904  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8676.104

-1.181928660D+05 1.438189710D+03-3.196131350D+00 1.465548163D-02-  
1.545537278D-05  
9.061235610D-09-2.135962274D-12 4.965317790D+04  
4.225608880D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
8676.104  
4.478136250D+06-1.154145714D+04 1.310143499D+01-1.862700578D-03  
4.006931250D-08  
3.710213600D-11-3.337266870D-15 1.325356168D+05-  
6.975964400D+01  
C2CL Gurvich,1991 pt1 p112 pt2 p85.  
2 tps91 C 2.00CL 1.00 0.00 0.00 0.00 0 59.47410  
534083.071  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
10780.626  
4.725889410D+04-8.980223610D+02 9.016877150D+00-6.333782830D-03  
1.087060050D-05  
-8.089068920D-09 2.248275223D-12 6.702215700D+04-  
2.354894160D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
10780.626  
2.137368408D+05-1.630519518D+03 8.623490250D+00-4.253517860D-04  
9.040018640D-08  
-1.007541495D-11 4.570764750D-16 7.171093280D+04-  
2.413015355D+01  
C2CL2 Gurvich,1991 pt1 p114 pt2 p86.  
2 tps91 C 2.00CL 2.00 0.00 0.00 0.00 0 94.92680  
200000.000  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
14592.612  
3.871169080D+04-9.336870730D+02 1.119377861D+01-3.746288200D-03  
6.770472560D-06  
-4.910388350D-09 1.299068749D-12 2.628230557D+04-  
3.310724640D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
14592.612  
2.961978472D+05-2.044286552D+03 1.187529315D+01-5.115011450D-04  
1.072661556D-07  
-1.183411171D-11 5.326498340D-16 3.316877050D+04-  
4.000823970D+01  
C2CL3 Gurvich,1991 pt1 p114 pt2 p87.  
2 tps91 C 2.00CL 3.00 0.00 0.00 0.00 0 130.37950  
190271.592  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
16150.258  
4.675016040D+04-8.851019640D+02 9.032270550D+00 1.242122796D-02-  
1.554614347D-05  
9.513887120D-09-2.341473263D-12 2.495863399D+04-  
1.779071189D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
16150.258  
-2.204028219D+05-1.072926248D+03 1.378367377D+01-3.093322915D-04  
6.777528950D-08  
-7.727301820D-12 3.566690220D-16 2.431020015D+04-  
4.342162850D+01  
C2CL4 Gurvich,1991 pt1 p115 pt2 p88.  
2 tps91 C 2.00CL 4.00 0.00 0.00 0.00 0 165.83220  
11000.000  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
19605.643

3.746258300D+04-8.481775630D+02 1.009156110D+01 1.845463613D-02-  
 2.390899444D-05  
 1.514828257D-08-3.841119320D-12 -1.070243179D+01-  
 2.368080605D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19605.643  
 -3.001315659D+05-1.132407598D+03 1.683072470D+01-3.288792490D-04  
 7.220907030D-08  
 -8.245332690D-12 3.810112780D-16 -7.052135540D+02-  
 5.980161160D+01  
 C2CL6 Gurvich,1991 pt1 p117 pt2 p90.  
 2 tpris91 C 2.00CL 6.00 0.00 0.00 0.00 0 236.73760 -  
 141500.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 27129.390  
 1.593451813D+05-2.606697136D+03 2.028011847D+01 1.769364822D-02-  
 3.133105185D-05  
 2.389395238D-08-6.893038300D-12 -8.232187460D+03-  
 7.953073760D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 27129.390  
 -5.577386320D+05-4.976491240D+02 2.237041989D+01-1.477759098D-04  
 3.257546580D-08  
 -3.727099210D-12 1.723801704D-16 -2.254641287D+04-  
 8.381732120D+01  
 C2F Gurvich,1991 pt1 p81 pt2 p59.  
 2 tpris91 C 2.00F 1.00 0.00 0.00 0.00 0 43.01980  
 353847.482  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10367.036  
 1.249797213D+04-3.483876750D+02 5.755084350D+00 8.528685380D-04  
 2.353546435D-06  
 -2.804737097D-09 9.083575640D-13 4.281525310D+04-  
 6.437200960D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10367.036  
 2.898776676D+05-2.016644658D+03 8.875045710D+00-5.166841130D-04  
 1.092094306D-07  
 -1.212216787D-11 5.482287680D-16 5.241287920D+04-  
 2.773089580D+01  
 C2FCL Gurvich,1991 pt1 p141 pt2 p113.  
 2 tpris91 C 2.00F 1.00CL 1.00 0.00 0.00 0 78.47250  
 33766.399  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13876.507  
 2.697675344D+04-7.414403180D+02 9.629604300D+00-3.865544930D-04  
 3.003347997D-06  
 -2.710191661D-09 7.737586890D-13 5.500620390D+03-  
 2.515775462D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13876.507  
 3.471454890D+05-2.348461100D+03 1.206875617D+01-5.804698230D-04  
 1.212734340D-07  
 -1.334214186D-11 5.992556610D-16 1.502061224D+04-  
 4.252446260D+01  
 C2FCL3 Gurvich,1991 pt1 p145 pt2 p119.  
 2 tpris91 C 2.00F 1.00CL 3.00 0.00 0.00 0 149.37790 -  
 166000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18731.914

1.237282217D+04-4.703961840D+02 7.581621790D+00 2.305727066D-02-  
 2.792144322D-05  
 1.679699826D-08-4.077572440D-12 -2.031333976D+04-  
 9.274646550D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18731.914  
 -2.829505545D+05-1.473853145D+03 1.707879074D+01-4.265213390D-04  
 9.357199850D-08  
 -1.067932796D-11 4.933261610D-16 -1.738433314D+04-  
 6.197055700D+01  
 C2F2 Gurvich,1991 pt1 p82 pt2 p60.  
 2 tpis91 C 2.00F 2.00 0.00 0.00 0.00 0 62.01821 -  
 144665.688  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13266.419  
 1.776313572D+04-6.113280940D+02 8.663606800D+00 9.156381210D-04  
 2.363808425D-06  
 -2.753750054D-09 8.713935970D-13 -1.649611017D+04-  
 2.165150307D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13266.419  
 4.193890940D+05-2.715359989D+03 1.230403413D+01-6.649305540D-04  
 1.385254301D-07  
 -1.520813764D-11 6.819821030D-16 -4.179221940D+03-  
 4.670386230D+01  
 C2F2CL2 Gurvich,1991 pt1 p143 pt2 p115. Eq1 mixture of isomers.  
 2 tpis91 C 2.00F 2.00CL 2.00 0.00 0.00 0 132.92361 -  
 337837.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17936.029  
 -1.150433214D+05 2.032113595D+03-1.119750271D+01 8.342451400D-02-  
 1.163698616D-04  
 7.833092890D-08-2.070004069D-11 -5.208256810D+04  
 8.888321470D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17936.029  
 -8.702565660D+05 7.264724480D+02 1.530689121D+01 3.045597224D-04-  
 7.045468040D-08  
 8.285924340D-12-3.898581070D-16 -5.208888710D+04-  
 4.998301430D+01  
 C2F3 Gurvich,1991 pt1 p83 pt2 p61.  
 2 tpis91 C 2.00F 3.00 0.00 0.00 0.00 0 81.01661 -  
 228181.093  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14163.567  
 -2.614775016D+04 2.101767714D+02 2.328625080D+00 2.368943293D-02-  
 2.416431591D-05  
 1.224916093D-08-2.488670434D-12 -3.028566585D+04  
 1.699608790D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14163.567  
 -1.242603837D+05-2.137292446D+03 1.455051371D+01-6.093891980D-04  
 1.331427672D-07  
 -1.515124358D-11 6.984112060D-16 -1.977146179D+04-  
 5.421039870D+01  
 C2F3CL Gurvich,1991 pt1 p142 pt2 p114.  
 2 tpis91 C 2.00F 3.00CL 1.00 0.00 0.00 0 116.46931 -  
 515200.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17128.149



-8.122270310D+03-1.574007092D+02 5.041810290D+00 2.621692321D-02-  
 2.843001445D-05  
 1.537643979D-08-3.360730670D-12 -6.354049950D+04  
 2.792298008D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17128.149  
 -2.162724659D+05-2.195103372D+03 1.759605428D+01-6.282617290D-04  
 1.374166610D-07  
 -1.565004037D-11 7.218309900D-16 -5.515109500D+04-  
 6.921932210D+01  
 C2F4 Gurvich,1991 pt1 p84 pt2 p62.  
 2 tps91 C 2.00F 4.00 0.00 0.00 0.00 0 100.01501 -  
 659500.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16330.554  
 -9.991530070D+03-1.291088427D+02 4.504229050D+00 2.592029640D-02-  
 2.630308720D-05  
 1.316489777D-08-2.625017169D-12 -8.090447080D+04  
 3.274241470D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16330.554  
 -1.629915758D+05-2.603903955D+03 1.788488423D+01-7.397038010D-04  
 1.614460340D-07  
 -1.835820392D-11 8.457641070D-16 -7.006371660D+04-  
 7.454165860D+01  
 C2F6 Gurvich,1991 pt1 p86 pt2 p64.  
 2 g12/99 C 2.00F 6.00 0.00 0.00 0.00 0 138.01182 -  
 1344000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 20272.040  
 -3.795371700D+04 7.998276400D+02-4.671561810D+00 7.501450990D-02-  
 9.812116100D-05  
 6.319807590D-08-1.622597311D-11 -1.675211878D+05  
 5.053759200D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 20272.040  
 -1.011551484D+06-9.422140710D+02 2.202553906D+01-1.314518750D-04  
 1.866045300D-08  
 -3.467118610D-12 2.488311205D-16 -1.657434402D+05-  
 9.302161150D+01  
 C2H Ervin, 1990. Jacox,1998. Peric,1990. Kanamori,1988.  
 2 g 6/01 C 2.00H 1.00 0.00 0.00 0.00 0 25.02934  
 566200.482  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10448.682  
 1.343669487D+04-5.067970720D+02 7.772107410D+00-6.512339820D-03  
 1.030117855D-05  
 -5.880147670D-09 1.226901861D-12 6.892269990D+04-  
 1.871881626D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10448.682  
 3.922334570D+06-1.204751703D+04 1.756172920D+01-3.655442940D-03  
 6.987685430D-07  
 -6.825162010D-11 2.719262793D-15 1.433266627D+05-  
 9.561634380D+01  
 C2HCL Gurvich,1991 pt1 p129 pt2 p99.  
 2 tps91 C 2.00H 1.00CL 1.00 0.00 0.00 0 60.48204  
 212856.775  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11788.381

1.329784835D+05-2.174541901D+03 1.497980728D+01-1.290343038D-02  
1.602596159D-05  
-9.152045650D-09 2.021222472D-12 3.441914590D+04-  
5.958237170D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
11788.381  
1.152144900D+06-4.461192150D+03 1.281366669D+01-6.797343570D-04  
1.151382029D-07  
-1.046641118D-11 3.949856700D-16 5.071060370D+04-  
5.320654020D+01  
C2HCL3 Gurvich,1991 pt1 p134 pt2 p105.  
2 g12/99 C 2.00H 1.00CL 3.00 0.00 0.00 0 131.38744 -  
19100.000  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
16604.624  
3.959231250D+04-5.178753580D+02 5.155028770D+00 2.816922486D-02-  
3.624741720D-05  
2.392074270D-08-6.362401960D-12 -1.726780931D+03  
1.209374516D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
16604.624  
6.049254660D+05-4.236992320D+03 1.846273557D+01-8.137195060D-04  
1.551211545D-07  
-1.584630634D-11 6.700932490D-16 1.829042084D+04-  
7.698368760D+01  
C2HF Gurvich,1991 pt1 p99 pt2 p73.  
2 tpis91 C 2.00H 1.00F 1.00 0.00 0.00 0 44.02774  
41692.304  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
11445.908  
9.161169110D+04-1.537245636D+03 1.133665074D+01-4.624729310D-03  
5.877985460D-06  
-2.690992345D-09 3.524719530D-13 1.085902820D+04-  
4.023994380D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
11445.908  
1.234347179D+06-4.819581960D+03 1.302337752D+01-7.495435820D-04  
1.285452942D-07  
-1.184559365D-11 4.536784760D-16 3.236811710D+04-  
5.640791820D+01  
C2HFCL2 Gurvich,1991 pt1 p155 pt2 p133. Eql mixture of isomers.  
2 tpis91 C 2.00H 1.00F 1.00CL 2.00 0.00 0 114.93314 -  
168648.000  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
16259.290  
3.117399823D+04-1.369505457D+02 1.176399869D+00 4.080776600D-02-  
5.418137800D-05  
3.613600660D-08-9.625862350D-12 -2.115142871D+04  
2.146432377D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
16259.290  
4.071243520D+05-3.808204520D+03 1.821144050D+01-7.278966060D-04  
1.381532849D-07  
-1.405342513D-11 5.920009720D-16 -2.676849943D+03-  
7.567354350D+01  
C2HF2CL Gurvich,1991 pt1 p153 pt2 p129. 1,1 cis & trans in  
equil.  
2 tpis91 C 2.00H 1.00F 2.00CL 1.00 0.00 0 98.47885 -  
333654.000  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
15262.754

1.704437675D+05-1.667236861D+03 4.788788500D+00 4.444830010D-02-  
 7.322197770D-05  
 5.629347550D-08-1.654638029D-11 -3.291809760D+04-  
 5.788598210D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15262.754  
 5.830374700D+05-3.810317410D+03 1.799003171D+01-5.888210860D-04  
 1.002861284D-07  
 -9.149788100D-12 3.459985160D-16 -2.205875409D+04-  
 7.590948990D+01  
 C2HF3 Gurvich,1991 pt1 p105 pt2 p79.  
 2 tpris91 C 2.00H 1.00F 3.00 0.00 0.00 0 82.02455 -  
 491000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14327.512  
 -1.410969036D+04 3.687624920D+02-1.144797568D+00 3.956306020D-02-  
 4.602001360D-05  
 2.785149385D-08-6.903760080D-12 -6.226410330D+04  
 3.289661690D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14327.512  
 6.917413780D+05-5.260301640D+03 1.915276614D+01-1.072493938D-03  
 2.099276744D-07  
 -2.195126633D-11 9.472702400D-16 -3.247640210D+04-  
 8.750456950D+01  
 C2H2,acetylene Hf:TRC(10/93) w-3040. Gurvich,1991 pt1 p47 pt2 p39.  
 2 g 1/91 C 2.00H 2.00 0.00 0.00 0.00 0 26.03728  
 228200.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10005.839  
 1.598112089D+05-2.216644118D+03 1.265707813D+01-7.979651080D-03  
 8.054992750D-06  
 -2.433307673D-09-7.529233180D-14 3.712619060D+04-  
 5.244338900D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10005.839  
 1.713847410D+06-5.929106660D+03 1.236127943D+01 1.314186993D-04-  
 1.362764431D-07  
 2.712655786D-11-1.302066204D-15 6.266578970D+04-  
 5.818960590D+01  
 C2H2,vinylidene Chen,1989. Osamura,1981.  
 2 g 5/01 C 2.00H 2.00 0.00 0.00 0.00 0 26.03728  
 414788.368  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10874.168  
 -1.466042239D+04 2.789475593D+02 1.276229776D+00 1.395015463D-02-  
 1.475702649D-05  
 9.476298110D-09-2.567602217D-12 4.736110180D+04  
 1.658225704D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10874.168  
 1.940838725D+06-6.892718150D+03 1.339582494D+01-9.368968670D-04  
 1.470804368D-07  
 -1.220040365D-11 4.122391660D-16 9.107112930D+04-  
 6.337502930D+01  
 C2H2CL2 Gurvich,1991 pt1 p130 pt2 p101. 1,1 cis & trans in  
 equil.  
 2 tpris91 C 2.00H 2.00CL 2.00 0.00 0.00 0 96.94268  
 3410.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14882.477

-1.203724514D+04 4.629031190D+02-1.318184584D+00 3.930449600D-02-  
4.851529020D-05  
3.178411460D-08-8.476938410D-12 -3.251806860D+03  
3.489217190D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
14882.477  
1.561121185D+06-7.358096350D+03 2.011869185D+01-1.310978834D-03  
2.411885716D-07  
-2.384166740D-11 9.785415750D-16 4.122200900D+04-  
9.550253640D+01  
C2H2FCL Gurvich,1991 pt1 p150 pt2 p125. 1,1 cis & trans in  
equil.  
2 tpris91 C 2.00H 2.00F 1.00CL 1.00 0.00 0 80.48838 -  
165082.000  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
13469.313  
2.260154427D+05-2.557428772D+03 9.236241200D+00 2.879408894D-02-  
5.163975470D-05  
4.252191030D-08-1.311612713D-11 -8.180627840D+03-  
3.234788140D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
13469.313  
1.527690968D+06-6.689712230D+03 1.950553830D+01-1.040920895D-03  
1.780587502D-07  
-1.633098515D-11 6.213465560D-16 1.705266451D+04-  
9.194078860D+01  
C2H2F2 Gurvich,1991 pt1 p101 pt2 p75. 1,1 cis & trans in  
equil.  
2 tpris91 C 2.00H 2.00F 2.00 0.00 0.00 0 64.03409 -  
336400.000  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
12479.683  
5.702935810D+04-6.762860400D+02 4.117411710D+00 1.822618762D-02-  
6.861331540D-06  
-3.295756740D-09 2.180965597D-12 -3.838650780D+04  
1.487528685D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
12479.683  
-8.227192750D+05-2.915718833D+03 1.830163995D+01-1.039630129D-03  
2.546725128D-07  
-3.157578705D-11 1.551540960D-15 -3.110028589D+04-  
8.400834700D+01  
CH2CO, ketene Wagman,1982. Moore,1963.  
2 g 7/00 C 2.00H 2.000 1.00 0.00 0.00 0 42.03668 -  
47700.000  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
11797.746  
3.503274040D+04-4.001693250D+02 3.691806430D+00 1.589408702D-02-  
1.733190594D-05  
1.161219965D-08-3.313412960D-12 -5.014866400D+03  
2.848266196D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
11797.746  
2.015132200D+06-8.200240060D+03 1.759005013D+01-1.460345107D-03  
2.684671350D-07  
-2.651382523D-11 1.087131348D-15 4.200517260D+04-  
8.836222940D+01  
C2H3, vinyl Radical. Ervin,1990.  
2 g 7/01 C 2.00H 3.00 0.00 0.00 0.00 0 27.04522  
299686.817

200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10521.791  
 -3.347896870D+04 1.064104103D+03-6.403857060D+00 3.934515480D-02-  
 4.760046090D-05  
 3.170071350D-08-8.633406430D-12 3.039122649D+04  
 5.809226180D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10521.791  
 2.718080093D+06-1.030956829D+04 1.836579807D+01-1.580131153D-03  
 2.680594939D-07  
 -2.439003999D-11 9.209096390D-16 9.765055590D+04-  
 9.760086860D+01  
 C2H3CL Gurvich,1991 pt1 p129 pt2 p100.  
 2 tpi91 C 2.00H 3.00CL 1.00 0.00 0.00 0 62.49792  
 23000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11819.647  
 -1.688895457D+04 8.545104550D+02-6.514967550D+00 4.944681930D-02-  
 6.117756670D-05  
 4.067293850D-08-1.101392611D-11 -1.949049652D+03  
 5.928434500D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11819.647  
 2.456176938D+06-1.047452327D+04 2.178736181D+01-1.816891849D-03  
 3.296369950D-07  
 -3.214395690D-11 1.302254061D-15 6.358255870D+04-  
 1.149890578D+02  
 C2H3F Gurvich,1991 pt1 p100 pt2 p74.  
 2 tpi91 C 2.00H 3.00F 1.00 0.00 0.00 0 46.04362 -  
 140100.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11335.928  
 -4.579134960D+04 1.411541724D+03-1.021500877D+01 5.775816570D-02-  
 7.080677490D-05  
 4.640850760D-08-1.240455865D-11 -2.402788827D+04  
 7.860828390D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11335.928  
 2.478832340D+06-1.075932307D+04 2.194796688D+01-1.869114110D-03  
 3.395280670D-07  
 -3.315382930D-11 1.345081799D-15 4.563455550D+04-  
 1.180410277D+02  
 CH3CN Acetonitrile. TRC(6/93) w9270. Koga,1984. Pavone,1990.  
 2 g 9/00 C 2.00H 3.00N 1.00 0.00 0.00 0 41.05196  
 66430.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12093.688  
 -9.965988380D+04 1.739278534D+03-7.898420820D+00 4.294894320D-02-  
 4.499973880D-05  
 2.717105086D-08-7.026117590D-12 -1.461161333D+03  
 6.852508420D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12093.688  
 2.923231393D+06-1.233792258D+04 2.324477222D+01-2.411565845D-03  
 4.622157170D-07  
 -4.740601240D-11 2.010639467D-15 8.058565550D+04-  
 1.292249087D+02  
 CH3CO,acetyl Radical. Hf:Niiranen,1992. Nimlos,1989.  
 2 g 6/96 C 2.00H 3.00O 1.00 0.00 0.00 0 43.04462 -  
 10000.000

200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13036.467  
 -7.193894130D+04 1.464465167D+03-6.632276130D+00 4.108468380D-02-  
 4.226256640D-05  
 2.485766819D-08-6.292558480D-12 -9.309370810D+03  
 6.422897620D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13036.467  
 2.485388150D+06-1.120714204D+04 2.277525438D+01-2.314260550D-03  
 4.536189170D-07  
 -4.742635550D-11 2.044663903D-15 6.380088410D+04-  
 1.215350925D+02  
 C2H4 TRC (4/88) w2600. Chao,1975. Knippers,1985.  
 2 g 1/00 C 2.00H 4.00 0.00 0.00 0.00 0 28.05316  
 52500.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10518.689  
 -1.163605836D+05 2.554851510D+03-1.609746428D+01 6.625779320D-02-  
 7.885081860D-05  
 5.125224820D-08-1.370340031D-11 -6.176191070D+03  
 1.093338343D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10518.689  
 3.408763670D+06-1.374847903D+04 2.365898074D+01-2.423804419D-03  
 4.431395660D-07  
 -4.352683390D-11 1.775410633D-15 8.820429380D+04-  
 1.371278108D+02  
 C2H4O, ethylen-o Ethylene Oxide. Shimanouchi,1972. Chase,1998 9/65.  
 2 g 8/88 C 2.00H 4.000 1.00 0.00 0.00 0 44.05256 -  
 52634.720  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10830.615  
 -1.728233345D+05 3.816678800D+03-2.629851977D+01 1.014103162D-01-  
 1.240578373D-04  
 8.034040350D-08-2.120942544D-11 -2.437519333D+04  
 1.654885056D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10830.615  
 3.151809957D+06-1.423646316D+04 2.708080476D+01-2.606238456D-03  
 4.853891930D-07  
 -4.852144760D-11 2.011778721D-15 7.662561440D+04-  
 1.563952401D+02  
 CH3CHO, ethanal Hf:TRC (6/78) w5300. Chao,1986.  
 2 g 8/88 C 2.00H 4.000 1.00 0.00 0.00 0 44.05256 -  
 166190.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12896.716  
 -1.373904369D+05 2.559937679D+03-1.340470172D+01 5.922128620D-02-  
 6.240006050D-05  
 3.703324410D-08-9.342697410D-12 -3.318731310D+04  
 1.007417652D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12896.716  
 3.321176590D+06-1.449719957D+04 2.708421279D+01-2.879320054D-03  
 5.556309920D-07  
 -5.732674880D-11 2.443965239D-15 6.507755640D+04-  
 1.536236027D+02  
 CH3COOH Acetic Acid. Chao,1978.  
 2 g 6/00 C 2.00H 4.000 2.00 0.00 0.00 0 60.05196 -  
 432249.040

200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13597.391  
 -3.219191980D+04 1.196329795D+03-8.705824020D+00 5.696257590D-02-  
 5.757887160D-05  
 3.352115220D-08-8.614438230D-12 -5.840112870D+04  
 7.282413920D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13597.391  
 2.103514223D+06-1.467822192D+04 3.382802830D+01-5.694858680D-03  
 1.343221353D-06  
 -1.606041158D-10 7.652794250D-15 2.924228407D+04-  
 1.935278850D+02  
 C2H5 Chen, 1990.  
 2 g 7/00 C 2.00H 5.00 0.00 0.00 0.00 0 29.06110  
 118658.240  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12185.226  
 -1.411312551D+05 2.714285088D+03-1.534977725D+01 6.451672580D-02-  
 7.259143960D-05  
 4.599116010D-08-1.218367535D-11 5.981418840D+02  
 1.090966520D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12185.226  
 4.169220400D+06-1.662982142D+04 2.795442134D+01-3.051715761D-03  
 5.685160040D-07  
 -5.682863600D-11 2.355648561D-15 1.137010087D+05-  
 1.639357995D+02  
 C2H5Br Bromoethane. TRC(6/79) tuv7650.  
 2 n 6/79 C 2.00H 5.00BR 1.00 0.00 0.00 0 108.96510 -  
 63600.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13569.000  
 -1.374172662D+05 2.861429418D+03-1.824108956D+01 8.566230600D-02-  
 1.047174473D-04  
 6.906074570D-08-1.862276022D-11 -2.198480205D+04  
 1.258435579D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13569.000  
 2.378649403D+06-1.267033647D+04 2.777558646D+01-2.010898783D-03  
 4.436083410D-07  
 -5.348198090D-11 2.639835850D-15 6.414062050D+04-  
 1.528277085D+02  
 C2H6 Ethane. Pamidimukkala, 1982.  
 2 g 7/00 C 2.00H 6.00 0.00 0.00 0.00 0 30.06904 -  
 83851.544  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11891.594  
 -1.862044161D+05 3.406191860D+03-1.951705092D+01 7.565835590D-02-  
 8.204173220D-05  
 5.061135800D-08-1.319281992D-11 -2.702932890D+04  
 1.298140496D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11891.594  
 5.025782130D+06-2.033022397D+04 3.322552930D+01-3.836703410D-03  
 7.238405860D-07  
 -7.319182500D-11 3.065468699D-15 1.115963950D+05-  
 2.039410584D+02  
 CH3N2CH3 Azomethane. Pamidumukkala, 1982.  
 2 g 8/88 C 2.00H 6.00N 2.00 0.00 0.00 0 58.08252  
 148699.360

200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16524.999  
 -3.738492320D+05 5.880453130D+03-2.986398524D+01 1.087380861D-01-  
 1.167950177D-04  
 6.916894890D-08-1.719950055D-11 -1.189984084D+04  
 1.948246342D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16524.999  
 4.993357090D+06-2.160996161D+04 3.964449920D+01-4.196450110D-03  
 8.023361980D-07  
 -8.212260020D-11 3.477237440D-15 1.449962610D+05-  
 2.372109724D+02  
 C2H5OH Hf:TRC(6/87) w5030. Chao,1986.  
 2 g 8/88 C 2.00H 6.00O 1.00 0.00 0.00 0 46.06844 -  
 234950.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14541.926  
 -2.342791392D+05 4.479180550D+03-2.744817302D+01 1.088679162D-01-  
 1.305309334D-04  
 8.437346400D-08-2.234559017D-11 -5.022229000D+04  
 1.764829211D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14541.926  
 4.694817650D+06-1.929798213D+04 3.447584040D+01-3.236165980D-03  
 5.784947720D-07  
 -5.564600270D-11 2.226226400D-15 8.601622710D+04-  
 2.034801732D+02  
 CH3OCH3 Dimethyl ether. Hf:TRC(6/91) w6040. Chao,1986.  
 2 g 7/00 C 2.00H 6.00O 1.00 0.00 0.00 0 46.06844 -  
 184110.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14354.379  
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 8.295671320D-05  
 4.801911510D-08-1.188699808D-11 -4.410237090D+04  
 1.467666934D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14354.379  
 4.933577190D+06-2.083094065D+04 3.629050610D+01-4.108351640D-03  
 7.903220310D-07  
 -8.131435630D-11 3.458166110D-15 1.013301012D+05-  
 2.185447466D+02  
 CCN Hf:Gurvich,1991 pt1 p222. Jacox,1998 p173.  
 2 g 7/00 C 2.00N 1.00 0.00 0.00 0.00 0 38.02814  
 804596.472  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11038.524  
 -1.696281385D+04 9.837891630D+01 3.812662940D+00 5.346894230D-03-  
 2.473598508D-06  
 -3.730564220D-10 4.481756860D-13 9.480072570D+04  
 5.553167150D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11038.524  
 7.948674890D+04-1.344786906D+03 8.309986460D+00-2.220105361D-04  
 1.753683113D-08  
 2.545998719D-12-2.645649117D-16 1.023187495D+05-  
 2.259793782D+01  
 CNC CNC radical. Gurvich,1991 pt1 p221 pt2 p209.  
 2 tpis91 C 2.00N 1.00 0.00 0.00 0.00 0 38.02814  
 684914.559



200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11356.611  
 -7.075192710D+04 1.007523898D+03-1.576789967D+00 2.052532634D-02-  
 2.278935009D-05  
 1.283362343D-08-2.933174091D-12 7.613324850D+04  
 3.487094290D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11356.611  
 -9.031313560D+04-8.313236500D+02 8.114735950D+00-2.447691991D-04  
 5.397508770D-08  
 -6.183984860D-12 2.865172411D-16 8.451833600D+04-  
 2.102937097D+01  
 C2N2 Gurvich,1979 pt1 p195 pt2 p220.  
 2 tpi579 C 2.00N 2.00 0.00 0.00 0.00 0 52.03488  
 309100.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12715.153  
 1.082404484D+05-1.928137871D+03 1.553891898D+01-1.821159329D-02  
 2.778840840D-05  
 -1.899434373D-08 4.949677720D-12 4.449097590D+04-  
 6.090964510D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12715.153  
 7.934423720D+05-3.997376270D+03 1.314497430D+01-8.747782000D-04  
 2.059156733D-07  
 -2.200469389D-11 9.974485770D-16 5.863632300D+04-  
 5.473201020D+01  
 C2O Hf:Gurvich,1991 pt1 p31. Jacox,1998.  
 2 g 8/00 C 2.00O 1.00 0.00 0.00 0.00 0 40.02080  
 291038.666  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10485.718  
 -3.959929420D+03-1.117516348D+02 4.593960060D+00 3.710602020D-03-  
 7.014760180D-07  
 -1.371129839D-09 7.123854000D-13 3.410109740D+04  
 4.622805600D-01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10485.718  
 -6.348056590D+05 1.184133091D+03 4.879173340D+00 1.757538773D-03-  
 3.957552270D-07  
 3.989179940D-11-1.546043135D-15 2.489803938D+04  
 9.809040590D-01  
 C2S2 TRC(6/01) p8150, tuvw-8150.  
 2 n 6/01 C 2.00S 2.00 0.00 0.00 0.00 0 88.15340  
 376660.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13760.000  
 4.192544750D+04-9.776562320D+02 1.085003376D+01-4.423407890D-03  
 1.067980519D-05  
 -8.781148100D-09 2.538862361D-12 4.789590500D+04-  
 3.097678451D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13760.000  
 8.629908790D+05-4.325413740D+03 1.460010162D+01-1.460638433D-03  
 2.778253364D-07  
 -2.755649209D-11 1.105350739D-15 6.839748750D+04-  
 5.986376450D+01  
 C3 Gurvich,1979 pt2 p23.  
 3 tpi579 C 3.00 0.00 0.00 0.00 0.00 0 36.03210  
 839948.646

200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12109.146  
 -4.354614480D+04 6.660183220D+02 1.451033157D+00 7.434513120D-03-  
 3.810152990D-06  
 -2.336961396D-11 4.407054530D-13 9.635170200D+04  
 2.025173297D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12109.146  
 4.508098930D+06-1.461033761D+04 2.281974644D+01-8.544340610D-03  
 2.146069341D-06  
 -2.103867761D-10 6.351589060D-15 1.911976065D+05-  
 1.271869723D+02  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12109.146  
 1.539589859D+08-2.089057498D+05 7.681111210D+01-8.939056190D-03  
 5.594033240D-07  
 -1.743774353D-11 2.181541208D-16 1.650801763D+06-  
 6.081693320D+02  
 C3H3,1-propynl TRC(4/98) tuv3140.  
 2 n 4/98 C 3.00H 3.00 0.00 0.00 0.00 0 39.05592  
 450000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12400.000  
 -6.505859350D+04 1.350858921D+03-5.825433930D+00 3.756610480D-02-  
 3.734903340D-05  
 2.117676603D-08-5.139113250D-12 4.656510530D+04  
 5.781477550D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12400.000  
 4.550654870D+06-1.640574172D+04 2.712605991D+01-4.474600380D-03  
 1.037712415D-06  
 -1.250211369D-10 6.026582050D-15 1.534087662D+05-  
 1.565931809D+02  
 C3H3,2-propynl TRC(4/98) tuv3140.  
 2 n 4/98 C 3.00H 3.00 0.00 0.00 0.00 0 39.05592  
 331800.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13230.000  
 6.188578320D+04-8.909578670D+02 6.347558820D+00 1.633173115D-02-  
 1.949975695D-05  
 1.417349778D-08-4.199866320D-12 4.271785830D+04-  
 1.231400729D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13230.000  
 2.989723833D+06-1.118954446D+04 2.222225052D+01-2.068106902D-03  
 4.121883640D-07  
 -4.438980590D-11 1.970824701D-15 1.061878289D+05-  
 1.186744583D+02  
 C3H4,allene TRC(4/84) w2750. Shimanouchi,1972 p115. Butcher,1973a.  
 2 g 2/00 C 3.00H 4.00 0.00 0.00 0.00 0 40.06386  
 190920.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12604.569  
 -1.645155745D+04 9.629457810D+02-7.532326680D+00 5.518219110D-02-  
 6.733585120D-05  
 4.532709050D-08-1.251837614D-11 1.772494269D+04  
 6.151969760D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12604.569  
 3.479355100D+06-1.430412453D+04 2.702534756D+01-2.557412369D-03  
 4.706646750D-07

-4.651688070D-11 1.908219044D-15 1.072312354D+05-  
 1.548846158D+02  
 C3H4, propyne Hf:TRC(10/93) w3040. Trambarulo,1950. Shimanouchi,1972.  
 2 g 1/00 C 3.00H 4.00 0.00 0.00 0.00 0 40.06386  
 184900.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13030.516  
 -3.563884400D+04 8.328139100D+02-4.073759440D+00 4.113929610D-02-  
 4.470444950D-05  
 2.847458197D-08-7.695298240D-12 1.710206236D+04  
 4.516720950D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13030.516  
 3.710441420D+06-1.489145507D+04 2.732397127D+01-2.645264770D-03  
 4.858300350D-07  
 -4.794128480D-11 1.964338121D-15 1.104898462D+05-  
 1.567992462D+02  
 C3H4, cyclo- Dorofeeva,1986.  
 2 g 5/90 C 3.00H 4.00 0.00 0.00 0.00 0 40.06386  
 277100.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11373.663  
 -1.969520627D+04 1.505379338D+03-1.418206573D+01 7.642632960D-02-  
 9.765583660D-05  
 6.612003820D-08-1.811251145D-11 2.625631782D+04  
 9.604631890D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11373.663  
 3.168399580D+06-1.371044699D+04 2.664303646D+01-2.420408050D-03  
 4.427994130D-07  
 -4.351820200D-11 1.775948955D-15 1.133683702D+05-  
 1.522619086D+02  
 C3H5, allyl Radical. Burcat,2001 p58.  
 2 g 3/01 C 3.00H 5.00 0.00 0.00 0.00 0 41.07180  
 163594.400  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12738.723  
 -4.315996140D+04 1.441600907D+03-1.197014426D+01 7.319796460D-02-  
 9.066357850D-05  
 6.077059450D-08-1.658826363D-11 1.232157460D+04  
 8.563173240D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12738.723  
 4.094570590D+06-1.676676186D+04 3.123006342D+01-2.885449982D-03  
 5.211343540D-07  
 -5.058284220D-11 2.039932554D-15 1.185720481D+05-  
 1.823070197D+02  
 C3H6, propylene Hf:TRC(4/88) w2600. Chao,1975.  
 2 g 2/00 C 3.00H 6.00 0.00 0.00 0.00 0 42.07974  
 20000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13550.558  
 -1.912462174D+05 3.542074240D+03-2.114878626D+01 8.901484790D-02-  
 1.001429154D-04  
 6.267959390D-08-1.637870781D-11 -1.529961824D+04  
 1.407641382D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13550.558  
 5.017620340D+06-2.086084035D+04 3.644156340D+01-3.881191170D-03  
 7.278677190D-07

-7.321204500D-11 3.052176369D-15 1.261245355D+05-  
 2.195715757D+02  
 C3H6, cyclo- Dorofeeva, 1986. Butcher, 1973b.  
 2 g 1/00 C 3.00H 6.00 0.00 0.00 0.00 0 42.07974  
 53300.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11409.981  
 -1.565787770D+05 4.111129870D+03-3.233447460D+01 1.306337881D-01-  
 1.645563833D-04  
 1.095708326D-07-2.956394783D-11 -1.245271686D+04  
 1.931559109D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11409.981  
 4.785000670D+06-2.042118175D+04 3.631495780D+01-3.561319440D-03  
 6.476241240D-07  
 -6.328430100D-11 2.568705857D-15 1.268274126D+05-  
 2.223729099D+02  
 C3H6O, propylox TRC (6/84) w6150. Swalen, 1957. Oetting, 1964.  
 Villarreal, 1975.  
 2 g 6/01 C 3.00H 6.000 1.00 0.00 0.00 0 58.07914 -  
 93720.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14405.453  
 -2.292808804D+05 4.495750540D+03-2.941117945D+01 1.213113827D-01-  
 1.440060464D-04  
 9.202051750D-08-2.416278343D-11 -3.317697210D+04  
 1.846878218D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14405.453  
 4.789729990D+06-2.106895971D+04 3.954647730D+01-3.910929980D-03  
 7.325531510D-07  
 -7.357085970D-11 3.060618500D-15 1.120344540D+05-  
 2.372004192D+02  
 C3H6O, acetone Chao, 1986. Chao, 1976.  
 2 g 6/97 C 3.00H 6.000 1.00 0.00 0.00 0 58.07914 -  
 217149.600  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16193.193  
 -2.277802525D+05 4.215280010D+03-2.415785316D+01 9.907483320D-02-  
 1.084940903D-04  
 6.583355960D-08-1.676046146D-11 -4.726243940D+04  
 1.607926432D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16193.193  
 5.001601920D+06-2.170155542D+04 3.964493990D+01-4.179945050D-03  
 7.962429530D-07  
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 2.368533477D+02  
 C3H6O, propanal Hf:TRC (6/78) w5300. Chao, 1986. Frankiss, 1974.  
 2 g 5/01 C 3.00H 6.000 1.00 0.00 0.00 0 58.07914 -  
 186000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17326.543  
 -2.649663905D+05 4.245478280D+03-2.108425317D+01 9.195034940D-02-  
 1.004998096D-04  
 6.136754150D-08-1.577443749D-11 -4.447480710D+04  
 1.456069724D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
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 4.830431830D+06-2.075367167D+04 3.924792260D+01-4.095258890D-03  
 7.881119620D-07

-8.107017850D-11 3.436792640D-15 9.944316710D+04-  
 2.316643347D+02  
 C3H7,n-propyl Radical. Tsang,1985.  
 2 g 7/01 C 3.00H 7.00 0.00 0.00 0.00 0 43.08768  
 100500.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14860.058  
 -1.895337073D+05 3.949517260D+03-2.606216089D+01 1.121920441D-01-  
 1.365292213D-04  
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 1.673705556D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14860.058  
 5.646512940D+06-2.291087136D+04 3.987275180D+01-4.106232870D-03  
 7.562557770D-07  
 -7.478263020D-11 3.068983677D-15 1.483006853D+05-  
 2.403781190D+02  
 C3H7,i-propyl Radical. Tsang,1985.  
 2 g 9/85 C 3.00H 7.00 0.00 0.00 0.00 0 43.08768  
 93300.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14807.207  
 -2.952063445D+05 5.294432300D+03-3.105287013D+01 1.143871563D-01-  
 1.291752393D-04  
 8.057843760D-08-2.093908432D-11 -1.476815514D+04  
 1.988082360D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14807.207  
 5.807002520D+06-2.411219997D+04 4.085288400D+01-4.517851330D-03  
 8.499427170D-07  
 -8.573514340D-11 3.583383960D-15 1.546504050D+05-  
 2.487098372D+02  
 C3H8 Hf:TRC(10/85) w1350. Chao,1973.  
 2 g 2/00 C 3.00H 8.00 0.00 0.00 0.00 0 44.09562 -  
 104680.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14741.218  
 -2.433144337D+05 4.656270810D+03-2.939466091D+01 1.188952745D-01-  
 1.376308269D-04  
 8.814823910D-08-2.342987994D-11 -3.540335270D+04  
 1.841749277D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14741.218  
 6.420731680D+06-2.659791134D+04 4.534356840D+01-5.020663920D-03  
 9.471216940D-07  
 -9.575405230D-11 4.009672880D-15 1.455582459D+05-  
 2.818374734D+02  
 C3H8O,1propanol Hf:TRC(6/87) w5030. Chao,1986.  
 2 g 2/00 C 3.00H 8.00O 1.00 0.00 0.00 0 60.09502 -  
 255200.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17518.759  
 -2.616973337D+05 5.192376660D+03-3.296481160D+01 1.354568128D-01-  
 1.593156164D-04  
 1.019498160D-07-2.688552974D-11 -5.612854350D+04  
 2.085024431D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
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 6.308672120D+06-2.642210376D+04 4.715112590D+01-4.642511930D-03  
 8.593465360D-07

-8.682091820D-11 3.642224010D-15 1.255003155D+05-  
 2.859463804D+02  
 C3H8O,2propanol Hf:TRC(6/87) w5030. Chao,1986.  
 2 g 2/00 C 3.00H 8.00O 1.00 0.00 0.00 0 60.09502 -  
 272700.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17264.775  
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 1.864354461D-04  
 1.213257738D-07-3.220433490D-11 -6.279959350D+04  
 2.334322610D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17264.775  
 6.001074750D+06-2.505876830D+04 4.622096120D+01-4.272466310D-03  
 7.693678770D-07  
 -7.450584840D-11 2.998959935D-15 1.148518732D+05-  
 2.796132222D+02  
 C3OS TRC(6/01) p8150, tuvw-8150.  
 2 n 6/01 C 3.00O 1.00S 1.00 0.00 0.00 0 84.09750  
 157330.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15720.000  
 1.173396837D+05-2.154246274D+03 1.739096818D+01-1.606951508D-02  
 2.815913738D-05  
 -2.144517776D-08 6.117883960D-12 2.690975728D+04-  
 6.715502020D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15720.000  
 4.650964090D+05-3.653583100D+03 1.589374854D+01-7.274431680D-04  
 1.507932631D-07  
 -1.250975180D-11 2.879103391D-16 3.664221650D+04-  
 6.509077530D+01  
 C3O2 Hf:Chase,1998 p690 6/68. Shimanouchi,1977 p1083.  
 2 g 7/88 C 3.00O 2.00 0.00 0.00 0.00 0 68.03090 -  
 93638.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15084.983  
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 2.978671986D-05  
 -2.182900022D-08 6.013797220D-12 -1.121054014D+03-  
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 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15084.983  
 6.968699890D+05-4.624733190D+03 1.663905725D+01-1.175486554D-03  
 2.478106444D-07  
 -2.745165984D-11 1.239566766D-15 1.252580069D+04-  
 7.275968780D+01  
 C3S2 TRC(6/01) p8150, tuvw-8150.  
 2 n 6/01 C 3.00S 2.00 0.00 0.00 0.00 0 100.16410  
 412500.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15990.000  
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 2.228897169D-05  
 -1.808702234D-08 5.421828530D-12 5.607264740D+04-  
 6.032258800D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15990.000  
 2.718212835D+05-2.941949284D+03 1.559075626D+01-8.093965740D-04  
 1.739434000D-07

-1.932034262D-11 8.570339980D-16 6.274672550D+04-  
6.207025890D+01  
C4 Gurvich,1991 pt1 p18 pt2 p16.  
3 g tpi C 4.00 0.00 0.00 0.00 0.00 0 48.04280  
1033903.742  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
13117.742  
3.903780500D+04-8.948280780D+02 1.050952925D+01-6.552894460D-03  
1.243940464D-05  
-8.645341370D-09 2.263638846D-12 1.266425869D+05-  
3.077594475D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
13117.742  
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1.779154772D-06  
2.589873632D-10-1.385553481D-14 1.334389611D+05-  
7.261148820D+00  
6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
13117.742  
-2.864752103D+07 1.765535487D+04 6.166598280D+00 8.098789030D-04-  
6.653483810D-08  
2.504726897D-12-3.585724180D-17 -2.082319291D+04  
4.331258920D+00  
C4H2,butadiyne 1,3-Butadiyne. Dorofeeva,1991.  
2 g 7/01 C 4.00H 2.00 0.00 0.00 0.00 0 50.05868  
450000.000  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
14393.860  
2.467542569D+05-3.897855640D+03 2.366080456D+01-2.208077805D-02  
2.781101140D-05  
-1.577340010D-08 3.423165460D-12 7.086907820D+04-  
1.109173560D+02  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
14393.860  
2.328179913D+06-8.925186090D+03 2.114326883D+01-1.368871276D-03  
2.327503159D-07  
-2.124517624D-11 8.053313020D-16 1.057788416D+05-  
1.088313574D+02  
C4H4,1,3-cyclo- 1,3-Cyclobutadiene. Dorofeeva,1986.  
2 g 8/00 C 4.00H 4.00 0.00 0.00 0.00 0 52.07456  
385000.000  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
12103.534  
-2.778428049D+04 1.768176915D+03-1.757895171D+01 9.383512920D-02-  
1.195524281D-04  
7.978086190D-08-2.152751100D-11 3.811627120D+04  
1.128478124D+02  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
12103.534  
2.991498949D+06-1.416781502D+04 3.001978876D+01-2.579200423D-03  
4.789990450D-07  
-4.775329710D-11 1.974923662D-15 1.274666920D+05-  
1.727532057D+02  
C4H6,butadiene 1,3-butadiene. TRC(10/92) tuv2820.  
2 n10/92 C 4.00H 6.00 0.00 0.00 0.00 0 54.09044  
110000.000  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
15130.000  
-9.181130530D+04 3.312570530D+03-2.985828611D+01 1.479201147D-01-  
2.056618326D-04

1.466496826D-07-4.145285730D-11 -2.077309444D+03  
 1.780687329D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15130.000  
 -2.361903188D+07 5.651323370D+04-3.275738320D+01 2.293070572D-02-  
 2.297106441D-06  
 4.292596210D-11 4.236766040D-15 -3.671358620D+05  
 3.013437302D+02  
 C4H6,1butyne TRC(10/93) tuv3040.  
 2 n10/93 C 4.00H 6.00 0.00 0.00 0.00 0 54.09044  
 165200.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16020.000  
 -5.597039970D+04 1.433191711D+03-9.691210720D+00 7.150002390D-02-  
 8.157967800D-05  
 5.290364970D-08-1.435655372D-11 1.184987013D+04  
 7.660225360D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16020.000  
 6.364402700D+06-2.392087731D+04 4.073750410D+01-3.176726490D-03  
 1.199856984D-07  
 3.201802510D-11-2.854392633D-15 1.634335546D+05-  
 2.460284791D+02  
 C4H6,2butyne TRC(10/93) tuv3040.  
 2 n10/93 C 4.00H 6.00 0.00 0.00 0.00 0 54.09044  
 145700.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16640.000  
 -2.650756405D+05 4.490728690D+03-2.400723889D+01 9.819579550D-02-  
 1.079717182D-04  
 6.675555770D-08-1.740766886D-11 -5.328363710D+03  
 1.595035268D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16640.000  
 3.981304330D+06-1.873032899D+04 3.654561490D+01-2.369686378D-03  
 3.990211810D-07  
 -3.698707270D-11 1.442072006D-15 1.261460214D+05-  
 2.155866205D+02  
 C4H6,cyclo- Cyclobutene. Dorofeeva,1986.  
 2 g 8/00 C 4.00H 6.00 0.00 0.00 0.00 0 54.09044  
 156700.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12557.564  
 -2.046707734D+05 4.919470570D+03-3.753278160D+01 1.497293031D-01-  
 1.860139375D-04  
 1.219909019D-07-3.254073590D-11 -3.915950540D+03  
 2.233282138D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12557.564  
 4.517367820D+06-2.097311985D+04 4.008039170D+01-3.949793980D-03  
 7.448484990D-07  
 -7.529754170D-11 3.153253502D-15 1.406469848D+05-  
 2.434836999D+02  
 C4H8,1-butene TRC(4/88) tuv2600.  
 2 n 4/88 C 4.00H 8.00 0.00 0.00 0.00 0 56.10632  
 540.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17120.000  
 -2.721492014D+05 5.100079250D+03-3.183786250D+01 1.317754442D-01-  
 1.527359339D-04



9.714761110D-08-2.560204470D-11 -2.523096386D+04  
 2.006932108D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17120.000  
 6.257948610D+06-2.660376305D+04 4.764920050D+01-4.383267110D-03  
 7.128838440D-07  
 -5.991020840D-11 2.051753504D-15 1.569252657D+05-  
 2.913869761D+02  
 C4H8,cis2-buten Cis2-butene TRC(4/88) tuv2600.  
 2 n 4/88 C 4.00H 8.00 0.00 0.00 0.00 0 56.10632 -  
 7400.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16800.000  
 -2.773870877D+05 5.382384040D+03-3.375188100D+01 1.322980623D-01-  
 1.490975922D-04  
 9.277722000D-08-2.408282948D-11 -2.715884347D+04  
 2.114462085D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16800.000  
 6.461018350D+06-2.775376432D+04 4.863532360D+01-4.862386350D-03  
 8.412626100D-07  
 -7.633890370D-11 2.861702826D-15 1.630856187D+05-  
 3.003105998D+02  
 C4H8,tr2-butene TRC(4/88) tuv2600.  
 2 n 4/88 C 4.00H 8.00 0.00 0.00 0.00 0 56.10632 -  
 11000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17510.000  
 -3.594644110D+05 5.930972080D+03-3.255825290D+01 1.254957780D-01-  
 1.374705365D-04  
 8.407341350D-08-2.163047345D-11 -3.113296523D+04  
 2.070081219D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17510.000  
 6.444758090D+06-2.750706151D+04 4.870329380D+01-4.952445460D-03  
 8.700135910D-07  
 -8.017471710D-11 3.052575093D-15 1.612137505D+05-  
 3.004419156D+02  
 C4H8,isobutene TRC(4/88) tuv2600.  
 2 n 4/88 C 4.00H 8.00 0.00 0.00 0.00 0 56.10632 -  
 17100.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17010.000  
 -2.327205032D+05 3.941994240D+03-2.224581184D+01 1.012790864D-01-  
 1.073194065D-04  
 6.454696910D-08-1.646330345D-11 -2.233766063D+04  
 1.479597621D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17010.000  
 6.484970990D+06-2.732504764D+04 4.836321080D+01-4.768004050D-03  
 8.233875840D-07  
 -7.449253000D-11 2.782303056D-15 1.595941773D+05-  
 2.982986237D+02  
 C4H8,cyclo- Cyclobutane. Dorofeeva,1986.  
 2 g 8/00 C 4.00H 8.00 0.00 0.00 0.00 0 56.10632  
 28400.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13534.163  
 -3.047655983D+05 6.519482730D+03-4.662987590D+01 1.743593052D-01-  
 2.090964176D-04

1.343528679D-07-3.542727400D-11 -2.700031171D+04  
 2.738348195D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13534.163  
 4.456213810D+06-2.301018492D+04 4.492448460D+01-3.080145176D-03  
 5.317165260D-07  
 -5.081079380D-11 2.048919092D-15 1.355487603D+05-  
 2.771801965D+02  
 (CH3COOH)<sub>2</sub> Acetic acid dimer. Chao,1978.  
 2 g10/00 C 4.00H 8.00O 4.00 0.00 0.00 0 120.10392 -  
 929015.360  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 28053.169  
 -3.094720023D+05 5.983338600D+03-3.573002920D+01 1.662525587D-01-  
 1.883866300D-04  
 1.154939386D-07-2.935166753D-11 -1.421493469D+05  
 2.295855147D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 28053.169  
 6.571327590D+06-3.036870720D+04 6.250376670D+01-5.732624710D-03  
 1.083461635D-06  
 -1.097963590D-10 4.609263380D-15 6.347426600D+04-  
 3.734555070D+02  
 C4H9,n-butyl TRC(10/84) tuvW1940.  
 2 n10/84 C 4.00H 9.00 0.00 0.00 0.00 0 57.11426  
 66530.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19797.000  
 -2.239560407D+05 4.676554100D+03-2.985424449D+01 1.345493704D-01-  
 1.600660350D-04  
 1.045338096D-07-2.812951048D-11 -1.525297704D+04  
 1.901651559D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19797.000  
 7.198686940D+06-2.959241524D+04 5.242042810D+01-5.441572440D-03  
 9.917758370D-07  
 -9.464455870D-11 3.729487040D-15 1.834566472D+05-  
 3.214209170D+02  
 C4H9,i-butyl 2-methylpropyl. TRC(10/84) tuvW1940.  
 2 n10/84 C 4.00H 9.00 0.00 0.00 0.00 0 57.11426  
 57320.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18317.000  
 -2.399461281D+05 4.697444540D+03-3.087472560D+01 1.391655831D-01-  
 1.670233968D-04  
 1.092423088D-07-2.936209962D-11 -1.638151036D+04  
 1.936662372D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18317.000  
 6.752936060D+06-2.837423721D+04 5.140687610D+01-4.982399010D-03  
 8.801506630D-07  
 -8.125738690D-11 3.099140009D-15 1.743448480D+05-  
 3.149940745D+02  
 C4H9,s-butyl 1-methylpropyl radical. Tsang,1985.  
 2 g 1/93 C 4.00H 9.00 0.00 0.00 0.00 0 57.11426  
 71000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17537.649  
 -3.351062890D+05 6.312945950D+03-4.003025260D+01 1.563875047D-01-  
 1.842331788D-04

1.182727848D-07-3.131156589D-11 -2.216045659D+04  
 2.481295714D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17537.649  
 7.224744350D+06-3.035291099D+04 5.288551830D+01-5.652083550D-03  
 1.060032692D-06  
 -1.066129835D-10 4.443810960D-15 1.883494279D+05-  
 3.255719880D+02  
 C4H9,t-butyl 1,1dimethylethyl radical. Tsang,1985.  
 2 g 1/93 C 4.00H 9.00 0.00 0.00 0.00 0 57.11426  
 51700.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17009.675  
 -4.723461950D+05 8.090198770D+03-4.683675340D+01 1.575300095D-01-  
 1.686559436D-04  
 9.981040130D-08-2.487608823D-11 -3.319367410D+04  
 2.894838706D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17009.675  
 7.151064950D+06-3.171224410D+04 5.442510320D+01-6.392331160D-03  
 1.241097612D-06  
 -1.287248300D-10 5.512618740D-15 1.934506997D+05-  
 3.399325290D+02  
 C4H10,n-butane Hf:TRC(10/85) w1350. Chen,1975.  
 2 g 12/00 C 4.00H 10.00 0.00 0.00 0.00 0 58.12220 -  
 125790.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19228.685  
 -3.175872540D+05 6.176331820D+03-3.891562120D+01 1.584654284D-01-  
 1.860050159D-04  
 1.199676349D-07-3.201670550D-11 -4.540363390D+04  
 2.379488665D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19228.685  
 7.682322450D+06-3.256051510D+04 5.736732750D+01-6.197916810D-03  
 1.180186048D-06  
 -1.221893698D-10 5.250635250D-15 1.774526560D+05-  
 3.587918760D+02  
 C4H10,isobutane TRC(10/85) w1350. Chen,1975.  
 2 g 8/00 C 4.00H 10.00 0.00 0.00 0.00 0 58.12220 -  
 134990.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17936.500  
 -3.834469330D+05 7.000039640D+03-4.440026900D+01 1.746183447D-01-  
 2.078195348D-04  
 1.339792433D-07-3.551681630D-11 -5.034018890D+04  
 2.658966497D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17936.500  
 7.528018920D+06-3.202517060D+04 5.700161000D+01-6.060013090D-03  
 1.143975809D-06  
 -1.157061835D-10 4.846042910D-15 1.728500802D+05-  
 3.576176890D+02  
 C4N2 Hf:TRC(12/93) w8992. Khanna,1987. Brown,1989.  
 2 g 6/01 C 4.00N 2.00 0.00 0.00 0.00 0 76.05628  
 529200.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17799.401  
 1.587802866D+05-2.987184206D+03 2.348081602D+01-2.607502448D-02  
 4.042830030D-05

-2.804912444D-08 7.397652050D-12 7.505299470D+04-  
 1.017578234D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17799.401  
 1.167686152D+06-6.198644180D+03 2.062070093D+01-1.518619449D-03  
 3.162361680D-07  
 -3.469922800D-11 1.555154128D-15 9.667409390D+04-  
 9.669734580D+01  
 C5 Gurvich,1991 pt1 p20 pt2 p18.  
 3 g 8/00 C 5.00 0.00 0.00 0.00 0.00 0 60.05350  
 1050924.332  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16191.831  
 -1.200801119D+04-5.553702910D+02 1.123828271D+01-4.347884520D-03  
 1.738987490D-05  
 -1.707945418D-08 5.574541910D-12 1.262404627D+05-  
 3.262308990D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16191.831  
 2.172055356D+05-2.958510027D+03 1.561080967D+01-8.200361920D-04  
 1.776898025D-07  
 -2.009853583D-11 9.222677770D-16 1.395208064D+05-  
 6.433077180D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16191.831  
 3.266863960D+06-2.666377675D+03 1.408383780D+01-6.620512140D-05  
 4.099789450D-09  
 -1.315689998D-13 1.711940703D-18 1.405413771D+05-  
 5.349354010D+01  
 C5H6,1,3cyclo- 1,3-Cyclopentadiene. Pedley,1986 p90. Dorofeeva,1986.  
 2 g 5/90 C 5.00H 6.00 0.00 0.00 0.00 0 66.10114  
 134300.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13535.529  
 -1.886259728D+05 4.738220870D+03-3.888958010D+01 1.667438533D-01-  
 2.141149581D-04  
 1.438132328D-07-3.906478110D-11 -5.667022010D+03  
 2.279898557D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13535.529  
 4.428478190D+06-2.123547976D+04 4.309819010D+01-3.914783460D-03  
 7.311847010D-07  
 -7.327241190D-11 3.044403403D-15 1.382542782D+05-  
 2.605959678D+02  
 C5H8,cyclo- Cyclopentene. Hf:TRC(10/92) w2840. Dorofeeva,1986.  
 2 g 1/93 C 5.00H 8.00 0.00 0.00 0.00 0 68.11702  
 33900.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14857.179  
 -2.631114588D+05 5.987753490D+03-4.522244600D+01 1.804626339D-01-  
 2.177216062D-04  
 1.402022671D-07-3.699094300D-11 -2.379504749D+04  
 2.660136401D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14857.179  
 4.569848100D+06-2.406018294D+04 4.881006460D+01-3.413054980D-03  
 6.047001660D-07  
 -5.927495780D-11 2.447865390D-15 1.413983093D+05-  
 2.989533527D+02  
 C5H10,1-pentene TRC(4/87) tuv2500.

2 n 4/87 C 5.00H 10.00 0.00 0.00 0.00 0 70.13290 -  
 21280.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 21680.000  
 -5.340548130D+05 9.298917380D+03-5.667792450D+01 2.123100266D-01-  
 2.571298290D-04  
 1.666834304D-07-4.434080470D-11 -4.790682180D+04  
 3.396036400D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 21680.000  
 3.744014970D+06-2.104485321D+04 4.736126990D+01-4.244201200D-04-  
 3.898975050D-08  
 1.367074243D-11-9.313194230D-16 1.154091373D+05-  
 2.786177449D+02  
 C5H10,cyclo- Cyclopentane. Dorofeeva,1986.  
 2 g 2/01 C 5.00H 10.00 0.00 0.00 0.00 0 70.13290 -  
 77100.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15023.337  
 -4.141119710D+05 8.627592800D+03-6.202959980D+01 2.259910921D-01-  
 2.682303330D-04  
 1.706289935D-07-4.464050920D-11 -4.931522140D+04  
 3.583916230D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15023.337  
 7.501938730D+06-3.505864850D+04 6.322480750D+01-6.940356580D-03  
 1.337306593D-06  
 -1.377905033D-10 5.867357640D-15 1.954925511D+05-  
 4.026550900D+02  
 C5H11,pentyl Radical. TRC(10/84) tuv1941.  
 2 n10/84 C 5.00H 11.00 0.00 0.00 0.00 0 71.14084  
 45810.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 24422.000  
 -4.653715920D+05 8.564220420D+03-5.295242890D+01 2.094288859D-01-  
 2.561602906D-04  
 1.692755961D-07-4.596788110D-11 -3.641704270D+04  
 3.196862240D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 24422.000  
 5.697252900D+06-2.891706175D+04 5.811029680D+01-3.593995010D-03  
 4.419967630D-07  
 -1.509664551D-11-6.626964430D-16 1.717009550D+05-  
 3.522477120D+02  
 C5H11,t-pentyl 1,1-dimethylpropyl radical. Tsang,1985.  
 2 g 1/93 C 5.00H 11.00 0.00 0.00 0.00 0 71.14084  
 32600.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19643.723  
 -5.152181980D+05 9.144327830D+03-5.602397890D+01 1.998204194D-01-  
 2.239112591D-04  
 1.375455547D-07-3.523833050D-11 -4.036266610D+04  
 3.402811000D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19643.723  
 8.602108260D+06-3.805205770D+04 6.649690370D+01-7.533860630D-03  
 1.451612787D-06  
 -1.495593207D-10 6.368022330D-15 2.281858805D+05-  
 4.169408550D+02  
 C5H12,n-pentane TRC(10/85) tuv1350.

2 n10/85 C 5.00H 12.00 0.00 0.00 0.00 0 72.14878 -  
 146760.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 24184.000  
 -2.768894625D+05 5.834283470D+03-3.617541480D+01 1.533339707D-01-  
 1.528395882D-04  
 8.191092000D-08-1.792327902D-11 -4.665375250D+04  
 2.265544053D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 24184.000  
 -2.530779286D+06-8.972593260D+03 4.536223260D+01-2.626989916D-03  
 3.135136419D-06  
 -5.318728940D-10 2.886896868D-14 1.484616529D+04-  
 2.516550384D+02  
 C5H12,i-pentane 2-Methylbutane. TRC(10/85) tuvwl350.  
 2 n10/85 C 5.00H 12.00 0.00 0.00 0.00 0 72.14878 -  
 153700.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22008.000  
 -4.231903390D+05 6.497189100D+03-3.681126970D+01 1.532424729D-01-  
 1.548790714D-04  
 8.749897120D-08-2.070547710D-11 -5.155416590D+04  
 2.309518218D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22008.000  
 1.156888594D+07-4.556246870D+04 7.495443630D+01-7.845415580D-03  
 1.444393314D-06  
 -1.464370213D-10 6.230285000D-15 2.544927135D+05-  
 4.801985780D+02  
 CH3C(CH3)2CH3 2,2-Dimethylpropane (neopentane). TRC(10/85) tuvwl350.  
 2 n10/85 C 5.00H 12.00 0.00 0.00 0.00 0 72.14878 -  
 167920.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 23179.000  
 -8.973222270D+06 1.289225617D+05-7.199344830D+02 2.056862183D+00-  
 2.953159699D-03  
 2.158893146D-06-6.268318770D-10 -6.394932020D+05  
 4.020806360D+03  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 23179.000  
 1.684705520D+07-5.979430570D+04 8.685451480D+01-9.621917600D-03  
 1.653363091D-06  
 -1.674727926D-10 7.372119360D-15 3.458496820D+05-  
 5.760466970D+02  
 C6D5,phenyl Radical-d5. Burcat,1985.  
 2 g 1/01 C 6.00D 5.00 0.00 0.00 0.00 0 82.13471  
 315740.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15919.077  
 2.012837008D+05-1.979349332D+03 2.628267500D+00 5.951865260D-02-  
 6.081280450D-05  
 3.381391650D-08-8.125429080D-12 4.697247490D+04  
 3.354700980D-01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15919.077  
 1.411628125D+06-1.362569472D+04 4.028984940D+01-3.490989270D-03  
 7.379612130D-07  
 -8.192244050D-11 3.705330970D-15 1.088073731D+05-  
 2.293621057D+02  
 C6D6 Benzene-d6. Burcat,1985.

2 g 1/01 C 6.00D 6.00 0.00 0.00 0.00 0 84.14881  
 58157.378  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16324.686  
 2.762911236D+05-2.865868902D+03 5.395070430D+00 5.939315170D-02-  
 6.023631180D-05  
 3.381398570D-08-8.306046370D-12 2.047083778D+04-  
 2.011790696D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16324.686  
 1.758057871D+06-1.572121558D+04 4.468162490D+01-4.003361920D-03  
 8.445434400D-07  
 -9.360556980D-11 4.228475530D-15 8.962045360D+04-  
 2.615332268D+02  
 C6H2 Dorofeeva,1991.  
 2 g 2/93 C 6.00H 2.00 0.00 0.00 0.00 0 74.08008  
 67000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19607.714  
 2.903722964D+05-4.929751500D+03 3.189323210D+01-3.119447315D-02  
 4.325763680D-05  
 -2.732517022D-08 6.674446110D-12 1.011898682D+05-  
 1.530593012D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19607.714  
 2.592848577D+06-1.083361978D+04 2.847459495D+01-1.876727704D-03  
 3.412134280D-07  
 -3.337392890D-11 1.356853889D-15 1.418517294D+05-  
 1.494853494D+02  
 C6H5,phenyl Radical.Hf:TRC(10/89) w4270. Jacox,1989. NASA ab  
 initio.  
 2 g 11/00 C 6.00H 5.00 0.00 0.00 0.00 0 77.10390  
 337200.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14154.633  
 -1.211278245D+05 3.529045580D+03-3.116903422D+01 1.467550630D-01-  
 1.831398296D-04  
 1.192576957D-07-3.149265860D-11 2.420972928D+04  
 1.868799946D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14154.633  
 3.670279230D+06-1.894601209D+04 4.180581820D+01-3.503914150D-03  
 6.561821740D-07  
 -6.594714450D-11 2.748094212D-15 1.476744628D+05-  
 2.475301142D+02  
 C6H5O,phenoxy Phenoxy radical. Burcat,1985.  
 2 g 8/00 C 6.00H 5.000 1.00 0.00 0.00 0 93.10330  
 47700.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16208.094  
 -1.292264217D+05 3.406740680D+03-2.911367361D+01 1.459180378D-01-  
 1.780202758D-04  
 1.138615885D-07-2.967142152D-11 -1.055026758D+04  
 1.770682011D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16208.094  
 3.678640340D+06-1.972980806D+04 4.541184410D+01-3.751064390D-03  
 7.114450780D-07  
 -7.233328850D-11 3.045637067D-15 1.163595961D+05-  
 2.681058539D+02

C6H6 TRC(10/86)w3200. Pliva,1982,1983,1984.  
Shimanouchi,1972.  
2 g 8/00 C 6.00H 6.00 0.00 0.00 0.00 0 78.11184  
82880.000  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
14195.691  
-1.677340902D+05 4.404500040D+03-3.717377910D+01 1.640509559D-01-  
2.020812374D-04  
1.307915264D-07-3.444284100D-11 -1.035455401D+04  
2.169853345D+02  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
14195.691  
4.538575720D+06-2.260502547D+04 4.694007300D+01-4.206676830D-03  
7.907994330D-07  
-7.968302100D-11 3.328212080D-15 1.391464686D+05-  
2.868751333D+02  
C6H5OH,phenol Burcat,1985.  
2 g 8/00 C 6.00H 6.000 1.00 0.00 0.00 0 94.11124 -  
96399.000  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
17496.700  
-1.209418144D+05 3.378292270D+03-2.991846148D+01 1.567802942D-01-  
1.970937198D-04  
1.291815064D-07-3.424351260D-11 -2.779387017D+04  
1.799708977D+02  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
17496.700  
4.462081570D+06-2.165521026D+04 4.815015050D+01-3.568282430D-03  
6.327175730D-07  
-6.039905720D-11 2.399168678D-15 1.113726204D+05-  
2.860454446D+02  
C6H10,cyclo- Cyclohexene. Dorofeeva,1986.  
2 g 1/93 C 6.00H 10.00 0.00 0.00 0.00 0 82.14360 -  
4600.000  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
17270.784  
-3.750282210D+05 7.643876750D+03-5.510434760D+01 2.166231405D-01-  
2.545452198D-04  
1.607607304D-07-4.185248410D-11 -3.661073010D+04  
3.202409460D+02  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
17270.784  
7.510128980D+06-3.556858210D+04 6.703034940D+01-7.045351870D-03  
1.358166400D-06  
-1.400074492D-10 5.964551700D-15 2.060274332D+05-  
4.238197660D+02  
C6H12,1-hexene TRC(4/87) tuv2500.  
2 n 4/87 C 6.00H 12.00 0.00 0.00 0.00 0 84.15948 -  
41950.000  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
26240.000  
-6.668831650D+05 1.176864939D+04-7.270998330D+01 2.709398396D-01-  
3.333246400D-04  
2.182347097D-07-5.859468820D-11 -6.215780540D+04  
4.286825640D+02  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
26240.000  
7.332906960D+05-1.448848641D+04 4.671215490D+01 3.172978470D-03-  
5.242646520D-07  
4.280355820D-11-1.472353254D-15 6.697740410D+04-  
2.623643854D+02



C6H12,cyclo- Cyclohexane. Dorofeeva,1986.

2 g 6/90 C 6.00H 12.00 0.00 0.00 0.00 0 84.15948 -  
123300.000  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
17544.814  
-5.679987040D+05 1.034238704D+04-6.800041250D+01 2.387797658D-01-  
2.511890049D-04  
1.425293184D-07-3.407833190D-11 -6.404635160D+04  
3.934808210D+02  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
17544.814  
5.225149470D+06-3.364194580D+04 7.174607470D+01-6.698979120D-03  
1.318443254D-06  
-1.390794789D-10 6.060102240D-15 1.732537609D+05-  
4.546814170D+02

C6H13,n-hexyl TRC(10/83) tuv1930.

2 n10/83 C 6.00H 13.00 0.00 0.00 0.00 0 85.16742  
25100.000  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
28983.000  
-1.427278220D+06 2.248828093D+04-1.297492240D+02 4.279797330D-01-  
5.556013180D-04  
3.791256940D-07-1.048462404D-10 -1.060261015D+05  
7.497186760D+02  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
28983.000  
5.967938620D+06-3.299023160D+04 6.869073440D+01-4.225009060D-03  
5.496523820D-07  
-2.292851471D-11-5.086341890D-16 1.906978683D+05-  
4.185362000D+02

C6H14,n-hexane TRC(4/85) tuv1440.

2 g 6/01 C 6.00H 14.00 0.00 0.00 0.00 0 86.17536 -  
166920.000  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
28702.000  
-5.815926700D+05 1.079097724D+04-6.633947030D+01 2.523715155D-01-  
2.904344705D-04  
1.802201514D-07-4.617223680D-11 -7.271544570D+04  
3.938283540D+02  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
28702.000  
-3.106625684D+06-7.346087920D+03 4.694131760D+01 1.693963977D-03  
2.068996667D-06  
-4.212141680D-10 2.452345845D-14 5.237503120D+02-  
2.549967718D+02

C7H7,benzyl Radical. Brouwer,1988. Hippler,1990.

2 g 7/01 C 7.00H 7.00 0.00 0.00 0.00 0 91.13048  
210500.000  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
18554.892  
-1.836764826D+05 4.102465660D+03-3.202406100D+01 1.588249575D-01-  
1.894466924D-04  
1.203649671D-07-3.136589637D-11 5.266333230D+03  
1.938751720D+02  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
18554.892  
5.297322160D+06-2.599909398D+04 5.509750790D+01-4.977661470D-03  
9.463152430D-07  
-9.639008860D-11 4.064470420D-15 1.738382912D+05-  
3.343829550D+02

C7H8 Hf:TRC(4/98) w3510. Hitchcock,1975. Rudolph,1967.

2 g 1/93 C 7.00H 8.00 0.00 0.00 0.00 0 92.13842  
 50170.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17940.345  
 -2.877962220D+05 6.133941520D+03-4.574706760D+01 1.936895724D-01-  
 2.304305304D-04  
 1.459301178D-07-3.790796100D-11 -2.308402499D+04  
 2.693915042D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17940.345  
 6.184538350D+06-2.990284056D+04 5.982005970D+01-5.696983960D-03  
 1.080748416D-06  
 -1.098702235D-10 4.624740220D-15 1.782047857D+05-  
 3.698082250D+02  
 C7H8O,cresol-mx Eql. mixture of isomers. Kudchadker,1978.  
 2 g12/00 C 7.00H 8.000 1.00 0.00 0.00 0 108.13782 -  
 132298.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 21838.344  
 -2.441417503D+05 5.080877840D+03-3.789048040D+01 1.864945070D-01-  
 2.269511868D-04  
 1.458989279D-07-3.822403350D-11 -4.093657830D+04  
 2.281352234D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 21838.344  
 6.017373450D+06-2.849882774D+04 6.081543070D+01-4.996807110D-03  
 9.134279950D-07  
 -8.979444110D-11 3.667756970D-15 1.472218400D+05-  
 3.674850140D+02  
 C7H14,1-heptene TRC(4/87) tuvW2500.  
 2 n 4/87 C 7.00H 14.00 0.00 0.00 0.00 0 98.18606 -  
 62760.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 30790.000  
 -7.449402840D+05 1.332179893D+04-8.281694380D+01 3.108065994D-01-  
 3.786779920D-04  
 2.446841042D-07-6.488763870D-11 -7.217885010D+04  
 4.856671490D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 30790.000  
 -1.927608174D+06-9.125024420D+03 4.748177970D+01 6.067660530D-03-  
 8.684859080D-07  
 5.813995260D-11-1.473979569D-15 2.600914656D+04-  
 2.562880707D+02  
 C7H15,n-heptyl TRC(10/83) tuvW1930.  
 2 n10/83 C 7.00H 15.00 0.00 0.00 0.00 0 99.19400  
 4390.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 33543.000  
 -1.671733521D+06 2.640010250D+04-1.526867707D+02 5.027121410D-01-  
 6.521014030D-04  
 4.443488110D-07-1.227815006D-10 -1.273754623D+05  
 8.783933320D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 33543.000  
 5.444527570D+06-3.456829290D+04 7.638651950D+01-3.298972000D-03  
 2.343496957D-07  
 2.467674021D-11-3.162012849D-15 1.939079354D+05-  
 4.641424660D+02  
 C7H16,n-heptane TRC(10/85) tuv1460. TRC(10/84) ptuv1010.

2 n10/85 C 7.00H 16.00 0.00 0.00 0.00 0 100.20194 -  
 187780.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 33221.000  
 -6.127432890D+05 1.184085437D+04-7.487188600D+01 2.918466052D-01-  
 3.416795490D-04  
 2.159285269D-07-5.655852730D-11 -8.013408940D+04  
 4.407213320D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 33221.000  
 9.135632470D+06-3.923319690D+04 7.889780850D+01-4.654251930D-03  
 2.071774142D-06  
 -3.442539300D-10 1.976834775D-14 2.050708295D+05-  
 4.851104020D+02  
 C7H16,2-methylh 2-methylhexane. TRC(10/85) tuvW1460.  
 2 n10/85 C 7.00H 16.00 0.00 0.00 0.00 0 100.20194 -  
 194600.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 30920.000  
 -7.104777770D+05 1.191251120D+04-7.345339440D+01 2.902952369D-01-  
 3.462767680D-04  
 2.260184498D-07-6.128813920D-11 -8.202147700D+04  
 4.320042290D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 30920.000  
 1.289912969D+06-1.784340963D+03 1.083537673D+01 5.270609240D-02-  
 1.886832314D-05  
 2.432255843D-09-1.135553789D-13 -1.637529884D+04-  
 2.981862410D+01  
 C8H8,styrene Ethenylbenzene. TRC(4/89) tuvW4490.  
 2 n 4/89 C 8.00H 8.00 0.00 0.00 0.00 0 104.14912  
 148300.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 20940.000  
 -2.686930520D+05 6.167999470D+03-4.836054940D+01 2.182873229D-01-  
 2.738561832D-04  
 1.810084981D-07-4.867750270D-11 -1.140639978D+04  
 2.817679014D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 20940.000  
 -6.629183620D+06 1.514594166D+04 1.609822364D+00 3.383318600D-02-  
 1.093737395D-05  
 1.338825116D-09-6.032534920D-14 -8.997324150D+04  
 4.311282790D+01  
 C8H10,ethylbenz Ethylbenzene. TRC(10/86) tuvW3200.  
 2 n10/86 C 8.00H 10.00 0.00 0.00 0.00 0 106.16500  
 29920.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22280.000  
 -4.694940000D+05 9.307168360D+03-6.521769470D+01 2.612080237D-01-  
 3.181753480D-04  
 2.051355473D-07-5.401817350D-11 -4.073870210D+04  
 3.780904360D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22280.000  
 5.551564100D+06-2.831380598D+04 6.061240720D+01 1.042112857D-03-  
 1.327426719D-06  
 2.166031743D-10-1.142545514D-14 1.642241062D+05-  
 3.691769820D+02  
 C8H16,1-octene TRC(4/87) tuvW2500.

2 n 4/87 C 8.00H 16.00 0.00 0.00 0.00 0 112.21264 -  
 83590.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 35350.000  
 -9.281905220D+05 1.640974476D+04-1.015939534D+02 3.748001410D-01-  
 4.590829400D-04  
 2.965335340D-07-7.840445210D-11 -8.952426080D+04  
 5.907594270D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 35350.000  
 -4.409336070D+06-4.383678800D+03 4.939154260D+01 7.912339630D-03-  
 7.888669510D-07  
 9.970212350D-12 1.913144872D-15 -1.122619342D+04-  
 2.577650649D+02  
 C8H17,n-octyl TRC(10/83) tuvwl930.  
 2 n10/83 C 8.00H 17.00 0.00 0.00 0.00 0 113.22058 -  
 16320.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 38103.000  
 -1.934340995D+06 3.054979830D+04-1.767903454D+02 5.801596650D-01-  
 7.517414010D-04  
 5.112469030D-07-1.410193662D-10 -1.498894706D+05  
 1.013724329D+03  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 38103.000  
 5.632173390D+06-3.821143670D+04 8.637927500D+01-3.608931580D-03  
 2.544260445D-07  
 2.908638837D-11-3.679549740D-15 2.103135470D+05-  
 5.262422830D+02  
 C8H18,n-octane TRC(4/85) tuvwl490.  
 2 n 4/85 C 8.00H 18.00 0.00 0.00 0.00 0 114.22852 -  
 208750.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 37780.000  
 -6.986647150D+05 1.338501096D+04-8.415165920D+01 3.271936660D-01-  
 3.777209590D-04  
 2.339836988D-07-6.010892650D-11 -9.026223250D+04  
 4.939222140D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 37780.000  
 6.365406950D+06-3.105364657D+04 6.969162340D+01 1.048059637D-02-  
 4.129621950D-06  
 5.543226320D-10-2.651436499D-14 1.500968785D+05-  
 4.169895650D+02  
 C8H18,isooctane 2,2,4-Trimethylpentane. TRC(4/85) tuvwl490.  
 2 n 4/85 C 8.00H 18.00 0.00 0.00 0.00 0 114.22852 -  
 224010.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 32170.000  
 -1.688758565D+05 3.126903227D+03-2.123502828D+01 1.489151508D-01-  
 1.151180135D-04  
 4.473216170D-08-5.554882070D-12 -4.468060620D+04  
 1.417455793D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 32170.000  
 1.352765032D+07-4.663370340D+04 7.795313180D+01 1.423729984D-02-  
 5.073593910D-06  
 7.248232970D-10-3.819190110D-14 2.541178017D+05-  
 4.933887190D+02  
 C9H19,n-nonyl TRC (10/83) tuvwl930.

2 n10/83 C 9.00H 19.00 0.00 0.00 0.00 0 127.24716 -  
 37030.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 42664.000  
 -2.194880612D+06 3.468565780D+04-2.009261419D+02 6.580503110D-01-  
 8.525930010D-04  
 5.794638960D-07-1.597637099D-10 -1.723194608D+05  
 1.149114017D+03  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 42664.000  
 5.277361740D+06-4.025701960D+04 9.457296720D+01-2.940301447D-03  
 6.978106990D-09  
 6.805250240D-11-5.907095330D-15 2.165320614D+05-  
 5.754449500D+02  
 C10H8,naphthale Naphthalene. Chen,1979.  
 2 g 3/01 C 10.00H 8.00 0.00 0.00 0.00 0 128.17052 -  
 150580.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 20713.076  
 -2.602845316D+05 6.237409570D+03-5.226095040D+01 2.397692776D-01-  
 2.912244803D-04  
 1.854944401D-07-4.816619270D-11 -1.114700880D+04  
 2.972139517D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 20713.076  
 5.906172110D+06-3.163229240D+04 7.030342030D+01-6.018865540D-03  
 1.142052144D-06  
 -1.161605689D-10 4.892844020D-15 1.962567046D+05-  
 4.347848950D+02  
 C10H21,n-decyl TRC(10/83) tuvwl930.  
 2 n10/83 C 10.00H 21.00 0.00 0.00 0.00 0 141.27374 -  
 57740.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 47224.000  
 -2.446511152D+06 3.870081300D+04-2.244388176D+02 7.343624970D-01-  
 9.513525600D-04  
 6.462970330D-07-1.781502862D-10 -1.941633889D+05  
 1.280987834D+03  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 47224.000  
 4.967237760D+06-4.242468440D+04 1.028853417D+02-2.324848180D-03-  
 2.284233900D-07  
 1.056127364D-10-8.068065900D-15 2.235429890D+05-  
 6.255191160D+02  
 C12H9,o-bipheny o-Biphenyl radical. Burcat,1985.  
 2 g 8/00 C 12.00H 9.00 0.00 0.00 0.00 0 153.19986 -  
 427730.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 26589.347  
 -3.595840820D+05 7.661378560D+03-5.873290460D+01 2.697557882D-01-  
 3.229756680D-04  
 2.032907100D-07-5.231316720D-11 1.458414642D+04  
 3.392687110D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 26589.347  
 6.736469420D+06-3.632194350D+04 8.210239600D+01-7.502342860D-03  
 1.456251733D-06  
 -1.507145019D-10 6.436470430D-15 2.555524521D+05-  
 5.042462970D+02  
 C12H10,biphenyl Burcat,1985.

2 g 8/00 C 12.00H 10.00 0.00 0.00 0.00 0 154.20780  
 182130.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 26783.523  
 -3.671034050D+05 8.128412590D+03-6.390994570D+01 2.901422744D-01-  
 3.509590740D-04  
 2.230989996D-07-5.788470290D-11 -1.679263066D+04  
 3.633464190D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 26783.523  
 7.480385360D+06-3.928087230D+04 8.661482220D+01-7.946398570D-03  
 1.531868544D-06  
 -1.576450171D-10 6.700602730D-15 2.438050641D+05-  
 5.381381490D+02  
 Ca Hf:Cox,1989. Sugar,1985. Gordon,1999.  
 3 g 8/97 CA 1.00 0.00 0.00 0.00 0.00 0 40.07800  
 177800.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 2.063892786D+04  
 4.384548330D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 7.547341240D+06-2.148642662D+04 2.530849567D+01-1.103773705D-02  
 2.293249636D-06  
 -1.209075383D-10-4.015333268D-15 1.585862323D+05-  
 1.609512955D+02  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 2.291781634D+09-1.608862960D+06 4.312466360D+02-5.396508990D-02  
 3.531856210D-06  
 -1.164403850D-10 1.527134223D-15 1.258651434D+07-  
 3.692101610D+03  
 Ca+ Sugar,1985. Gordon,1999.  
 3 g 1/98 CA 1.00E -1.00 0.00 0.00 0.00 0 40.07745  
 773827.728  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 9.232417790D+04  
 5.077674980D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 3.747070820D+06-1.174707738D+04 1.672546969D+01-8.334797710D-03  
 2.394593294D-06  
 -2.988243468D-10 1.356563002D-14 1.664329088D+05-  
 9.582821260D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 9.117128410D+08-6.220428460D+05 1.683741136D+02-2.140862670D-02  
 1.452947686D-06  
 -4.920790880D-11 6.575369235D-16 4.959472060D+06-  
 1.422600719D+03  
 CaBr Gurvich,1996a pt1 p471 pt2 p367.  
 2 tpi96 CA 1.00BR 1.00 0.00 0.00 0.00 0 119.98200 -  
 24868.681  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9856.119

5.693832620D+02-1.257513537D+02 5.001508330D+00-1.039868753D-03  
 1.377594927D-06  
 -8.949013960D-10 2.395658928D-13 -3.728103980D+03  
 1.784864847D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9856.119  
 2.783236402D+06-8.458203730D+03 1.431756560D+01-5.430781680D-03  
 1.522218659D-06  
 -1.831824807D-10 7.864288660D-15 4.931270680D+04-  
 6.537001100D+01  
 CaBr2 Gurvich,1996a pt1 p474 pt2 p369.  
 2 tpis96 CA 1.00BR 2.00 0.00 0.00 0.00 0 199.88600 -  
 387197.300  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15603.200  
 1.572504318D+03-2.238551236D+02 8.388457890D+00-1.944164774D-03  
 2.397926088D-06  
 -1.556572350D-09 4.124309580D-13 -4.772106610D+04-  
 1.074965233D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15603.200  
 -2.219846426D+04-4.463155330D+00 7.503755110D+00-1.641654626D-06  
 3.879428060D-10  
 -4.683424260D-14 2.259325541D-18 -4.885436820D+04-  
 5.590324250D+00  
 CaCL Gurvich,1996a pt1 p464 pt2 p363.  
 2 tpis96 CA 1.00CL 1.00 0.00 0.00 0.00 0 75.53070 -  
 103772.885  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9595.115  
 6.395335260D+03-2.249042269D+02 5.283278390D+00-1.447983237D-03  
 1.643742771D-06  
 -9.430104280D-10 2.237516133D-13 -1.270169000D+04-  
 1.391970247D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9595.115  
 1.629182545D+06-4.766223020D+03 9.658929770D+00-2.523044131D-03  
 5.833542160D-07  
 -4.101726990D-11 8.813177640D-17 1.662599241D+04-  
 3.398731770D+01  
 CaCL+ Gurvich,1996a pt1 p466 pt2 p364.  
 2 tpis96 CA 1.00CL 1.00E -1.00 0.00 0.00 0 75.53015  
 467190.513  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9361.113  
 2.285284542D+03-2.002872721D+02 4.936990190D+00-3.860973030D-04  
 8.686661880D-08  
 1.470205680D-10-7.689315870D-14 5.588277950D+04-  
 6.359874920D-01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9361.113  
 1.770280396D+05-5.891372390D+02 5.103368800D+00-2.356761168D-04  
 5.483732870D-08  
 2.137973112D-14-5.572887310D-16 5.853417250D+04-  
 2.191259602D+00  
 CaCL2 Gurvich,1996a pt1 p470 pt2 p366.  
 2 tpis96 CA 1.00CL 2.00 0.00 0.00 0.00 0 110.98340 -  
 485243.477  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14857.023

1.106802030D+04-4.249108250D+02 9.134711860D+00-3.497185310D-03  
4.242184630D-06  
-2.719673231D-09 7.138268630D-13 -5.850346760D+04-  
1.808679105D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
14857.023  
-3.595768780D+04-8.796495630D+00 7.507256910D+00-3.129465934D-06  
7.322886480D-10  
-8.776403220D-14 4.210486040D-18 -6.066779660D+04-  
8.553531560D+00  
CaF Gurvich,1996a pt1 p456 pt2 p359.  
2 tpris96 CA 1.00F 1.00 0.00 0.00 0.00 0 59.07640 -  
276403.790  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
9132.110  
3.184235400D+04-4.918235090D+02 5.701120890D+00-1.465138218D-03  
9.092930810D-07  
-1.367585222D-10-5.106323380D-14 -3.197694110D+04-  
5.996662260D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
9132.110  
5.195882670D+05-1.512321567D+03 5.869276250D+00-3.882524480D-04-  
2.484582298D-08  
3.749915960D-11-3.470976450D-15 -2.488814584D+04-  
8.614663700D+00  
CaF+ Gurvich,1996a pt1 p460 pt2 p360.  
2 tpris96 CA 1.00F 1.00E -1.00 0.00 0.00 0 59.07585  
260664.608  
298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
9003.108  
4.158340800D+04-5.627661660D+02 5.687522150D+00-1.264710572D-03  
6.669086480D-07  
-6.926752820D-11-3.978714620D-14 3.305119500D+04-  
6.974485010D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
9003.108  
-1.398670845D+05 2.191526375D+02 4.214324340D+00 2.142798048D-04-  
5.778672600D-08  
9.985756310D-12-6.059621880D-16 2.841605897D+04  
2.740342729D+00  
CaF2 Gurvich,1996a pt1 p462 pt2 p362.  
2 tpris96 CA 1.00F 2.00 0.00 0.00 0.00 0 78.07481 -  
790828.409  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
12811.591  
5.909352290D+04-1.019733042D+03 1.013165309D+01-5.503506440D-03  
5.629319980D-06  
-3.115401465D-09 7.205525940D-13 -9.192608190D+04-  
2.639505950D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
12811.591  
-8.280409440D+04-3.115950071D+01 7.023577370D+00-9.521000020D-06  
2.118160895D-09  
-2.440713888D-13 1.135135468D-17 -9.729466770D+04-  
7.546243340D+00  
CaH Gurvich,1996a pt1 p447 pt2 p353.  
2 tpris96 CA 1.00H 1.00 0.00 0.00 0.00 0 41.08594  
229409.105  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
8705.105



-4.513782230D+04 7.629429210D+02-1.280874223D+00 1.318774659D-02-  
 1.481595334D-05  
 8.536573220D-09-1.989958945D-12 2.300378814D+04  
 3.053421525D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8705.105  
 -2.696952529D+06 8.607059750D+03-7.027454820D+00 7.467916310D-03-  
 2.318610699D-06  
 3.423072420D-10-1.892679792D-14 -2.773819107D+04  
 7.845822010D+01  
 CaI Gurvich,1996a pt1 p474 pt2 p370.  
 2 tpis96 CA 1.00I 1.00 0.00 0.00 0.00 0 166.98247  
 12183.320  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10018.120  
 -8.261790180D+02-8.508975900D+01 4.864171690D+00-7.863169650D-04  
 1.100493506D-06  
 -7.348030610D-10 2.010892767D-13 5.236753440D+02  
 3.585391680D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10018.120  
 1.771071309D+06-5.683643730D+03 1.153857476D+01-4.194020200D-03  
 1.291359961D-06  
 -1.730043579D-10 8.380762350D-15 3.583293200D+04-  
 4.405917570D+01  
 CaI2 Gurvich,1996a pt1 p477 pt2 p372.  
 2 tpis96 CA 1.00I 2.00 0.00 0.00 0.00 0 293.88694 -  
 259319.505  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16050.995  
 -1.097851401D+03-1.459821761D+02 8.089341840D+00-1.305332923D-03  
 1.624199331D-06  
 -1.061194001D-09 2.825551217D-13 -3.272692980D+04-  
 6.981714940D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16050.995  
 -1.623727104D+04-2.859530722D+00 7.502432190D+00-1.071178707D-06  
 2.544559095D-10  
 -3.083631004D-14 1.491836724D-18 -3.346341170D+04-  
 3.567305740D+00  
 CaO Gurvich,1996a pt1 p443 pt2 p349.  
 3 tpis96 CA 1.000 1.00 0.00 0.00 0.00 0 56.07740  
 38005.308  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8953.108  
 3.889733070D+04-4.835677350D+02 5.077713250D+00 3.076235250D-04-  
 1.159759897D-06  
 8.493433340D-10-1.495333366D-13 5.937643480D+03-  
 3.955320730D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8953.108  
 -4.913106170D+07 1.495865950D+05-1.681654149D+02 9.381950260D-02-  
 2.455529428D-05  
 3.074980720D-09-1.485914237D-13 -9.461511720D+05  
 1.235694769D+03  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8953.108  
 -3.504055130D+08 2.083212387D+05-3.978209270D+01 5.039268720D-03-  
 3.220707680D-07  
 1.057379426D-11-1.396044154D-16 -1.662378721D+06  
 3.934491930D+02

CaO+ Gurvich,1996a pt1 p445 pt2 p351.

3 tpis96 CA 1.000 1.00E -1.00 0.00 0.00 0 56.07685 -  
710237.542  
298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
9163.110  
1.098060332D+05-1.459992448D+03 9.880777940D+00-9.157564600D-03  
8.707582560D-06  
-4.390411080D-09 9.264854660D-13 9.150057350D+04-  
3.009947701D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
9163.110  
9.397843130D+05-2.993362243D+03 8.336191820D+00-2.303295087D-03  
7.373967530D-07  
-1.052888279D-10 5.257138410D-15 1.028098401D+05-  
2.461547836D+01  
6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
9163.110  
-7.648645260D+07 1.739245253D+04 8.420288710D+00-1.168386844D-03  
8.413684900D-08  
-2.770799280D-12 3.569474430D-17 -8.643489770D+04-  
2.376513061D+01

CaOH Gurvich,1996a pt1 p451 pt2 p355.

2 tpis96 CA 1.000 1.00H 1.00 0.00 0.00 0 57.08534 -  
173307.350  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
11049.697  
4.620028900D+04-9.285672820D+02 9.175828770D+00-3.962828800D-03  
2.505447308D-06  
3.852068210D-11-3.352778470D-13 -1.798009717D+04-  
2.533704850D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
11049.697  
1.979972994D+06-5.598880990D+03 1.151348706D+01-1.668264707D-03  
3.312573910D-07  
-1.789056647D-11-3.580716410D-16 1.340196822D+04-  
4.646084260D+01

CaOH+ Gurvich,1996a pt1 p452 pt2 p356.

2 tpis96 CA 1.000 1.00H 1.00E -1.00 0.00 0 57.08479 -  
372938.100  
298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
11097.719  
4.884342660D+04-9.832415100D+02 9.610182950D+00-5.204360660D-03  
4.263049820D-06  
-1.197590878D-09 9.028411890D-15 4.795056340D+04-  
2.827077334D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
11097.719  
8.637615370D+05-2.347302046D+03 7.981911200D+00 1.003160947D-04-  
6.240074170D-08  
1.019540904D-11-5.698925280D-16 5.830580120D+04-  
2.152181937D+01

Ca(OH)2 Gurvich,1996a pt1 p455 pt2 p358.

2 tpis96 CA 1.000 2.00H 2.00 0.00 0.00 0 74.09268 -  
598338.869  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
16592.281  
8.389257540D+04-1.791902135D+03 1.621891031D+01-7.840857170D-03  
5.095111610D-06  
-6.955487550D-11-6.132152640D-13 -6.600405630D+04-  
6.070913920D+01

1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16592.281  
 1.721854884D+06-4.702217670D+03 1.396947691D+01 1.983791405D-04-  
 1.243050592D-07  
 2.033402404D-11-1.137157819D-15 -4.443761350D+04-  
 5.287444860D+01  
 CaS Gurvich,1996a pt1 p480 pt2 p374.  
 2 tpis96 CA 1.00S 1.00 0.00 0.00 0.00 0 72.14400  
 121475.313  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9360.113  
 2.320990615D+04-4.518446080D+02 6.172333750D+00-3.598852020D-03  
 4.823731710D-06  
 -3.631733540D-09 1.212849867D-12 1.554597691D+04-  
 7.686915670D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9360.113  
 -1.568353214D+07 5.293855810D+04-6.322467240D+01 4.027726380D-02-  
 1.114855081D-05  
 1.464389344D-09-7.376078970D-14 -3.172022670D+05  
 4.799606220D+02  
 Ca2 Gurvich,1996a pt1 p439 pt2 p347.  
 2 tpis96 CA 2.00 0.00 0.00 0.00 0.00 0 80.15600  
 341765.336  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11273.136  
 -8.582228620D+04 1.588188960D+02 1.103952055D+01-3.333196760D-02  
 5.345938810D-05  
 -4.011573240D-08 1.160486682D-11 3.770350800D+04-  
 2.397744561D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11273.136  
 2.405966267D+05 5.775803820D+01 2.347436675D+00 1.199275034D-04-  
 4.329150310D-08  
 7.015302690D-12-3.705660320D-16 4.081875400D+04  
 1.895399607D+01  
 Cd Hf:Cox,1989. Moore,1971. Gordon,1999.  
 3 g 7/97 CD 1.00 0.00 0.00 0.00 0.00 0 112.41100  
 111800.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 -1.081751543D-04 1.816433041D-06 2.499999989D+00 3.129989231D-11-  
 4.600710160D-14  
 3.407048740D-17-9.989497436D-21 1.270099766D+04  
 5.931549760D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 -2.699757467D+05 7.866001140D+02 1.628169079D+00 4.594123290D-04-  
 1.150420443D-07  
 1.074836707D-11 8.790199555D-17 7.675148260D+03  
 1.220006052D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 -1.336284287D+09 9.320949110D+05-2.490956222D+02 3.302878610D-02-  
 2.200384347D-06  
 7.425712550D-11-1.026730246D-15 -7.267528990D+06  
 2.167946107D+03  
 Cd+ Moore,1971. Gordon,1999.  
 3 g 7/97 CD 1.00E -1.00 0.00 0.00 0.00 0 112.41045  
 985754.328

298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 4.098344940D-04-4.343581620D-06 2.500000019D+00-4.389036810D-11  
 5.563969200D-14  
 -3.638228260D-17 9.607881995D-21 1.178129439D+05  
 6.624689450D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 1.484880812D+04-4.669153680D+01 2.557883006D+00-3.624701700D-05  
 1.213747570D-08  
 -2.072802814D-12 1.420665367D-16 1.181070109D+05  
 6.216414480D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 -6.428364400D+07 4.740395160D+04-1.165755517D+01 2.220273739D-03-  
 1.964219980D-07  
 9.262295070D-12-1.560026961D-16 -2.489244513D+05  
 1.263946278D+02  
 CL Hf:Cox,1989. Moore,1971. Moore,1970a. Gordon,1999.  
 3 g 7/97 CL 1.00 0.00 0.00 0.00 0.00 0 35.45270  
 121301.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6271.588  
 2.276215854D+04-2.168413293D+02 2.745185115D+00 2.451101694D-03-  
 5.458011990D-06  
 4.417986880D-09-1.288134004D-12 1.501357068D+04  
 3.102950764D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6271.588  
 -1.697932930D+05 6.081726460D+02 2.128664090D+00 1.307367034D-04-  
 2.644883596D-08  
 2.842504775D-12-1.252911731D-16 9.934387400D+03  
 8.844759410D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6271.588  
 -7.139687070D+07 4.499936330D+04-9.264315350D+00 1.657437964D-03-  
 1.326219399D-07  
 5.533998870D-12-8.390301878D-17 -3.405333030D+05  
 1.069111299D+02  
 CL+ Moore,1971. Moore,1970a. Gordon,1999.  
 3 g 1/98 CL 1.00E -1.00 0.00 0.00 0.00 0 35.45215  
 1378799.635  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6386.335  
 1.034697859D+05-1.293758873D+03 8.186702690D+00-9.916014600D-03  
 9.208472370D-06  
 -4.507426240D-09 9.182127880D-13 1.714758780D+05-  
 2.766419200D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6386.335  
 4.056409480D+04-4.960165720D+01 3.101653630D+00-5.868738290D-04  
 2.252039316D-07  
 -3.299703020D-11 1.708780842D-15 1.652982337D+05  
 2.574929905D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6386.335  
 -3.078099946D+06-6.858418280D+02 3.092289282D+00-1.922260015D-05  
 3.805551560D-10  
 -1.571848967D-13 8.442513880D-18 1.683434405D+05  
 1.334394541D+00  
 CL- Hotop,1985. Gordon,1999.

3 g 4/97 CL 1.00E 1.00 0.00 0.00 0.00 0 35.45325 -  
 233957.972  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.888389093D+04  
 4.200629330D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.888389093D+04  
 4.200629330D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.888389093D+04  
 4.200629330D+00  
 CLCN Gurvich,1991 pt1 p230 pt2 p218  
 2 g 6/95 CL 1.00C 1.00N 1.00 0.00 0.00 0 61.47014  
 134200.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10669.042  
 7.274043430D+04-1.297344947D+03 1.107676527D+01-1.108430216D-02  
 1.614009477D-05  
 -1.088916772D-08 2.830952246D-12 2.084388986D+04-  
 3.597370680D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10669.042  
 3.467573120D+05-1.957857370D+03 8.807806150D+00-4.388362780D-04  
 1.024761895D-07  
 -1.110675026D-11 4.986179420D-16 2.581923944D+04-  
 2.636885997D+01  
 CLF Gurvich,1989 pt1 p190 pt2 p97.  
 2 tpi89 CL 1.00F 1.00 0.00 0.00 0.00 0 54.45110 -  
 55700.993  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8908.107  
 3.352210810D+04-3.688311900D+02 4.272288620D+00 2.549434508D-03-  
 4.456830890D-06  
 3.413854120D-09-9.838685200D-13 -5.839369690D+03  
 2.317931556D-01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8908.107  
 3.045867173D+06-9.979328260D+03 1.684162254D+01-7.465850620D-03  
 2.336213612D-06  
 -3.365865460D-10 1.763082415D-14 5.447120800D+04-  
 8.707987920D+01  
 CLF3 Gurvich,1989 pt1 p193 pt2 p98.  
 2 tpi89 CL 1.00F 3.00 0.00 0.00 0.00 0 92.44791 -  
 164600.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13728.449  
 1.285175171D+05-2.140445721D+03 1.493096474D+01-6.042471040D-03  
 3.718968610D-06  
 -8.053201100D-10-7.985600530D-14 -1.138459640D+04-  
 5.594838840D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13728.449

-2.294956235D+05-1.220741000D+02 1.009124644D+01-3.649724750D-05  
 8.058910750D-09  
 -9.230849950D-13 4.272569490D-17 -2.282840447D+04-  
 2.511605966D+01  
 CLF5 Gurvich,1989 pt1 p194 pt2 p99.  
 2 tpris89 CL 1.00F 5.00 0.00 0.00 0.00 0 130.44472 -  
 238000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17930.396  
 2.459703939D+05-4.315348070D+03 2.727005972D+01-1.670193839D-02  
 1.421668208D-05  
 -6.426479740D-09 1.183099799D-12 -1.071423726D+04-  
 1.267466871D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17930.396  
 -4.269327450D+05-2.058057390D+02 1.615465278D+01-6.212688180D-05  
 1.376637959D-08  
 -1.581335709D-12 7.336422490D-17 -3.361466600D+04-  
 5.757531520D+01  
 CLO Gurvich,1989 pt1 p180 pt2 p90.  
 2 tpris89 CL 1.000 1.00 0.00 0.00 0.00 0 51.45210  
 101621.115  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9522.115  
 -1.687268145D+04 2.573812247D+02 2.175846120D+00 6.432061130D-03-  
 8.568249500D-06  
 5.764971250D-09-1.545771209D-12 9.829518980D+03  
 1.386009628D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9522.115  
 4.093760520D+05-1.765985112D+03 7.087900630D+00-1.828450169D-03  
 7.103818100D-07  
 -1.209332942D-10 7.076441040D-15 2.151891784D+04-  
 1.668646423D+01  
 CLO2 Gurvich,1989 pt1 p182 pt2 p91.  
 2 g 7/93 CL 1.000 2.00 0.00 0.00 0.00 0 67.45150  
 105000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10800.646  
 -1.127277696D+04 3.903032030D+02-3.843018530D-01 2.108677947D-02-  
 2.793137755D-05  
 1.841289286D-08-4.839779150D-12 9.756933670D+03  
 2.913262033D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10800.646  
 -1.633793802D+05-3.161480670D+02 7.009787260D+00 2.837971144D-04-  
 1.179925338D-07  
 2.920383252D-11-2.024030202D-15 1.184946452D+04-  
 1.091169494D+01  
 CL2 Ref-Elm. Gurvich,1989 pt1 p177 pt2 p88.  
 2 tpris89 CL 2.00 0.00 0.00 0.00 0.00 0 70.90540  
 0.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9181.110  
 3.462815170D+04-5.547126520D+02 6.207589370D+00-2.989632078D-03  
 3.173027290D-06  
 -1.793629562D-09 4.260043590D-13 1.534069331D+03-  
 9.438343800D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9181.110

6.092569420D+06-1.949627662D+04 2.854535795D+01-1.449968764D-02  
 4.463890770D-06  
 -6.358525860D-10 3.327360290D-14 1.212117724D+05-  
 1.690778951D+02  
 CL20 Gurvich,1989 pt1 p184 pt2 p92.  
 2 tpris89 CL 2.000 1.00 0.00 0.00 0.00 0 86.90480  
 79000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11695.482  
 7.798855400D+04-1.182537879D+03 9.526514660D+00-2.596163176D-03  
 8.696781310D-07  
 4.484098270D-10-3.044511967D-13 1.376729572D+04-  
 2.484691754D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11695.482  
 -1.271743461D+05-6.741963220D+01 7.050022450D+00-1.988084386D-05  
 4.366209050D-09  
 -4.978580680D-13 2.295679186D-17 7.387289300D+03-  
 8.797487610D+00  
 Co Hf:Hultgren,1973. Sugar,1985. Gordon,1999.  
 3 g 7/97 CO 1.00 0.00 0.00 0.00 0.00 0 58.93320  
 428441.600  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6359.768  
 -2.598939184D+03 2.461989844D+02-6.106058370D-01 1.393005772D-02-  
 2.210012979D-05  
 1.623755261D-08-4.534904351D-12 4.984613760D+04  
 2.257584199D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6359.768  
 1.381841305D+06-3.756036680D+03 6.657130650D+00-1.269246675D-03  
 1.464092329D-07  
 6.574946570D-12-1.102384178D-15 7.494442910D+04-  
 2.258500836D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6359.768  
 -5.468015750D+08 4.037704950D+05-1.142413163D+02 1.663014422D-02-  
 1.156228007D-06  
 3.862515150D-11-5.002032746D-16 -3.076031798D+06  
 1.003028648D+03  
 Co+ Sugar,1985. Gordon,1999.  
 3 g 7/97 CO 1.00E -1.00 0.00 0.00 0.00 0 58.93265  
 1193003.307  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6291.507  
 1.028494160D+05-8.744731260D+02 4.279500280D+00 2.225857835D-03-  
 7.457274570D-06  
 7.279221950D-09-2.347541963D-12 1.474895959D+05-  
 5.679019220D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6291.507  
 2.907386174D+06-8.619705750D+03 1.188134934D+01-3.510647420D-03  
 5.748004680D-07  
 -2.534065135D-11 2.976607469D-16 1.977419221D+05-  
 6.096533440D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6291.507  
 2.701785479D+09-1.604232092D+06 3.687314770D+02-4.041150820D-02  
 2.371848586D-06  
 -7.119952160D-11 8.635423717D-16 1.293631390D+07-  
 3.201662470D+03

Co- Hotop,1985. Gordon,1999.

3 g 9/97 CO 1.00E 1.00 0.00 0.00 0.00 0 58.93375  
358414.372  
298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6306.772  
3.459493760D+04-1.355041712D+02 1.116330898D+00 9.042761830D-03-  
1.454296726D-05  
9.994940630D-09-2.595633259D-12 4.337037820D+04  
1.270494975D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6306.772  
-5.741394170D+05 1.763109207D+03 1.415561988D+00 3.776869690D-04-  
7.534179980D-08  
7.995701540D-12-3.490440000D-16 3.083493114D+04  
1.634360353D+01  
6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6306.772  
-7.121795840D+05 7.962447120D+02 2.328870839D+00 1.919463732D-05-  
1.179708474D-09  
3.764228600D-14-4.875340940D-19 3.689285080D+04  
9.511282720D+00

Cr Hf:Chase,1998 p963 6/79. Sugar,1985. Gordon,1999.

3 g 7/97 CR 1.00 0.00 0.00 0.00 0.00 0 51.99610  
397480.000  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428  
1.335658217D+03-2.102424026D+01 2.631908173D+00-4.246263250D-04  
7.439194160D-07  
-6.763931630D-10 2.507855625D-13 4.715866640D+04  
6.005425450D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428  
-1.120220789D+07 3.401163690D+04-3.657062170D+01 2.110296902D-02-  
5.518180140D-06  
7.173601710D-10-3.505127367D-14 -1.688993440D+05  
2.864481267D+02  
6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428  
3.900886930D+09-2.462918543D+06 5.915632640D+02-6.697121640D-02  
3.946957790D-06  
-1.166504597D-10 1.367279456D-15 1.955381984D+07-  
5.133510550D+03

Cr+ Sugar,1985. Gordon,1999.

3 g 7/97 CR 1.00E -1.00 0.00 0.00 0.00 0 51.99555  
1056546.728  
298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428  
1.819187467D+02-2.188843517D+00 2.510676511D+00-2.706791825D-05  
3.768492630D-08  
-2.736784742D-11 8.115389932D-15 1.263380825D+05  
6.506276170D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428  
3.342330790D+06-1.064261051D+04 1.557884307D+01-7.708971480D-03  
2.158300274D-06  
-2.368108110D-10 8.952805604D-15 1.932997670D+05-  
8.604356670D+01  
6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428  
4.853867040D+08-4.114535830D+05 1.242898882D+02-1.610102894D-02  
1.147677369D-06



-4.099673600D-11 5.728606039D-16 3.281645810D+06-  
1.034723629D+03

Cr- Hotop,1985. Gordon,1999.  
3 g10/97 CR 1.00E 1.00 0.00 0.00 0.00 0 51.99665  
327023.428  
298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428  
0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 3.858627870D+04  
6.566835370D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428  
0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 3.858627870D+04  
6.566835370D+00  
6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428  
0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 3.858627870D+04  
6.566835370D+00

CrN Chase,1998 p967.  
2 j12/73 CR 1.00N 1.00 0.00 0.00 0.00 0 66.00284  
505008.800  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
8777.789  
-8.239129220D+03 3.008144202D+02 5.147874920D-01 1.129636791D-02-  
1.515183504D-05  
1.010997229D-08-2.687775750D-12 5.845628120D+04  
2.298028787D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
8777.789  
1.110672490D+06-3.690478540D+03 8.599056680D+00-2.125587223D-03  
5.282358480D-07  
-4.921139150D-11 1.404331106D-15 8.254804580D+04-  
2.799968320D+01

CrO Gurvich,1982 pt1 p13 pt2 p17.  
3 tpis82 CR 1.00O 1.00 0.00 0.00 0.00 0 67.99550  
186581.318  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
9849.118  
9.373334110D+03 1.369743818D+02 1.621443428D+00 8.814095960D-03-  
1.232845360D-05  
8.497960940D-09-2.315804197D-12 2.090948871D+04  
1.781935787D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
9849.118  
1.092367332D+06-3.749758650D+03 9.007870210D+00-2.545445236D-03  
6.928051680D-07  
-6.390831950D-11 1.659741645D-15 4.447098210D+04-  
2.942600453D+01  
6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
9849.118  
5.600191720D+08-3.409592350D+05 7.971428300D+01-7.045904880D-03  
3.311256200D-07  
-8.196877430D-12 8.487479810D-17 2.738393714D+06-  
6.629641700D+02

CrO2 Gurvich,1982 pt1 p16 pt2 p19.

2 tpis82 CR 1.000 2.00 0.00 0.00 0.00 0 83.99490 -  
 108043.235  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10693.869  
 3.548629900D+04-2.298628537D+02 2.286289393D+00 1.616929338D-02-  
 2.345198910D-05  
 1.631365714D-08-4.444269620D-12 -1.278912840D+04  
 1.442954956D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10693.869  
 -4.327109140D+05 1.915584657D+02 7.188247370D+00-5.694846190D-04  
 3.546366130D-07  
 -5.655123060D-11 2.908946349D-15 -1.743339545D+04-  
 1.006424720D+01  
 CrO3 Gurvich,1982 pt1 p17 pt2 p20.  
 2 tpis82 CR 1.000 3.00 0.00 0.00 0.00 0 99.99430 -  
 322037.084  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13040.072  
 4.183020060D+04-5.059348850D+02 4.432715670D+00 1.995079387D-02-  
 2.920597649D-05  
 2.039330280D-08-5.580086630D-12 -3.769702400D+04  
 8.653827280D-01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13040.072  
 -6.283314010D+05 6.928158180D+02 8.971274600D+00 6.823365640D-04-  
 2.235048825D-07  
 3.366785790D-11-1.614026492D-15 -4.723880200D+04-  
 1.945305345D+01  
 CrO3- Gurvich,1982 pt1 p18 pt2 p21.  
 2 tpis82 CR 1.000 3.00E 1.00 0.00 0.00 0 99.99485 -  
 632850.845  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13423.739  
 1.873455703D+05-2.300722991D+03 1.343953022D+01-1.663085846D-03-  
 1.443973096D-06  
 2.045898933D-09-6.837555300D-13 -6.630111580D+04-  
 4.930644200D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13423.739  
 -6.499682030D+05 4.522017620D+02 9.980575900D+00-4.214136730D-04  
 2.631277945D-07  
 -4.594543650D-11 2.659097549D-15 -8.350019730D+04-  
 2.464810900D+01  
 Cs Hf:Cox,1989. Moore,1971. Moore,1970a. Gordon,1999.  
 3 g 7/97 CS 1.00 0.00 0.00 0.00 0.00 0 132.90545  
 76500.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 5.466584070D+01-8.279346040D-01 2.504942210D+00-1.494620690D-05  
 2.425976774D-08  
 -2.013172322D-11 6.704271991D-15 8.459321390D+03  
 6.848825772D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 6.166040900D+06-1.896175522D+04 2.483229903D+01-1.251977234D-02  
 3.309017390D-06  
 -3.354012020D-10 9.626500908D-15 1.285111231D+05-  
 1.522942188D+02  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428

-9.566231720D+08 4.321690420D+05-6.371801020D+01 5.246260580D-03-  
 2.366560159D-07  
 5.848488480D-12-6.169370441D-17 -3.585268840D+06  
 6.156618174D+02  
 Cs+ Moore,1971. Gordon,1999.  
 3 g 1/98 CS 1.00E -1.00 0.00 0.00 0.00 0 132.90490  
 458401.828  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 5.438737820D+04  
 6.182757992D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 5.438737820D+04  
 6.182757992D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 -2.479469300D+08 1.405115456D+05-2.805027359D+01 3.087928133D-03-  
 1.273598265D-07  
 -3.748818380D-13 1.214944533D-16 -1.072498017D+06  
 2.756827325D+02  
 Cs- Hotop,1985. Gordon,1999.  
 3 g10/97 CS 1.00E 1.00 0.00 0.00 0.00 0 132.90600  
 24797.228  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 2.237029001D+03  
 6.182770382D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 2.237029001D+03  
 6.182770382D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 2.237029001D+03  
 6.182770382D+00  
 CsBO2 Gurvich,1982 pt1 p505 pt2 p526.  
 2 tpris82 CS 1.00B 1.000 2.00 0.00 0.00 0 175.71525 -  
 686901.906  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14466.094  
 4.193609580D+04-6.664237400D+02 8.134835880D+00 2.902960302D-03-  
 7.881467920D-07  
 -8.327694540D-10 4.441719110D-13 -8.122320070D+04-  
 1.121622595D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14466.094  
 8.975579890D+04-1.656134283D+03 1.116468934D+01-4.476366990D-04  
 9.621091810D-08  
 -1.081470115D-11 4.938446740D-16 -7.610479670D+04-  
 3.036616012D+01

CsBr Gurvich,1982 pt1 p490 pt2 p512.  
 2 tpris82 CS 1.00BR 1.00 0.00 0.00 0.00 0 212.80945 -  
 206828.875  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10406.125  
 1.639263647D+03-6.947477970D+01 4.860058720D+00-8.587780150D-04  
 1.375177550D-06  
 -9.891766980D-10 2.895433432D-13 -2.589550471D+04  
 4.465355690D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10406.125  
 -1.528329963D+05 1.259712657D+03 1.704268408D+00 2.776255318D-03-  
 1.228389838D-06  
 2.698111786D-10-1.983534480D-14 -3.327842030D+04  
 2.484116659D+01

CsCL Gurvich,1982 pt1 p487 pt2 p509.  
 2 tpris82 CS 1.00CL 1.00 0.00 0.00 0.00 0 168.35815 -  
 242228.878  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10131.122  
 -2.538165292D+04 2.972839326D+02 2.667813848D+00 5.583272410D-03-  
 8.529005090D-06  
 6.595191390D-09-1.989715823D-12 -3.189251450D+04  
 1.511365442D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10131.122  
 -3.674923480D+06 1.186152941D+04-1.063287842D+01 9.804117920D-03-  
 3.277797460D-06  
 5.534233390D-10-3.401231500D-14 -1.048658658D+05  
 1.114096037D+02

CsF Gurvich,1982 pt1 p483 pt2 p506.  
 2 tpris82 CS 1.00F 1.00 0.00 0.00 0.00 0 151.90385 -  
 364214.884  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9645.116  
 1.843685799D+04-4.042409390D+02 6.383178860D+00-4.674323370D-03  
 6.630134010D-06  
 -4.760905530D-09 1.374569797D-12 -4.318489590D+04-  
 7.226593230D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9645.116  
 -1.850863231D+06 5.625298800D+03-2.250022212D+00 4.109243540D-03-  
 1.250243837D-06  
 1.941483152D-10-1.071166179D-14 -8.079827790D+04  
 5.135559450D+01

CsH Gurvich,1982 pt1 p477 pt2 p501.  
 2 tpris82 CS 1.00H 1.00 0.00 0.00 0.00 0 133.91339  
 115950.106  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8846.106  
 1.620544411D+04-7.087016280D+01 2.480847135D+00 7.021985990D-03-  
 1.007126309D-05  
 7.090639030D-09-1.950395735D-12 1.342777328D+04  
 9.894247170D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8846.106  
 -9.112146650D+05 3.576472750D+03-1.258058765D+00 4.314855150D-03-  
 1.407820502D-06  
 2.154598897D-10-1.254525606D-14 -9.158717270D+03  
 3.908800030D+01

CsI Gurvich,1982 pt1 p494 pt2 p515.

2 tpis82 CS 1.00I 1.00 0.00 0.00 0.00 0 259.80992 -  
 152319.873  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10550.127  
 -4.072685650D+03 2.330073667D+01 4.387277690D+00 3.412084290D-04-  
 2.175588153D-07  
 8.906787000D-11-2.182639837D-15 -1.978766885D+04  
 8.074657820D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10550.127  
 4.511259050D+06-1.341706362D+04 1.980984712D+01-8.359855550D-03  
 2.348201245D-06  
 -2.874285248D-10 1.208087750D-14 6.573439130D+04-  
 1.021032592D+02  
 CsLi Gurvich,1982 pt1 p505 pt2 p527.  
 2 tpis82 CS 1.00LI 1.00 0.00 0.00 0.00 0 139.84645  
 162146.324  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10341.124  
 1.368709568D+03-7.451297060D+01 4.845620930D+00-5.573667210D-04  
 4.953326760D-07  
 4.369068910D-10-4.608145770D-13 1.850577392D+04  
 2.112012017D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10341.124  
 7.481630230D+06-2.885297839D+04 4.631104990D+01-2.784288108D-02  
 8.787413490D-06  
 -1.264901197D-09 6.720186280D-14 1.945137819D+05-  
 2.857846194D+02  
 CsNO2 Gurvich,1982 pt1 p499 pt2 p520.  
 2 tpis82 CS 1.00N 1.000 2.00 0.00 0.00 0 178.91099 -  
 210339.828  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15980.172  
 -7.106010440D+04 1.272448257D+03-2.447362349D+00 3.064441948D-02-  
 3.699225940D-05  
 2.259121812D-08-5.580635910D-12 -3.313370920D+04  
 4.954693370D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15980.172  
 -1.633503154D+05-8.468879580D+02 1.062853461D+01-2.508799215D-04  
 5.541255770D-08  
 -6.355591950D-12 2.946880031D-16 -2.403040739D+04-  
 2.443488854D+01  
 CsNO3 Gurvich,1982 pt1 p501 pt2 p522.  
 2 tpis82 CS 1.00N 1.000 3.00 0.00 0.00 0 194.91039 -  
 318486.390  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16563.610  
 -2.677219779D+04 9.011692690D+02-3.265340820D+00 4.298377700D-02-  
 5.386751380D-05  
 3.384527520D-08-8.565223660D-12 -4.405304140D+04  
 5.118862720D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16563.610  
 -3.147517676D+05-1.367011655D+03 1.401012848D+01-4.018647130D-04  
 8.853614700D-08  
 -1.013466457D-11 4.691758730D-16 -3.549026670D+04-  
 4.500692760D+01  
 CsNa Gurvich,1982 pt1 p506 pt2 p528.

2 tpis82 CS 1.00NA 1.00 0.00 0.00 0.00 0 155.89522  
 125907.329  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10702.129  
 2.521738609D+04-4.295362490D+02 7.223094740D+00-8.460463000D-03  
 1.443905157D-05  
 -1.143624855D-08 3.183721930D-12 1.579099265D+04-  
 8.838790300D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10702.129  
 3.879556790D+06-1.780167288D+04 3.491355800D+01-2.320080793D-02  
 7.861975840D-06  
 -1.171011257D-09 6.323927370D-14 1.195776556D+05-  
 2.001754433D+02  
 CsO Gurvich,1982 pt1 p471 pt2 p493.  
 2 tpis82 CS 1.00O 1.00 0.00 0.00 0.00 0 148.90485  
 37587.318  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9835.118  
 8.683958810D+03 4.250278170D+02-3.484055300D+00 3.801969830D-02-  
 6.651927560D-05  
 5.173472190D-08-1.512567066D-11 1.969690015D+03  
 4.240796140D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9835.118  
 8.375544350D+05-2.418205772D+03 8.908065350D+00-3.378180040D-03  
 1.312755917D-06  
 -2.150508925D-10 1.219138980D-14 1.809493447D+04-  
 2.460858580D+01  
 CsOH Gurvich,1997.  
 2 g 9/97 CS 1.00O 1.00H 1.00 0.00 0.00 0 149.91279 -  
 256000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11834.689  
 9.386960790D+03-5.009354260D+02 8.301351980D+00-3.235596840D-03  
 2.612406777D-06  
 -4.950613410D-10-1.038364927D-13 -3.025722427D+04-  
 1.742194837D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11834.689  
 8.967171130D+05-2.323978587D+03 7.959644870D+00 1.101149275D-04-  
 6.466013970D-08  
 1.045968201D-11-5.822514170D-16 -1.736258234D+04-  
 1.864239624D+01  
 CsRb Gurvich,1982 pt1 p508 pt2 p530.  
 2 tpis82 CS 1.00RB 1.00 0.00 0.00 0.00 0 218.37325  
 111477.332  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10972.132  
 -4.910922680D+03-9.209015550D+00 5.193377890D+00-4.390246990D-03  
 1.254790436D-05  
 -1.414878514D-08 5.101441310D-12 1.200498171D+04  
 5.361542930D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10972.132  
 -1.328693378D+07 3.414579470D+04-2.373696406D+01 7.070465400D-03  
 3.863450970D-07  
 -3.158132986D-10 2.667747207D-14 -2.124008997D+05  
 2.239970251D+02  
 Cs2 Gurvich,1982 pt1 p467 pt2 p492.

2 tpis82 CS 2.00 0.00 0.00 0.00 0.00 0 265.81090  
 109404.333  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11029.133  
 -4.674158730D+04 5.952019510D+02 1.895333975D+00 4.082065810D-03  
 2.531487119D-06  
 -9.085139030D-09 4.290179930D-12 8.857282570D+03  
 2.391592727D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11029.133  
 -2.592739590D+07 7.539818910D+04-7.484086800D+01 3.692866790D-02-  
 8.082497240D-06  
 8.171850730D-10-3.089285900D-14 -4.715045720D+05  
 5.860933750D+02  
 Cs2Br2 Gurvich,1982 pt1 p491 pt2 p513.  
 2 tpis82 CS 2.00BR 2.00 0.00 0.00 0.00 0 425.61890 -  
 565828.869  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22113.130  
 -6.321285180D+03-1.213153529D+01 1.004967112D+01-1.102100044D-04  
 1.365293456D-07  
 -8.856957070D-11 2.339447704D-14 -7.099771710D+04-  
 7.539424790D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22113.130  
 -7.545846650D+03-2.087093009D-01 1.000018042D+01-8.034260730D-08  
 1.923604258D-11  
 -2.344698140D-15 1.139365834D-19 -7.105883540D+04-  
 7.251793040D+00  
 Cs2CO3 Gurvich,1982 pt1 p503 pt2 p524.  
 2 tpis82 CS 2.00C 1.000 3.00 0.00 0.00 0 325.81980 -  
 806447.939  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 21179.061  
 -4.673130000D+04 9.436549060D+02-2.374670436D-01 4.168484610D-02-  
 5.094372210D-05  
 3.132078394D-08-7.780421670D-12 -1.039162411D+05  
 4.055853980D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 21179.061  
 -3.037149985D+05-1.517078400D+03 1.711941656D+01-4.449700120D-04  
 9.798325240D-08  
 -1.121256063D-11 5.189734780D-16 -9.420414770D+04-  
 5.682006260D+01  
 Cs2CL2 Gurvich,1982 pt1 p487 pt2 p510.  
 2 tpis82 CS 2.00CL 2.00 0.00 0.00 0.00 0 336.71630 -  
 644658.398  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 20944.712  
 -1.077956357D+04-5.346106950D+01 1.021710683D+01-4.789687030D-04  
 5.908946530D-07  
 -3.821416520D-10 1.006995985D-13 -8.029515170D+04-  
 1.207856753D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 20944.712  
 -1.625143966D+04-9.006137350D-01 1.000077173D+01-3.416194080D-07  
 8.144968080D-11  
 -9.897475280D-15 4.798330810D-19 -8.056513220D+04-  
 1.081977604D+01  
 Cs2F2 Gurvich,1982 pt1 p484 pt2 p507.

2 tpis82 CS 2.00F 2.00 0.00 0.00 0.00 0 303.80771 -  
 891858.506  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19388.600  
 -9.942677480D+03-2.536723355D+02 1.100684073D+01-2.185640152D-03  
 2.664791874D-06  
 -1.708229209D-09 4.471151980D-13 -1.090582601D+05-  
 2.000699602D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19388.600  
 -3.677946420D+04-4.355753480D+00 1.000366687D+01-1.603814186D-06  
 3.791469740D-10  
 -4.578687430D-14 2.209385787D-18 -1.103456448D+05-  
 1.415086452D+01  
 Cs2I2 Gurvich,1982 pt1 p495 pt2 p516.  
 2 tpis82 CS 2.00I 2.00 0.00 0.00 0.00 0 519.61984 -  
 454033.097  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22584.903  
 -4.449286970D+03-5.321793660D+00 1.002183919D+01-4.853374850D-05  
 6.019338400D-08  
 -3.908226390D-11 1.032981014D-14 -5.757823380D+04-  
 5.271267090D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22584.903  
 -4.983376010D+03-9.461179880D-02 1.000008229D+01-3.680962040D-08  
 8.844660910D-12  
 -1.081178562D-15 5.266141980D-20 -5.760501040D+04-  
 5.144864890D+00  
 Cs2O Gurvich,1982 pt1 p473 pt2 p496.  
 2 tpis82 CS 2.00O 1.00 0.00 0.00 0.00 0 281.81030 -  
 142855.345  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14089.855  
 1.910533804D+04-4.962181530D+02 8.759606300D+00-3.511622790D-03  
 4.016479830D-06  
 -2.450899853D-09 6.172404890D-13 -1.677664956D+04-  
 1.159258822D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14089.855  
 -4.119147410D+04-1.079255391D+01 7.008500470D+00-3.542955780D-06  
 8.081699120D-10  
 -9.499419930D-14 4.489122540D-18 -1.934377850D+04-  
 1.203970450D+00  
 Cs2O+ Gurvich,1982 pt1 p474 pt2 p497.  
 2 tpis82 CS 2.00O 1.00E -1.00 0.00 0.00 0 281.80975 -  
 283699.926  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14447.726  
 6.837056090D+02-2.435575007D+02 7.783037470D+00-1.414552725D-03  
 1.470799739D-06  
 -8.218821330D-10 1.911749489D-13 3.324194870D+04-  
 4.750423560D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14447.726  
 -3.153085844D+04-5.771559030D+00 7.004482630D+00-1.848241331D-06  
 4.180882300D-10  
 -4.882376270D-14 2.295419936D-18 3.196227310D+04-  
 5.434350690D-02  
 Cs2O2 Gurvich,1982 pt1 p476 pt2 p499.



2 tpi82 CS 2.000 2.00 0.00 0.00 0.00 0 297.80970 -  
 247069.104  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17426.496  
 2.274505180D+04-5.667912570D+02 1.001728332D+01 2.547081016D-03-  
 4.909216690D-06  
 3.848788910D-09-1.124566008D-12 -2.947334360D+04-  
 1.841275291D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17426.496  
 -1.190032094D+05-9.261075260D+01 1.006915777D+01-2.766227147D-05  
 6.110752960D-09  
 -7.003595480D-13 3.243742520D-17 -3.255610740D+04-  
 1.724868948D+01  
 Cs2O2H2 Gurvich,1997.  
 2 g 9/97 CS 2.000 2.00H 2.00 0.00 0.00 0 299.82558 -  
 653000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 23937.353  
 -1.085981041D+04-6.883068420D+02 1.643543354D+01-4.039220580D-03  
 2.331117156D-06  
 8.439651630D-10-6.859309730D-13 -7.939476230D+04-  
 4.906196810D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 23937.353  
 1.802857941D+06-4.656354750D+03 1.693566597D+01 2.117402535D-04-  
 1.272249096D-07  
 2.066555839D-11-1.152390667D-15 -5.190813690D+04-  
 5.849719160D+01  
 Cs2SO4 Gurvich,1982 pt1 p497 pt2 p518.  
 2 g10/99 CS 2.00S 1.00O 4.00 0.00 0.00 0 361.87450 -  
 1117651.834  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 23988.166  
 6.153637870D+04-6.381374330D+02 6.894772090D+00 3.960182910D-02-  
 5.529862010D-05  
 3.736332520D-08-9.973241830D-12 -1.339760310D+05-  
 1.284428443D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 23988.166  
 -5.223397520D+05-9.444155250D+02 1.970476453D+01-2.821225990D-04  
 6.240792280D-08  
 -7.163464070D-12 3.322667190D-16 -1.364179983D+05-  
 6.820406380D+01  
 Cu Hf:Cox,1989. Sugar,1990. Gordon,1999.  
 3 g12/97 CU 1.00 0.00 0.00 0.00 0.00 0 63.54600  
 337400.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 7.713133150D+01-1.169236206D+00 2.506987803D+00-2.116434879D-05  
 3.441714710D-08  
 -2.862608999D-11 9.559250991D-15 3.983981210D+04  
 5.730813220D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 2.308090411D+06-8.503261000D+03 1.467859102D+01-8.467136520D-03  
 2.887821016D-06  
 -4.270659180D-10 2.304265084D-14 9.207535620D+04-  
 7.854701560D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428

-6.490595890D+08 4.240323360D+05-1.028965806D+02 1.297259934D-02-  
 7.766697680D-07  
 2.220446727D-11-2.441532031D-16 -3.305304580D+06  
 9.198622920D+02  
 Cu+ Sugar,1990. Gordon,1999.  
 3 g 3/98 CU 1.00E -1.00 0.00 0.00 0.00 0 63.54545  
 1089079.728  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 -2.452340093D-03 2.606893531D-05 2.499999890D+00 2.351922485D-10-  
 2.669362382D-13  
 1.510315123D-16-3.278224814D-20 1.302400621D+05  
 5.075940770D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 -2.181443016D+06 7.217858190D+03-6.941154750D+00 6.208248920D-03-  
 2.139340497D-06  
 3.566431440D-10-2.081198501D-14 8.516456660D+04  
 7.116800670D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 2.994686480D+09-1.831416099D+06 4.294926960D+02-4.801927720D-02  
 2.836504248D-06  
 -8.452189040D-11 1.013018211D-15 1.468809255D+07-  
 3.729918010D+03  
 Cu- Hotop,1985. Gordon,1999.  
 3 g10/97 CU 1.00E 1.00 0.00 0.00 0.00 0 63.54655  
 212718.628  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 2.483864954D+04  
 5.075966030D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 2.483864954D+04  
 5.075966030D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 2.483864954D+04  
 5.075966030D+00  
 CuCL Chase,1998 p748.  
 2 j 3/66 CU 1.00CL 1.00 0.00 0.00 0.00 0 98.99870  
 91090.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9471.175  
 1.469847736D+04-3.393167250D+02 5.723459590D+00-2.417296132D-03  
 2.858019864D-06  
 -1.757900548D-09 4.455047290D-13 1.131714015D+04-  
 4.527357140D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9471.175  
 -2.577122410D+04-7.106346060D+00 4.505623180D+00 5.394548270D-05  
 5.386417960D-10  
 -6.348482770D-14 3.006622062D-18 9.566192870D+03  
 2.680063018D+00

CuF Chase,1998 p1013.  
 2 j12/77 CU 1.00F 1.00 0.00 0.00 0.00 0 82.54440 -  
 12550.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9083.091  
 3.761385410D+04-5.468104900D+02 5.832351720D+00-1.695312068D-03  
 1.218150880D-06  
 -3.713285280D-10 2.002276589D-14 5.865140720D+01-  
 7.156930090D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9083.091  
 5.094154830D+05-1.415009870D+03 5.632349380D+00-1.629128410D-04-  
 1.156611499D-07  
 5.066034080D-11-4.153205110D-15 6.305506600D+03-  
 7.407773610D+00  
 CuF2 Chase,1998 p1017.  
 2 j12/77 CU 1.00F 2.00 0.00 0.00 0.00 0 101.54281 -  
 266940.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12055.910  
 6.573311280D+04-8.962430840D+02 7.917560940D+00 1.345667904D-03-  
 4.162400010D-06  
 3.716181090D-09-1.155537597D-12 -2.916887325D+04-  
 1.587076153D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12055.910  
 -1.650355082D+06 3.775362120D+03 3.889116550D+00 6.821912640D-04  
 1.875979026D-07  
 -5.677368110D-11 3.823248730D-15 -5.953371700D+04  
 1.522659664D+01  
 CuO Chase,1998 p1020.  
 2 j12/77 CU 1.00O 1.00 0.00 0.00 0.00 0 79.54540  
 306270.000  
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 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
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 Cu2 Chase,1998 p1022.  
 2 j 9/66 CU 2.00 0.00 0.00 0.00 0.00 0 127.09200  
 485340.000  
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 1.105391325D+00  
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 9930.154  
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 6.914502170D+00  
 Cu3CL3 Chase,1998 p874.

2 j 3/66 CU 3.00CL 3.00 0.00 0.00 0.00 0 296.99610 -  
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 28723.690  
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 1.302748507D-09  
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 D D0 (D2): Herzberg,1970. Moore,1972. Gordon,1999.  
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 0.000000000D+00 0.000000000D+00 2.592128700D+04  
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 2.726201602D+02  
 D+ Moore,1972. Gordon,1999.  
 3 g 9/96 D 1.00E -1.00 0.00 0.00 0.00 0 2.01355  
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 0.000000000D+00 0.000000000D+00 1.845120037D+05-  
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 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
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 0.000000000D+00 0.000000000D+00 1.845120037D+05-  
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 0.000000000D+00 0.000000000D+00 1.845120037D+05-  
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 D- Hotop,1985. Gordon,1999.  
 3 g 8/96 D 1.00E 1.00 0.00 0.00 0.00 0 2.01465  
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0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00
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1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
6197.428
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0.000000000D+00
0.000000000D+00 0.000000000D+00 1.642373393D+04-
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6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
6197.428
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0.000000000D+00
0.000000000D+00 0.000000000D+00 1.642373393D+04-
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DBr Gurvich,1989 pt1 p206 pt2 p107.
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-6.591160280D-09 2.093769216D-12 -6.560074400D+03
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8668.104
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2.894201105D-07
-3.152037514D-11 1.011011776D-15 1.037813140D+04-
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DCL Gurvich,1989 pt1 p188 pt2 p95.
2 tpis89 D 1.00CL 1.00 0.00 0.00 0.00 0 37.46680 -
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DF Gurvich,1989 pt1 p172 pt2 p80.
3 tpis89 D 1.00F 1.00 0.00 0.00 0.00 0 21.01251 -
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-6.941812690D-09 1.538525476D-12 -3.069230024D+04-
1.932760992D+01
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8638.104
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```

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 1.978551386D-08  
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 1.428958225D+02  
 DOCL D0 estimated from HOCL. Jacox, 1998 p155.  
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 F- Hotop,1985. Gordon,1999.  
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 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
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 0.000000000D+00 0.000000000D+00 -3.142572443D+04  
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 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
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 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.142572443D+04  
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 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
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 -1.280287231D-11 5.733807190D-16 1.588449451D+04-  
 2.984971849D+01  
 FCO Hf:Gurvich,1991 pt1 p87. Jacox,1998 p193.  
 2 g12/99 F 1.00C 1.00O 1.00 0.00 0.00 0 47.00850 -  
 179418.150  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10387.955  
 1.132662744D+04-5.397918500D+01 2.966927601D+00 7.559959350D-03-  
 6.211773580D-06  
 2.403781550D-09-3.369507750D-13 -2.240369579D+04  
 1.092652142D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10387.955  
 -6.085851580D+04-1.022397533D+03 7.527322560D+00-1.057942328D-04-  
 1.365311093D-09  
 2.484612871D-12-9.997916800D-17 -1.805098416D+04-  
 1.630331278D+01  
 FO Chase,1996b p582.

2 j 9/95 F 1.000 1.00 0.00 0.00 0.00 0 34.99780  
 109012.100  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9388.000  
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 2.095210771D-05  
 1.382740666D-08-3.664524950D-12 8.375525230D+03  
 3.383325720D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9388.000  
 -1.597940503D+06 4.377376380D+03-4.897507640D-01 2.682336321D-03-  
 6.900804850D-07  
 7.246479680D-11-2.726912632D-15 -1.644248211D+04  
 3.559923610D+01  
 FO2,FOO Chase,1996b p582.  
 2 j 9/95 F 1.000 2.00 0.00 0.00 0.00 0 50.99720  
 25400.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11255.812  
 5.821564000D+03-2.347363967D+02 5.437338760D+00 2.165855252D-03  
 3.671472190D-07  
 -2.071530827D-09 9.431066850D-13 2.694856027D+03-  
 1.168202057D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11255.812  
 -1.213166895D+06 2.493397189D+03 4.465065740D+00 9.416104040D-04-  
 6.426472260D-08  
 -1.085643277D-11 1.216995394D-15 -1.596800286D+04  
 8.655193180D+00  
 FO2,OFO Chase,1996b p583.  
 2 j 9/95 F 1.000 2.00 0.00 0.00 0.00 0 50.99720  
 378600.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10538.382  
 -7.734106400D+04 1.663800209D+03-9.612815160D+00 4.989156870D-02-  
 6.946217130D-05  
 4.707787800D-08-1.258890729D-11 3.697092730D+04  
 7.795943040D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10538.382  
 -6.211867340D+05 9.369474590D+02 6.401558750D+00 2.136110846D-04-  
 4.337977650D-08  
 4.667312240D-12-2.059767432D-16 3.638357270D+04-  
 6.150264330D+00  
 F2 Ref-Elm. Gurvich,1989. pt1 p157 pt2 p73.  
 2 tpris89 F 2.00 0.00 0.00 0.00 0.00 0 37.99681  
 0.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8825.106  
 1.018176308D+04 2.274241183D+01 1.971353040D+00 8.151604010D-03-  
 1.148960090D-05  
 7.958652530D-09-2.167079526D-12 -9.586943000D+02  
 1.130600296D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8825.106  
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 2.241007605D-06  
 2.915845236D-10-1.425033974D-14 -6.071005610D+04  
 8.423835080D+01  
 F2O Gurvich,1989 pt1 p161 pt2 p76.

2 g 4/99 F 2.000 1.00 0.00 0.00 0.00 0 53.99621  
 24500.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
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 2.345633734D-05  
 1.679619314D-08-4.703560330D-12 3.055185332D+03  
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 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10911.521  
 -1.885374518D+05-2.100729689D+02 7.151239160D+00 1.327687906D-04  
 1.804705706D-08  
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 1.257858336D+01  
 F2O2 FOOF. Chase,1996b p585.  
 2 j 9/95 F 2.000 2.00 0.00 0.00 0.00 0 69.99561  
 19200.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13778.453  
 5.612270460D+04-9.985952230D+02 8.980649390D+00 6.421900870D-03-  
 9.888516020D-06  
 6.858061010D-09-1.842137493D-12 5.298712590D+03-  
 2.239292195D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13778.453  
 -2.190563532D+05-3.910920810D+02 1.029107144D+01-1.163345202D-04  
 2.570922521D-08  
 -2.949199983D-12 1.367386916D-16 8.278020940D+02-  
 2.756752555D+01  
 FS2F Difluorodisulfane. Chase,1998 p1146.  
 2 j 6/76 F 2.00S 2.00 0.00 0.00 0.00 0 102.12881 -  
 336435.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14595.300  
 1.144462280D+05-1.853247564D+03 1.394098518D+01-4.043689370D-03  
 1.370970316D-06  
 6.711903100D-10-4.624954960D-13 -3.351068330D+04-  
 4.849212420D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14595.300  
 -2.077097921D+05-1.094539831D+02 1.008136946D+01-3.239537910D-05  
 7.125225270D-09  
 -8.134787410D-13 3.755022410D-17 -4.349446060D+04-  
 2.346913121D+01  
 Fe Hf:Hultgren,1973. Sugar,1985. Gordon,1999.  
 3 g 5/97 FE 1.00 0.00 0.00 0.00 0.00 0 55.84500  
 415471.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6850.327  
 6.790822660D+04-1.197218407D+03 9.843393310D+00-1.652324828D-02  
 1.917939959D-05  
 -1.149825371D-08 2.832773807D-12 5.466995940D+04-  
 3.383946260D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6850.327  
 -1.954923682D+06 6.737161100D+03-5.486410970D+00 4.378803450D-03-  
 1.116286672D-06  
 1.544348856D-10-8.023578182D-15 7.137370060D+03  
 6.504979860D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6850.327

1.216352511D+09-5.828563930D+05 9.789634510D+01-5.370704430D-03  
3.192037920D-08  
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8.697289770D+02

Fe+ Sugar,1985. Gordon,1999.

3 g 3/98 FE 1.00E -1.00 0.00 0.00 0.00 0 55.84445  
1184217.849

298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6935.749

-5.691231620D+04 1.847134390D+02 4.196972120D+00-5.978275970D-03

1.054267912D-05

-8.059804320D-09 2.256925874D-12 1.401206571D+05-

3.602542580D-01

1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6935.749

-8.176450090D+05 1.925359408D+03 1.717387154D+00 3.385338980D-04-

9.813533120D-08

2.228179208D-11-1.483964439D-15 1.286352466D+05

1.500256262D+01

6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6935.749

1.065217491D+08-2.883923997D+04-2.821752459D+00 2.712846797D-03-

3.107069182D-07

1.543726493D-11-2.725133516D-16 4.142981690D+05

4.053497330D+01

Fe- Hotop,1985. Gordon,1999.

3 g 9/97 FE 1.00E 1.00 0.00 0.00 0.00 0 55.84555  
393338.036

298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6641.836

1.341276767D+05-1.775438064D+03 1.084366935D+01-1.499440282D-02

1.412129744D-05

-6.942189050D-09 1.410953082D-12 5.519472530D+04-

4.140886490D+01

1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6641.836

-1.237808631D+05 8.249279070D+02 1.912936452D+00 2.280194065D-04-

4.942014160D-08

5.591493490D-12-2.566386941D-16 4.156251610D+04

1.265367627D+01

6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6641.836

-1.008467687D+06 7.642402360D+02 2.332880311D+00 1.892649914D-05-

1.170322571D-09

3.749758920D-14-4.871021520D-19 4.111417150D+04

9.680921840D+00

Fe(CO)5 Chase,1998 p698.

2 j 3/78 FE 1.00C 5.000 5.00 0.00 0.00 0 195.89550 -  
727850.000

200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
33145.399

3.797805710D+05-7.285928160D+03 5.400236180D+01-6.935400750D-02

1.026705717D-04

-7.207373130D-08 1.958981996D-11 -5.854580480D+04-

2.604377836D+02

1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
33145.399

1.116600852D+06-8.067074730D+03 3.652942410D+01-2.047190300D-03

4.441967750D-07

-4.932507130D-11 2.235704865D-15 -4.860661250D+04-

1.754566113D+02

FeCL Chase,1998 p761.  
 2 j 6/65 FE 1.00CL 1.00 0.00 0.00 0.00 0 91.29770  
 251040.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10377.153  
 1.117340353D+04-5.402144290D+01 3.486057920D+00 6.879837140D-03-  
 1.273679557D-05  
 1.025321859D-08-3.051544011D-12 2.928681990D+04  
 9.428958050D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10377.153  
 5.288700220D+05-1.282897413D+03 5.798441690D+00-2.896589776D-04  
 3.343903810D-08  
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 FeCL2 Chase,1998 p822.  
 2 j12/70 FE 1.00CL 2.00 0.00 0.00 0.00 0 126.75040 -  
 141000.800  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14277.338  
 2.301121607D+04-5.858044060D+02 9.322903480D+00-3.006298824D-03  
 2.590788666D-06  
 -1.080178662D-09 2.341239608D-13 -1.621041276D+04-  
 1.816753103D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14277.338  
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 8.624218250D-07  
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 1.116896991D+01  
 FeCL3 Chase,1998 p879.  
 2 j 6/65 FE 1.00CL 3.00 0.00 0.00 0.00 0 162.20310 -  
 1059104.288  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18214.073  
 4.284772100D+03-5.741705370D+02 1.220667256D+01-4.680434120D-03  
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 2.887584913D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18214.073  
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 8.545873640D-10  
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 1.598495003D+01  
 FeO Chase,1998 p1239.  
 2 j 9/66 FE 1.00O 1.00 0.00 0.00 0.00 0 71.84440  
 251040.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8837.031  
 1.569282213D+04-6.460188880D+01 2.458925470D+00 7.016047360D-03-  
 1.021405947D-05  
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 1.326115545D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8837.031  
 -1.195971480D+05-3.624864780D+02 5.518880750D+00-9.978856890D-04  
 4.376913830D-07  
 -6.790629460D-11 3.639292680D-15 3.037985806D+04-  
 3.633655420D+00  
 Fe(OH)2 Chase,1998 p1230.

2 j12/66 FE 1.000 2.00H 2.00 0.00 0.00 0 89.85968 -  
 330536.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14209.461  
 4.443027200D+05-6.795140890D+03 3.894726210D+01-5.973005680D-02  
 7.046165430D-05  
 -4.087859510D-08 9.368766340D-12 -9.051420860D+03-  
 1.931304058D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14209.461  
 1.612519190D+06-6.533241990D+03 1.842922816D+01-2.073249635D-03  
 4.265874360D-07  
 -4.564063130D-11 1.990105746D-15 -2.992568633D+03-  
 8.445940590D+01  
 Fe2CL4 Chase,1998 p891.  
 2 j12/70 FE 2.00CL 4.00 0.00 0.00 0.00 0 253.50080 -  
 431370.400  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 29849.201  
 1.501308814D+03-6.617096510D+02 1.826924882D+01-4.181494660D-03  
 4.196535050D-06  
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 4.935641390D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 29849.201  
 1.402450973D+05 6.936064410D+02 1.313800410D+01 2.754333070D-03-  
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 1.752492221D+01  
 Fe2CL6 Chase,1998 p928.  
 2 j 6/65 FE 2.00CL 6.00 0.00 0.00 0.00 0 324.40620 -  
 654377.600  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 40447.854  
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 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 40447.854  
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 1.226831608D-09  
 -1.473195806D-13 7.078272330D-18 -8.551496190D+04-  
 6.143758030D+01  
 Ga Hf:Gurvich,1996a. Moore,1971. Johansson,1966.  
 Gordon,1999.  
 3 g12/98 GA 1.00 0.00 0.00 0.00 0.00 0 69.72300  
 272000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
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 1.932327565D-05  
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 7.547172760D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6551.115  
 -5.544186520D+04 8.808624420D+02 1.760717716D+00 2.993259460D-04-  
 5.610827310D-08  
 2.682832239D-12 3.132134914D-16 2.684351822D+04  
 1.252212023D+01

6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6551.115  
 2.288759836D+08-6.759297920D+04 2.526821493D+00 1.463058875D-03-  
 1.250892936D-07  
 3.820116110D-12-3.997883065D-17 6.402915740D+05-  
 8.083504020D+00  
 Ga+ IP:Johansson,1966. Moore,1971. Gordon,1999.  
 3 g12/98 GA 1.00E -1.00 0.00 0.00 0.00 0 69.72245  
 856688.428  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 4.098344940D-04-4.343581620D-06 2.500000019D+00-4.389036810D-11  
 5.563969200D-14  
 -3.638228260D-17 9.607881995D-21 1.022899726D+05  
 5.215090460D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 3.566607140D+04-1.108845546D+02 2.635517951D+00-8.338973520D-05  
 2.734243614D-08  
 -4.555673740D-12 3.035050101D-16 1.029897430D+05  
 4.257075410D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 1.880791061D+08-1.410890480D+05 4.500268850D+01-6.445582900D-03  
 5.005999840D-07  
 -1.789454995D-11 2.439723414D-16 1.191428220D+06-  
 3.545671850D+02  
 GaBr Gurvich,1996a pt1 p239 pt2 p193  
 2 tpis96 GA 1.00BR 1.00 0.00 0.00 0.00 0 149.62700 -  
 17967.880  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9932.119  
 -2.185275415D+03-7.672232970D+01 4.770805670D+00-4.497881060D-04  
 5.579853600D-07  
 -3.065156457D-10 7.042946040D-14 -3.138004818D+03  
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 9932.119  
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 2 tpis96 GA 1.00BR 2.00 0.00 0.00 0.00 0 229.53100 -  
 149180.952  
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 1.162714892D+00  
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 19037.337  
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 -9.175147260D-14 4.391186940D-18 -3.833402150D+04-  
 1.410315914D+01  
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 2 tpris96 GA 1.00CL 1.00 0.00 0.00 0.00 0 105.17570 -  
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 1.864959150D+01  
 GaF Gurvich,1996a pt1 p224 pt2 p179  
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 12115.659  
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 8673.104  
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 2.224032244D+01  
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 9.820900220D+01  
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 44871.122

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 4.928964650D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10109.122  
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 8.658040510D-07  
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 3.227359770D+01  
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 14470.935  
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 4.250516810D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
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 3.611531540D-10  
 -4.350978870D-14 2.095704875D-18 -1.700058453D+04-  
 1.090291552D+01  
 GaO Gurvich,1996a pt1 p214 pt2 p174  
 2 tpris96 GA 1.00O 1.00 0.00 0.00 0.00 0 85.72240  
 146823.607  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8925.107  
 7.325543910D+04-9.804269510D+02 7.844122760D+00-7.171072850D-03  
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 1.799742951D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8925.107  
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 143630.495

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 10583.608  
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 5.943068910D-08  
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 136963.692  
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 4.427520690D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 30591.766  
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 6.146455950D-10  
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 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 27315.392  
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 1.721694751D-09  
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 4.147281510D+01  
 Ga2CL6 Gurvich,1996a pt1 p238 pt2 p192.  
 2 tpis96 GA 2.00CL 6.00 0.00 0.00 0.00 0 352.16220 -  
 962463.532  
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 6.745333650D+01  
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 17147.856  
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 1.908325521D+01  
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 22653.242  
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 Ga2F6 Gurvich,1996a pt1 p230 pt2 p185.  
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 2017623.843  
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 -1.601732039D-12 7.407584420D-17 -2.494298707D+05-  
 7.787635830D+01  
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 13520.947  
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 21497.947  
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 3.535333010D-07  
 -2.289632389D-10 6.040085360D-14 -1.233174068D+03-  
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 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 21497.947  
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 Ga2I4 Gurvich,1996a pt1 p253 pt2 p205.  
 2 tpris96 GA 2.00I 4.00 0.00 0.00 0.00 0 647.06388 -  
 159267.987  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 32583.813  
 -1.769495991D+04-1.354871509D+02 1.654625333D+01-1.199014713D-03  
 1.473754848D-06  
 -9.504796570D-10 2.499380837D-13 -2.333405795D+04-  
 3.325712890D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 32583.813  
 -3.171299760D+04-2.287068836D+00 1.600194812D+01-8.588964380D-07  
 2.041966602D-10  
 -2.476145769D-14 1.198551944D-18 -2.401940505D+04-  
 3.008672521D+01  
 Ga2I6 Gurvich,1996a pt1 p253 pt2 p206.  
 2 tpris96 GA 2.00I 6.00 0.00 0.00 0.00 0 900.87282 -  
 317294.623

200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 43573.378  
 -2.110891458D+04-3.695404160D+02 2.346811836D+01-3.189178210D-03  
 3.890339040D-06  
 -2.494830378D-09 6.532007280D-13 -4.301188090D+04-  
 6.014811500D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 43573.378  
 -6.015698150D+04-6.329209230D+00 2.200533040D+01-2.332008629D-06  
 5.513868480D-10  
 -6.659445350D-14 3.213670430D-18 -4.488699380D+04-  
 5.161008750D+01  
 Ga20 Gurvich,1996a pt1 p216 pt2 p175.  
 2 tpis96 GA 2.000 1.00 0.00 0.00 0.00 0 155.44540 -  
 99457.457  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12162.595  
 5.697197180D+04-8.074085990D+02 7.733061540D+00 1.478450874D-03-  
 4.097743430D-06  
 3.581158920D-09-1.107073202D-12 -9.512216820D+03-  
 1.256149299D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12162.595  
 -1.193874986D+05-8.719341610D+01 7.064678200D+00-2.571524542D-05  
 5.651108490D-09  
 -6.448190540D-13 2.975374645D-17 -1.393694796D+04-  
 6.942801300D+00  
 Ge Hf:Gurvich,1991 pt1 p311. Sugar,1993. Gordon,1999.  
 3 g 3/99 GE 1.00 0.00 0.00 0.00 0.00 0 72.61000  
 367800.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7398.584  
 -2.059215242D+04-1.432022103D+02 4.506002330D+00 1.547187840D-03-  
 8.518296550D-06  
 8.243824460D-09-2.566167305D-12 4.363070860D+04-  
 6.225268510D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7398.584  
 -8.565413840D+05 3.917958660D+03-1.809888212D+00 2.276482224D-03-  
 5.365627550D-07  
 5.984958090D-11-2.541700646D-15 1.956518798D+04  
 3.841346790D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7398.584  
 2.423965136D+07-2.543605174D+04 1.456087539D+01-2.592562254D-03  
 2.658628502D-07  
 -1.122785077D-11 1.620997559D-16 2.295812461D+05-  
 8.953585860D+01  
 Ge+ Sugar,1993. Gordon,1999.  
 3 g 3/99 GE 1.00E -1.00 0.00 0.00 0.00 0 72.60945  
 1134984.385  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6205.785  
 -3.453666430D+05 4.008449710D+03-1.522395737D+01 3.626030020D-02-  
 3.351367260D-05  
 1.431059219D-08-2.236976459D-12 1.157058042D+05  
 1.090151986D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6205.785  
 -2.244860570D+06 5.165531140D+03-3.867516510D-01 8.528730940D-04-  
 1.386040003D-07

1.155945775D-11-3.784413134D-16 1.006823985D+05  
2.965783448D+01  
6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6205.785  
5.768056240D+07-3.078606210D+04 8.706291820D+00-4.942233500D-04-  
2.690467703D-11  
1.853441677D-12-5.082067525D-17 3.857785420D+05-  
4.842599100D+01  
Ge- Hotop,1985. Gordon,1999.  
3 g 3/99 GE 1.00E 1.00 0.00 0.00 0.00 0 72.61055  
245402.540  
298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6980.940  
2.989142308D+03 8.657417230D+01 2.191868507D+00 5.900795270D-04-  
6.375800580D-07  
3.661132150D-10-8.689778450D-14 2.835695190D+04  
9.417004020D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6980.940  
1.352040246D+04-5.048518780D-01 2.500140247D+00-3.652944160D-09-  
6.716722200D-12  
1.378119925D-15-8.475212940D-20 2.881739757D+04  
7.577334250D+00  
6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6980.940  
1.079877187D+04 1.149969180D+00 2.499738027D+00 3.051383052D-08-  
1.930296476D-12  
6.305166240D-17-8.327676240D-22 2.880429709D+04  
7.580847710D+00  
GeBr Gurvich,1991 pt1 p333 pt2 p287.  
2 tpis91 GE 1.00BR 1.00 0.00 0.00 0.00 0 152.51400  
137438.119  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
9864.119  
-5.680774630D+04 9.173361260D+02-2.224809366D+00 2.171239242D-02-  
3.035490868D-05  
2.011776305D-08-5.202915040D-12 1.104192901D+04  
4.107836480D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
9864.119  
2.256750476D+05-7.310715460D+02 6.263283810D+00-1.198085447D-03  
4.000377770D-07  
-5.429937880D-11 2.510481953D-15 1.942863606D+04-  
6.106802870D+00  
GeBr2 Gurvich,1991 pt1 p334 pt2 p288.  
2 tpis91 GE 1.00BR 2.00 0.00 0.00 0.00 0 232.41800 -  
60962.897  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
14193.463  
-1.649285325D+03-2.296262116D+02 7.900144680D+00-1.936685504D-03  
2.345776175D-06  
-1.496279368D-09 3.901453500D-13 -8.316624210D+03-  
6.918349740D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
14193.463  
-2.636655245D+04-3.990509020D+00 7.003327440D+00-1.445749787D-06  
3.401591360D-10  
-4.093457030D-14 1.969987842D-18 -9.484999250D+03-  
1.673810702D+00  
GeBr3 Gurvich,1991 pt1 p335 pt2 p289.

2 tpis91 GE 1.00BR 3.00 0.00 0.00 0.00 0 312.32200 -  
 119031.308  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18549.492  
 2.725568677D+03-5.186213260D+02 1.199957754D+01-4.251024530D-03  
 5.103629720D-06  
 -3.233706250D-09 8.388358860D-13 -1.477988251D+04-  
 2.534570086D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18549.492  
 -5.433926700D+04-9.280327950D+00 1.000765019D+01-3.297322150D-06  
 7.712929260D-10  
 -9.241571850D-14 4.432876230D-18 -1.742697092D+04-  
 1.366960704D+01  
 GeBr4 Gurvich,1991 pt1 p336 pt2 p290.  
 2 tpis91 GE 1.00BR 4.00 0.00 0.00 0.00 0 392.22600 -  
 291000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 23963.218  
 5.431940390D+03-6.777748800D+02 1.560015305D+01-5.507788880D-03  
 6.594764290D-06  
 -4.170146140D-09 1.080116643D-12 -3.557606400D+04-  
 4.209134400D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 23963.218  
 -6.977757910D+04-1.179873115D+01 1.300953955D+01-4.024938750D-06  
 9.203567210D-10  
 -1.076853369D-13 5.040954800D-18 -3.904148160D+04-  
 2.689447543D+01  
 GeCL Gurvich,1991 pt1 p328 pt2 p283.  
 2 tpis91 GE 1.00CL 1.00 0.00 0.00 0.00 0 108.06270  
 69029.915  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9599.115  
 1.069724739D+04-2.241238266D+01 1.987371070D+00 1.368270905D-02-  
 2.358294414D-05  
 1.786756020D-08-5.102503250D-12 7.440683390D+03  
 1.505795136D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9599.115  
 -3.784193250D+05 1.429309204D+03 3.194854640D+00 8.119939120D-04-  
 2.652459954D-07  
 5.151957880D-11-3.534214570D-15 -2.087046335D+03  
 1.384991767D+01  
 GeCL2 Gurvich,1991 pt1 p330 pt2 p284.  
 2 tpis91 GE 1.00CL 2.00 0.00 0.00 0.00 0 143.51540 -  
 171000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13276.791  
 1.838536673D+04-5.827205340D+02 9.161404660D+00-4.464786030D-03  
 5.244873550D-06  
 -3.268067210D-09 8.367575420D-13 -1.975798598D+04-  
 1.734353609D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13276.791  
 -4.890128920D+04-1.126210418D+01 7.009063530D+00-3.839180730D-06  
 8.865633570D-10  
 -1.052000540D-13 5.008422220D-18 -2.275254424D+04-  
 4.656961090D+00  
 GeCL3 Hf:Gurvich,1991 pt1 p331. Gurvich,1979 pt2 p287.



2 g 6/01 GE 1.00CL 3.00 0.00 0.00 0.00 0 178.96810 -  
 266950.589  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17559.437  
 1.935859579D+04-8.342020000D+02 1.312702530D+01-6.511390020D-03  
 7.696277480D-06  
 -4.818541730D-09 1.238399959D-12 -3.097218753D+04-  
 3.552573080D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17559.437  
 -7.574499820D+04-1.579213420D+01 1.001278835D+01-5.441738310D-06  
 1.260936724D-09  
 -1.500137106D-13 7.156400810D-18 -3.525131720D+04-  
 1.719745840D+01  
 GeCL4 Gurvich,1991 pt1 p332 pt2 p286.  
 2 tpris91 GE 1.00CL 4.00 0.00 0.00 0.00 0 214.42080 -  
 500000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 21136.625  
 6.502870410D+04-1.652482760D+03 1.881327000D+01-1.152426810D-02  
 1.310809980D-05  
 -7.961956110D-09 1.997505040D-12 -5.570052390D+04-  
 6.754459960D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 21136.625  
 -1.376261210D+05-3.603769500D+01 1.302816670D+01-1.164956960D-05  
 2.636193380D-09  
 -3.072926720D-13 1.439808750D-17 -6.426281780D+04-  
 3.318180130D+01  
 GeF Gurvich,1991 pt1 p324 pt2 p279.  
 2 tpris91 GE 1.00F 1.00 0.00 0.00 0.00 0 91.60840 -  
 70592.990  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9144.110  
 5.017097820D+04-4.395552520D+02 2.990864513D+00 1.252766738D-02-  
 2.337593226D-05  
 1.841631179D-08-5.398492260D-12 -7.093516400D+03  
 7.063757790D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9144.110  
 -5.150480580D+05 1.659711777D+03 2.999610299D+00 8.198511680D-04-  
 2.271982948D-07  
 3.624183860D-11-2.133840473D-15 -2.051529487D+04  
 1.373105116D+01  
 GeF2 Gurvich,1991 pt1 p326 pt2 p280.  
 2 tpris91 GE 1.00F 2.00 0.00 0.00 0.00 0 110.60681 -  
 574000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11787.485  
 7.543097080D+04-1.108456469D+03 9.078898270D+00-1.445630636D-03-  
 6.575322320D-07  
 1.475344103D-09-5.811220270D-13 -6.510685550D+04-  
 2.200497813D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11787.485  
 -1.275327716D+05-7.162591350D+01 7.053002370D+00-2.101910441D-05  
 4.607893700D-09  
 -5.246394670D-13 2.416218951D-17 -7.112637630D+04-  
 8.484248230D+00  
 GeF3 Hf:Gurvich,1991 pt1 p327. Gurvich,1979 v2 pt2 p283.

2 g 6/01 GE 1.00F 3.00 0.00 0.00 0.00 0 129.60521 -  
 806332.833  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14678.187  
 1.114121569D+05-1.776908030D+03 1.352166477D+01-2.983622949D-03-  
 3.612749750D-08  
 1.621528436D-09-7.199011780D-13 -9.038262960D+04-  
 4.568794740D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14678.187  
 -2.069580129D+05-1.110233803D+02 1.008234122D+01-3.271676260D-05  
 7.183896700D-09  
 -8.190388120D-13 3.776322440D-17 -9.999749090D+04-  
 2.303500657D+01  
 GeF4 Gurvich,1991 pt1 p328 pt2 p282.  
 2 tpi91 GE 1.00F 4.00 0.00 0.00 0.00 0 148.60361 -  
 1190150.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17293.025  
 1.119818968D+05-1.636859630D+03 1.231371005D+01 1.025446325D-02-  
 1.893783072D-05  
 1.476849261D-08-4.325174110D-12 -1.374265128D+05-  
 4.104232670D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17293.025  
 -3.253032680D+05-2.538279448D+02 1.318792173D+01-7.460058550D-05  
 1.637384721D-08  
 -1.866482733D-12 8.605530500D-17 -1.466176526D+05-  
 4.122267840D+01  
 GeH4 Barin,1989 pt1 p628.  
 2 bar89 GE 1.00H 4.00 0.00 0.00 0.00 0 76.64176  
 90793.000  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 -2.568398191D+05-4.132811450D+01 7.755116280D+00 2.129640783D-03  
 7.255053610D-07  
 -5.096314010D-10 1.431608261D-13 7.881538040D+03-  
 2.030166702D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 -3.809805880D+06 1.093167093D+04-5.149675410D+00 9.485931370D-03-  
 1.649459859D-06  
 1.419674126D-10-5.004639750D-15 -6.158518520D+04  
 7.168902570D+01  
 GeI Gurvich,1991 pt1 p337 pt2 p291.  
 2 tpi91 GE 1.00I 1.00 0.00 0.00 0.00 0 199.51447  
 210969.120  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10005.120  
 -7.438308220D+04 1.033759595D+03-1.520491112D+00 1.555125152D-02-  
 1.683415215D-05  
 8.383557810D-09-1.550875391D-12 1.912920413D+04  
 3.959372920D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10005.120  
 -2.133148437D+05-2.953079008D+02 6.876607360D+00-2.102579132D-03  
 8.596299380D-07  
 -1.447692760D-10 8.401042790D-15 2.452326136D+04-  
 8.550009280D+00  
 GeO Gurvich,1991 pt1 p315 pt2 p274.

2 tpis91 GE 1.000 1.00 0.00 0.00 0.00 0 88.60940 -  
 37694.307  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8782.106  
 -6.781225630D+03 2.791946972D+02 6.198952860D-01 1.111378013D-02-  
 1.501027092D-05  
 1.006783003D-08-2.687101932D-12 -6.711847430D+03  
 2.156390251D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8782.106  
 -1.044508485D+06 2.734866048D+03 1.298071298D+00 1.832638634D-03-  
 5.060986350D-07  
 6.374958020D-11-2.172371872D-15 -2.362104658D+04  
 2.350855275D+01  
 GeO2 Gurvich,1991 pt1 p323 pt2 p278.  
 2 tpis91 GE 1.000 2.00 0.00 0.00 0.00 0 104.60880 -  
 106171.998  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11258.002  
 -3.824173830D+03 1.563451633D+02 1.694198285D+00 1.756205059D-02-  
 2.418270032D-05  
 1.632388154D-08-4.368957860D-12 -1.477534880D+04  
 1.556883504D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11258.002  
 -1.727347526D+05-2.961154443D+02 7.720726250D+00-8.824933390D-05  
 1.949874702D-08  
 -2.235834829D-12 1.036128507D-16 -1.387983288D+04-  
 1.669888706D+01  
 GeS Gurvich,1991 pt1 p344 pt2 p297.  
 2 tpis91 GE 1.00S 1.00 0.00 0.00 0.00 0 104.67600  
 92525.110  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9141.110  
 3.661018430D+04-5.659653500D+02 6.152936410D+00-2.746908039D-03  
 2.733435196D-06  
 -1.460209187D-09 3.278709470D-13 1.274175754D+04-  
 7.706074970D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9141.110  
 -2.351367441D+06 7.211581860D+03-4.362526310D+00 5.451737750D-03-  
 1.721002774D-06  
 2.632908084D-10-1.394374040D-14 -3.583317250D+04  
 6.505525340D+01  
 GeS2 Gurvich,1991 pt1 p347 pt2 p299.  
 2 tpis91 GE 1.00S 2.00 0.00 0.00 0.00 0 136.74200  
 118817.831  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13067.831  
 5.543683600D+04-1.024826697D+03 1.057594552D+01-5.287883910D-03  
 5.295803080D-06  
 -2.872529530D-09 6.519027550D-13 1.735579668D+04-  
 2.991750248D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13067.831  
 -8.970980360D+04-3.364377000D+01 7.525433720D+00-1.026368137D-05  
 2.282230718D-09  
 -2.628748770D-13 1.222218614D-17 1.195232103D+04-  
 1.135201328D+01  
 Ge2 Gurvich,1991 pt1 p313 pt2 p273.

2 tpi91 GE 2.00 0.00 0.00 0.00 0.00 0 145.22000  
 471498.929  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10696.129  
 2.161978929D+05-3.079621733D+03 1.888047728D+01-2.604825861D-02  
 2.279151350D-05  
 -9.028351270D-09 1.146806387D-12 7.032402550D+04-  
 7.901157930D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10696.129  
 1.969461258D+06-5.248687100D+03 1.058277303D+01-3.336551510D-03  
 1.052745838D-06  
 -1.484534793D-10 7.475431760D-15 8.925665990D+04-  
 3.750295910D+01  
 H D0 (H2): Herzberg, 1970. Moore, 1972. Gordon, 1999.  
 3 g 6/97 H 1.00 0.00 0.00 0.00 0.00 0 1.00794  
 217998.828  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 2.547370801D+04-  
 4.466828530D-01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 6.078774250D+01-1.819354417D-01 2.500211817D+00-1.226512864D-07  
 3.732876330D-11  
 -5.687744560D-15 3.410210197D-19 2.547486398D+04-  
 4.481917770D-01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 2.173757694D+08-1.312035403D+05 3.399174200D+01-3.813999680D-03  
 2.432854837D-07  
 -7.694275540D-12 9.644105630D-17 1.067638086D+06-  
 2.742301051D+02  
 H+ IP (H): Moore, 1972. Gordon, 1999.  
 3 g10/00 H 1.00E -1.00 0.00 0.00 0.00 0 1.00739  
 1536245.928  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 1.840214877D+05-  
 1.140646644D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 1.840214877D+05-  
 1.140646644D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 1.840214877D+05-  
 1.140646644D+00  
 H- Hotop, 1985. Gordon, 1999.  
 3 g 9/96 H 1.00E 1.00 0.00 0.00 0.00 0 1.00849  
 139031.328  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428

```

0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00
0.000000000D+00
0.000000000D+00 0.000000000D+00 1.597615494D+04-
1.139013868D+00
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
6197.428
0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00
0.000000000D+00
0.000000000D+00 0.000000000D+00 1.597615494D+04-
1.139013868D+00
6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
6197.428
0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00
0.000000000D+00
0.000000000D+00 0.000000000D+00 1.597615494D+04-
1.139013868D+00
HALO Gurvich,1996a pt1 p147 pt2 p111.
2 tpis96 AL 1.000 1.00H 1.00 0.00 0.00 0 43.98888
1821.114
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
9935.217
2.668671568D+04-4.663214590D+02 5.383800210D+00 2.902425002D-03-
2.243677610D-07
-1.516294323D-09 6.951737660D-13 1.235914473D+03-
6.508837520D+00
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
9935.217
7.847467050D+04-1.515628850D+03 8.572776230D+00-4.142611440D-04
8.935081700D-08
-1.007036446D-11 4.608017250D-16 6.663241890D+03-
2.672948642D+01
HALO2 Gurvich,1996a pt1 p148 pt2 p112.
2 tpis96 H 1.00AL 1.000 2.00 0.00 0.00 0 59.98828 -
355473.551
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
11980.604
3.544598910D+03 1.159819104D+02 8.637970690D-01 2.460875785D-02-
3.423160120D-05
2.373182987D-08-6.467608830D-12 -4.449506140D+04
2.012317065D+01
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
11980.604
6.985705440D+05-2.864935042D+03 1.086721494D+01-5.368312700D-05-
2.836877559D-08
6.291641190D-12-3.889033110D-16 -2.764392495D+04-
3.775886340D+01
HBO Boron oxide-hydride Gurvich,1996 pt1 p39,pt2 p23.
2 tpis96 H 1.00B 1.000 1.00 0.00 0.00 0 27.81834 -
210621.205
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
9166.898
6.360975030D+04-8.001557590D+02 6.218816130D+00-7.801679980D-04
3.141286759D-06
-2.031853478D-09 3.738552890D-13 -2.240282910D+04-
1.326952393D+01
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
9166.898
8.861860230D+05-3.913068050D+03 9.888644800D+00-8.222269140D-04
1.621530554D-07
-1.703550237D-11 7.372740020D-16 -3.161852029D+03-
4.036812720D+01

```

HBO+ Chase,1998 p223 12/75.

3 g 1/01 H 1.00B 1.000 1.00E -1.00 0.00 0 27.81779  
1175219.729  
298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
9094.629  
6.524471470D+04-7.047337360D+02 5.294271870D+00 1.308494598D-03  
2.088343622D-06  
-2.564100339D-09 8.198981250D-13 1.439293436D+05-  
6.816749230D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
9094.629  
1.836083606D+04-1.212975446D+03 6.822901960D+00 9.142272500D-04-  
2.665355457D-07  
3.297049810D-11-1.530684082D-15 1.463617504D+05-  
1.699646159D+01  
6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
9094.629  
-2.428406068D+07 1.188114816D+04 5.641928570D+00 1.354130653D-04-  
2.943428505D-09  
-3.120357467D-14 1.432576207D-18 3.883449210D+04-  
3.069802126D+00

HBO2 Gurvich,1996a pt1 p42 pt2 p26.

2 tpi96 H 1.00B 1.000 2.00 0.00 0.00 0 43.81774 -  
560210.053  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
10918.102  
6.225087470D+03 7.566153690D+01 1.253406833D+00 1.748006535D-02-  
1.982688351D-05  
1.229656460D-08-3.153609847D-12 -6.878588780D+04  
1.767793507D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
10918.102  
1.049369185D+06-4.479145480D+03 1.197755861D+01-4.735743400D-04  
6.080207140D-08  
-3.641565440D-12 6.155973170D-17 -4.221149470D+04-  
4.911366820D+01

HBS Chase,1998 p227 12/75. Jacox,1994.

2 g 2/01 H 1.00B 1.00S 1.00 0.00 0.00 0 43.88494  
50208.000  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
9286.259  
5.649966210D+04-5.466409950D+02 3.636458390D+00 9.963657670D-03-  
1.395090386D-05  
1.032834167D-08-3.047186722D-12 7.919860530D+03  
1.182489495D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
9286.259  
-2.021836183D+05-5.052026620D+02 6.415218280D+00 1.049432932D-03-  
3.683146690D-07  
5.342968310D-11-2.154140451D-15 6.485475620D+03-  
1.331376446D+01

HBS+ Chase,1998 p228 12/75. Jacox,1998 p141.

3 g 1/01 H 1.00B 1.00S 1.00E -1.00 0.00 0 43.88439  
1129458.967  
298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
10135.990  
1.489509163D+05-1.847661736D+03 1.147458020D+01-9.476828370D-03  
1.110746739D-05  
-6.175558610D-09 1.336853512D-12 1.437822395D+05-  
4.113509080D+01

1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10135.990  
 6.610658360D+05-2.791498527D+03 9.131267640D+00-5.063795290D-04  
 7.751213140D-08  
 -4.191132930D-12 2.687149095D-17 1.510734114D+05-  
 3.081422748D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10135.990  
 -9.547637920D+06 7.401763110D+03 4.866419360D+00 4.143886550D-04-  
 2.488064459D-08  
 6.972990680D-13-7.714953540D-18 7.555300990D+04  
 3.822672190D+00  
 HBr Gurvich,1989 pt1 p205 pt2 p106.  
 2 tpis89 H 1.00BR 1.00 0.00 0.00 0.00 0 80.91194 -  
 36290.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8648.104  
 2.527222498D+04-4.065110270D+02 6.043116610D+00-7.717882870D-03  
 1.149123213D-05  
 -7.293633280D-09 1.747406491D-12 -3.510414550D+03-  
 9.903186290D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8648.104  
 1.170033949D+06-3.786521010D+03 7.503148050D+00-1.284963943D-03  
 3.206257190D-07  
 -3.444925160D-11 1.126758417D-15 1.856413349D+04-  
 2.562712911D+01  
 HCN Hf: East,1993. Gurvich,1991 pt1 p226.  
 2 g 6/01 H 1.00C 1.00N 1.00 0.00 0.00 0 27.02538  
 133082.460  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9235.463  
 9.098286930D+04-1.238657512D+03 8.721307870D+00-6.528242940D-03  
 8.872700830D-06  
 -4.808886670D-09 9.317898500D-13 2.098915450D+04-  
 2.746677854D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9235.463  
 1.236889278D+06-4.446732410D+03 9.738874850D+00-5.855182640D-04  
 1.072791440D-07  
 -1.013313244D-11 3.348247980D-16 4.221513770D+04-  
 4.005773850D+01  
 HCO Hf:Terentis,1996. Jacox,1998 p146.  
 2 g 1/01 H 1.00C 1.00O 1.00 0.00 0.00 0 29.01804  
 42397.850  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9989.450  
 -1.189851887D+04 2.151536111D+02 2.730224028D+00 1.806516108D-03  
 4.984300570D-06  
 -5.814567920D-09 1.869689894D-12 2.905755640D+03  
 1.136772540D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9989.450  
 6.949606120D+05-3.656223380D+03 9.604731170D+00-1.117129278D-03  
 2.875328019D-07  
 -3.626247740D-11 1.808329595D-15 2.543704440D+04-  
 3.582473720D+01  
 HCO+ Formyl ion. Hf:Chase,1998 p603 12/70. Jacox,1998 p145.  
 3 g 1/01 H 1.00C 1.00O 1.00E -1.00 0.00 0 29.01749  
 833034.000

298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9045.992  
 1.573442506D+05-1.867692159D+03 1.099235423D+01-1.211637888D-02  
 1.659091514D-05  
 -1.016592642D-08 2.391234771D-12 1.084930280D+05-  
 4.078261620D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9045.992  
 1.219060653D+06-4.714294890D+03 1.021192493D+01-8.854517070D-04  
 1.667408026D-07  
 -1.683285548D-11 7.040051780D-16 1.277989027D+05-  
 4.351158460D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9045.992  
 -4.593151930D+05-1.132568857D+03 7.739065200D+00-2.648464060D-05  
 1.613280824D-09  
 -5.113217500D-14 6.588027500D-19 1.032813937D+05-  
 2.458716820D+01  
 HCCN Gurvich,1989 pt1 p228 pt2 p216.  
 2 tpris89 H 1.00C 2.00N 1.00 0.00 0.00 0 39.03608  
 610430.628  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11865.731  
 2.994114377D+03-4.404660680D+02 6.940036410D+00 3.846304960D-03-  
 1.264728529D-06  
 -3.639235130D-10 2.748929104D-13 7.370878640D+04-  
 1.315302437D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11865.731  
 9.395620310D+05-4.091067750D+03 1.272233302D+01-6.874405310D-04  
 1.231169968D-07  
 -1.186956238D-11 4.760610350D-16 9.585164820D+04-  
 5.248695640D+01  
 HCCO Ketenyl rad. Osborn,1997. Szalay,1996. Jacox,1998 p156.  
 2 g 6/01 H 1.00C 2.00O 1.00 0.00 0.00 0 41.02874  
 176568.100  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11664.994  
 6.959612700D+04-1.164594402D+03 9.456616260D+00-2.331240632D-03  
 5.161873600D-06  
 -3.526169970D-09 8.599143230D-13 2.535003992D+04-  
 2.726355351D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11664.994  
 1.093922002D+06-4.498228210D+03 1.246446433D+01-6.343317400D-04  
 1.108549019D-07  
 -1.125488678D-11 5.689151940D-16 4.652280300D+04-  
 5.099070430D+01  
 HCL Gurvich,1989 pt1 p186 pt2 p93.  
 2 tpris89 H 1.00CL 1.00 0.00 0.00 0.00 0 36.46064 -  
 92310.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8640.104  
 2.062588287D+04-3.093368855D+02 5.275418850D+00-4.828874220D-03  
 6.195794600D-06  
 -3.040023782D-09 4.916790030D-13 -1.067782299D+04-  
 7.309317750D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8640.104  
 9.157749510D+05-2.770550211D+03 5.973539790D+00-3.629810060D-04  
 4.735529190D-08



2.810262054D-12-6.656104220D-16 5.674958050D+03-  
 1.642827056D+01  
 HD Gurvich,1989 pt1 p144 pt2 p53.  
 3 tpis89 H 1.00D 1.00 0.00 0.00 0.00 0 3.02204  
 323.302  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8509.102  
 2.519120338D+04-2.761004999D+02 4.644441290D+00-2.082376844D-03  
 1.418070803D-06  
 2.839893835D-10-3.202331030D-13 3.913616430D+02-  
 9.395396120D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8509.102  
 8.455830000D+05-1.956578537D+03 4.404373870D+00 5.751681090D-04-  
 2.131983152D-07  
 4.036126680D-11-2.727170705D-15 1.227254163D+04-  
 1.084742878D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8509.102  
 4.829960940D+08-3.077144916D+05 7.864816510D+01-8.332990910D-03  
 4.732254110D-07  
 -1.372721571D-11 1.614120677D-16 2.431070386D+06-  
 6.569437060D+02  
 HD+ Chase,1998 p1034.  
 3 j 9/77 H 1.00D 1.00E -1.00 0.00 0.00 0 3.02149  
 1496792.618  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8614.000  
 -8.070073050D+04 8.796432580D+02 5.968932160D-02 5.418181010D-03-  
 2.021515155D-06  
 -4.945261650D-10 4.092935650D-13 1.744992497D+05  
 1.934281193D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8614.000  
 1.340083030D+06-5.730069570D+03 1.213836576D+01-5.243338120D-03  
 1.976302344D-06  
 -3.306573530D-10 1.937902763D-14 2.135348051D+05-  
 6.128758390D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8614.000  
 6.116880040D+06-1.884939608D+04 1.741572175D+01-2.495631471D-03  
 1.746560021D-07  
 -5.815870420D-12 7.638706130D-17 3.018292196D+05-  
 1.105093671D+02  
 HDO Gurvich,1989 pt1 p145 pt2 p55.  
 2 g 5/99 H 1.00D 1.000 1.00 0.00 0.00 0 19.02144 -  
 245280.477  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9925.723  
 -2.737795356D+04 4.310503900D+02 1.558479899D+00 5.764969150D-03-  
 4.855129360D-06  
 3.382990170D-09-1.040863879D-12 -3.273226450D+04  
 1.487751891D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9925.723  
 1.711376798D+06-5.322872300D+03 9.124351520D+00-3.400664150D-04  
 4.152343520D-08  
 -4.780768570D-14-1.468035170D-16 3.245224680D+03-  
 3.774600680D+01  
 HDO2 Gurvich,1989 pt1 p146 pt2 p56.

2 g 5/99 H 1.00D 1.000 2.00 0.00 0.00 0 35.02084 -  
 140241.635  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11334.965  
 -3.216476650D+04 7.492334460D+02-1.957676212D+00 2.412802791D-02-  
 2.915946684D-05  
 1.930016324D-08-5.226986310D-12 -2.151059175D+04  
 3.672406740D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11334.965  
 1.313180619D+06-5.175637120D+03 1.216490975D+01-6.136699480D-04  
 1.227560176D-07  
 -1.079624939D-11 3.874013720D-16 1.303209670D+04-  
 5.085276870D+01  
 HF Gurvich,1989 pt1 p162 pt2 p77.  
 3 tpi89 H 1.00F 1.00 0.00 0.00 0.00 0 20.00634 -  
 273300.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8599.103  
 -3.192098970D+03 5.986807720D+01 3.055113902D+00 1.684673783D-03-  
 3.287394830D-06  
 3.095923617D-09-9.764691610D-13 -3.418443160D+04  
 3.294904120D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8599.103  
 7.257089040D+05-1.484797741D+03 3.855527470D+00 7.138989850D-04-  
 2.106757333D-07  
 3.050092453D-11-1.639495583D-15 -2.355456660D+04-  
 3.203856830D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8599.103  
 1.764588423D+08-8.789998060D+04 1.886524859D+01-6.850866180D-04-  
 1.403468022D-08  
 1.503711045D-12-2.717518148D-17 6.853573220D+05-  
 1.393231574D+02  
 HI Chase,1998 p1265.  
 2 j 9/61 H 1.00I 1.00 0.00 0.00 0.00 0 127.91241  
 26359.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8656.500  
 1.872881730D+04-3.431788840D+02 5.956712430D+00-8.543439600D-03  
 1.454780274D-05  
 -1.049104164D-08 2.839734003D-12 3.682950720D+03-  
 8.149756090D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8656.500  
 4.724921450D+05-1.923465741D+03 5.758048970D+00-4.066266380D-04  
 9.474332050D-08  
 -1.033534431D-11 4.611614790D-16 1.394857037D+04-  
 1.182487652D+01  
 HNC Hf:Gurvich,1991 pt1 p227. Jacox,1998 p145.  
 2 g 6/01 H 1.00N 1.00C 1.00 0.00 0.00 0 27.02538  
 194378.121  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10000.724  
 4.870620640D+04-9.891456250D+02 9.722153890D+00-1.113593916D-02  
 1.668862707D-05  
 -1.113940941D-08 2.893600868D-12 2.664679758D+04-  
 3.104826122D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10000.724

1.198791660D+06-3.918941860D+03 9.118020090D+00-3.417761100D-04  
3.314809680D-08  
-5.701574740D-13-7.789455390D-17 4.658810300D+04-  
3.468575660D+01

HNCO Hf:East,1993. Jacox,1998 p236.

2 g 7/00 H 1.00N 1.00C 1.00O 1.00 0.00 0 43.02478 -  
118056.529

200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
10966.126

7.542460080D+04-9.550937770D+02 6.725705870D+00 4.705687500D-03-  
4.959475510D-06

3.694255120D-09-1.164859121D-12 -1.068149742D+04-  
1.365584623D+01

1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
10966.126

1.253216926D+06-5.021091540D+03 1.247789314D+01-6.891655250D-04  
1.097738448D-07

-9.306403800D-12 3.242606950D-16 1.453155559D+04-  
5.306419680D+01

HNO Gurvich,1989 pt1 p362 pt2 p227. Jacox,1998 p151.

2 g10/01 H 1.00N 1.00O 1.00 0.00 0.00 0 31.01408  
102032.725

200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
9941.880

-6.854764860D+04 9.551627200D+02-6.000720210D-01 7.995176750D-03-  
6.547079160D-07

-3.670513400D-09 1.783392519D-12 6.435351260D+03  
3.048166372D+01

1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
9941.880

-5.795614980D+06 1.945457427D+04-2.152568374D+01 1.797428992D-02-  
4.976040670D-06

6.397924170D-10-3.142619368D-14 -1.104192372D+05  
1.818650357D+02

HNO2 Cis-trans. Gurvich,1989 pt1 p363 pt2 p228.

2 tpi89 H 1.00N 1.00O 2.00 0.00 0.00 0 47.01348 -  
78451.922

200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
11597.285

8.591985060D+03 1.203644046D+02 9.412979120D-01 1.942891839D-02-  
2.253174194D-05

1.384587594D-08-3.473550460D-12 -1.106337202D+04  
2.073967459D+01

1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
11597.285

8.787904130D+05-3.990455030D+03 1.187349269D+01-4.881900610D-04  
7.133636790D-08

-5.376303340D-12 1.581778986D-16 1.246343241D+04-  
4.608874560D+01

HNO3 Gurvich,1989 pt1 p367 pt2 p231.

2 g 5/99 H 1.00N 1.00O 3.00 0.00 0.00 0 63.01288 -  
133912.869

200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
11876.390

9.202869010D+03 1.093774496D+02-4.521042450D-01 2.984914503D-02-  
3.190635500D-05

1.720931528D-08-3.782649830D-12 -1.764048507D+04  
2.746644974D+01

1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
11876.390

-9.497809640D+04-2.733024468D+03 1.449426995D+01-7.821868050D-04  
 1.702693665D-07  
 -1.930543961D-11 8.870455120D-16 -4.882517780D+03-  
 5.928392890D+01  
 HOCL Hf:Gurvich,1989 pt1 p187. Jacox,1998 p155.  
 2 g 1/01 H 1.000 1.00CL 1.00 0.00 0.00 0 52.46004 -  
 75740.032  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10224.626  
 -9.739307430D+03 3.547569520D+02 1.539514254D-01 1.617051795D-02-  
 2.179693631D-05  
 1.509103049D-08-4.125383510D-12 -1.176323791D+04  
 2.473256901D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10224.626  
 8.530457810D+05-2.847760552D+03 7.948329040D+00-1.048782013D-04-  
 1.482405043D-08  
 4.591678270D-12-3.060073987D-16 7.250964950D+03-  
 2.249832548D+01  
 HOF Gurvich,1989 pt1 p171 pt2 p79.  
 2 tpris89 H 1.000 1.00F 1.00 0.00 0.00 0 36.00574 -  
 96898.221  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10088.435  
 -3.696888300D+04 7.809006660D+02-2.077685317D+00 2.038690173D-02-  
 2.586919999D-05  
 1.713797538D-08-4.551281870D-12 -1.631720064D+04  
 3.645052500D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10088.435  
 8.812018230D+05-3.120013169D+03 8.223710070D+00-2.298036315D-04  
 1.459115709D-08  
 1.095883303D-12-1.404445608D-16 6.300546710D+03-  
 2.590150427D+01  
 HO2 Hf:Hills,1984. Jacox,1998 p153.  
 2 g 5/99 H 1.000 2.00 0.00 0.00 0.00 0 33.00674  
 12552.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10002.162  
 -7.598882540D+04 1.329383918D+03-4.677388240D+00 2.508308202D-02-  
 3.006551588D-05  
 1.895600056D-08-4.828567390D-12 -5.809366430D+03  
 5.193602140D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10002.162  
 -1.810669724D+06 4.963192030D+03-1.039498992D+00 4.560148530D-03-  
 1.061859447D-06  
 1.144567878D-10-4.763064160D-15 -3.194418740D+04  
 4.066850920D+01  
 HO2- Gurvich,1989 pt1 p121 pt2 p35.  
 2 tpris89 H 1.000 2.00E 1.00 0.00 0.00 0 33.00729 -  
 97629.980  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10017.620  
 5.980517650D+02 4.532183650D+02-7.885641820D-01 1.660606821D-02-  
 2.000303995D-05  
 1.273201256D-08-3.271493480D-12 -1.467223832D+04  
 2.880195356D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10017.620

8.883563120D+05-3.269606190D+03 8.381873830D+00-3.027048578D-04  
 3.189230840D-08  
 -9.694896340D-13-4.235596680D-17 7.066473970D+03-  
 2.750636195D+01  
 HPO Hf:Gurvich,1989 pt1 p424. Jacox,1994 p46.  
 2 tpis89 H 1.00P 1.000 1.00 0.00 0.00 0 47.98110 -  
 56868.759  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10065.343  
 -3.816314120D+04 7.927641870D+02-1.889940652D+00 1.800907425D-02-  
 1.857631793D-05  
 1.018768867D-08-2.355583619D-12 -1.157641240D+04  
 3.692925910D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10065.343  
 3.842459450D+05-2.434951707D+03 8.582173920D+00-4.058448570D-04-  
 1.669488740D-08  
 2.253640566D-11-1.943063011D-15 5.761632120D+03-  
 2.649097544D+01  
 HSO3F Chase,1998 p1057.  
 2 j 6/72 H 1.00S 1.000 3.00F 1.00 0.00 0 100.07054 -  
 753120.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15014.174  
 6.896242130D+03-9.305810750D+01 1.570331788D+00 3.780820750D-02-  
 4.872720780D-05  
 3.160796011D-08-8.189782930D-12 -9.180240820D+04  
 1.716317476D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15014.174  
 5.544047080D+05-3.974424320D+03 1.778869264D+01-4.409322030D-04  
 5.944411390D-08  
 -3.927015810D-12 8.891284000D-17 -7.153438270D+04-  
 7.613126350D+01  
 H2 Ref-Elm. Gurvich,1978 pt1 p103 pt2 p31.  
 3 tpis78 H 2.00 0.00 0.00 0.00 0.00 0 2.01588  
 0.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8468.102  
 4.078323210D+04-8.009186040D+02 8.214702010D+00-1.269714457D-02  
 1.753605076D-05  
 -1.202860270D-08 3.368093490D-12 2.682484665D+03-  
 3.043788844D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8468.102  
 5.608128010D+05-8.371504740D+02 2.975364532D+00 1.252249124D-03-  
 3.740716190D-07  
 5.936625200D-11-3.606994100D-15 5.339824410D+03-  
 2.202774769D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8468.102  
 4.966884120D+08-3.147547149D+05 7.984121880D+01-8.414789210D-03  
 4.753248350D-07  
 -1.371873492D-11 1.605461756D-16 2.488433516D+06-  
 6.695728110D+02  
 H2+ Gurvich,1978 pt1 p107 pt2 p33.  
 3 tpis78 H 2.00E -1.00 0.00 0.00 0.00 0 2.01533  
 1494672.430  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8583.103

-3.120886060D+04 2.304622909D+02 3.335564420D+00-2.419056763D-03  
 7.006022340D-06  
 -5.610010660D-09 1.564169746D-12 1.774104638D+05-  
 8.278523760D-01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8583.103  
 1.672225964D+06-6.595184990D+03 1.279321925D+01-5.509345260D-03  
 2.030669412D-06  
 -3.351027480D-10 1.946089104D-14 2.189999548D+05-  
 6.792710780D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8583.103  
 -1.822070983D+08 1.018196269D+05-1.245831898D+01 1.076647496D-03-  
 3.932290360D-08  
 6.285405030D-13-2.094721880D-18 -6.513101500D+05  
 1.471415370D+02  
 H2- Chase,1998 p1312.  
 2 j 9/77 H 2.00E 1.00 0.00 0.00 0.00 0 2.01643  
 235168.362  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8620.592  
 -9.753565670D+04 1.221166236D+03-2.264588838D+00 1.237202227D-02-  
 1.127100020D-05  
 5.367239950D-09-1.049420160D-12 2.121399948D+04  
 3.050556136D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8620.592  
 9.599275620D+04-9.144682880D+02 5.149418810D+00-1.016559478D-04  
 5.446919560D-08  
 -6.155174450D-12 2.822451181D-16 3.234105180D+04-  
 1.440780980D+01  
 HBOH Gurvich,1996a pt1 p44 pt2 p27.  
 2 g 9/98 H 2.00B 1.000 1.00 0.00 0.00 0 28.82628 -  
 48724.364  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10940.536  
 -6.159644190D+04 1.223483035D+03-5.460370510D+00 3.555388680D-02-  
 4.675020140D-05  
 3.236008850D-08-8.986053320D-12 -1.263659051D+04  
 5.422352290D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10940.536  
 1.534611049D+06-5.753666430D+03 1.270893665D+01-7.059628250D-04  
 1.027679375D-07  
 -7.670926740D-12 2.211854768D-16 2.779370419D+04-  
 5.608860080D+01  
 HCHO,formaldehy Hf:TRC(6/78) w-5300. Gurvich,1991 pt1 p62 pt2 p47.  
 2 g 5/01 H 2.00C 1.000 1.00 0.00 0.00 0 30.02598 -  
 108580.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10019.717  
 -1.173916343D+05 1.873628846D+03-6.890288570D+00 2.641561665D-02-  
 2.186389299D-05  
 1.005693006D-08-2.023476949D-12 -2.307351768D+04  
 6.420420550D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10019.717  
 1.700825405D+06-7.620853840D+03 1.472447547D+01-1.649111754D-03  
 3.292144720D-07  
 -3.495049770D-11 1.526135000D-15 3.146812947D+04-  
 7.386478500D+01



6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9934.466  
 -2.040922112D+07-1.072691716D+03 1.131977392D+01-7.364445000D-04  
 5.416450200D-08  
 -1.900872342D-12 2.604761558D-17 1.042565942D+05-  
 5.467272320D+01  
 H2O2 Hf:Gurvich,1989 pt1 p127. Gurvich,1978 pt1 p121.  
 2 g 6/99 H 2.000 2.00 0.00 0.00 0.00 0 34.01468 -  
 135880.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11158.835  
 -9.279533580D+04 1.564748385D+03-5.976460140D+00 3.270744520D-02-  
 3.932193260D-05  
 2.509255235D-08-6.465045290D-12 -2.494004728D+04  
 5.877174180D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11158.835  
 1.489428027D+06-5.170821780D+03 1.128204970D+01-8.042397790D-05-  
 1.818383769D-08  
 6.947265590D-12-4.827831900D-16 1.418251038D+04-  
 4.650855660D+01  
 H2S Gurvich,1989 pt1 p298 pt2 p181.  
 2 g 4/01 H 2.00S 1.00 0.00 0.00 0.00 0 34.08188 -  
 20600.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9958.421  
 9.543808810D+03-6.875175080D+01 4.054921960D+00-3.014557336D-04  
 3.768497750D-06  
 -2.239358925D-09 3.086859108D-13 -3.278457280D+03  
 1.415238703D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9958.421  
 1.430040220D+06-5.284028650D+03 1.016182124D+01-9.703849960D-04  
 2.154003405D-07  
 -2.169695700D-11 9.318163070D-16 2.908696214D+04-  
 4.349155990D+01  
 H2SO4 Gurvich,1989 pt1 p300 pt2 p182.  
 2 tpi89 H 2.00S 1.000 4.00 0.00 0.00 0 98.07948 -  
 732731.721  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16508.589  
 -4.129150050D+04 6.681589890D+02-2.632753507D+00 5.415382480D-02-  
 7.067502230D-05  
 4.684611420D-08-1.236791238D-11 -9.315660120D+04  
 3.961097730D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16508.589  
 1.437877914D+06-6.614902530D+03 2.157662058D+01-4.806255970D-04  
 3.010775121D-08  
 2.334842469D-12-2.946330375D-16 -5.259092950D+04-  
 1.023603571D+02  
 H2BOH Gurvich,1996a pt1 p46 pt2 p29.  
 2 tpi96 H 3.00B 1.000 1.00 0.00 0.00 0 29.83422 -  
 289633.898  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10622.306  
 -8.686766780D+04 1.820335089D+03-1.032373881D+01 4.922801060D-02-  
 5.978619910D-05  
 3.946062730D-08-1.068442257D-11 -4.415238150D+04  
 7.986177290D+01



1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10622.306  
 2.294795193D+06-9.382923560D+03 1.798228329D+01-1.506116214D-03  
 2.635641095D-07  
 -2.483163637D-11 9.736759120D-16 2.039738953D+04-  
 9.448201210D+01  
 HB(OH)2 Gurvich,1996a pt1 p47 pt2 p30.  
 2 tpis96 H 3.00B 1.000 2.00 0.00 0.00 0 45.83362 -  
 644438.724  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12157.532  
 -2.067044022D+04 9.534459160D+02-8.088956520D+00 5.972425290D-02-  
 8.071336320D-05  
 5.612118350D-08-1.553607566D-11 -8.264270810D+04  
 6.539571640D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12157.532  
 2.122674609D+06-8.615948940D+03 1.966179520D+01-8.148411500D-04  
 8.955082040D-08  
 -3.344830510D-12-6.919578140D-17 -2.788790377D+04-  
 9.983559610D+01  
 H3B03 Gurvich,1996a pt1 p50 pt2 p32.  
 2 tpis96 H 3.00B 1.000 3.00 0.00 0.00 0 61.83302 -  
 1004360.442  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13559.958  
 2.568901843D+04 1.138029495D+02-4.045096580D+00 5.924521680D-02-  
 8.148028410D-05  
 5.658593290D-08-1.549277050D-11 -1.221702050D+05  
 4.132220140D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13559.958  
 2.297369132D+06-8.933571790D+03 2.193496552D+01-3.094783490D-04-  
 5.064052990D-08  
 1.482296684D-11-9.764420900D-16 -6.970298470D+04-  
 1.122292829D+02  
 H3B303 Gurvich,1996a pt1 p53 pt2 p34.  
 2 tpis96 H 3.00B 3.000 3.00 0.00 0.00 0 83.45502 -  
 1203760.987  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15603.321  
 -1.985284188D+05 4.104132090D+03-2.827215617D+01 1.269639253D-01-  
 1.558505781D-04  
 9.966304070D-08-2.603677650D-11 -1.648494375D+05  
 1.763917407D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15603.321  
 1.286220713D+06-1.093258784D+04 3.213518670D+01-2.595402269D-03  
 5.353766470D-07  
 -5.833567380D-11 2.600757913D-15 -8.752856890D+04-  
 1.770847815D+02  
 H3B306 Gurvich,1996a pt1 p55 pt2 p35.  
 2 tpis96 H 3.00B 3.000 6.00 0.00 0.00 0 131.45322 -  
 2263687.611  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 23696.853  
 -2.067031503D+04 7.083391540D+02-7.123820950D+00 1.025049979D-01-  
 1.295004602D-04  
 8.322737590D-08-2.145746724D-11 -2.778049216D+05  
 6.063597630D+01

1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 23696.853  
 1.952433352D+06-1.154932896D+04 3.892676110D+01-1.113852280D-03  
 1.280317726D-07  
 -5.728464820D-12-2.214529572D-17 -2.120927136D+05-  
 2.075566801D+02  
 H3F3 Gurvich,1989 pt1 p166 pt2 p309.  
 2 tpi89 H 3.00F 3.00 0.00 0.00 0.00 0 60.01903 -  
 883676.790  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15263.022  
 9.888562650D+04-1.380212880D+03 8.980458470D+00 1.871609057D-02-  
 3.127862508D-05  
 2.589436165D-08-8.040372270D-12 -1.013661491D+05-  
 2.585302557D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15263.022  
 2.515790373D+06-8.789423320D+03 2.023933445D+01-1.131704646D-03  
 1.692779921D-07  
 -1.308662105D-11 3.978322000D-16 -5.471713650D+04-  
 9.907787640D+01  
 H3O+ Gurvich,1989 pt1 p130 pt2 p41.  
 3 tpi89 H 3.00O 1.00E -1.00 0.00 0.00 0 19.02267  
 598000.000  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10046.427  
 -6.447640150D+04 1.181817922D+03-3.801893060D+00 2.220628313D-02-  
 2.445343237D-05  
 1.573297747D-08-4.158836410D-12 6.530613320D+04  
 4.282723130D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10046.427  
 2.955126200D+06-9.185669410D+03 1.341398696D+01-5.590339210D-04  
 1.138387119D-08  
 7.259927210D-12-6.133734360D-16 1.290534257D+05-  
 7.021828180D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10046.427  
 -1.591228592D+07 4.898727210D+03 8.881336820D+00 1.299244015D-04-  
 8.169245590D-09  
 2.649115685D-13-3.472865280D-18 2.090178405D+04-  
 3.217683350D+01  
 (HCOOH)2 Formic acid dimer. Chao,1978.  
 2 g 6/01 H 4.00C 2.000 4.00 0.00 0.00 0 92.05076 -  
 820942.640  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19631.909  
 -2.001447991D+05 3.502457370D+03-1.853488051D+01 9.547467130D-02-  
 1.059184484D-04  
 6.323086900D-08-1.567561216D-11 -1.172621688D+05  
 1.319646887D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19631.909  
 3.308188420D+06-1.633668256D+04 3.751348820D+01-3.148108995D-03  
 6.008707760D-07  
 -6.144462500D-11 2.600562474D-15 -6.265894440D+03-  
 2.107476941D+02  
 H4F4 Gurvich,1989 pt1 p167 pt2 p310.  
 2 tpi89 H 4.00F 4.00 0.00 0.00 0.00 0 80.02537 -  
 1186932.336

200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 21654.080  
 1.315109024D+05-1.840361560D+03 1.264093152D+01 2.495407360D-02-  
 4.170394610D-05  
 3.452523840D-08-1.072034360D-11 -1.364003454D+05-  
 4.122913530D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 21654.080  
 3.354037990D+06-1.171922040D+04 2.765243565D+01-1.508934621D-03  
 2.257027572D-07  
 -1.744867255D-11 5.304351740D-16 -7.420213160D+04-  
 1.388603332D+02  
 H5F5 Gurvich,1989 pt1 p168 pt2 p311.  
 2 tpris89 H 5.00F 5.00 0.00 0.00 0.00 0 100.03172 -  
 1490187.882  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 28045.138  
 1.641361897D+05-2.300510396D+03 1.630140545D+01 3.119205422D-02-  
 5.212926350D-05  
 4.315611240D-08-1.340031413D-11 -1.714345408D+05-  
 5.682157380D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 28045.138  
 4.192290730D+06-1.464903043D+04 3.506554920D+01-1.886170471D-03  
 2.821289954D-07  
 -2.181090984D-11 6.630474160D-16 -9.368704200D+04-  
 1.788592044D+02  
 H6F6 Gurvich,1989 pt1 p169 pt2 p312.  
 2 tpris89 H 6.00F 6.00 0.00 0.00 0.00 0 120.03806 -  
 1805545.131  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 34334.493  
 1.956886618D+05-2.753909880D+03 1.975625055D+01 3.807717010D-02-  
 6.341218880D-05  
 5.219233290D-08-1.612185649D-11 -2.079269410D+05-  
 7.113607980D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 34334.493  
 5.024520320D+06-1.742817868D+04 4.214870500D+01-2.084564791D-03  
 2.930051519D-07  
 -2.052079159D-11 5.206937300D-16 -1.154497653D+05-  
 2.163947001D+02  
 H7F7 Gurvich,1989 pt1 p170 pt2 p313.  
 2 tpris89 H 7.00F 7.00 0.00 0.00 0.00 0 140.04440 -  
 2099698.974  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 40827.254  
 2.293867477D+05-3.220807860D+03 2.362235212D+01 4.366801880D-02-  
 7.297990340D-05  
 6.041786420D-08-1.876025627D-11 -2.418637479D+05-  
 8.838812260D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 40827.254  
 5.868789830D+06-2.050863473D+04 4.989176110D+01-2.640634895D-03  
 3.949796330D-07  
 -3.053515088D-11 9.282601780D-16 -1.330177809D+05-  
 2.592385142D+02  
 He Ref-Elm. Moore,1971. Moore,1970a. Gordon,1999.  
 3 g 5/97 HE 1.00 0.00 0.00 0.00 0.00 0 4.00260  
 0.000

200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -7.453750000D+02  
 9.287239740D-01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -7.453750000D+02  
 9.287239740D-01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 3.396845420D+06-2.194037652D+03 3.080231878D+00-8.068957550D-05  
 6.252784910D-09  
 -2.574990067D-13 4.429960218D-18 1.650518960D+04-  
 4.048814390D+00  
 He+ Moore,1971; Moore,1970a. Gordon,1999.  
 3 g 3/97 HE 1.00E -1.00 0.00 0.00 0.00 0 4.00205  
 2378521.473  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 2.853233739D+05  
 1.621665557D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 2.853233739D+05  
 1.621665557D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 2.853233739D+05  
 1.621665557D+00  
 Hg Hf:Cox,1989. Moore,1971. Gordon,1999.  
 3 g 1/98 HG 1.00 0.00 0.00 0.00 0.00 0 200.59000  
 61380.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 6.636900080D+03  
 6.800201540D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 5.146573510D+04-1.681269855D+02 2.718343098D+00-1.445026192D-04  
 5.158977660D-08  
 -9.472485010D-12 7.034797406D-16 7.688684930D+03  
 5.271236090D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 5.358443930D+08-4.433853810D+05 1.463223992D+02-2.318441669D-02  
 1.916335174D-06  
 -7.419662000D-11 1.067224054D-15 3.391999920D+06-  
 1.201225990D+03  
 Hg+ Moore,1971. Gordon,1999.

3 g 7/97 HG 1.00E -1.00 0.00 0.00 0.00 0 200.58945  
1074643.128  
298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428  
4.098344940D-04-4.343581620D-06 2.500000019D+00-4.389036810D-11  
5.563969200D-14  
-3.638228260D-17 9.607881995D-21 1.285037483D+05  
7.493344500D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428  
-1.229984728D+04 2.732269908D+01 2.484182160D+00-4.426797610D-06  
7.489685860D-09  
-2.549887287D-12 2.819873366D-16 1.283188257D+05  
7.625244570D+00  
6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428  
-5.498617710D+07 3.775543500D+04-7.155545550D+00 1.170310234D-03-  
7.931471440D-08  
4.029174000D-12-7.741071633D-17 -1.676894201D+05  
9.116750020D+01

HgBr2 Hf: Pankratz,1984. Chase,1998 p485 3/62.  
2 g12/00 HG 1.00BR 2.00 0.00 0.00 0.00 0 360.39800 -  
91311.616  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
15658.384  
-1.991826537D+03-1.902186083D+02 8.246401260D+00-1.607089392D-03  
1.947654549D-06  
-1.242873546D-09 3.241818310D-13 -1.230723096D+04-  
8.716659300D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
15658.384  
-2.243649290D+04-3.312652270D+00 7.502765170D+00-1.202360213D-06  
2.830526999D-10  
-3.407686700D-14 1.640497921D-18 -1.327483366D+04-  
4.368555600D+00

I Hf:Cox,1989. Moore,1971. Moore,1970a. Gordon,1999.  
3 g 3/97 I 1.00 0.00 0.00 0.00 0.00 0 126.90447  
106760.000  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428  
1.698199675D+02-2.716437233D+00 2.517385557D+00-5.730692070D-05  
1.031716184D-07  
-9.670641930D-11 3.706471651D-14 1.210750090D+04  
7.405823130D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428  
-7.785860570D+05 2.303279568D+03 2.886686091D-03 1.180878463D-03-  
2.264074866D-07  
1.963511339D-11-6.243525941D-16 -2.616792742D+03  
2.558922997D+01  
6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428  
4.747630780D+07-8.681111190D+04 3.950617020D+01-6.514063250D-03  
5.380695340D-07  
-1.969145066D-11 2.643177163D-16 6.384843030D+05-  
2.972997119D+02

I+ Moore,1971. Moore,1970a. Gordon,1999.  
3 g10/97 I 1.00E -1.00 0.00 0.00 0.00 0 126.90392  
1121351.028  
298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428

-8.014969010D+02 8.139052610D+00 2.470174760D+00 4.161393820D-05  
 7.133397860D-09  
 -7.105950140D-11 4.873766102D-14 1.340794213D+05  
 7.903420090D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 -7.788385330D+05 2.404962651D+03-1.791751142D-01 1.227311979D-03-  
 1.801494030D-07  
 9.923983960D-12-9.775286439D-17 1.188531631D+05  
 2.710544347D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 -6.314420010D+08 3.971131910D+05-9.860191990D+01 1.358236563D-02-  
 9.920747650D-07  
 3.684927700D-11-5.301687095D-16 -3.001474591D+06  
 8.790468740D+02  
 I- Hotop,1985. Gordon,1999.  
 3 g10/97 I 1.00E 1.00 0.00 0.00 0.00 0 126.90502 -  
 194595.572  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.414970936D+04  
 6.113465380D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.414970936D+04  
 6.113465380D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.414970936D+04  
 6.113465380D+00  
 IF5 Gurvich,1989 pt1 p232 pt2 p123.  
 2 tpi89 I 1.00F 5.00 0.00 0.00 0.00 0 221.89649 -  
 841000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 20044.142  
 2.026184530D+05-3.598183170D+03 2.530349738D+01-1.348602458D-02  
 1.105687229D-05  
 -4.707939510D-09 7.864411470D-13 -8.700147250D+04-  
 1.112719941D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 20044.142  
 -3.620506260D+05-1.639236093D+02 1.612272743D+01-4.914431550D-05  
 1.086015052D-08  
 -1.244672691D-12 5.763593620D-17 -1.061642293D+05-  
 5.398773360D+01  
 IF7 Gurvich,1989 pt1 p234 pt2 p124.  
 2 tpi89 I 1.00F 7.00 0.00 0.00 0.00 0 259.89329 -  
 961500.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 24123.333  
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1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
9752.117



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 18306.773  
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 -1.518261505D-13 7.226562770D-18 -4.758974170D+04-  
 1.669761621D+01  
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 12588.776

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 863079.566  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
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 4.885515130D+00  
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 3.297697490D+01  
 InI2 Gurvich,1996a pt1 p300 pt2 p243.  
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 14912.757  
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1.211411745D+01  
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InO Gurvich,1996a pt1 p261 pt2 p212  
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145993.109  
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3.500742460D+00  
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21434.943

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 -1.425555379D+04-2.866009341D+02 1.713866292D+01-2.473506655D-03  
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 43096.728  
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 -5.125076850D-09 1.324324755D-12 -7.027688140D+04-  
 5.582666180D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 29456.525

-8.503771790D+04-1.552464614D+01 1.601269668D+01-5.441549870D-06  
 1.267594997D-09  
 -1.514110365D-13 7.245404540D-18 -7.461921740D+04-  
 3.691151100D+01  
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 2 tpris96 IN 2.00CL 6.00 0.00 0.00 0.00 0 442.35220 -  
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 38423.462  
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 1.475341213D-05  
 -9.252689200D-09 2.381233885D-12 -1.048828300D+05-  
 9.788405250D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 38423.462  
 -1.499400484D+05-2.988680816D+01 2.202425362D+01-1.033652301D-05  
 2.397911922D-09  
 -2.855307516D-13 1.363051661D-17 -1.130110233D+05-  
 6.293986290D+01  
 In2F2 Gurvich,1996a pt1 p276 pt2 p221.  
 2 tpris96 IN 2.00F 2.00 0.00 0.00 0.00 0 267.63281 -  
 532234.300  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18039.900  
 7.255717100D+03-6.448265650D+02 1.247539512D+01-5.246089620D-03  
 6.283616210D-06  
 -3.974342340D-09 1.029559356D-12 -6.384892450D+04-  
 3.108004586D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18039.900  
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 9.608828320D-10  
 -1.150013486D-13 5.511437480D-18 -6.714277850D+04-  
 1.661718474D+01  
 In2F4 Gurvich,1996a pt1 p277 pt2 p222.  
 2 tpris96 IN 2.00F 4.00 0.00 0.00 0.00 0 305.62961 -  
 1284788.126  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 24763.074  
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 -7.181673930D-09 1.648386404D-12 -1.466942111D+05-  
 8.943560050D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 24763.074  
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 5.329582790D-09  
 -6.144609570D-13 2.859099598D-17 -1.595716347D+05-  
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 2 tpris96 IN 2.00F 6.00 0.00 0.00 0.00 0 343.62642 -  
 1960000.000  
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 33567.102  
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 1.892443162D-05  
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 -9.191681700D-13 4.278494150D-17 -2.426661118D+05-  
 7.155328560D+01  
 In2I2 Gurvich,1996a pt1 p303 pt2 p246.  
 2 tpris96 IN 2.00I 2.00 0.00 0.00 0.00 0 483.44494 -  
 27813.524  
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 1.628373589D-07  
 -1.056087811D-10 2.788963879D-14 -6.279602600D+03-  
 7.291130980D+00  
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 22058.476  
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 2.242988180D-11  
 -2.732299303D-15 1.327135699D-19 -6.352651500D+03-  
 6.947725420D+00  
 In2I4 Gurvich,1996a pt1 p304 pt2 p247.  
 2 tpris96 IN 2.00I 4.00 0.00 0.00 0.00 0 737.25388 -  
 199143.181  
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 33468.979  
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 1.065671801D-06  
 -6.879252680D-10 1.810240886D-13 -2.830388443D+04-  
 2.986294828D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 33468.979  
 -2.505699251D+04-1.642155234D+00 1.600140149D+01-6.187066280D-07  
 1.472308565D-10  
 -1.786593333D-14 8.652338780D-19 -2.879655333D+04-  
 2.757790375D+01  
 In2I6 Gurvich,1996a pt1 p305 pt2 p248.  
 2 tpris96 IN 2.00I 6.00 0.00 0.00 0.00 0 991.06282 -  
 319720.040  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 45088.120  
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 2.161510393D-06  
 -1.392400447D-09 3.658171880D-13 -4.412547680D+04-  
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 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 45088.120  
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 3.012121900D-10  
 -3.649676710D-14 1.765530622D-18 -4.513820270D+04-  
 4.806868370D+01  
 In2O Gurvich,1996a pt1 p264 pt2 p213.  
 2 tpris96 IN 2.000 1.00 0.00 0.00 0.00 0 245.63540 -  
 34763.707  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12796.504  
 5.065653500D+04-8.070363670D+02 8.642067270D+00-1.533035446D-03  
 2.866419382D-07  
 4.981134970D-10-2.554320291D-13 -1.924908459D+03-  
 1.490718759D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12796.504

-9.232786360D+04-5.201127280D+01 7.038723620D+00-1.543821179D-05  
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4.421820410D+00

K Hf:Cox,1989. Sugar,1985. Gordon 1999.

3 g 7/97 K 1.00 0.00 0.00 0.00 0.00 0 39.09830  
89000.000

200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428

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-3.439722110D-12 1.131569009D-15 9.959493490D+03  
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1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428

-3.566422360D+06 1.085289825D+04-1.054134898D+01 8.009801350D-03-  
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4.715294150D-10-2.976897350D-14 -5.875337010D+04  
9.738551240D+01

6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428

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1.430294866D-06

-4.409335020D-11 5.366769166D-16 5.395082190D+06-  
1.622158805D+03

K+ Sugar,1985. Gordon 1999.

3 g 6/97 K 1.00E -1.00 0.00 0.00 0.00 0 39.09775  
514007.528

298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428

0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
0.000000000D+00

0.000000000D+00 0.000000000D+00 6.107516860D+04  
4.347404440D+00

1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428

0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
0.000000000D+00

0.000000000D+00 0.000000000D+00 6.107516860D+04  
4.347404440D+00

6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428

2.177901245D+07-1.415076630D+04 6.248954270D+00-5.187436800D-04  
3.959640680D-08

-1.584335542D-12 2.603558905D-17 1.722753576D+05-  
2.781728990D+01

K- Hotop,1985. Gordon 1999.

3 g 9/97 K 1.00E 1.00 0.00 0.00 0.00 0 39.09885  
34418.128

298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428

0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
0.000000000D+00

0.000000000D+00 0.000000000D+00 3.394150710D+03  
4.347446530D+00

1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428

0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
0.000000000D+00

0.000000000D+00 0.000000000D+00 3.394150710D+03  
4.347446530D+00

6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 3.394150710D+03  
 4.347446530D+00  
 KALF4 Gurvich,1982 pt1 p417 pt2 p441.  
 2 tpi82 K 1.00AL 1.00F 4.00 0.00 0.00 0 142.07345 -  
 1907856.822  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 21421.391  
 1.199327246D+05-2.156457352D+03 1.815348004D+01 3.115762809D-03-  
 9.511991670D-06  
 8.431756230D-09-2.615583061D-12 -2.222545809D+05-  
 6.823299970D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 21421.391  
 -3.435135370D+05-2.420680834D+02 1.618029250D+01-7.193817680D-05  
 1.585712708D-08  
 -1.814017733D-12 8.388391180D-17 -2.339658121D+05-  
 5.233898700D+01  
 KBO2 Gurvich,1982 pt1 p415 pt2 p439.  
 2 tpi82 K 1.00B 1.00O 2.00 0.00 0.00 0 81.90810 -  
 668023.297  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14090.703  
 4.296308650D+04-7.209616430D+02 8.349639350D+00 2.407820401D-03-  
 1.680003427D-07  
 -1.231930486D-09 5.479951640D-13 -7.868523470D+04-  
 1.476077068D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14090.703  
 8.890726600D+04-1.671432436D+03 1.117483930D+01-4.513760260D-04  
 9.699003460D-08  
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 3.274749370D+01  
 KBr Gurvich,1982 pt1 p396 pt2 p423.  
 2 tpi82 K 1.00BR 1.00 0.00 0.00 0.00 0 119.00230 -  
 179250.878  
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 10109.122  
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 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10109.122  
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 4.401923850D-07  
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 2.864647026D+01  
 KCN Chase,1998 p620.  
 2 j 3/66 K 1.00C 1.00N 1.00 0.00 0.00 0 65.11574  
 79496.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12456.334  
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 1.751014980D-05  
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 2.594060197D+01



1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12456.334  
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 9.249499710D-08  
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 2.281619149D+01  
 KCL Gurvich,1982 pt1 p393 pt2 p420.  
 2 tpris82 K 1.00CL 1.00 0.00 0.00 0.00 0 74.55100 -  
 214574.881  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9885.119  
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 4.130983060D-06  
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 3.677982890D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9885.119  
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 5.834260780D-07  
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 1.401864032D+01  
 KF Gurvich,1982 pt1 p389 pt2 p417.  
 2 tpris82 K 1.00F 1.00 0.00 0.00 0.00 0 58.09670 -  
 328444.886  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9455.114  
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 3.265915640D-06  
 -2.210110860D-09 6.212042050D-13 -3.914254420D+04-  
 5.810999620D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9455.114  
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 1.093902537D-06  
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 4.088635920D+01  
 KH Gurvich,1982 pt1 p383 pt2 p412.  
 2 tpris82 K 1.00H 1.00 0.00 0.00 0.00 0 40.10624  
 125399.106  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8795.106  
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 1.341218171D-05  
 9.034529940D-09-2.409887770D-12 1.338250358D+04  
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 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8795.106  
 -3.752276520D+06 1.172778444D+04-1.014137678D+01 8.854548900D-03-  
 2.517188074D-06  
 3.344072360D-10-1.701157835D-14 -6.025103300D+04  
 1.010304590D+02  
 KI Gurvich,1982 pt1 p400 pt2 p426.  
 2 tpris82 K 1.00I 1.00 0.00 0.00 0.00 0 166.00277 -  
 128455.877  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10244.123  
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 1.336737911D-06  
 -1.000530992D-09 3.004503956D-13 -1.650340769D+04  
 3.552594820D+00

1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10244.123  
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 7.859123370D+01  
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 170702.323  
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 1.207990165D-06  
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 1.912285942D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10197.123  
 1.211296843D+07-4.081004870D+04 5.683792120D+01-3.128695515D-02  
 8.975062200D-06  
 -1.189303691D-09 5.880129180D-14 2.738792595D+05-  
 3.669693600D+02  
 KNO2 Gurvich,1982 pt1 p406 pt2 p431.  
 2 tpis82 K 1.00N 1.000 2.00 0.00 0.00 0 85.10384 -  
 192497.394  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15342.606  
 -7.246236930D+04 1.226722811D+03-2.258926457D+00 3.019643903D-02-  
 3.640259950D-05  
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 4.537172620D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15342.606  
 -1.689414093D+05-8.515973150D+02 1.063209586D+01-2.523254810D-04  
 5.573644410D-08  
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 2.755200361D+01  
 KNO3 Gurvich,1982 pt1 p409 pt2 p433.  
 2 tpis82 K 1.00N 1.000 3.00 0.00 0.00 0 101.10324 -  
 315832.888  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15917.112  
 -2.596112303D+04 8.200606610D+02-2.886015624D+00 4.207288900D-02-  
 5.270323090D-05  
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 4.603187390D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15917.112  
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 8.900847780D-08  
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 132404.327  
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 10574.127  
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1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10574.127  
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 8.232705790D-06  
 -1.128503590D-09 5.663264890D-14 1.697274909D+05-  
 2.664117219D+02  
 KO Gurvich,1982 pt1 p375 pt2 p404.  
 2 tpis82 K 1.000 1.00 0.00 0.00 0.00 0 55.09770  
 64733.314  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9481.114  
 1.462562908D+04-3.384765650D+02 5.716607640D+00-2.363265083D-03  
 2.848716276D-06  
 -1.739858233D-09 4.431006520D-13 8.141835380D+03-  
 4.022101520D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9481.114  
 6.960103380D+05-3.304835290D+03 1.005743444D+01-4.331112000D-03  
 1.747281632D-06  
 -3.012370548D-10 1.790827870D-14 2.604972496D+04-  
 3.448781520D+01  
 KOH Gurvich,1997.  
 2 g 9/97 K 1.000 1.00H 1.00 0.00 0.00 0 56.10564 -  
 232000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11674.650  
 1.770684196D+04-6.153205220D+02 8.684075720D+00-3.962849510D-03  
 3.408650590D-06  
 -9.601972220D-10 8.494054970D-15 -2.677903261D+04-  
 2.174495666D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11674.650  
 8.917271950D+05-2.334179072D+03 7.972578710D+00 1.038863156D-04-  
 6.315893470D-08  
 1.027938106D-11-5.736685820D-16 -1.443696469D+04-  
 2.076401416D+01  
 K2 Gurvich,1982 pt1 p370 pt2 p402.  
 2 tpis82 K 2.00 0.00 0.00 0.00 0.00 0 78.19660  
 126546.329  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10741.129  
 1.524169293D+04-3.301789360D+02 7.070795950D+00-9.767072460D-03  
 2.021535863D-05  
 -1.886092452D-08 6.112974640D-12 1.533402849D+04-  
 9.101035800D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10741.129  
 -2.734470745D+07 6.562180010D+04-4.476350440D+01 8.938859150D-03  
 2.984557092D-06  
 -1.064158914D-09 8.334936930D-14 -4.226243830D+05  
 3.867142510D+02  
 K2+ Gurvich,1982 pt1 p374 pt2 p403.  
 2 tpis82 K 2.00E -1.00 0.00 0.00 0.00 0 78.19605  
 524660.731  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10861.131  
 5.196036570D+04-6.113382530D+02 7.264990540D+00-5.810634820D-03  
 6.567496500D-06  
 -2.378020865D-09-1.318637581D-13 6.479820270D+04-  
 1.042370517D+01

1000.000 3000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10861.131  
 1.107950739D+07-4.177483820D+04 6.448659840D+01-4.024998030D-02  
 1.360587923D-05  
 -2.361920107D-09 1.673430610D-13 3.177612050D+05-  
 4.105063100D+02  
 K2Br2 Gurvich,1982 pt1 p397 pt2 p424.  
 2 tpi82 K 2.00BR 2.00 0.00 0.00 0.00 0 238.00460 -  
 538744.193  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 20951.806  
 -1.093040504D+04-4.856651480D+01 1.019754923D+01-4.363157100D-04  
 5.387173660D-07  
 -3.486116500D-10 9.190702950D-14 -6.758073240D+04-  
 1.294944706D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 20951.806  
 -1.589229976D+04-8.101379460D-01 1.000069442D+01-3.074491521D-07  
 7.331024160D-11  
 -8.908944780D-15 4.319245430D-19 -6.782595440D+04-  
 1.180425726D+01  
 K2CO3 Gurvich,1982 pt1 p411 pt2 p435.  
 2 tpi82 K 2.00C 1.000 3.00 0.00 0.00 0 138.20550 -  
 811649.163  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19515.837  
 -4.407406700D+04 7.069815440D+02 6.931482470D-01 3.967831320D-02-  
 4.850958300D-05  
 2.976635787D-08-7.374761530D-12 -1.033913232D+05  
 2.980651689D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19515.837  
 -3.264263160D+05-1.521168973D+03 1.712283562D+01-4.464580710D-04  
 9.833379630D-08  
 -1.125478371D-11 5.210069120D-16 -9.488275100D+04-  
 6.215220630D+01  
 K2C2N2 Chase,1998 p678.  
 2 j 3/66 K 2.00C 2.00N 2.00 0.00 0.00 0 130.23148 -  
 8368.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 24786.242  
 4.627789480D+03-9.729810620D+02 1.996665910D+01-1.953015081D-02  
 3.275330460D-05  
 -2.393985120D-08 6.596548240D-12 -7.774411260D+02-  
 6.755613540D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 24786.242  
 7.269599500D+05-3.492108680D+03 1.835676822D+01-8.785475140D-04  
 1.845532919D-07  
 -2.038717568D-11 9.185420990D-16 1.582600773D+04-  
 6.728483960D+01  
 K2CL2 Gurvich,1982 pt1 p393 pt2 p421.  
 2 tpi82 K 2.00CL 2.00 0.00 0.00 0.00 0 149.10200 -  
 615393.663  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19963.448  
 -1.328526456D+04-1.241832429D+02 1.050035730D+01-1.097776004D-03  
 1.348871402D-06  
 -8.697215120D-10 2.286584080D-13 -7.644363150D+04-  
 1.790150656D+01

1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19963.448  
 -2.614611331D+04-2.096229095D+00 1.000178456D+01-7.864803710D-07  
 1.869281152D-10  
 -2.266272348D-14 1.096790704D-18 -7.707189330D+04-  
 1.499721406D+01  
 K2F2 Gurvich,1982 pt1 p389 pt2 p418.  
 2 tpi82 K 2.00F 2.00 0.00 0.00 0.00 0 116.19341 -  
 859875.481  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18125.626  
 -1.611833856D+03-5.135644890D+02 1.199922511D+01-4.280109550D-03  
 5.165387540D-06  
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 3.039925079D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18125.626  
 -5.740892530D+04-9.046182110D+00 1.000750685D+01-3.250764840D-06  
 7.630064590D-10  
 -9.165649530D-14 4.405048440D-18 -1.065413546D+05-  
 1.874037620D+01  
 K2I2 Gurvich,1982 pt1 p401 pt2 p427.  
 2 tpi82 K 2.00I 2.00 0.00 0.00 0.00 0 332.00554 -  
 418915.452  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 21456.548  
 -8.977752440D+03-2.776460169D+01 1.011331014D+01-2.508421994D-04  
 3.102352114D-07  
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 1.032092509D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 21456.548  
 -1.179634729D+04-4.724761550D-01 1.000040695D+01-1.807689054D-07  
 4.320560970D-11  
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 9.664440500D+00  
 K2O Gurvich,1982 pt1 p377 pt2 p407.  
 2 tpi82 K 2.00O 1.00 0.00 0.00 0.00 0 94.19600 -  
 74086.902  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13858.298  
 2.392044068D+04-5.445358390D+02 8.826403230D+00-3.481429430D-03  
 3.834542070D-06  
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 1.663099064D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13858.298  
 -4.611464580D+04-1.363119524D+01 7.010530440D+00-4.323658260D-06  
 9.747788420D-10  
 -1.135283694D-13 5.325860600D-18 -1.107222244D+04-  
 5.768718720D+00  
 K2O+ Gurvich,1982 pt1 p379 pt2 p408.  
 2 tpi82 K 2.00O 1.00E -1.00 0.00 0.00 0 94.19545  
 368390.321  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14138.121  
 7.201102730D+03-3.336526400D+02 8.050730350D+00-1.869353797D-03  
 1.921291874D-06  
 -1.064020951D-09 2.457514799D-13 4.389986360D+04-  
 1.073204150D+01

1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14138.121  
 -3.780033500D+04-8.849537390D+00 7.006847890D+00-2.815510856D-06  
 6.355001500D-10  
 -7.408551990D-14 3.478334960D-18 4.214519680D+04-  
 4.418276610D+00  
 K2O2 Gurvich,1982 pt1 p381 pt2 p410.  
 2 tpi82 K 2.000 2.00 0.00 0.00 0.00 0 110.19540 -  
 191566.301  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16289.803  
 4.810870610D+04-1.003601504D+03 1.154229002D+01-4.546332520D-04-  
 1.516606209D-06  
 1.799426090D-09-6.128337290D-13 -2.057151920D+04-  
 3.181199790D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16289.803  
 -1.476073073D+05-1.021932040D+02 1.007664713D+01-3.076517991D-05  
 6.815252810D-09  
 -7.828654450D-13 3.632506100D-17 -2.592056324D+04-  
 2.162287184D+01  
 K2O2H2 Gurvich,1997.  
 2 g 9/97 K 2.000 2.00H 2.00 0.00 0.00 0 112.21128 -  
 641000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22384.933  
 8.174788370D+03-1.130630680D+03 1.815303256D+01-7.737431080D-03  
 6.837614010D-06  
 -2.054691111D-09 7.672877510D-14 -7.574965170D+04-  
 6.391759470D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22384.933  
 1.773523196D+06-4.665292470D+03 1.694308128D+01 2.085297143D-04-  
 1.264714762D-07  
 2.057506565D-11-1.148042134D-15 -5.051263310D+04-  
 6.334773920D+01  
 K2SO4 Gurvich,1982 pt1 p404 pt2 p429.  
 2 g10/99 K 2.00S 1.000 4.00 0.00 0.00 0 174.26020 -  
 1095851.121  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22283.879  
 6.271492310D+04-8.152049920D+02 7.455413720D+00 3.849909780D-02-  
 5.400630980D-05  
 3.654656800D-08-9.760223570D-12 -1.304692568D+05-  
 1.034633909D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22283.879  
 -5.446125640D+05-9.590667230D+02 1.971591285D+01-2.866586009D-04  
 6.342480640D-08  
 -7.281462540D-12 3.377886930D-16 -1.337873384D+05-  
 7.399102690D+01  
 Kr Ref-Elm. Sugar,1991.  
 3 g 8/97 KR 1.00 0.00 0.00 0.00 0.00 0 83.80000  
 0.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -7.453750000D+02  
 5.490956510D+00

1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 2.643639057D+02-7.910050820D-01 2.500920585D+00-5.328164110D-07  
 1.620730161D-10  
 -2.467898017D-14 1.478585040D-18 -7.403488940D+02  
 5.484398150D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 -1.375531087D+09 9.064030530D+05-2.403481435D+02 3.378312030D-02-  
 2.563103877D-06  
 9.969787790D-11-1.521249677D-15 -7.111667370D+06  
 2.086866326D+03  
 Kr+ Sugar,1991. Gordon,1999.  
 3 g 7/97 KR 1.00E -1.00 0.00 0.00 0.00 0 83.79945  
 1356953.918  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 -5.650402860D+03 6.930740810D+01 2.157028132D+00 8.711228930D-04-  
 1.181609730D-06  
 7.862198630D-10-1.832589387D-13 1.621164118D+05  
 8.818242260D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 -2.216567015D+05 1.166167840D+03 4.869655320D-01 1.429223599D-03-  
 3.949628610D-07  
 4.982853510D-11-2.406719258D-15 1.556002861D+05  
 2.059230986D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 -3.319875960D+07 1.797953100D+04-7.155015940D-01 2.671088984D-04-  
 6.196251880D-09  
 -4.107025960D-13 2.000619351D-17 1.648114259D+04  
 3.620325750D+01  
 Li Hf:Cox,1989. Moore,1971. Gordon,1999.  
 3 g 7/97 LI 1.00 0.00 0.00 0.00 0.00 0 6.94100  
 159300.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 1.841390197D+04  
 2.447622965D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 1.125610652D+06-3.463536730D+03 6.566611920D+00-2.260983356D-03  
 5.922289160D-07  
 -6.281635100D-11 2.884948238D-15 4.034637400D+04-  
 2.655918195D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 2.604352623D+09-1.521952201D+06 3.454400500D+02-3.779674850D-02  
 2.222420069D-06  
 -6.691570800D-11 8.088023606D-16 1.217791847D+07-  
 3.006680193D+03  
 Li+ Moore,1971. Gordon,1999.  
 3 g 3/97 LI 1.00E -1.00 0.00 0.00 0.00 0 6.94045  
 685719.428  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00

0.000000000D+00 0.000000000D+00 8.172724550D+04  
 1.754357228D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 8.172724550D+04  
 1.754357228D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 8.172724550D+04  
 1.754357228D+00  
 Li- Hotop,1985. Gordon,1999.  
 3 g 1/98 LI 1.00E 1.00 0.00 0.00 0.00 0 6.94155  
 93474.728  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 1.049698659D+04  
 1.754594332D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 1.049698659D+04  
 1.754594332D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 1.049698659D+04  
 1.754594332D+00  
 LiAlF4 Gurvich,1982 pt1 p300 pt2 p333.  
 2 tpis82 LI 1.00AL 1.00F 4.00 0.00 0.00 0 109.91615 -  
 1857287.824  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19534.389  
 1.761529360D+05-2.999300134D+03 2.079739570D+01-1.742914656D-03-  
 4.266642090D-06  
 5.362829770D-09-1.866817087D-12 -2.117947828D+05-  
 8.762725890D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19534.389  
 -4.020700930D+05-2.783355146D+02 1.620791185D+01-8.316341570D-05  
 1.836905690D-08  
 -2.104932808D-12 9.747253020D-17 -2.278696416D+05-  
 5.597304840D+01  
 LiBO2 Gurvich,1982 pt1 p299 pt2 p332.  
 2 tpis82 LI 1.00B 1.00O 2.00 0.00 0.00 0 49.75080 -  
 652352.276  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13427.724  
 6.518987570D+04-1.060320845D+03 9.548049960D+00-5.469576070D-05  
 2.658687599D-06  
 -2.931603694D-09 9.663029730D-13 -7.506204110D+04-  
 2.490883998D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13427.724



8.554404520D+04-1.731920898D+03 1.121462090D+01-4.659162170D-04  
 9.999875690D-08  
 -1.122880592D-11 5.123529460D-16 -7.154743820D+04-  
 3.612397290D+01  
 LiBr Gurvich,1982 pt1 p285 pt2 p318.  
 2 tpris82 LI 1.00BR 1.00 0.00 0.00 0.00 0 86.84500 -  
 151162.890  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9173.110  
 3.805620470D+04-6.129614990D+02 6.577369550D+00-4.219891760D-03  
 5.391423370D-06  
 -3.693144810D-09 1.049158761D-12 -1.637487617D+04-  
 1.128654012D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9173.110  
 6.380191420D+04-2.597050764D+02 4.656768870D+00 1.022867706D-04-  
 5.178252340D-08  
 2.058203991D-11-1.942190308D-15 -1.793363752D+04-  
 2.290806613D-01  
 LiCl Gurvich,1982 pt1 p281 pt2 p314.  
 2 tpris82 LI 1.00CL 1.00 0.00 0.00 0.00 0 42.39370 -  
 193779.891  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9060.109  
 4.964399500D+04-7.187346620D+02 6.785147030D+00-4.522145460D-03  
 5.748483700D-06  
 -3.966255670D-09 1.137911398D-12 -2.091014703D+04-  
 1.406384962D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9060.109  
 -2.352769705D+05 6.120046920D+02 3.634293730D+00 6.810973320D-04-  
 2.174238799D-07  
 4.220403610D-11-2.848628426D-15 -2.862358494D+04  
 5.618500520D+00  
 LiF Gurvich,1982 pt1 p275 pt2 p310.  
 2 tpris89 LI 1.00F 1.00 0.00 0.00 0.00 0 25.93940 -  
 340944.894  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8828.106  
 2.912537320D+04-2.531413159D+02 3.539727980D+00 3.695917040D-03-  
 4.829466150D-06  
 2.944090711D-09-6.838794740D-13 -4.064849660D+04  
 2.325294408D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8828.106  
 -3.784246490D+05 7.668062460D+02 3.585473400D+00 6.031084350D-04-  
 1.588764206D-07  
 2.569397177D-11-1.406798386D-15 -4.756469450D+04  
 4.385163290D+00  
 LiH Gurvich,1982 pt1 p265 pt2 p301.  
 2 tpris82 LI 1.00H 1.00 0.00 0.00 0.00 0 7.94894  
 139264.104  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8686.104  
 -4.913731570D+04 7.756092190D+02-1.011102377D+00 1.145479597D-02-  
 1.151038734D-05  
 5.875068960D-09-1.196789735D-12 1.204858910D+04  
 2.568801877D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8686.104

-2.633686357D+06 6.996429170D+03-3.233533060D+00 4.033935980D-03-  
 9.099579640D-07  
 8.775909870D-11-2.889490251D-15 -2.990043016D+04  
 4.971984500D+01  
 LiI Gurvich,1982 pt1 p289 pt2 p322.  
 2 tpi82 LI 1.00I 1.00 0.00 0.00 0.00 0 133.84547 -  
 85269.888  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9290.112  
 4.071976370D+04-6.667289470D+02 7.064257530D+00-5.480041020D-03  
 6.905790160D-06  
 -4.537168520D-09 1.226373296D-12 -8.235487020D+03-  
 1.296236234D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9290.112  
 1.616342632D+06-4.877717080D+03 9.987186550D+00-2.889137815D-03  
 8.037313770D-07  
 -9.028172610D-11 3.078321954D-15 1.937718764D+04-  
 3.729276310D+01  
 LiN Chase,1998 p1500.  
 2 j12/66 LI 1.00N 1.00 0.00 0.00 0.00 0 20.94774  
 334720.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8999.148  
 3.764959200D+04-4.883457630D+02 5.187373450D+00 2.275252171D-04-  
 1.416337564D-06  
 1.450236258D-09-4.790014330D-13 4.161915310D+04-  
 5.952154380D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8999.148  
 -5.993489980D+04-4.031134550D+01 4.529624210D+00 8.744156930D-05  
 2.557428364D-09  
 -2.905751800D-13 1.336125922D-17 3.894831130D+04-  
 1.214950032D+00  
 LiNO2 Gurvich,1982 pt1 p294 pt2 p327.  
 2 tpi82 LI 1.00N 1.000 2.00 0.00 0.00 0 52.94654 -  
 202031.208  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13368.792  
 -3.133773859D+04 5.389940810D+02-2.059877081D-02 2.610777454D-02-  
 3.209235040D-05  
 1.974344044D-08-4.892199160D-12 -2.838214963D+04  
 2.710019642D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13368.792  
 -2.196671160D+05-8.610042710D+02 1.063956465D+01-2.554392587D-04  
 5.644478540D-08  
 -6.476140050D-12 3.003536591D-16 -2.313547535D+04-  
 3.238276990D+01  
 LiNO3 Gurvich,1982 pt1 p296 pt2 p329.  
 2 tpi82 LI 1.00N 1.000 3.00 0.00 0.00 0 68.94594 -  
 311584.675  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13915.325  
 1.967205518D+04 9.052795260D+01-5.109770400D-01 3.756605950D-02-  
 4.782738650D-05  
 3.029277805D-08-7.708013150D-12 -3.907563990D+04  
 2.746873120D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13915.325

-3.559402450D+05-1.447644737D+03 1.406684061D+01-4.236371280D-04  
 9.320824510D-08  
 -1.065894872D-11 4.930780620D-16 -3.434827460D+04-  
 5.275382610D+01  
 LiO Gurvich,1982 pt1 p256 pt2 p294.  
 2 tpi82 LI 1.000 1.00 0.00 0.00 0.00 0 22.94040  
 72914.313  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9362.113  
 3.627029760D+04-3.499363230D+02 4.394933180D+00 1.079712984D-03-  
 8.724038810D-07  
 5.607962970D-10-2.054288457D-13 9.533330530D+03-  
 9.058149610D-01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9362.113  
 1.612392133D+06-5.551312340D+03 1.120573851D+01-3.437226880D-03  
 9.133194660D-07  
 -1.027902258D-10 3.822991000D-15 4.201575470D+04-  
 4.857354580D+01  
 LiOF Chase,1998 p1069.  
 2 j 9/65 LI 1.000 1.00F 1.00 0.00 0.00 0 41.93880 -  
 92048.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10827.363  
 5.510110690D+04-5.770688170D+02 4.424954930D+00 1.102425422D-02-  
 1.710493381D-05  
 1.234361201D-08-3.453693000D-12 -9.278986980D+03  
 1.238830687D-01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10827.363  
 -1.833563281D+05-2.110049301D+02 7.156818170D+00-6.249462010D-05  
 1.376567002D-08  
 -1.574099067D-12 7.277167140D-17 -1.254530277D+04-  
 1.272130479D+01  
 LiOH Gurvich,1996b.  
 2 g12/96 LI 1.000 1.00H 1.00 0.00 0.00 0 23.94834 -  
 229000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11336.961  
 4.574190120D+03-1.030949027D+02 4.272407370D+00 8.465219230D-03-  
 1.386148524D-05  
 1.101099795D-08-3.291248210D-12 -2.848728855D+04-  
 8.775745780D-01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11336.961  
 8.500751370D+05-2.430540791D+03 8.055314620D+00 6.895680880D-05-  
 5.527207460D-08  
 9.368054030D-12-5.313785680D-16 -1.365894396D+04-  
 2.457598093D+01  
 LiON Chase,1998 p1501.  
 2 j 9/66 LI 1.000 1.00N 1.00 0.00 0.00 0 36.94714  
 179912.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11300.979  
 -9.412672670D+03 1.009332300D+02 3.006187607D+00 9.890462200D-03-  
 1.128294343D-05  
 6.410291740D-09-1.466806373D-12 1.978348318D+04  
 1.016334975D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11300.979

-9.740629140D+04-5.111560940D+02 7.378493870D+00-1.508777884D-04  
 3.329914980D-08  
 -3.817514290D-12 1.769558455D-16 2.211006635D+04-  
 1.454104878D+01  
 Li2 Chase,1998 p1505.  
 2 j12/83 LI 2.00 0.00 0.00 0.00 0.00 0 13.88200  
 215900.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9675.116  
 6.778481580D+03-2.246205832D+02 5.296037440D+00-1.272412017D-03  
 1.205843729D-06  
 -9.818544590D-11-2.416702607D-13 2.573638186D+04-  
 6.869257580D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9675.116  
 3.767645400D+07-1.185747185D+05 1.482167789D+02-8.378532110D-02  
 2.424919798D-05  
 -3.275820240D-09 1.652000081D-13 7.723072010D+05-  
 1.021697298D+03  
 Li2+ Gurvich,1982 pt1 p249 pt2 p292.  
 2 tpis82 LI 2.00E -1.00 0.00 0.00 0.00 0 13.88145  
 721611.420  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9989.120  
 -1.040056453D+04 2.675405642D+01 4.247271750D+00 1.057450777D-03-  
 1.281715096D-06  
 1.067477239D-09-2.759413508D-13 8.529811310D+04  
 5.298189960D-01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9989.120  
 1.279931073D+07-3.492861390D+04 3.844785360D+01-1.380635397D-02  
 2.531394250D-06  
 -2.197815991D-10 7.087669250D-15 3.117964450D+05-  
 2.509543641D+02  
 Li2Br2 Gurvich,1982 pt1 p286 pt2 p319.  
 2 tpis82 LI 2.00BR 2.00 0.00 0.00 0.00 0 173.69000 -  
 495833.524  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16950.476  
 2.786312863D+04-1.005641437D+03 1.370963066D+01-7.633663300D-03  
 8.942905920D-06  
 -5.561135090D-09 1.421736784D-12 -5.762845840D+04-  
 4.121843760D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16950.476  
 -8.900983360D+04-1.988916335D+01 1.001596418D+01-6.749134050D-06  
 1.556299963D-09  
 -1.844693069D-13 8.774879920D-18 -6.279989960D+04-  
 1.943063525D+01  
 Li2CL2 Gurvich,1982 pt1 p282 pt2 p315.  
 2 tpis82 LI 2.00CL 2.00 0.00 0.00 0.00 0 84.78740 -  
 597538.789  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15906.322  
 5.313398610D+04-1.427266759D+03 1.512410161D+01-1.032824906D-02  
 1.190773317D-05  
 -7.312991160D-09 1.851289430D-12 -6.769860400D+04-  
 5.285132610D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15906.322

-1.179571272D+05-3.027126342D+01 1.002397711D+01-1.003660907D-05  
 2.297007564D-09  
 -2.706930258D-13 1.281817017D-17 -7.506822590D+04-  
 2.264971291D+01  
 Li2F2 Gurvich,1982 pt1 p276 pt2 p311.  
 2 tpris82 LI 2.00F 2.00 0.00 0.00 0.00 0 51.87881 -  
 935323.076  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13766.030  
 1.443166185D+05-2.466874678D+03 1.702863290D+01-1.145541210D-02  
 1.086098792D-05  
 -5.569754280D-09 1.193819664D-12 -1.026070133D+05-  
 7.000386610D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13766.030  
 -2.188931683D+05-9.259814530D+01 1.006970757D+01-2.803632163D-05  
 6.217549520D-09  
 -7.146267020D-13 3.316857300D-17 -1.156611527D+05-  
 2.729853181D+01  
 Li2I2 Gurvich,1982 pt1 p290 pt2 p323.  
 2 tpris82 LI 2.00I 2.00 0.00 0.00 0.00 0 267.69094 -  
 362801.349  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17658.652  
 1.014872266D+04-7.120421010D+02 1.270392960D+01-5.685536810D-03  
 6.770340380D-06  
 -4.263304890D-09 1.100658186D-12 -4.313063860D+04-  
 3.303950980D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17658.652  
 -6.973587060D+04-1.316825508D+01 1.001074855D+01-4.600203780D-06  
 1.070510527D-09  
 -1.277717768D-13 6.110612240D-18 -4.677470050D+04-  
 1.721894034D+01  
 Li2O Gurvich,1982 pt1 p259 pt2 p296.  
 2 tpris82 LI 2.00O 1.00 0.00 0.00 0.00 0 29.88140 -  
 167338.920  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12792.080  
 2.636601597D+04-1.798629279D+02 4.051115220D+00 1.189981375D-02-  
 1.730095793D-05  
 1.205584550D-08-3.292733880D-12 -2.061907963D+04  
 1.605995610D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12792.080  
 7.261487040D+05-9.543783720D+03 2.887491643D+01-1.959494099D-02  
 8.086339840D-06  
 -1.370211764D-09 8.111727190D-14 2.990726399D+04-  
 1.564517822D+02  
 Li2O+ Gurvich,1982 pt1 p260 pt2 p297.  
 2 tpris82 LI 2.00O 1.00E -1.00 0.00 0.00 0 29.88085 -  
 439095.089  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13028.689  
 1.081044623D+05-1.261961355D+03 9.692011290D+00-1.793477428D-03  
 3.380326900D-07  
 4.143395150D-10-1.990530222D-13 5.754976040D+04-  
 2.915719946D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13028.689

-1.302166086D+05-1.466759528D+02 7.610729450D+00-4.469426690D-05  
9.947160640D-09  
-1.147038806D-12 5.339241470D-17 5.098762310D+04-  
1.528011047D+01  
Li2O2 Gurvich,1982 pt1 p262 pt2 p299.  
2 tps82 LI 2.000 2.00 0.00 0.00 0.00 0 45.88080 -  
279397.988  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
13548.012  
1.392619730D+05-1.764036747D+03 1.029649198D+01 7.605949950D-03-  
1.538519312D-05  
1.238199941D-08-3.685431570D-12 -2.638056746D+04-  
3.437710560D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
13548.012  
-2.939232153D+05-2.359107937D+02 1.017463402D+01-6.931624360D-05  
1.521202834D-08  
-1.733841909D-12 7.993154620D-17 -3.618481910D+04-  
2.904221044D+01  
Li2O2H2 Gurvich,1996b.  
2 g12/96 LI 2.000 2.00H 2.00 0.00 0.00 0 47.89668 -  
737000.000  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
15579.040  
1.894413579D+05-2.779117524D+03 1.530234911D+01 1.070738317D-02-  
2.510075145D-05  
2.224910575D-08-6.949359580D-12 -7.702776920D+04-  
6.514116940D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
15579.040  
1.215377492D+06-3.982057440D+03 1.585877373D+01 7.509145680D-04-  
2.585218184D-07  
3.646841700D-11-1.904139406D-15 -6.738748380D+04-  
6.647208400D+01  
Li2SO4 Chase,1998 p1522.  
2 j12/78 LI 2.00S 1.000 4.00 0.00 0.00 0 109.94560 -  
1041816.000  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
19652.538  
1.006318702D+05-1.543457217D+03 9.670054910D+00 3.390757380D-02-  
4.823483810D-05  
3.267368920D-08-8.702518510D-12 -1.201939538D+05-  
2.911715271D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
19652.538  
-6.038750870D+05-1.064550976D+03 1.979557349D+01-3.188978250D-04  
7.062411120D-08  
-8.114439070D-12 3.766830210D-16 -1.268908595D+05-  
8.014315310D+01  
Li3+ Gurvich,1982 pt1 p251 pt2 p293.  
2 tps82 LI 3.00E -1.00 0.00 0.00 0.00 0 20.82245 -  
756590.836  
298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
13289.409  
-6.873222290D+03-2.820780467D+02 7.922697480D+00-1.687949474D-03  
1.771718993D-06  
-9.972535400D-10 2.332934849D-13 9.027963650D+04-  
1.619319856D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
13289.409

-4.355098060D+04-6.056432750D+00 7.004722890D+00-1.953320933D-06  
 4.429152230D-10  
 -5.181983190D-14 2.439894871D-18 8.879902870D+04-  
 1.066880792D+01  
 Li3Br3 Gurvich,1982 pt1 p287 pt2 p320.  
 2 tpris82 LI 3.00BR 3.00 0.00 0.00 0.00 0 260.53500 -  
 824639.193  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 26036.807  
 6.431966250D+04-1.823743601D+03 2.243492856D+01-1.279418260D-02  
 1.459200355D-05  
 -8.884688150D-09 2.233708050D-12 -9.480677670D+04-  
 8.206864420D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 26036.807  
 -1.584670201D+05-4.041360940D+01 1.603177633D+01-1.322713911D-05  
 3.014221791D-09  
 -3.540292160D-13 1.672030783D-17 -1.042470448D+05-  
 4.405478160D+01  
 Li3CL3 Gurvich,1982 pt1 p283 pt2 p316.  
 2 tpris82 LI 3.00CL 3.00 0.00 0.00 0.00 0 127.18110 -  
 976107.121  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 24560.546  
 9.867429000D+04-2.324074851D+03 2.378484564D+01-1.483522400D-02  
 1.634495612D-05  
 -9.675366520D-09 2.377033859D-12 -1.103839177D+05-  
 9.474115440D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 24560.546  
 -2.005930356D+05-5.939400190D+01 1.604590929D+01-1.885890854D-05  
 4.253517370D-09  
 -4.955560940D-13 2.325408214D-17 -1.224927071D+05-  
 4.844414690D+01  
 Li3F3 Gurvich,1982 pt1 p278 pt2 p312.  
 2 tpris82 LI 3.00F 3.00 0.00 0.00 0.00 0 77.81821 -  
 1524596.926  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 20536.734  
 1.823874443D+05-3.163786240D+03 2.287811928D+01-7.544903890D-03  
 3.446790230D-06  
 2.690705228D-10-5.250840960D-13 -1.712446093D+05-  
 9.973654990D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 20536.734  
 -3.618664990D+05-1.937051395D+02 1.614457133D+01-5.775628500D-05  
 1.274057038D-08  
 -1.458168875D-12 6.744850030D-17 -1.882081974D+05-  
 5.633612880D+01  
 Li3I3 Gurvich,1982 pt1 p290 pt2 p324.  
 2 tpris82 LI 3.00I 3.00 0.00 0.00 0.00 0 401.53641 -  
 612457.307  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 27232.694  
 3.611764690D+04-1.392033487D+03 2.110791892D+01-1.046866587D-02  
 1.222589173D-05  
 -7.584135430D-09 1.935199180D-12 -7.153084580D+04-  
 7.093882030D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 27232.694

-1.266696511D+05-2.783891914D+01 1.602228068D+01-9.399364930D-06  
2.163919735D-09  
-2.561731922D-13 1.217394107D-17 -7.869550680D+04-  
4.091724060D+01

Mg Hf:Cox,1989. Kaufman,1991a. Gordon,1999.

3 g 6/97 MG 1.00 0.00 0.00 0.00 0.00 0 24.30500  
147100.000  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428  
0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 1.694658761D+04  
3.634330140D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428  
-5.364831550D+05 1.973709576D+03-3.633776900D-01 2.071795561D-03-  
7.738051720D-07  
1.359277788D-10-7.766898397D-15 4.829188110D+03  
2.339104998D+01  
6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428  
2.166012586D+09-1.008355665D+06 1.619680021D+02-8.790130350D-03-  
1.925690961D-08  
1.725045214D-11-4.234946112D-16 8.349525900D+06-  
1.469355261D+03

Mg+ Kaufman,1991a. Gordon,1999.

3 g 6/97 MG 1.00E -1.00 0.00 0.00 0.00 0 24.30445  
891047.000  
298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428  
0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 1.064223354D+05  
4.327443460D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428  
-1.914758821D+04 4.877347920D+01 2.457662661D+00 1.218104674D-05  
1.897261686D-09  
-1.580433756D-12 2.135732238D-16 1.061022394D+05  
4.646442860D+00  
6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428  
4.015949550D+08-2.281591735D+05 5.421745710D+01-5.983017190D-03  
3.657189130D-07  
-1.020737688D-11 1.024202854D-16 1.932463961D+06-  
4.480157830D+02

MgBr Gurvich,1996a pt1 p417 pt2 p331.

2 tpris96 MG 1.00BR 1.00 0.00 0.00 0.00 0 104.20900  
6163.315  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
9588.115  
7.361419140D+03-2.395789881D+02 5.360560420D+00-1.667141829D-03  
1.981137765D-06  
-1.201637202D-09 3.032148099D-13 5.915634440D+02-  
1.421771179D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
9588.115  
2.477604216D+04-6.417687520D+02 6.019932090D+00-1.391004302D-03  
6.443330960D-07  
-1.197734078D-10 7.421644240D-15 2.824060334D+03-  
6.264439920D+00



MgBr2 Gurvich,1996a pt1 p420 pt2 p333.

2 tpris96 MG 1.00BR 2.00 0.00 0.00 0.00 0 184.11300 -  
306743.219  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
14757.281  
2.148477999D+04-5.154528900D+02 9.273258750D+00-3.470049040D-03  
3.921840790D-06  
-2.377174864D-09 5.967025560D-13 -3.652443850D+04-  
1.791077763D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
14757.281  
-4.326899010D+04-1.283036001D+01 7.510024300D+00-4.152332400D-06  
9.426499180D-10  
-1.103873928D-13 5.201104310D-18 -3.919886020D+04-  
7.409168030D+00

MgCL Gurvich,1996a pt1 p412 pt2 p328.

2 tpris96 MG 1.00CL 1.00 0.00 0.00 0.00 0 59.75770 -  
54704.887  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
9363.113  
2.043995280D+04-4.072155160D+02 5.880372300D+00-2.594175042D-03  
2.945953528D-06  
-1.750648628D-09 4.337959330D-13 -5.851444950D+03-  
6.023553280D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
9363.113  
1.041328453D+06-3.380158330D+03 8.637775470D+00-2.447789643D-03  
7.841969440D-07  
-1.126409380D-10 5.810620730D-15 1.327188977D+04-  
2.703803148D+01

MgCL+ Chase,1998 p786 6/68.

3 g 1/01 MG 1.00CL 1.00E -1.00 0.00 0.00 0 59.75715  
646339.332  
298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
9515.732  
8.182385120D+03-2.622253760D+02 5.419863430D+00-1.774129606D-03  
2.185811127D-06  
-1.418143432D-09 3.918898580D-13 7.770403710D+04-  
3.780946370D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
9515.732  
-1.268391921D+07 3.478824540D+04-3.004222950D+01 1.481739497D-02-  
2.470965605D-06  
1.424433718D-10 2.789613105D-16 -1.487013740D+05  
2.552015042D+02  
6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
9515.732  
1.382463416D+08-6.324735630D+04 2.090164490D+01-1.924320270D-03  
1.303442285D-07  
-4.354246510D-12 5.852012920D-17 5.856144100D+05-  
1.379609299D+02

MgCL2 Gurvich,1996a pt1 p416 pt2 p330.

2 tpris96 MG 1.00CL 2.00 0.00 0.00 0.00 0 95.21040 -  
399169.896  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
13900.604  
3.637824680D+04-7.307844960D+02 9.661030510D+00-3.660212940D-03  
3.610819350D-06  
-1.928769286D-09 4.309912350D-13 -4.646914570D+04-  
2.360113219D+01

1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13900.604  
 -6.835217010D+04-2.490899393D+01 7.518783200D+00-7.564518260D-06  
 1.679293770D-09  
 -1.931706275D-13 8.971657820D-18 -5.032686910D+04-  
 1.053269327D+01  
 MgF Gurvich,1996a pt1 p408 pt2 p325.  
 2 tpi96 MG 1.00F 1.00 0.00 0.00 0.00 0 43.30340 -  
 232266.792  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8969.108  
 3.823001620D+04-4.803310390D+02 5.068468940D+00 5.212029300D-04-  
 1.874026347D-06  
 1.759241129D-09-5.609403190D-13 -2.659114296D+04-  
 3.768969210D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8969.108  
 -1.695883782D+05 3.588757630D+02 3.936001650D+00 4.813044140D-04-  
 1.658385409D-07  
 3.336052290D-11-2.270104205D-15 -3.169323990D+04  
 4.410565900D+00  
 MgF+ Chase,1998 p1071 12/75.  
 3 g 2/01 MG 1.00F 1.00E -1.00 0.00 0.00 0 43.30285  
 516867.775  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8969.375  
 6.413293840D+05-8.518532610D+03 4.814216910D+01-1.163071535D-01  
 1.622560562D-04  
 -1.063484590D-07 2.634809398D-11 1.024308480D+05-  
 2.450074295D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8969.375  
 -1.056852362D+07 2.077122379D+04-6.119523560D+00 2.245834831D-03-  
 9.515738610D-08  
 -2.263502341D-11 2.284524246D-15 -8.331549880D+04  
 8.727102380D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8969.375  
 5.735804460D+07-2.157378345D+04 6.572317550D+00 1.887605214D-04-  
 1.860864600D-08  
 6.862191460D-13-8.597821080D-18 2.477615733D+05-  
 1.922750114D+01  
 MgF2 Gurvich,1996a pt1 p411 pt2 p327.  
 2 tpi96 MG 1.00F 2.00 0.00 0.00 0.00 0 62.30181 -  
 735498.060  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12622.440  
 4.338429550D+04-6.616511770D+02 7.453448520D+00 3.520814050D-03-  
 6.955764580D-06  
 5.619923480D-09-1.688028906D-12 -8.687183670D+04-  
 1.545476790D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12622.440  
 -1.244419584D+05-8.687343750D+01 7.563581230D+00-2.499267978D-05  
 5.440129140D-09  
 -6.158245760D-13 2.822792666D-17 -9.060019440D+04-  
 1.420796990D+01  
 MgF2+ Chase,1998 p1122 12/75.  
 3 g 2/01 MG 1.00F 2.00E -1.00 0.00 0.00 0 62.30126  
 582692.164

298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12415.064  
 7.832220260D+04-1.176632752D+03 1.025829767D+01-3.755272890D-03  
 3.016621585D-06  
 -1.327098871D-09 2.465289749D-13 7.413228550D+04-  
 2.990883551D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12415.064  
 -1.502316870D+05 7.725289560D+01 7.271569360D+00 2.237529770D-04-  
 1.003070865D-07  
 1.996274309D-11-1.233278721D-15 6.699117500D+04-  
 1.094528006D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12415.064  
 2.601903911D+07-5.388879260D+03 5.218198280D+00 7.632535320D-04-  
 6.606231900D-08  
 2.428649361D-12-3.341900910D-17 1.228640353D+05  
 3.390783040D+00  
 MgH Gurvich,1996a pt1 p401 pt2 p320.  
 2 tpris96 MG 1.00H 1.00 0.00 0.00 0.00 0 25.31294  
 229786.104  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8682.104  
 -4.958679150D+04 7.500278650D+02-6.442047500D-01 9.826301010D-03-  
 8.789822440D-06  
 3.823353520D-09-6.003725760D-13 2.302279383D+04  
 2.657165344D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8682.104  
 -1.005748598D+05 1.952890106D+03-1.317191549D+00 5.603665800D-03-  
 2.137334980D-06  
 3.324880500D-10-1.824672746D-14 1.598582755D+04  
 3.431233160D+01  
 MgI Gurvich,1996a pt1 p420 pt2 p334.  
 2 tpris96 MG 1.00I 1.00 0.00 0.00 0.00 0 151.20947  
 61206.317  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9741.117  
 2.943889099D+03-1.690248574D+02 5.147251830D+00-1.321186997D-03  
 1.623056505D-06  
 -1.005114222D-09 2.567337785D-13 6.845890270D+03  
 8.593132250D-01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9741.117  
 -2.370562811D+06 6.916452480D+03-3.183894490D+00 4.051551140D-03-  
 9.774290750D-07  
 1.023329400D-10-3.790304870D-15 -3.818551110D+04  
 5.993104380D+01  
 MgI2 Gurvich,1996a pt1 p423 pt2 p336.  
 2 tpris96 MG 1.00I 2.00 0.00 0.00 0.00 0 278.11394 -  
 171706.029  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15294.471  
 1.594739709D+04-4.160412720D+02 9.010638320D+00-3.090359024D-03  
 3.621264260D-06  
 -2.260138392D-09 5.809055550D-13 -2.080441400D+04-  
 1.412175736D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15294.471  
 -3.340299180D+04-9.343511780D+00 7.507468540D+00-3.147707890D-06  
 7.241336470D-10

-8.567664950D-14 4.069691700D-18 -2.294555505D+04-  
5.241272590D+00

MgN Chase,1998 p1535.  
2 j 3/64 MG 1.00N 1.00 0.00 0.00 0.00 0 38.31174  
288696.000  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
8988.881  
3.759538640D+04-4.853164280D+02 5.163054240D+00 2.591539493D-04-  
1.518993975D-06  
1.522840476D-09-4.992531450D-13 3.607294610D+04-  
3.813907210D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
8988.881  
-6.018589100D+04-4.010864780D+01 4.529498950D+00 4.760490910D-05  
2.547271298D-09  
-2.894058118D-13 1.330639131D-17 3.341285700D+04  
7.925265870D-01

MgO Gurvich,1996a pt1 p398 pt2 p318.  
3 tpi96 MG 1.00O 1.00 0.00 0.00 0.00 0 40.30440  
32261.307  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
8909.107  
3.513659740D+05-5.287197160D+03 3.382060060D+01-8.400489630D-02  
1.210016160D-04  
-7.630795020D-08 1.701022862D-11 2.790679519D+04-  
1.624886199D+02  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
8909.107  
-1.586738367D+07 3.420468100D+04-1.774087677D+01 7.004963050D-03-  
1.104138249D-06  
8.957488530D-11-3.052513649D-15 -2.300504434D+05  
1.738984472D+02  
6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
8909.107  
2.290059050D+06-2.073499632D+04 1.444150005D+01-1.490609900D-03  
1.052119343D-07  
-3.523030610D-12 4.613111760D-17 1.490218815D+05-  
8.007281730D+01

MgOH Gurvich,1996a pt1 p404 pt2 p322.  
2 tpi96 MG 1.00O 1.00H 1.00 0.00 0.00 0 41.31234 -  
132428.980  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
11124.284  
3.839851620D+04-7.367383640D+02 7.920664460D+00-5.950940590D-04-  
2.112941162D-06  
3.228282110D-09-1.214159329D-12 -1.392326188D+04-  
1.916078109D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
11124.284  
6.648664750D+05-1.770750355D+03 7.269999270D+00 5.336842760D-04-  
1.980894443D-07  
3.025677088D-11-1.554849476D-15 -6.149114560D+03-  
1.671027009D+01

MgOH+ Chase,1998 p1285 12/75.  
3 g 1/01 MG 1.00O 1.00H 1.00E -1.00 0.00 0 41.31179  
615769.370  
298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
10188.370  
1.170224573D+05-1.735933343D+03 1.164059613D+01-8.449876220D-03  
7.351713740D-06

-2.790223071D-09 3.514982130D-13 8.118807670D+04-  
 4.271174370D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10188.370  
 8.296339540D+05-2.459700177D+03 8.118732020D+00 3.500579100D-05-  
 4.670574750D-08  
 8.312358260D-12-4.802836220D-16 8.801661710D+04-  
 2.438155217D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10188.370  
 -6.691779770D+06 2.437864449D+03 6.949387850D+00 6.355744850D-05-  
 3.980850170D-09  
 1.287525303D-13-1.684735436D-18 4.948972630D+04-  
 1.400323314D+01  
 Mg(OH)2 Gurvich,1996a pt1 p407 pt2 p324.  
 2 tpis96 MG 1.000 2.00H 2.00 0.00 0.00 0 58.31968 -  
 551995.808  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17131.558  
 5.245894670D+04-1.289056383D+03 1.389327642D+01-7.806693670D-04-  
 4.151257230D-06  
 6.109473040D-09-2.274138833D-12 -6.295089150D+04-  
 5.015353340D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17131.558  
 1.713709254D+06-4.730005350D+03 1.448925967D+01 1.907819857D-04-  
 1.226834131D-07  
 2.015343753D-11-1.128993279D-15 -3.887724670D+04-  
 5.840498120D+01  
 MgS Gurvich,1996a pt1 p425 pt2 p338.  
 2 tpis96 MG 1.00S 1.00 0.00 0.00 0.00 0 56.37100  
 120649.311  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9234.111  
 -9.565788090D+03 1.443637798D+02 1.813794717D+00 1.147168775D-02-  
 2.220170412D-05  
 1.995344981D-08-6.090688740D-12 1.276501517D+04  
 1.461335754D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9234.111  
 2.650794328D+07-7.711355860D+04 8.463771680D+01-3.644250680D-02  
 8.403084420D-06  
 -9.539882170D-10 4.264658030D-14 5.078931170D+05-  
 5.834655830D+02  
 Mg2 Gurvich,1996a pt1 p393 pt2 p316.  
 2 tpis96 MG 2.00 0.00 0.00 0.00 0.00 0 48.61000  
 286513.315  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9542.115  
 4.545195590D+03 4.115850040D+02 4.841196170D-01 4.891969650D-03-  
 6.395536840D-06  
 4.299764550D-09-1.164624418D-12 3.181641790D+04  
 2.640432143D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9542.115  
 3.038224994D+04 5.945240460D+01 2.352706666D+00 1.378537924D-04-  
 5.895692040D-08  
 1.104045317D-11-6.558868290D-16 3.351036560D+04  
 1.588177377D+01  
 Mg2F4 Chase,1998 p1178.

2 j12/75 MG 2.00F 4.00 0.00 0.00 0.00 0 124.60361 -  
 1718369.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 21143.314  
 1.511956137D+05-3.122595912D+03 2.517715088D+01-1.558723757D-02  
 1.552195619D-05  
 -8.408729050D-09 1.911618525D-12 -1.953078883D+05-  
 1.085103537D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 21143.314  
 -2.980610166D+05-1.201299868D+02 1.609110864D+01-3.687456290D-05  
 8.220317050D-09  
 -9.488869780D-13 4.419795330D-17 -2.117349690D+05-  
 5.308655470D+01  
 Mn Hf:Desai,1987. Sugar,1985. Gordon,1999.  
 3 g 7/97 MN 1.00 0.00 0.00 0.00 0.00 0 54.93805  
 282400.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 1.034061359D-01-1.551537349D-03 2.500009148D+00-2.723162066D-08  
 4.333897430D-11  
 -3.511093890D-14 1.136032201D-17 3.321935190D+04  
 6.649325463D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 5.855155820D+03 8.838588440D+02-3.648662580D-02 2.703720687D-03-  
 1.324971998D-06  
 2.872603290D-10-1.923633570D-14 2.867803487D+04  
 2.292541198D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 3.936189040D+09-2.353549748D+06 5.377244800D+02-5.824812570D-02  
 3.330475100D-06  
 -9.689631050D-11 1.133286034D-15 1.879530161D+07-  
 4.690097890D+03  
 Mn+ Sugar,1985. Gordon,1999.  
 3 g 6/97 MN 1.00E -1.00 0.00 0.00 0.00 0 54.93750  
 1005871.328  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 3.458017700D+02-4.251151330D+00 2.521281028D+00-5.565087280D-05  
 8.037162210D-08  
 -6.093550970D-11 1.900014268D-14 1.202533602D+05  
 6.683468162D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 6.471314100D+05-2.403796253D+03 5.937715750D+00-2.341014594D-03  
 7.464165640D-07  
 -9.075969730D-11 4.467879847D-15 1.349902108D+05-  
 1.702666341D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 1.717119921D+09-9.029185830D+05 1.784788847D+02-1.566770206D-02  
 7.346534410D-07  
 -1.750673350D-11 1.667889239D-16 7.443546080D+06-  
 1.568005804D+03  
 Mo Hf:Desai,1987. Sugar,1988. Gordon,1999.  
 3 g 7/97 MO 1.00 0.00 0.00 0.00 0.00 0 95.94000  
 658500.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428

7.646367910D+01-1.159269043D+00 2.506929462D+00-2.099249725D-05  
 3.414779430D-08  
 -2.841269591D-11 9.492443321D-15 7.845899800D+04  
 7.601835660D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 5.573271000D+06-1.662365811D+04 2.135147077D+01-1.003069377D-02  
 2.409784357D-06  
 -1.811267352D-10 1.034189087D-15 1.842646473D+05-  
 1.275326434D+02  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 6.205038910D+09-3.855961600D+06 9.371595060D+02-1.108164544D-01  
 6.929123900D-06  
 -2.199865715D-10 2.798315513D-15 3.062163602D+07-  
 8.122811340D+03  
 Mo+ Sugar,1988. Gordon,1999.  
 3 g 7/97 MO 1.00E -1.00 0.00 0.00 0.00 0 95.93945  
 1349012.928  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 1.298236623D+02-1.560279908D+00 2.507600281D+00-1.923789063D-05  
 2.673316651D-08  
 -1.937174292D-11 5.729735412D-15 1.615103759D+05  
 7.442543460D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 1.298891120D+07-3.948276230D+04 4.866599780D+01-2.605352326D-02  
 7.215431920D-06  
 -8.719164960D-10 3.788423040D-14 4.118948570D+05-  
 3.216791030D+02  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 -1.731253943D+09 8.776685240D+05-1.669716753D+02 1.732439603D-02-  
 9.372726850D-07  
 2.593422324D-11-2.913787941D-16 -6.989098130D+06  
 1.517101780D+03  
 Mo- Hotop,1985. Gordon,1999.  
 3 g10/97 MO 1.00E 1.00 0.00 0.00 0.00 0 95.94055  
 580324.628  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 6.905123690D+04  
 7.485659540D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 6.905123690D+04  
 7.485659540D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 6.905123690D+04  
 7.485659540D+00  
 MoO Gurvich,1982 pt1 p25 pt2 p30.  
 3 tpis89 MO 1.00O 1.00 0.00 0.00 0.00 0 111.93940  
 358005.323

200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10253.123  
 -2.801152706D+04 5.139883480D+02 1.075385931D+00 8.681048470D-03-  
 1.111118984D-05  
 7.234349330D-09-1.893138381D-12 3.941374080D+04  
 2.272230239D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10253.123  
 1.573131992D+06-5.241483580D+03 1.102656868D+01-3.902996620D-03  
 1.147334134D-06  
 -1.358975691D-10 5.775268580D-15 7.448972000D+04-  
 4.253612930D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10253.123  
 2.846838911D+08-1.710122789D+05 4.036556200D+01-2.750495204D-03  
 8.916821240D-08  
 -1.248340135D-12 3.675821910D-18 1.408558917D+06-  
 3.171602770D+02  
 MoO2 Gurvich,1982 pt1 p28 pt2 p33.  
 2 tpris82 MO 1.000 2.00 0.00 0.00 0.00 0 127.93880 -  
 15558.079  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10707.025  
 3.247183220D+04-1.904783783D+02 2.120771647D+00 1.650280086D-02-  
 2.381696822D-05  
 1.652371586D-08-4.494452430D-12 -1.862932837D+03  
 1.640582056D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10707.025  
 3.096143654D+05-1.932750274D+03 9.428673180D+00-1.630508855D-03  
 5.752760170D-07  
 -7.590457470D-11 3.461337780D-15 7.327725180D+03-  
 2.533315948D+01  
 MoO3 Gurvich,1982 pt1 p31 pt2 p35.  
 2 tpris82 MO 1.000 3.00 0.00 0.00 0.00 0 143.93820 -  
 364412.371  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13192.785  
 5.977385360D+04-7.684557830D+02 5.881844440D+00 1.686119817D-02-  
 2.582485043D-05  
 1.850382718D-08-5.152249850D-12 -4.155872390D+04-  
 6.529162160D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13192.785  
 -4.097597270D+05 2.379066513D+02 9.311100800D+00 6.579338910D-04-  
 2.895307725D-07  
 5.692637260D-11-3.489657310D-15 -4.923738720D+04-  
 2.114864892D+01  
 MoO3- Gurvich,1982 pt1 p32 pt2 p36.  
 2 tpris82 MO 1.000 3.00E 1.00 0.00 0.00 0 143.93875 -  
 655242.501  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13560.083  
 1.821617352D+05-2.224656970D+03 1.320405967D+01-1.249800352D-03-  
 1.864166983D-06  
 2.276579470D-09-7.366564570D-13 -6.938986000D+04-  
 4.699377210D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13560.083  
 -4.881098720D+05 1.848536991D+01 1.042644941D+01-6.265557910D-04  
 3.020554347D-07



-4.733195890D-11 2.527517727D-15 -8.337815500D+04-  
2.701522825D+01

Mo206 Gurvich,1982 pt1 p33 pt2 p37.  
2 tpris82 MO 2.000 6.00 0.00 0.00 0.00 0 287.87640 -  
1149446.813  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
25763.499  
1.568375811D+05-2.159930184D+03 1.522500503D+01 3.194198900D-02-  
5.063877150D-05  
3.689371820D-08-1.037872908D-11 -1.309931161D+05-  
5.408918500D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
25763.499  
-6.312238160D+05-6.642827550D+02 2.249383570D+01-1.968470329D-04  
4.336740610D-08  
-4.959777990D-12 2.293212733D-16 -1.430573250D+05-  
8.669628540D+01

Mo309 Gurvich,1982 pt1 p34 pt2 p38.  
2 tpris82 MO 3.000 9.00 0.00 0.00 0.00 0 431.81460 -  
1902031.349  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
40784.119  
1.483386187D+05-1.863895133D+03 1.738405871D+01 6.233012320D-02-  
9.328441350D-05  
6.613638790D-08-1.830607518D-11 -2.248945631D+05-  
5.826669470D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
40784.119  
-9.230290540D+05-1.076171759D+03 3.480007260D+01-3.189633800D-04  
7.028397040D-08  
-8.039642640D-12 3.717879530D-16 -2.357422166D+05-  
1.448769485D+02

Mo4012 Gurvich,1982 pt1 p36 pt2 p39.  
2 tpris82 MO 4.000 12.00 0.00 0.00 0.00 0 575.75280 -  
2625526.773  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
54893.850  
2.234876437D+05-2.996203728D+03 2.682458827D+01 7.597345720D-02-  
1.155247012D-04  
8.256472570D-08-2.296764551D-11 -3.084619476D+05-  
1.065236386D+02  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
54893.850  
-1.225283388D+06-1.368141197D+03 4.701687810D+01-4.052910200D-04  
8.928472390D-08  
-1.021091158D-11 4.721091690D-16 -3.256477770D+05-  
2.047486535D+02

Mo5015 Gurvich,1982 pt1 p38 pt2 p40.  
2 tpris82 MO 5.000 15.00 0.00 0.00 0.00 0 719.69100 -  
3329108.437  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
68917.342  
2.768903251D+05-3.757933100D+03 3.408197760D+01 9.485414960D-02-  
1.442672100D-04  
1.031163900D-07-2.868600013D-11 -3.913507030D+05-  
1.426449143D+02  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
68917.342  
-1.535389516D+06-1.710367122D+03 5.927125780D+01-5.066836290D-04  
1.116223706D-07

-1.276562233D-11 5.902318910D-16 -4.128972380D+05-  
2.651287167D+02

N Hf:Cox,1989. Moore,1975. Gordon,1999.  
3 g 5/97 N 1.00 0.00 0.00 0.00 0.00 0 14.00674  
472680.000  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428  
0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 5.610463780D+04  
4.193909320D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428  
8.876501380D+04-1.071231500D+02 2.362188287D+00 2.916720081D-04-  
1.729515100D-07  
4.012657880D-11-2.677227571D-15 5.697351330D+04  
4.865235790D+00  
6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428  
5.475181050D+08-3.107574980D+05 6.916782740D+01-6.847988130D-03  
3.827572400D-07  
-1.098367709D-11 1.277986024D-16 2.550585618D+06-  
5.848769710D+02

N+ Moore,1975. Gordon,1999.  
3 g 6/97 N 1.00E -1.00 0.00 0.00 0.00 0 14.00619  
1882127.624  
298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
7116.524  
5.237079210D+03 2.299958315D+00 2.487488821D+00 2.737490756D-05-  
3.134447576D-08  
1.850111332D-11-4.447350984D-15 2.256284738D+05  
5.076835070D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
7116.524  
2.904970374D+05-8.557908610D+02 3.477389290D+00-5.288267190D-04  
1.352350307D-07  
-1.389834122D-11 5.046166279D-16 2.310809984D+05-  
1.994142261D+00  
6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
7116.524  
1.646092148D+07-1.113165218D+04 4.976986640D+00-2.005393583D-04  
1.022481356D-08  
-2.691430863D-13 3.539931593D-18 3.136284696D+05-  
1.706645952D+01

N- Hotop,1985. Chase,1998 p1602. Gordon,1999.  
3 j12/82 N 1.00E 1.00 0.00 0.00 0.00 0 14.00729  
473537.545  
298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6498.345  
1.445682471D+03 7.335205110D+00 2.476680939D+00 4.227869180D-05-  
4.426293320D-08  
2.490985431D-11-5.831608090D-15 5.617625000D+04  
5.145758260D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6498.345  
2.404189576D+03 2.954965336D-01 2.499789368D+00 8.307564970D-08-  
1.829942770D-11  
2.100136461D-15-9.754986710D-20 5.621413890D+04  
5.006488440D+00  
6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6498.345

1.884379470D+03 3.905516910D-01 2.499914043D+00 9.818512540D-09-  
6.126037340D-13  
1.980010689D-17-2.593295116D-22 5.621304520D+04  
5.005651890D+00

NCO Hf:East,1993. Jacox,1998 p184.

2 g 6/01 N 1.00C 1.000 1.00 0.00 0.00 0 42.01684  
131847.241

200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
10198.245

1.136503036D+04-2.444613367D+02 4.671376100D+00 2.309387548D-03  
2.798649599D-06

-4.546357380D-09 1.692880931D-12 1.577649188D+04-  
2.171462623D-01

1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
10198.245

1.089445289D+05-1.735459316D+03 8.655610330D+00-4.053229260D-04  
7.599716410D-08

-7.253804150D-12 3.244872410D-16 2.365792776D+04-  
2.619532827D+01

ND Hf:est. from NH,H&D data. Chase,1998 p1037 6/77.

2 g 4/01 N 1.00D 1.00 0.00 0.00 0.00 0 16.02084  
355738.797

200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
8648.000

2.290155757D+04-3.957388510D+02 6.179010330D+00-8.847806970D-03  
1.441582970D-05

-1.006647227D-08 2.654403586D-12 4.355913430D+04-  
1.180413697D+01

1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
8648.000

5.439657960D+05-2.084583507D+03 5.834089720D+00-4.189393360D-04  
9.768929530D-08

-1.056317654D-11 4.683079210D-16 5.466633410D+04-  
1.480810564D+01

ND2 Hf:est. from NH2,H,&D data. Jacox,1998 p133.

2 g 4/01 N 1.00D 2.00 0.00 0.00 0.00 0 18.03494  
184836.570

200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
9962.325

1.935222164D+04-2.130631713D+02 4.844017600D+00-2.516949288D-03  
7.616381540D-06

-5.464501770D-09 1.292736999D-12 2.211998374D+04-  
3.171709090D+00

1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
9962.325

1.631308357D+06-6.564637490D+03 1.280547961D+01-3.094456779D-03  
9.181660230D-07

-1.241119284D-10 6.226299860D-15 6.108929580D+04-  
6.124502360D+01

ND3 Hf:est. from NH3,H,&D data. Chase,1998 p1047 6/77.

2 g 4/01 N 1.00D 3.00 0.00 0.00 0.00 0 20.04905 -  
54752.106

200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
10234.000

1.045120370D+04 1.610166943D+02 8.574963230D-01 1.319688794D-02-  
1.153090144D-05

7.142495560D-09-2.109194351D-12 -8.220948900D+03  
1.675921598D+01

1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
10234.000

2.599516958D+06-1.013420124D+04 1.798028169D+01-3.582609800D-03  
 1.009922000D-06  
 -1.537638609D-10 9.106175650D-15 5.397205660D+04-  
 9.810988270D+01  
 NF Gurvich,1989 pt1 p372 pt2 p234. Gurvich,1978 pt2 p243.  
 2 tpis89 N 1.00F 1.00 0.00 0.00 0.00 0 33.00514  
 232990.500  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8738.105  
 -3.504927750D+04 6.674502990D+02-1.201665982D+00 1.452074253D-02-  
 1.822873148D-05  
 1.160136864D-08-2.973416333D-12 2.395414002D+04  
 3.089260613D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8738.105  
 8.002987330D+05-3.237696580D+03 8.703408870D+00-2.701025798D-03  
 9.150042110D-07  
 -1.365256630D-10 7.234624410D-15 4.642819450D+04-  
 3.019933066D+01  
 NF2 Gurvich,1989 pt1 p373. McBride,1992 METHOD NRRAO1.  
 2 g 4/99 N 1.00F 2.00 0.00 0.00 0.00 0 52.00355  
 34421.447  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10581.605  
 1.511831104D+04 9.196389940D+01 4.947301790D-01 2.001847323D-02-  
 2.767712684D-05  
 1.872924867D-08-5.020318040D-12 2.839279606D+03  
 2.270515785D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10581.605  
 -1.945010078D+05-3.536034070D+02 7.263494360D+00-8.402380400D-05  
 2.326721111D-08  
 -2.667577562D-12 1.236070614D-16 3.435440590D+03-  
 1.336102396D+01  
 NF3 Gurvich,1989 pt1 p375. McBride,1992 METHOD NRRAO2.  
 2 g 4/99 N 1.00F 3.00 0.00 0.00 0.00 0 71.00195 -  
 131700.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11854.511  
 8.757149280D+04-9.031832890D+02 4.027417270D+00 2.314439555D-02-  
 3.415106470D-05  
 2.409483651D-08-6.633464190D-12 -1.237232074D+04  
 3.026439163D-01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11854.511  
 -3.496268760D+05-4.973728670D+02 1.036866128D+01 8.900687650D-05  
 5.882654360D-08  
 -3.157737664D-12 1.714329953D-16 -1.713183352D+04-  
 3.098920773D+01  
 NH Hf:Anderson,1989. Gurvich,1978 pt2 p223.  
 3 g 4/99 N 1.00H 1.00 0.00 0.00 0.00 0 15.01468  
 357032.001  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8601.103  
 1.359651320D+04-1.900296604D+02 4.518496790D+00-2.432776899D-03  
 2.377587464D-06  
 -2.592797084D-10-2.659680792D-13 4.280972190D+04-  
 3.886557620D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8601.103

1.958141991D+06-5.782861300D+03 9.335742020D+00-2.292910311D-03  
 6.076092480D-07  
 -6.647942750D-11 2.384234783D-15 7.898912340D+04-  
 4.116970000D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8601.103  
 9.524636790D+07-8.585826910D+04 2.980445181D+01-2.979563697D-03  
 1.656334158D-07  
 -4.744791840D-12 5.570148290D-17 6.961434270D+05-  
 2.229027379D+02  
 NH+ Hf:Gibson,1985. Gurvich,1989 pt2 p216.  
 3 g 5/99 N 1.00H 1.00E -1.00 0.00 0.00 0 15.01413  
 1665787.914  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9495.114  
 4.253656850D+03-2.458222206D+02 6.708919490D+00-1.038489430D-02  
 1.509008623D-05  
 -9.580512190D-09 2.333206758D-12 2.001077797D+05-  
 1.395057232D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9495.114  
 1.405709438D+06-4.136215710D+03 7.632014480D+00-1.228325778D-03  
 2.721187746D-07  
 -2.010098289D-11 3.717190180D-17 2.258975960D+05-  
 2.786784834D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9495.114  
 2.392941759D+08-1.741658624D+05 5.107907910D+01-5.567623700D-03  
 3.273391600D-07  
 -9.797978060D-12 1.186543279D-16 1.554705305D+06-  
 4.065968920D+02  
 NHF Gurvich,1989 pt1 p386 pt2 p247.  
 2 tpris89 N 1.00H 1.00F 1.00 0.00 0.00 0 34.01308  
 112000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10029.728  
 -5.110659820D+04 9.612256430D+02-2.706446594D+00 2.036562680D-02-  
 2.425558952D-05  
 1.551553017D-08-4.058458260D-12 7.909628340D+03  
 4.099317300D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10029.728  
 9.013902720D+05-3.463397050D+03 8.705804860D+00-4.018963410D-04  
 2.322774501D-08  
 6.280487330D-12-6.283095690D-16 3.337065340D+04-  
 2.900483458D+01  
 NHF2 Gurvich,1989 pt1 p388 pt2 p249.  
 2 tpris89 N 1.00H 1.00F 2.00 0.00 0.00 0 53.01149 -  
 103000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10807.439  
 -5.626113420D+04 1.205756556D+03-6.017529420D+00 3.760027690D-02-  
 4.619198600D-05  
 2.942475570D-08-7.598732360D-12 -1.897014374D+04  
 5.901715020D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10807.439  
 7.394278990D+05-4.004471770D+03 1.221322320D+01-6.970437730D-04  
 1.271073981D-07  
 -1.247136898D-11 5.086517590D-16 9.134195980D+03-  
 4.867843850D+01



NH4+ Gurvich,1989 pt1 p355 pt2 p220.  
 2 tpis89 N 1.00H 4.00E -1.00 0.00 0.00 0 18.03795  
 644904.945  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9978.772  
 -2.668315752D+05 3.763020690D+03-1.571327725D+01 4.548820210D-02-  
 4.379962120D-05  
 2.464478293D-08-5.961532330D-12 5.823284720D+04  
 1.112087189D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9978.772  
 4.141889000D+06-1.442072042D+04 2.011893564D+01-1.971492619D-03  
 3.112721421D-07  
 -2.602979969D-11 8.894342130D-16 1.664196236D+05-  
 1.201535728D+02

NO Gurvich,1978,1989 pt1 p326 pt2 p203.  
 3 tpis89 N 1.00O 1.00 0.00 0.00 0.00 0 30.00614  
 91271.310  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9179.110  
 -1.143916503D+04 1.536467592D+02 3.431468730D+00-2.668592368D-03  
 8.481399120D-06  
 -7.685111050D-09 2.386797655D-12 9.098214410D+03  
 6.728727490D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9179.110  
 2.239018716D+05-1.289651623D+03 5.433936030D+00-3.656034900D-04  
 9.880966450D-08  
 -1.416076856D-11 9.380184620D-16 1.750317656D+04-  
 8.501667090D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9179.110  
 -9.575303540D+08 5.912434480D+05-1.384566826D+02 1.694339403D-02-  
 1.007351096D-06  
 2.912584076D-11-3.295109350D-16 -4.677501240D+06  
 1.242081218D+03

NO+ Cp,S,IP(NO): Gurvich,1989 pt1 p330 pt2 p205.  
 3 g 5/99 N 1.00O 1.00E -1.00 0.00 0.00 0 30.00559  
 990809.704  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8670.104  
 1.398106635D+03-1.590446941D+02 5.122895400D+00-6.394388620D-03  
 1.123918342D-05  
 -7.988581260D-09 2.107383677D-12 1.187495132D+05-  
 4.398431810D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8670.104  
 6.069876900D+05-2.278395427D+03 6.080324670D+00-6.066847580D-04  
 1.432002611D-07  
 -1.747990522D-11 8.935014060D-16 1.322709615D+05-  
 1.519879837D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8670.104  
 2.676400347D+09-1.832948690D+06 5.099249390D+02-7.113819280D-02  
 5.317659880D-06  
 -1.963208212D-10 2.805268230D-15 1.443308939D+07-  
 4.324044460D+03

NOCL Gurvich,1989 pt1 p389. McBride,1992 METHOD PANDK.  
 2 g 4/99 N 1.00O 1.00CL 1.00 0.00 0.00 0 65.45884  
 52698.828

200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11364.488  
 2.308835209D+04-5.495983840D+02 7.730463360D+00-5.073910900D-03  
 1.062996184D-05  
 -8.793249700D-09 2.648180166D-12 7.389898390D+03-  
 1.318393617D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11364.488  
 -6.133413330D+05-3.919298830D+02 9.138917220D+00-2.605664613D-03  
 1.295687247D-06  
 -2.215378352D-10 1.280394898D-14 4.517328420D+03-  
 2.307323931D+01  
 NOF Gurvich,1989 pt1 p382. McBride,1992 METHOD NRRAO2.  
 2 g 4/99 N 1.000 1.00F 1.00 0.00 0.00 0 49.00454 -  
 65000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10720.271  
 4.755024260D+04-7.253904170D+02 7.213996360D+00-2.532427181D-03  
 6.377743900D-06  
 -5.518305880D-09 1.681935713D-12 -5.609722520D+03-  
 1.289663494D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10720.271  
 1.889069274D+06-6.731022660D+03 1.419018767D+01-3.693124620D-03  
 9.938575140D-07  
 -1.080748188D-10 4.210354430D-15 3.209900780D+04-  
 6.370266840D+01  
 NOF3 Gurvich,1989 pt1 p385 pt2 p246.  
 2 tpis89 N 1.000 1.00F 3.00 0.00 0.00 0 87.00135 -  
 187000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13697.653  
 1.488360135D+05-2.241049812D+03 1.302355027D+01 5.463976680D-03-  
 8.641865250D-06  
 5.913659030D-09-1.577009169D-12 -1.328342568D+04-  
 4.877320670D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13697.653  
 -2.785625217D+05-1.252321663D+03 1.390824337D+01-3.566687500D-04  
 7.785011060D-08  
 -8.850411970D-12 4.075980030D-16 -2.025651446D+04-  
 5.106881790D+01  
 NO2 Gurvich,1989 pt1 p332 pt2 p207.  
 2 g 4/99 N 1.000 2.00 0.00 0.00 0.00 0 46.00554  
 34193.019  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10208.175  
 -5.642038780D+04 9.633085720D+02-2.434510974D+00 1.927760886D-02-  
 1.874559328D-05  
 9.145497730D-09-1.777647635D-12 -1.547925037D+03  
 4.067851340D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10208.175  
 7.213001570D+05-3.832615200D+03 1.113963285D+01-2.238062246D-03  
 6.547723430D-07  
 -7.611335900D-11 3.328361050D-15 2.502497403D+04-  
 4.305129910D+01  
 NO2- Gurvich,1989 pt1 p334 pt2 p208.  
 2 tpis89 N 1.000 2.00E 1.00 0.00 0.00 0 46.00609 -  
 200035.591



298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10177.009  
 -1.282067858D+04 6.990138180D+02-2.812596273D+00 2.412894252D-02-  
 2.831606689D-05  
 1.670509365D-08-3.983330130D-12 -2.809915579D+04  
 4.063271640D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10177.009  
 1.325710335D+05-1.557032129D+03 8.126721920D+00-2.728626780D-04-  
 4.707541800D-08  
 2.826729008D-11-2.353985481D-15 -1.715795217D+04-  
 2.228575913D+01  
 NO2CL Gurvich,1989 pt1 p391. McBride,1992 METHOD NRRA01.  
 2 g 4/99 N 1.000 2.00CL 1.00 0.00 0.00 0 81.45824  
 12500.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12204.839  
 8.508370340D+03-1.805383762D+02 3.785388560D+00 1.414934934D-02-  
 1.423946765D-05  
 7.028226180D-09-1.374688214D-12 9.156246470D+02  
 6.958899670D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12204.839  
 -1.086773327D+05-1.452231167D+03 1.105656962D+01-4.000099280D-04  
 9.101543040D-08  
 -1.036656913D-11 4.781664810D-16 6.294267320D+03-  
 3.521240160D+01  
 NO2F Gurvich,1989 pt1 p349. McBride,1992 METHOD NRRA01. -  
 2 g 4/99 N 1.000 2.00F 1.00 0.00 0.00 0 65.00394 -  
 109000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11346.581  
 5.667856950D+04-6.538251950D+02 4.472771520D+00 1.368870672D-02-  
 1.460533236D-05  
 7.779227940D-09-1.689355106D-12 -1.102179443D+04  
 3.292083540D-01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11346.581  
 -1.008577842D+05-1.704722752D+03 1.122954945D+01-4.685215970D-04  
 1.047692566D-07  
 -1.189150595D-11 5.470307120D-16 -6.891719180D+03-  
 3.849788400D+01  
 NO3 Chase,1998 p1607.  
 2 j12/64 N 1.000 3.00 0.00 0.00 0.00 0 62.00494  
 71128.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10958.914  
 3.405398410D+04 2.266670652D+02-3.793081630D+00 4.170732700D-02-  
 5.709913270D-05  
 3.834158110D-08-1.021969284D-11 7.088112200D+03  
 4.273091810D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10958.914  
 -3.943872710D+05-8.244263530D+02 1.061325843D+01-2.448749816D-04  
 5.406060320D-08  
 -6.195466750D-12 2.870000149D-16 8.982011730D+03-  
 3.444666500D+01  
 NO3- Gurvich,1989 pt1 p335 pt2 p209.  
 2 tpris89 N 1.000 3.00E 1.00 0.00 0.00 0 62.00549 -  
 310779.531

298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10773.105  
 9.204813610D+04-3.911171150D+02-2.354356764D-01 2.836042108D-02-  
 3.461324080D-05  
 2.081787460D-08-5.021601270D-12 -3.576411500D+04  
 2.299942405D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10773.105  
 -3.110005758D+05-1.369087552D+03 1.101342913D+01-4.036878820D-04  
 8.902086470D-08  
 -1.019733480D-11 4.723330790D-16 -3.364321090D+04-  
 3.878432560D+01  
 NO3F Gurvich,1989 pt1 p384 pt2 p245.  
 2 tpris89 N 1.000 3.00F 1.00 0.00 0.00 0 81.00334  
 15000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14444.156  
 6.472832030D+04-8.213134310D+02 6.194917440D+00 1.805438628D-02-  
 1.996693240D-05  
 1.124482018D-08-2.680013077D-12 4.206661790D+03-  
 7.016103560D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14444.156  
 -3.411793300D+05-2.353908798D+03 1.628114887D+01-1.910415273D-03  
 4.690873560D-07  
 -5.686040140D-11 2.720906921D-15 9.760583980D+03-  
 6.558153610D+01  
 N2 Ref-Elm. Gurvich,1978 pt1 p280 pt2 p207.  
 3 tpris78 N 2.00 0.00 0.00 0.00 0.00 0 28.01348  
 0.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8670.104  
 2.210371497D+04-3.818461820D+02 6.082738360D+00-8.530914410D-03  
 1.384646189D-05  
 -9.625793620D-09 2.519705809D-12 7.108460860D+02-  
 1.076003316D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8670.104  
 5.877124060D+05-2.239249073D+03 6.066949220D+00-6.139685500D-04  
 1.491806679D-07  
 -1.923105485D-11 1.061954386D-15 1.283210415D+04-  
 1.586639599D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8670.104  
 8.310139160D+08-6.420733540D+05 2.020264635D+02-3.065092046D-02  
 2.486903333D-06  
 -9.705954110D-11 1.437538881D-15 4.938707040D+06-  
 1.672099736D+03  
 N2+ Gurvich,1989 pt1 p323 pt2 p200.  
 3 tpris89 N 2.00E -1.00 0.00 0.00 0.00 0 28.01293  
 1509508.424  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8671.100  
 -3.474047470D+04 2.696222703D+02 3.164916370D+00-2.132239781D-03  
 6.730476400D-06  
 -5.637304970D-09 1.621756000D-12 1.790004424D+05  
 6.832978450D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8671.100  
 -2.845599002D+06 7.058893030D+03-2.884886385D+00 3.068677059D-03-  
 4.361652310D-07

2.102514545D-11 5.411996470D-16 1.340388483D+05  
 5.090897450D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8671.100  
 -3.712829770D+08 3.139287234D+05-9.603518050D+01 1.571193286D-02-  
 1.175065525D-06  
 4.144441230D-11-5.621893090D-16 -2.217361867D+06  
 8.436270990D+02  
 N2- Chase,1998 p1623.  
 3 j 9/77 N 2.00E 1.00 0.00 0.00 0.00 0 28.01403  
 148183.282  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8674.282  
 -8.146227110D+04 9.063600790D+02-1.520054079D-01 6.023190840D-03-  
 2.897138445D-06  
 -4.129106680D-11 3.206989770D-13 1.218808548D+04  
 2.638069283D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8674.282  
 2.169637706D+05-1.275098516D+03 5.391095700D+00-3.198907510D-04  
 7.311051350D-08  
 -8.202017370D-12 3.740044700D-16 2.424964308D+04-  
 9.014930010D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8674.282  
 1.345850786D+06-1.060565497D+03 4.732026850D+00-5.091450050D-06  
 1.628212099D-09  
 -5.224243560D-14 6.796651250D-19 2.394627677D+04-  
 4.297857260D+00  
 NCN Hf:Gurvich,1991 pt1 p219. Jacox,1998 p180.  
 2 g 6/01 N 2.00C 1.00 0.00 0.00 0.00 0 40.02418  
 500456.573  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10180.177  
 -5.634680700D+04 7.323804580D+02-7.821401840D-01 1.838552441D-02-  
 1.950836491D-05  
 1.035712021D-08-2.208158483D-12 5.539789700D+04  
 2.905309285D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10180.177  
 -1.641880975D+05-7.767840750D+02 7.999981870D+00-1.659081508D-04  
 2.983403318D-08  
 -3.120157047D-12 1.992698720D-16 6.184424480D+04-  
 2.149108520D+01  
 N2D2,cis Hf:Use NASA data for N2H2,H,&D. Chase,1998 p1044 6/77.  
 2 g 6/01 N 2.00D 2.00 0.00 0.00 0.00 0 32.04168  
 202857.330  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10308.037  
 -2.743733656D+04 7.149808830D+02-2.223247620D+00 2.088722282D-02-  
 1.821711897D-05  
 8.844079940D-09-1.918010649D-12 2.011115649D+04  
 3.637100570D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10308.037  
 8.798074710D+05-5.299362040D+03 1.355007485D+01-1.316635227D-03  
 2.755816197D-07  
 -3.036294387D-11 1.365324117D-15 5.356311890D+04-  
 6.271215500D+01  
 N2F2 Gurvich,1989 pt1 p377 pt2 p237.

2 tpi89 N 2.00F 2.00 0.00 0.00 0.00 0 66.01029  
 62373.546  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12868.756  
 1.543893150D+04-2.183635130D+02 3.890284250D+00 1.674017740D-02-  
 2.056393090D-05  
 1.258692110D-08-3.110498290D-12 7.052038700D+03  
 5.265868260D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12868.756  
 -1.824883860D+05-9.534029960D+02 1.069795480D+01-2.759968700D-04  
 6.055439700D-08  
 -6.911215080D-12 3.192587230D-16 9.283466960D+03-  
 3.246968590D+01  
 N2F4 Gurvich,1989 pt1 p380 pt2 p240.  
 2 tpi89 N 2.00F 4.00 0.00 0.00 0.00 0 104.00709 -  
 22000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17811.571  
 1.162914512D+05-1.538660418D+03 9.054033050D+00 2.862113563D-02-  
 4.332286990D-05  
 3.067642499D-08-8.455474110D-12 2.865277526D+03-  
 2.476492891D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17811.571  
 -5.188594710D+05-6.702256510D+02 1.650109262D+01-2.006404436D-04  
 4.436752510D-08  
 -5.089808880D-12 2.359374159D-16 -5.281488900D+03-  
 6.040513320D+01  
 N2H2 Gurvich,1989 pt1 p356.Trans,cis,& 1,1 in equilibrium.  
 2 g 5/99 N 2.00H 2.00 0.00 0.00 0.00 0 30.02936  
 211858.756  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9996.961  
 -1.504005163D+05 2.346687716D+03-9.405430290D+00 3.284299800D-02-  
 3.121920401D-05  
 1.721283190D-08-4.014537220D-12 1.319384041D+04  
 7.832383030D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9996.961  
 6.217567870D+06-1.753952096D+04 2.022730509D+01-9.757297660D-04-  
 4.208416740D-07  
 1.117921171D-10-7.627102210D-15 1.374152574D+05-  
 1.199559128D+02  
 NH2NO2 Aminyl Nitrite. Gurvich,1989 pt1 p370 pt2 p233.  
 2 tpi89 N 2.00H 2.000 2.00 0.00 0.00 0 62.02816 -  
 26000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12163.853  
 -4.573035060D+04 1.201365987D+03-8.105984110D+00 5.402715200D-02-  
 6.438074450D-05  
 4.025097920D-08-1.025154190D-11 -9.615785160D+03  
 6.867353550D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12163.853  
 1.654040575D+06-8.125220880D+03 2.021742772D+01-1.244291821D-03  
 2.122804183D-07  
 -1.948359653D-11 7.439351360D-16 4.230822580D+04-  
 1.016190160D+02  
 N2H4 Gurvich,1989 pt1 p360 pt2 p225.

2 g 4/99 N 2.00H 4.00 0.00 0.00 0.00 0 32.04524  
 95180.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11449.304  
 -1.660756354D+05 3.035416736D+03-1.736889823D+01 7.159834020D-02-  
 8.866799300D-05  
 5.798970280D-08-1.530037218D-11 -3.731927230D+03  
 1.190002255D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11449.304  
 3.293486700D+06-1.199850628D+04 2.104406814D+01-1.399381724D-03  
 1.933173351D-07  
 -1.318016127D-11 3.166400170D-16 8.348433700D+04-  
 1.155750987D+02  
 N20 Gurvich,1989 pt1 p337 pt2 p210.  
 2 g 4/99 N 2.00O 1.00 0.00 0.00 0.00 0 44.01288  
 81600.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9580.935  
 4.288225970D+04-6.440118440D+02 6.034351430D+00 2.265394436D-04  
 3.472782850D-06  
 -3.627748640D-09 1.137969552D-12 1.179405506D+04-  
 1.003128297D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9580.935  
 3.438448040D+05-2.404557558D+03 9.125636220D+00-5.401667930D-04  
 1.315124031D-07  
 -1.414215100D-11 6.381066870D-16 2.198632638D+04-  
 3.147804743D+01  
 N20+ Chase,1998 p1625.  
 2 j12/70 N 2.00O 1.00E -1.00 0.00 0.00 0 44.01233  
 1332956.507  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10623.407  
 -5.624147080D+04 6.696211610D+02 8.781456190D-02 1.524476027D-02-  
 1.527290811D-05  
 7.827237390D-09-1.646739623D-12 1.557295192D+05  
 2.562355058D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10623.407  
 -2.983553254D+04-1.179455967D+03 8.300186690D+00-2.887267217D-04  
 5.705105010D-08  
 -5.958885120D-12 2.835725557D-16 1.646021769D+05-  
 2.287356344D+01  
 N203 Gurvich,1989 pt1 p338 pt2 p211.  
 2 g 4/99 N 2.00O 3.00 0.00 0.00 0.00 0 76.01168  
 86630.595  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17120.855  
 -9.204444170D+04 9.295520150D+02 3.203664810D+00 1.356473078D-02-  
 6.262966070D-06  
 -1.402915559D-09 1.431620930D-12 3.313622080D+03  
 1.844431111D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17120.855  
 7.783881860D+05-4.483024660D+03 1.666668024D+01-2.062143878D-03  
 5.309541710D-07  
 -6.190451220D-11 2.692956658D-15 3.360912450D+04-  
 6.739212230D+01  
 N204 Gurvich,1989 pt1 p342 pt2 p212.

2 tpis89 N 2.000 4.00 0.00 0.00 0.00 0 92.01108  
 11110.919  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16741.231  
 -3.804751440D+04 5.612828890D+02-2.083648324D-01 3.887087820D-02-  
 4.422412260D-05  
 2.498812310D-08-5.679102380D-12 -3.310794730D+03  
 2.963924970D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16741.231  
 -4.582843760D+05-1.604749805D+03 1.674102133D+01-5.091385080D-04  
 1.143634670D-07  
 -1.316288176D-11 5.976316620D-16 4.306900520D+03-  
 6.569450250D+01  
 N205 Gurvich,1989 pt1 p343 pt2 p213.  
 2 g 4/99 N 2.000 5.00 0.00 0.00 0.00 0 108.01048  
 13300.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 20797.425  
 4.007828170D+04-8.769675120D+02 1.055932981D+01 1.394613859D-02-  
 8.884346920D-06  
 8.500431150D-10 7.791550910D-13 3.038962037D+03-  
 2.386831749D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 20797.425  
 -5.325578960D+04-3.109277389D+03 2.036088958D+01-9.959901140D-04  
 2.401398635D-07  
 -3.057161911D-11 1.495915511D-15 1.336957281D+04-  
 8.298623230D+01  
 N3 Gurvich,1989 pt1 p325 pt2 p202.  
 2 tpis89 N 3.00 0.00 0.00 0.00 0.00 0 42.02022  
 436000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9570.906  
 3.337406790D+04-2.965683604D+02 3.314279150D+00 6.721685360D-03-  
 4.181126390D-06  
 8.618442360D-10 6.883352530D-14 5.298840620D+04  
 5.312780770D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9570.906  
 2.529264658D+05-2.362876591D+03 9.135267130D+00-6.212870850D-04  
 1.324094351D-07  
 -1.478989640D-11 6.721230470D-16 6.412695390D+04-  
 3.135825545D+01  
 N3H Gurvich,1989 pt1 p362 pt2 p226.  
 2 g 4/99 N 3.00H 1.00 0.00 0.00 0.00 0 43.02816  
 294000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10947.183  
 3.242576060D+03 6.692664890D+01 1.766142217D+00 1.487411419D-02-  
 1.539086440D-05  
 9.172303550D-09-2.337205474D-12 3.392069700D+04  
 1.513752475D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10947.183  
 1.170469241D+06-5.102451990D+03 1.278288910D+01-8.409487160D-04  
 1.592142834D-07  
 -1.512289051D-11 6.102906630D-16 6.428344470D+04-  
 5.513118690D+01  
 Na Hf:Cox,1989. Martin,1981. Gordon,1999.

3 g 8/97 NA 1.00 0.00 0.00 0.00 0.00 0 22.98977  
107500.000  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428  
0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 1.218382949D+04  
4.244028180D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428  
9.525723380D+05-2.623807254D+03 5.162596620D+00-1.210218586D-03  
2.306301844D-07  
-1.249597843D-11 7.226771190D-16 2.912963564D+04-  
1.519717061D+01  
6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428  
1.592533392D+09-9.717836660D+05 2.238443963D+02-2.380930558D-02  
1.352018117D-06  
-3.936971110D-11 4.630689121D-16 7.748677260D+06-  
1.939615505D+03

Na+ Martin,1981. Gordon,1999.

3 g 1/98 NA 1.00E -1.00 0.00 0.00 0.00 0 22.98922  
609542.928  
298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428  
0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 7.256537070D+04  
3.550845080D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428  
0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 7.256537070D+04  
3.550845080D+00  
6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428  
3.401202990D+04-2.137774622D+01 2.505443851D+00-7.186631690D-07  
5.188796390D-11  
-1.944511626D-15 2.959355125D-20 7.273413620D+04  
3.503904060D+00

Na- Hotop,1985. Gordon,1999.

3 g 4/97 NA 1.00E 1.00 0.00 0.00 0.00 0 22.99032  
48453.428  
298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428  
0.000000000D+00 0.000000000D+00 2.500000001D+00 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 5.082199670D+03  
3.550916790D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428  
0.000000000D+00 0.000000000D+00 2.500000001D+00 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 5.082199670D+03  
3.550916790D+00  
6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428  
0.000000000D+00 0.000000000D+00 2.500000001D+00 0.000000000D+00  
0.000000000D+00

0.000000000D+00 0.000000000D+00 5.082199670D+03  
 3.550916790D+00  
 NaAlF4 Gurvich,1982 pt1 p359 pt2 p393.  
 2 tpris82 NA 1.00AL 1.00F 4.00 0.00 0.00 0 125.96492 -  
 1857841.546  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 20808.667  
 1.315359536D+05-2.394685695D+03 1.909539612D+01 1.044339733D-03-  
 6.949754130D-06  
 6.769098140D-09-2.176199098D-12 -2.150512366D+05-  
 7.505102130D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 20808.667  
 -3.571177930D+05-2.496543879D+02 1.618634511D+01-7.449049300D-05  
 1.644510872D-08  
 -1.883696066D-12 8.719877450D-17 -2.279533538D+05-  
 5.370665140D+01  
 NaBO2 Gurvich,1982 pt1 p358 pt2 p392.  
 2 tpris82 NA 1.00B 1.00O 2.00 0.00 0.00 0 65.79957 -  
 633449.330  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13682.670  
 5.046867360D+04-8.699970600D+02 8.942208240D+00 1.092655824D-03  
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 8.595814050D+04-1.691902222D+03 1.118847517D+01-4.564202310D-04  
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 -1.101655008D-11 5.029172760D-16 -6.949292060D+04-  
 3.416353130D+01  
 NaBr Gurvich,1982 pt1 p342 pt2 p379.  
 2 tpris82 NA 1.00BR 1.00 0.00 0.00 0.00 0 102.89377 -  
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 9821.118  
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 2.457391648D-06  
 1.739334522D-09-4.796701380D-13 -1.926491755D+04  
 6.404382860D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9821.118  
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 1.856478949D+01  
 NaCN Chase,1998 p634.  
 2 j 3/66 NA 1.00C 1.00N 1.00 0.00 0.00 0 49.00721  
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 12125.972  
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 -1.319387974D-08 3.589766560D-12 1.297820493D+04-  
 2.988519559D+01  
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 12125.972  
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 9.362229310D-08



-1.033071320D-11 4.650466810D-16 2.010926347D+04-  
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 NaCl Gurvich,1982 pt1 p337 pt2 p375.  
 2 tpris82 NA 1.00CL 1.00 0.00 0.00 0.00 0 58.44247 -  
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 -9.667032250D-09 2.746261290D-12 -1.950409477D+04-  
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 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9615.116  
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 1.491128988D-08  
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 2 tpris82 NA 1.00F 1.00 0.00 0.00 0.00 0 41.98817 -  
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 -4.820425730D-09 1.364849175D-12 -3.352940890D+04-  
 1.403212229D+01  
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 9225.111  
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 NaH Gurvich,1982 pt1 p326 pt2 p366.  
 2 tpris82 NA 1.00H 1.00 0.00 0.00 0.00 0 23.99771  
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 2.990041189D-06  
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 1.222070060D+02  
 NaI Gurvich,1982 pt1 p345 pt2 p382.  
 2 tpris82 NA 1.00I 1.00 0.00 0.00 0.00 0 149.89424 -  
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 5.566881310D-06  
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 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
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-2.285837754D-10 1.195889950D-14 3.253893620D+04-  
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 NaLi Gurvich,1982 pt1 p363 pt2 p396.  
 2 tpris82 NA 1.00LI 1.00 0.00 0.00 0.00 0 29.93077  
 178598.320  
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 1.965726597D-06  
 2.086472026D-09-8.195988110D-13 2.016224293D+04  
 1.413253322D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9993.120  
 1.091664860D+07-3.480010640D+04 4.614311920D+01-2.260951051D-02  
 5.685324370D-06  
 -6.458143300D-10 2.696508992D-14 2.394431755D+05-  
 2.961780126D+02  
 NaNO2 Gurvich,1982 pt1 p352 pt2 p387.  
 2 g10/99 NA 1.00N 1.000 2.00 0.00 0.00 0 68.99531 -  
 166292.779  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14807.221  
 -6.934460610D+04 1.115432670D+03-1.816284973D+00 2.916366016D-02-  
 3.505788520D-05  
 2.128602855D-08-5.226211990D-12 -2.707275053D+04  
 4.121853340D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14807.221  
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 NaNO3 Gurvich,1982 pt1 p355 pt2 p389.  
 2 tpris82 NA 1.00N 1.000 3.00 0.00 0.00 0 84.99471 -  
 285528.711  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15401.289  
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 5.141702580D-05  
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 4.174749530D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15401.289  
 -3.225592190D+05-1.396782195D+03 1.403092409D+01-4.098161770D-04  
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 NaO Gurvich,1982 pt1 p318 pt2 p358.  
 2 tpris82 NA 1.000 1.00 0.00 0.00 0.00 0 38.98917  
 106505.317  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9753.117  
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 6.330775390D-06  
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NaOH Gurvich,1996b.  
2 g12/96 NA 1.000 1.00H 1.00 0.00 0.00 0 39.99711 -  
191000.000  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
11397.671  
3.442036740D+04-7.923218180D+02 8.997932300D+00-4.079844520D-03  
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-5.119189340D-10-1.541016409D-13 -2.086951091D+04-  
2.510590090D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
11397.671  
8.753787760D+05-2.342514649D+03 7.978469890D+00 1.016451512D-04-  
6.268531950D-08  
1.022715136D-11-5.713286410D-16 -9.509901710D+03-  
2.202310401D+01

NaOH+ Chase,1998 p1297 12/71. Jacox,1994.  
3 g 2/01 NA 1.000 1.00H 1.00E -1.00 0.00 0 39.99656  
683862.371  
298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
11694.871  
2.278039363D+04-6.672194220D+02 8.921593120D+00-4.481263270D-03  
3.951883920D-06  
-1.173341234D-09 2.041806631D-14 8.363382190D+04-  
2.258912262D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
11694.871  
8.815413650D+05-2.363159755D+03 8.053203930D+00 7.271279740D-05-  
5.897417890D-08  
1.007487881D-11-5.474406210D-16 9.584441650D+04-  
2.079484012D+01  
6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
11694.871  
-2.839326542D+07 1.778338286D+04 2.821047612D+00 5.793749100D-04-  
3.328793850D-08  
9.421248450D-13-1.072317149D-17 -6.175194270D+04  
2.465488033D+01

Na2 Gurvich,1982 pt1 p314 pt2 p357.  
2 tpis82 NA 2.00 0.00 0.00 0.00 0.00 0 45.97954  
142339.125  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
10403.125  
6.848628680D+03-1.530836599D+02 5.325230390D+00-1.944906088D-03  
2.657477888D-06  
-9.096841120D-10-2.448756730D-13 1.649170574D+04-  
2.653564394D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
10403.125  
1.929940758D+07-6.269280120D+04 8.267682110D+01-4.565137810D-02  
1.259515667D-05  
-1.560445735D-09 7.024677170D-14 4.090820800D+05-  
5.509970890D+02

Na2Br2 Gurvich,1982 pt1 p342 pt2 p380.  
2 tpis82 NA 2.00BR 2.00 0.00 0.00 0.00 0 205.78754 -  
480848.453  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
19591.547  
-1.384946731D+04-1.573241177D+02 1.063192589D+01-1.383418339D-03  
1.697156537D-06

-1.092992547D-09 2.870988020D-13 -6.010391820D+04-  
1.861473856D+01  
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19591.547  
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2.358676253D-10  
-2.857194816D-14 1.381909879D-18 -6.090039920D+04-  
1.494517863D+01  
Na2CL2 Gurvich,1982 pt1 p338 pt2 p376.  
2 tpris82 NA 2.00CL 2.00 0.00 0.00 0.00 0 116.88494 -  
564401.783  
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18699.327  
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3.286359480D-06  
-2.105377639D-09 5.508056610D-13 -6.938675430D+04-  
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18699.327  
-4.412105230D+04-5.393491280D+00 1.000453407D+01-1.981155641D-06  
4.680188200D-10  
-5.648940680D-14 2.724721177D-18 -7.098063410D+04-  
1.787231167D+01  
Na2F2 Gurvich,1982 pt1 p333 pt2 p372.  
2 tpris82 NA 2.00F 2.00 0.00 0.00 0.00 0 83.97635 -  
834062.776  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
16682.330  
2.351580802D+04-1.000737062D+03 1.375845076D+01-7.838346980D-03  
9.276288700D-06  
-5.813612970D-09 1.495354820D-12 -9.835831880D+04-  
4.381148090D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
16682.330  
-9.030750690D+04-1.893938035D+01 1.001535518D+01-6.539675450D-06  
1.516333603D-09  
-1.804877459D-13 8.613474920D-18 -1.034896664D+05-  
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Na2I2 Gurvich,1982 pt1 p346 pt2 p383.  
2 tpris82 NA 2.00I 2.00 0.00 0.00 0.00 0 299.78848 -  
356869.932  
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20246.068  
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1.487509548D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
20246.068  
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1.360287207D-10  
-1.650916036D-14 7.996149680D-19 -4.596921750D+04-  
1.276523965D+01  
Na2O Gurvich,1982 pt1 p321 pt2 p361.  
2 tpris82 NA 2.00O 1.00 0.00 0.00 0.00 0 61.97894 -  
16559.830  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
14410.170  
3.901149290D+04-7.266207890D+02 9.623710780D+00-3.556418640D-03  
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-1.835177736D-09 4.062134710D-13 -4.593073250D+02-  
 2.349565832D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14410.170  
 -6.600525160D+04-2.569021634D+01 7.519385420D+00-7.811635240D-06  
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 -1.996634558D-13 9.276433550D-18 -4.297339650D+03-  
 1.063530214D+01  
 Na2O+ Gurvich,1982 pt1 p322 pt2 p362.  
 2 tpris82 NA 2.000 1.00E -1.00 0.00 0.00 0 61.97839  
 520833.968  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14606.568  
 2.647969755D+04-5.969062160D+02 9.294129530D+00-3.080702005D-03  
 3.080460653D-06  
 -1.669452593D-09 3.789784140D-13 6.347310250D+04-  
 2.025274459D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14606.568  
 -5.740909330D+04-1.989178143D+01 7.515295260D+00-6.258333230D-06  
 1.407321045D-09  
 -1.635833952D-13 7.662445130D-18 6.032977470D+04-  
 9.426526740D+00  
 Na2O2 Gurvich,1982 pt1 p324 pt2 p364.  
 2 tpris82 NA 2.000 2.00 0.00 0.00 0.00 0 77.97834 -  
 123930.345  
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 15565.255  
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 1.003950603D-09-4.447732070D-13 -1.058858918D+04-  
 4.021811780D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15565.255  
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 7.577721890D-09  
 -8.701256730D-13 4.036061390D-17 -1.780300574D+04-  
 2.386789190D+01  
 Na2O2H2 Gurvich,1996b.  
 2 g 8/01 NA 2.000 2.00H 2.00 0.00 0.00 0 79.99422 -  
 624000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19346.141  
 1.089414289D+05-2.634822704D+03 2.306608858D+01-1.689310193D-02  
 1.673483190D-05  
 -7.821166010D-09 1.475034470D-12 -6.593137330D+04-  
 9.802987580D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
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 1.236951748D-07  
 2.025311778D-11-1.132991623D-15 -4.856245570D+04-  
 6.813480980D+01  
 Na2SO4 Gurvich,1982 pt1 p349 pt2 p385.  
 2 tpris82 NA 2.00S 1.000 4.00 0.00 0.00 0 142.04314 -  
 1040132.302  
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 20971.698  
 8.344283210D+04-1.210880769D+03 8.742353000D+00 3.600796630D-02-  
 5.117645960D-05

3.481569040D-08-9.321931220D-12 -1.217387045D+05-  
 2.061504729D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 20971.698  
 -5.754483110D+05-9.817060340D+02 1.973310397D+01-2.936395520D-04  
 6.498708170D-08  
 -7.462479400D-12 3.462491660D-16 -1.270597762D+05-  
 7.667870540D+01  
 Na3CL3 Gurvich,1982 pt1 p339 pt2 p377.  
 2 tpis82 NA 3.00CL 3.00 0.00 0.00 0.00 0 175.32741 -  
 912674.509  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 29477.157  
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 5.646438220D-06  
 -3.604760320D-09 9.405556240D-13 -1.119270172D+05-  
 5.290105730D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 29477.157  
 -7.160297970D+04-9.573493810D+00 1.600799614D+01-3.478356970D-06  
 8.190943690D-10  
 -9.863210030D-14 4.749005350D-18 -1.147252948D+05-  
 4.031342930D+01  
 Na3F3 Gurvich,1982 pt1 p334 pt2 p373.  
 2 tpis82 NA 3.00F 3.00 0.00 0.00 0.00 0 125.96452 -  
 1348015.386  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 25602.274  
 5.247030350D+04-1.775597273D+03 2.250927609D+01-1.333033615D-02  
 1.555790239D-05  
 -9.646011460D-09 2.460254271D-12 -1.580736389D+05-  
 8.580122370D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 25602.274  
 -1.553995698D+05-3.551970190D+01 1.602841159D+01-1.198056094D-05  
 2.757248730D-09  
 -3.263300970D-13 1.550483212D-17 -1.672141773D+05-  
 4.753780680D+01  
 Nb Hf:Gurvich,1982. Moore,1971. Moore,1970a. Gordon,1999.  
 3 g 3/98 NB 1.00 0.00 0.00 0.00 0.00 0 92.90638  
 723113.099  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8354.099  
 7.889660670D+04-1.212813914D+03 1.034579819D+01-1.676630056D-02  
 1.979119979D-05  
 -1.218224409D-08 3.058098336D-12 9.165315140D+04-  
 3.594742850D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8354.099  
 -1.096553196D+06 2.546650713D+03 2.236054882D+00-1.280029198D-03  
 8.464237990D-07  
 -1.486269508D-10 8.714309406D-15 6.879124550D+04  
 1.398169030D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8354.099  
 1.818626365D+09-1.032414940D+06 2.308238005D+02-2.445004311D-02  
 1.395626888D-06  
 -4.087233010D-11 4.826490497D-16 8.359622560D+06-  
 1.997797290D+03  
 Nb+ Moore,1971. Moore,1970a. Gordon,1999.

3 g 7/97 NB 1.00E -1.00 0.00 0.00 0.00 0 92.90583  
 1393604.675  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8589.075  
 1.314447859D+05-2.000135035D+03 1.505024212D+01-2.996583942D-02  
 3.729868630D-05  
 -2.269869569D-08 5.449089902D-12 1.760054029D+05-  
 6.224595520D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8589.075  
 -1.077639646D+06 2.159046421D+03 2.310604767D+00-5.363991760D-04  
 5.057915090D-07  
 -1.032401533D-10 6.629241280D-15 1.517945546D+05  
 1.210678502D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8589.075  
 1.876113970D+07-2.202847919D+04 1.427004521D+01-2.295936786D-03  
 2.430819459D-07  
 -1.116131589D-11 1.836221996D-16 3.245415600D+05-  
 8.494555710D+01  
 Nb- Hotop,1985. Gordon,1999.  
 3 g 9/97 NB 1.00E 1.00 0.00 0.00 0.00 0 92.90693  
 631054.008  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8653.808  
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 7.401859030D-06  
 -5.016302070D-09 1.314100719D-12 7.178828870D+04  
 5.155510070D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8653.808  
 1.117458019D+05 1.340072834D+02 2.391474129D+00 4.524813430D-05-  
 1.025345000D-08  
 1.195577988D-12-5.606330450D-17 7.473996750D+04  
 9.675315610D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8653.808  
 -1.279446680D+05 1.664265071D+02 2.463334336D+00 4.161717840D-06-  
 2.573750764D-10  
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 9.186188470D+00  
 NbCL5 Chase,1998 p918.  
 2 j12/74 NB 1.00CL 5.00 0.00 0.00 0.00 0 270.16988 -  
 703330.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 26343.163  
 7.348277970D+04-1.919172996D+03 2.290799567D+01-1.404352774D-02  
 1.638106985D-05  
 -1.018941843D-08 2.612266639D-12 -7.974118810D+04-  
 8.439637920D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 26343.163  
 -1.563816638D+05-4.450521280D+01 1.603544630D+01-1.489949737D-05  
 3.420777920D-09  
 -4.041124420D-13 1.917266128D-17 -8.962815120D+04-  
 4.374583440D+01  
 NbO Gurvich,1982 pt1 p76 pt2 p78.  
 3 tpris82 NB 1.00O 1.00 0.00 0.00 0.00 0 108.90578  
 210988.706  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8780.106

-6.797834360D+03 2.839767438D+02 5.645708400D-01 1.134928619D-02-  
1.549821141D-05  
1.047624988D-08-2.762937835D-12 2.317993893D+04  
2.365708974D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
8780.106  
5.532258780D+05-1.287669306D+03 4.980066040D+00 1.116014163D-04  
4.031838680D-08  
1.048773710D-11-1.893595022D-15 3.268457790D+04-  
1.868958549D+00  
6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
8780.106  
5.210846640D+07-7.508889140D+04 3.023869608D+01-2.881829240D-03  
1.595446362D-07  
-4.532772640D-12 5.266479160D-17 5.788974420D+05-  
2.169255418D+02  
NbOCL3 Barin,1989. Wagman,1982.  
2 bar 89 NB 1.000 1.00CL 3.00 0.00 0.00 0 215.26388 -  
752300.000  
298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
20631.000  
-1.108482359D+05 1.173066983D+02 1.165558433D+01 1.287422064D-03-  
1.659778281D-06  
1.102107826D-09-2.949903264D-13 -9.504023920D+04-  
2.386450719D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
20631.000  
-1.515551427D+05 5.305545230D+01 1.228915282D+01-1.527366571D-04  
6.778576440D-08  
-9.365170650D-12 4.670036930D-16 -9.490768120D+04-  
2.745264461D+01  
NbO2 Gurvich,1982 pt1 p80 pt2 p81.  
2 tpi82 NB 1.000 2.00 0.00 0.00 0.00 0 124.90518 -  
201266.752  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
10654.352  
1.739046582D+04 3.881029440D+01 9.024299120D-01 1.909523319D-02-  
2.667013583D-05  
1.813901051D-08-4.872365880D-12 -2.528518558D+04  
2.289323379D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
10654.352  
-6.851859900D+05 9.112249320D+02 6.339199840D+00-8.230080300D-05  
1.984439605D-07  
-3.261171490D-11 1.602430854D-15 -3.325027320D+04-  
3.559556550D+00  
Ne Ref-Elm. Moore,1971. Moore,1970a. Gordon,1999.  
3 g 5/97 NE 1.00 0.00 0.00 0.00 0.00 0 20.17970  
0.000  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428  
0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -7.453750000D+02  
3.355322720D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428  
0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -7.453750000D+02  
3.355322720D+00



6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 -1.238252746D+07 6.958579580D+03 1.016709287D+00 1.424664555D-04-  
 4.803933930D-09  
 -1.170213183D-13 8.415153652D-18 -5.663933630D+04  
 1.648438697D+01  
 Ne+ Moore,1971. Moore,1970a. Gordon,1999.  
 3 g 3/97 NE 1.00E -1.00 0.00 0.00 0.00 0 20.17915  
 2086965.946  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6304.214  
 7.281551480D+04-8.695697990D+02 6.108646970D+00-5.841356930D-03  
 5.041044170D-06  
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 1.673449355D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6304.214  
 -1.112742658D+05 4.765697970D+02 2.196650531D+00 1.102593151D-04-  
 2.287564425D-08  
 2.510218183D-12-1.126646096D-16 2.472536944D+05  
 7.466140540D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6304.214  
 -5.615474110D+04 1.418980160D+02 2.475716842D+00 1.944430992D-06-  
 6.323099200D-11  
 -1.313313446D-16 3.534699010D-20 2.494452217D+05  
 5.366882220D+00  
 Ni Hf:Hultgren,1973. Litzen,1993. Gordon,1999.  
 3 g 8/97 NI 1.00 0.00 0.00 0.00 0.00 0 58.69340  
 430116.605  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6825.013  
 -3.235810550D+04 6.015264620D+02-1.079270657D+00 1.089505519D-02-  
 1.369578748D-05  
 8.317725790D-09-2.019206968D-12 4.813810810D+04  
 2.718829200D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6825.013  
 -4.938262210D+05 1.092909991D+03 2.410485014D+00-1.599071827D-05-  
 1.047414069D-08  
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 9.677195600D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6825.013  
 3.492669880D+08-1.654227575D+05 3.349869360D+01-3.527085900D-03  
 3.240060240D-07  
 -1.604177606D-11 2.935430214D-16 1.409017848D+06-  
 2.672455567D+02  
 Ni+ Sugar,1985. Gordon,1999.  
 3 g 8/97 NI 1.00E -1.00 0.00 0.00 0.00 0 58.69285  
 1172594.573  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6205.773  
 -8.969386030D+04 1.173601500D+03-3.410620410D+00 1.390739137D-02-  
 1.501714923D-05  
 7.896337900D-09-1.648686761D-12 1.345589500D+05  
 4.031495160D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6205.773  
 -3.961999320D+06 1.017084853D+04-6.029331290D+00 2.770858029D-03-  
 8.902077700D-08

-5.541000580D-11 5.235342833D-15 7.340395120D+04  
7.137503100D+01  
6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6205.773  
5.286662360D+07-3.719827100D+04 1.470794435D+01-1.489309517D-03  
8.648712770D-08  
-1.705443550D-12 5.049635419D-18 4.253204090D+05-  
9.590502160D+01

Ni- Hotop,1985. Gordon,1999.  
3 g 9/97 NI 1.00E 1.00 0.00 0.00 0.00 0 58.69395  
311764.357  
298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6207.157  
-8.437624750D+04 1.135476552D+03-3.380615830D+00 1.423003786D-02-  
1.582586302D-05  
8.608840410D-09-1.875316029D-12 3.124307590D+04  
3.998061300D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6207.157  
-5.433424800D+05 1.182645330D+03 2.126441240D+00 3.730455940D-05  
6.953608430D-09  
-1.945719381D-12 1.271571579D-16 2.854759122D+04  
1.043462235D+01  
6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6207.157  
2.235741343D+06-7.539321100D+02 2.675777011D+00-2.056834268D-05  
1.297167360D-09  
-4.210909080D-14 5.520885950D-19 4.359114370D+04  
5.724516640D+00

NiCL Chase,1998 p794.  
2 j 9/77 NI 1.00CL 1.00 0.00 0.00 0.00 0 94.14610  
182004.000  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
9464.921  
-2.357997085D+04 2.205491630D+02 2.714260287D+00 4.453598470D-03-  
2.849162229D-06  
-1.691898007D-10 5.156699260D-13 1.957229490D+04  
1.423642590D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
9464.921  
-3.905769190D+06 9.961533990D+03-3.839432340D+00 2.767979391D-03-  
7.005959380D-08  
-5.741403660D-11 5.307635800D-15 -4.505397050D+04  
6.769402070D+01

NiCL2 Chase,1998 p840.  
2 j 9/77 NI 1.00CL 2.00 0.00 0.00 0.00 0 129.59880 -  
73931.000  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
14206.546  
7.109976530D+04-1.218958288D+03 1.208750596D+01-8.674403140D-03  
1.043608104D-05  
-6.298493010D-09 1.485857653D-12 -5.006998710D+03-  
3.499472730D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
14206.546  
1.585889817D+05-1.161488738D+03 9.608015380D+00-9.461224510D-04  
2.608172043D-07  
-3.264637250D-11 1.525950893D-15 -4.578985540D+03-  
2.212398041D+01

NiO Pedley,1983 p1012 p1019.

2 g12/00 NI 1.000 1.00 0.00 0.00 0.00 0 74.69280  
 297064.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8866.569  
 2.320630462D+04-1.907136094D+02 3.190178620D+00 5.291383490D-03-  
 8.080210430D-06  
 5.839812760D-09-1.639499596D-12 3.576711120D+04  
 7.841265670D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8866.569  
 -7.234091940D+04-8.035554270D+01 4.559221020D+00 2.305154510D-05  
 5.139832820D-09  
 -5.853474910D-13 2.697077329D-17 3.461143850D+04  
 1.209414814D+00  
 NiS Chase,1998 p1707.  
 2 j12/76 NI 1.00S 1.00 0.00 0.00 0.00 0 90.75940  
 357419.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9218.527  
 -1.272488974D+04 1.432801381D+02 2.471951556D+00 5.505271120D-03-  
 3.418355280D-06  
 -3.099052241D-10 6.268154670D-13 4.117716080D+04  
 1.517983488D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9218.527  
 -7.358128980D+05 1.178231095D+03 4.837865580D+00-3.931201390D-04  
 1.341974852D-07  
 -1.569591708D-11 6.677045060D-16 3.275565940D+04  
 3.690668810D+00  
 O D0(O2):Brix,1954. Moore,1976. Gordon,1999.  
 3 g 5/97 O 1.00 0.00 0.00 0.00 0.00 0 15.99940  
 249175.003  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6725.403  
 -7.953611300D+03 1.607177787D+02 1.966226438D+00 1.013670310D-03-  
 1.110415423D-06  
 6.517507500D-10-1.584779251D-13 2.840362437D+04  
 8.404241820D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6725.403  
 2.619020262D+05-7.298722030D+02 3.317177270D+00-4.281334360D-04  
 1.036104594D-07  
 -9.438304330D-12 2.725038297D-16 3.392428060D+04-  
 6.679585350D-01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6725.403  
 1.779004264D+08-1.082328257D+05 2.810778365D+01-2.975232262D-03  
 1.854997534D-07  
 -5.796231540D-12 7.191720164D-17 8.890942630D+05-  
 2.181728151D+02  
 O+ Martin,1993. Gordon,1999.  
 3 g 8/97 O 1.00E -1.00 0.00 0.00 0.00 0 15.99885  
 1568787.228  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 1.879352842D+05  
 4.393376760D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428

-2.166513208D+05 6.665456150D+02 1.702064364D+00 4.714992810D-04-  
 1.427131823D-07  
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 1.005690382D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 -2.143835383D+08 1.469518523D+05-3.680864540D+01 5.036164540D-03-  
 3.087873854D-07  
 9.186834870D-12-1.074163268D-16 -9.614208960D+05  
 3.426193080D+02  
 O- Gurvich,1989 pt1 p93. Hotop,1985. Gordon,1999.  
 3 g 1/97 O 1.00E 1.00 0.00 0.00 0.00 0 15.99995  
 101846.192  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6570.792  
 -5.695857110D+03 1.099287334D+02 2.184719661D+00 5.326359800D-04-  
 5.298878440D-07  
 2.870216236D-10-6.524692740D-14 1.093287498D+04  
 6.729863860D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6570.792  
 9.769363180D+03 7.159604780D+00 2.494961726D+00 1.968240938D-06-  
 4.304174850D-10  
 4.912083080D-14-2.271600083D-18 1.149554438D+04  
 4.837036440D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6570.792  
 5.662391000D+02 7.572340320D+00 2.498352500D+00 1.862632395D-07-  
 1.151227211D-11  
 3.688814210D-16-4.793297600D-21 1.148426000D+04  
 4.813406590D+00  
 OD Gurvich,1989 pt1 p135 pt2 p47.  
 2 tpi89 O 1.00D 1.00 0.00 0.00 0.00 0 18.01350  
 37221.508  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8999.108  
 2.118691536D+04-2.785982360D+02 5.456210120D+00-6.148119830D-03  
 9.117670560D-06  
 -5.527812710D-09 1.239794711D-12 4.711375030D+03-  
 7.616618910D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8999.108  
 7.832473160D+05-2.532992554D+03 5.952124650D+00-3.743595280D-04  
 4.959527620D-08  
 3.454454730D-12-7.380626800D-16 1.955142652D+04-  
 1.568898441D+01  
 OD- Gurvich,1989 pt1 p137 pt2 p48.  
 2 tpi89 O 1.00D 1.00E 1.00 0.00 0.00 0 18.01405 -  
 145382.896  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8642.104  
 5.606128320D+04-7.514156150D+02 7.544188470D+00-1.092083064D-02  
 1.503688938D-05  
 -9.351665840D-09 2.246466046D-12 -1.489548282D+04-  
 2.106498377D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8642.104  
 3.029467029D+05-1.079684654D+03 4.211417380D+00 6.260830070D-04-  
 2.411665054D-07  
 4.248425540D-11-2.387099102D-15 -1.162776255D+04-  
 4.724898790D+00

OH Gurvich,1978 pt1 p110 pt2 p37.

3 tps78 O 1.00H 1.00 0.00 0.00 0.00 0 17.00734  
39344.106  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
8813.106  
-1.998858990D+03 9.300136160D+01 3.050854229D+00 1.529529288D-03-  
3.157890998D-06  
3.315446180D-09-1.138762683D-12 3.239683480D+03  
4.674110790D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
8813.106  
1.017393379D+06-2.509957276D+03 5.116547860D+00 1.305299930D-04-  
8.284322260D-08  
2.006475941D-11-1.556993656D-15 2.044487130D+04-  
1.101282337D+01  
6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
8813.106  
2.847234193D+08-1.859532612D+05 5.008240900D+01-5.142374980D-03  
2.875536589D-07  
-8.228817960D-12 9.567229020D-17 1.468642377D+06-  
4.023555580D+02

OH+ Gurvich,1978 pt2 p39. Gurvich,1989 pt1 p117.

3 g 6/99 O 1.00H 1.00E -1.00 0.00 0.00 0 17.00679  
1290331.503  
298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
8603.103  
6.031630860D+04-7.573520300D+02 7.307752930D+00-9.506881670D-03  
1.202555795D-05  
-6.829026100D-09 1.501588659D-12 1.578579989D+05-  
1.950106996D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
8603.103  
5.040729100D+05-1.380052958D+03 4.125462200D+00 8.331948840D-04-  
3.442856290D-07  
6.792853950D-11-4.363872130D-15 1.633157066D+05-  
3.997058490D+00  
6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
8603.103  
1.158286700D+09-6.841280390D+05 1.576194558D+02-1.618421339D-02  
8.846128780D-07  
-2.475038507D-11 2.807730875D-16 5.615528970D+06-  
1.351879042D+03

OH- Gurvich,1989 pt1 p118 pt2 p32.

2 tps89 O 1.00H 1.00E 1.00 0.00 0.00 0 17.00789 -  
143190.296  
298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
8606.104  
2.910880827D+04-3.216904940D+02 4.851029050D+00-2.579035357D-03  
2.004980024D-06  
-7.956852960D-11-2.320495634D-13 -1.664039310D+04-  
7.121591300D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
8606.104  
4.711331170D+05-8.572336690D+02 3.166181210D+00 1.233581296D-03-  
3.999244580D-07  
6.239081670D-11-3.354343220D-15 -1.200002214D+04  
1.487736260D+00

O2 Ref-Elm. Gurvich,1989 pt1 p94 pt2 p9.

3 tps89 O 2.00 0.00 0.00 0.00 0.00 0 31.99880  
0.000

200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8680.104  
 -3.425563420D+04 4.847000970D+02 1.119010961D+00 4.293889240D-03-  
 6.836300520D-07  
 -2.023372700D-09 1.039040018D-12 -3.391454870D+03  
 1.849699470D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8680.104  
 -1.037939022D+06 2.344830282D+03 1.819732036D+00 1.267847582D-03-  
 2.188067988D-07  
 2.053719572D-11-8.193467050D-16 -1.689010929D+04  
 1.738716506D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8680.104  
 4.975294300D+08-2.866106874D+05 6.690352250D+01-6.169959020D-03  
 3.016396027D-07  
 -7.421416600D-12 7.278175770D-17 2.293554027D+06-  
 5.530621610D+02  
 O2+ Gurvich,1989 pt1 p98 pt2 p11.  
 3 tpi89 O 2.00E -1.00 0.00 0.00 0.00 0 31.99825  
 1171828.436  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9311.112  
 -8.607205450D+04 1.051875934D+03-5.432380470D-01 6.571166540D-03-  
 3.274263750D-06  
 5.940645340D-11 3.238784790D-13 1.345544668D+05  
 2.902709750D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9311.112  
 7.384654880D+04-8.459559540D+02 4.985164160D+00-1.611010890D-04  
 6.427083990D-08  
 -1.504939874D-11 1.578465409D-15 1.446321044D+05-  
 5.811230650D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9311.112  
 -1.562125524D+09 1.161406778D+06-3.302504720D+02 4.710937520D-02-  
 3.354461380D-06  
 1.167968599D-10-1.589754791D-15 -8.857866270D+06  
 2.852035602D+03  
 O2- Gurvich,1989 pt1 p100 pt2 p13.  
 2 g11/99 O 2.00E 1.00 0.00 0.00 0.00 0 31.99935 -  
 48027.921  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9349.611  
 1.883874344D+04 1.149551768D+02 1.518876821D+00 8.016111380D-03-  
 9.850571030D-06  
 6.044196210D-09-1.486439845D-12 -7.101538760D+03  
 1.501210380D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9349.611  
 -5.655208050D+04-2.367815862D+02 4.675833670D+00-2.197245300D-05  
 1.711509280D-08  
 -1.757645062D-12 8.248172790D-17 -5.960177750D+03-  
 2.436885556D+00  
 O3 Gurvich,1989 pt1 p101 pt2 p15.  
 2 g 8/01 O 3.00 0.00 0.00 0.00 0.00 0 47.99820  
 141800.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10366.305  
 -1.282314507D+04 5.898216640D+02-2.547496763D+00 2.690121526D-02-  
 3.528258340D-05

2.312290922D-08-6.044893270D-12 1.348368701D+04  
 3.852218580D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10366.305  
 -3.869662480D+07 1.023344994D+05-8.961551600D+01 3.706144970D-02-  
 4.137638740D-06  
 -2.725018591D-10 5.248188110D-14 -6.517918180D+05  
 7.029109520D+02  
 P Hf:Cox,1989. Martin,1985. Gordon,1999.  
 3 g 5/97 P 1.00 0.00 0.00 0.00 0.00 0 30.97376  
 316500.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 5.040866570D+01-7.639418650D-01 2.504563992D+00-1.381689958D-05  
 2.245585515D-08  
 -1.866399889D-11 6.227063395D-15 3.732421910D+04  
 5.359303481D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 1.261794642D+06-4.559838190D+03 8.918079310D+00-4.381401460D-03  
 1.454286224D-06  
 -2.030782763D-10 1.021022887D-14 6.541723960D+04-  
 3.915974795D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 -2.215392545D+07-4.566911180D+04 2.837245428D+01-4.483244040D-03  
 3.579413080D-07  
 -1.255311557D-11 1.590290483D-16 3.370905760D+05-  
 2.056960928D+02  
 P+ Martin,1985. Gordon,1999.  
 3 g 4/97 P 1.00E -1.00 0.00 0.00 0.00 0 30.97321  
 1336453.460  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8141.860  
 -7.316908110D+04 9.627979140D+02-3.693938050D-01 4.766778340D-03-  
 4.574768580D-06  
 2.371262331D-09-5.131314900D-13 1.549406849D+05  
 2.376640762D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8141.860  
 -5.594249360D+05 1.722576545D+03 8.430381090D-01 6.287368940D-04-  
 6.317195460D-08  
 -1.810842484D-12 4.318112570D-16 1.490493431D+05  
 1.845275207D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8141.860  
 1.362531054D+07-8.717502380D+03 4.747426280D+00-1.620871933D-04-  
 3.935548100D-10  
 4.845613020D-13-7.448402970D-18 2.284649718D+05-  
 1.346454894D+01  
 P- Hotop,1985. Gordon,1999.  
 3 g 4/97 P 1.00E 1.00 0.00 0.00 0.00 0 30.97431  
 238826.765  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6747.865  
 -1.008949093D+04 1.826468403D+02 1.962456304D+00 9.197377540D-04-  
 9.214998630D-07  
 5.012872360D-10-1.142677121D-13 2.703082432D+04  
 9.478137822D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6747.865

1.543488016D+04 9.495009340D+00 2.493170861D+00 2.700167711D-06-  
5.949210390D-10  
6.823766290D-14-3.166959910D-18 2.797572693D+04  
6.246793872D+00  
6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6747.865  
1.724147889D+03 1.074832503D+01 2.497654940D+00 2.655333078D-07-  
1.642839012D-11  
5.268015350D-16-6.849362660D-21 2.795482976D+04  
6.215849262D+00  
PCL Gurvich,1989 pt1 p431 pt2 p282.  
2 tpris89 P 1.00CL 1.00 0.00 0.00 0.00 0 66.42646  
134615.112  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
9291.112  
3.488861700D+04-5.603119340D+02 6.264568480D+00-3.183364370D-03  
3.495326840D-06  
-2.091034291D-09 5.418758600D-13 1.774653764D+04-  
8.074578922D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
9291.112  
-3.471681510D+05 9.935557930D+02 3.399430270D+00 4.019711700D-04  
8.295588390D-08  
-3.090212484D-11 2.106384858D-15 8.433591150D+03  
1.064901561D+01  
PCL2 Gurvich,1989 pt1 p432 pt2 p283.  
2 tpris89 P 1.00CL 2.00 0.00 0.00 0.00 0 101.87916 -  
54292.353  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
12248.757  
5.190084500D+04-1.060904200D+03 1.058549940D+01-6.879917530D-03  
7.620773180D-06  
-4.530115470D-09 1.116671660D-12 -3.220331180D+03-  
2.753519242D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
12248.757  
-8.349833970D+04-2.625249470D+01 7.020361810D+00-8.388768680D-06  
1.896784740D-09  
-2.214879920D-13 1.041653550D-17 -8.742993680D+03-  
6.234032024D+00  
PCL2- Gurvich,1989 pt1 p433 pt2 p284.  
2 tpris89 P 1.00CL 2.00E 1.00 0.00 0.00 0 101.87971 -  
356285.253  
298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
12453.247  
4.934832770D+04-9.601590540D+02 9.884769700D+00-4.950202950D-03  
4.946217870D-06  
-2.678675201D-09 6.076723610D-13 -3.998072400D+04-  
2.413132578D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
12453.247  
-8.564986760D+04-3.185555940D+01 7.024494960D+00-1.002251172D-05  
2.253747944D-09  
-2.619657192D-13 1.227059658D-17 -4.503811430D+04-  
6.721531195D+00  
PCL3 Gurvich,1989 pt1 p433 pt2 p285.  
2 tpris89 P 1.00CL 3.00 0.00 0.00 0.00 0 137.33186 -  
289500.000  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
15932.466



7.717745470D+04-1.617650860D+03 1.536080470D+01-1.011077050D-02  
 1.103408340D-05  
 -6.476121020D-09 1.579151140D-12 -2.955893640D+04-  
 5.244339671D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15932.466  
 -1.333076930D+05-4.145883210D+01 1.003186060D+01-1.301946160D-05  
 2.922916890D-09  
 -3.391869240D-13 1.586425530D-17 -3.800336680D+04-  
 2.050738661D+01  
 PCL5 Gurvich,1989 pt1 p435 pt2 p286.  
 2 tpris89 P 1.00CL 5.00 0.00 0.00 0.00 0 208.23726 -  
 376000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 23305.466  
 1.029070200D+05-2.515707460D+03 2.430114970D+01-1.564610690D-02  
 1.709873030D-05  
 -1.006011430D-08 2.460158790D-12 -3.722582370D+04-  
 9.816336250D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 23305.466  
 -2.255906890D+05-6.938542820D+01 1.605359630D+01-2.202156960D-05  
 4.971392290D-09  
 -5.799860050D-13 2.725970770D-17 -5.034234220D+04-  
 4.872455950D+01  
 PF Gurvich,1989 pt1 p425 pt2 p276.  
 2 tpris89 P 1.00F 1.00 0.00 0.00 0.00 0 49.97216 -  
 47944.793  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8891.107  
 2.227866728D+04-1.727508706D+02 3.085366934D+00 5.489718230D-03-  
 8.247972540D-06  
 5.868882910D-09-1.617252113D-12 -5.809279650D+03  
 7.709718850D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8891.107  
 -1.132572282D+06 3.200038550D+03 7.780502370D-01 1.969518902D-03-  
 4.365818970D-07  
 5.243648570D-11-2.618755712D-15 -2.766773009D+04  
 2.759312302D+01  
 PF+ Chase,1998 p1086.  
 3 j 6/77 P 1.00F 1.00E -1.00 0.00 0.00 0 49.97162  
 901518.000  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9429.848  
 -1.779138157D+04 3.909991270D+02 1.257434156D+00 7.861363750D-03-  
 9.342312680D-06  
 5.630915650D-09-1.370669924D-12 1.054873882D+05  
 1.901676576D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9429.848  
 -4.011525180D+04-1.597504413D+02 4.621397480D+00-2.378072183D-05  
 1.431831329D-08  
 -2.300109157D-12 1.694069882D-16 1.078633756D+05-  
 4.072343950D-02  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9429.848  
 -2.628686921D+07 1.300876535D+04 2.564713658D+00 3.269650350D-05  
 1.867188317D-08  
 -9.293307220D-13 1.456723674D-17 -2.640503508D+02  
 1.921588661D+01

PF- Chase,1998 p1087.

3 j 6/77 P 1.00F 1.00E 1.00 0.00 0.00 0 49.97271 -  
164046.000  
298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
9515.643  
7.705210950D+03-1.152432706D+02 4.254952310D+00 1.163521526D-03-  
1.627947259D-06  
1.084382815D-09-2.809490132D-13 -2.035558966D+04  
2.217923793D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
9515.643  
-1.303793388D+05 2.715526386D+02 4.137619810D+00 2.728610614D-04-  
7.644416250D-08  
1.182073001D-11-6.083906640D-16 -2.290799827D+04  
3.748526100D+00  
6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
9515.643  
-2.589702487D+07 2.274827883D+04-2.913204829D+00 1.134351740D-03-  
7.184766090D-08  
2.254067861D-12-2.781608692D-17 -1.940751937D+05  
6.372454240D+01

PFCL Gurvich,1989 pt1 p437 pt2 p288.

2 tpis89 P 1.00F 1.00CL 1.00 0.00 0.00 0 85.42486 -  
283184.119  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
11630.381  
5.490188530D+04-8.658679480D+02 7.944467650D+00 9.503779100D-04-  
3.339090210D-06  
3.023977817D-09-9.450377540D-13 -3.132843217D+04-  
1.440427413D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
11630.381  
-1.282143211D+05-9.739043550D+01 7.072661660D+00-2.903614134D-05  
6.408504490D-09  
-7.338993770D-13 3.396723170D-17 -3.600649260D+04-  
7.626498303D+00

PFCL- Gurvich,1989 pt1 p438 pt2 p289.

2 tpis89 P 1.00F 1.00CL 1.00E 1.00 0.00 0 85.42541 -  
529269.107  
298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
11742.793  
8.934336850D+04-1.266972513D+03 9.912194530D+00-3.877928300D-03  
3.036692411D-06  
-1.296559380D-09 2.324226580D-13 -5.894505710D+04-  
2.617050987D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
11742.793  
-1.231565150D+05-9.765861110D+01 7.074029570D+00-2.997070692D-05  
6.685280620D-09  
-7.722262200D-13 3.599382300D-17 -6.558817220D+04-  
8.208883327D+00

PFCL2 Gurvich,1989 pt1 p440 pt2 p292.

2 tpis89 P 1.00F 1.00CL 2.00 0.00 0.00 0 120.87756 -  
511925.340  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
14867.760  
8.266560560D+04-1.512138928D+03 1.303404207D+01-2.903247162D-03  
7.836652970D-07  
6.458340660D-10-3.737641820D-13 -5.644237870D+04-  
4.100906413D+01

1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14867.760  
 -1.864589813D+05-1.148004379D+02 1.008599754D+01-3.447456520D-05  
 7.627972010D-09  
 -8.753097430D-13 4.057788350D-17 -6.450472190D+04-  
 2.174055308D+01  
 PFCL4 Gurvich,1989 pt1 p442 pt2 p295.  
 2 tpis89 P 1.00F 1.00CL 4.00 0.00 0.00 0 191.78296 -  
 635016.440  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 21733.860  
 1.412071573D+05-2.882471080D+03 2.387345233D+01-1.239510207D-02  
 1.141290085D-05  
 -5.705483820D-09 1.195229703D-12 -6.613478650D+04-  
 9.859694489D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 21733.860  
 -2.954375880D+05-1.325154294D+02 1.610005380D+01-4.035359170D-05  
 8.971130740D-09  
 -1.033288810D-12 4.804468350D-17 -8.135719400D+04-  
 5.062404859D+01  
 PF2 Gurvich,1989 pt1 p426 pt2 p277.  
 2 tpis89 P 1.00F 2.00 0.00 0.00 0.00 0 68.97057 -  
 513103.659  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11081.447  
 5.524765720D+04-6.280517800D+02 5.137437920D+00 9.120673350D-03-  
 1.468773760D-05  
 1.081268450D-08-3.064944490D-12 -5.977541470D+04-  
 1.689589472D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11081.447  
 -1.708467120D+05-1.692051540D+02 7.125491600D+00-4.990852850D-05  
 1.097335230D-08  
 -1.252870260D-12 5.784791140D-17 -6.338295840D+04-  
 1.041715673D+01  
 PF2- Gurvich,1989 pt1 p426 pt2 p278.  
 2 tpis89 P 1.00F 2.00E 1.00 0.00 0.00 0 68.97112 -  
 709337.947  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11044.553  
 1.404793057D+05-1.699945753D+03 1.036823971D+01-3.599587690D-03  
 1.961925800D-06  
 -3.829329870D-10-3.375549520D-14 -7.810434510D+04-  
 3.217375182D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11044.553  
 -1.653976056D+05-1.640604822D+02 7.124091520D+00-5.015431400D-05  
 1.117302152D-08  
 -1.289308601D-12 6.004706670D-17 -8.700223320D+04-  
 1.109074866D+01  
 PF2CL Gurvich,1989 pt1 p439 pt2 p290.  
 2 tpis89 P 1.00F 2.00CL 1.00 0.00 0.00 0 104.42327 -  
 735076.682  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13876.318  
 8.397590160D+04-1.318075883D+03 1.017203515D+01 5.571231220D-03-  
 1.100920478D-05  
 8.726383180D-09-2.567714099D-12 -8.381656170D+04-  
 2.766013382D+01

1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13876.318  
 -2.409281185D+05-2.033484670D+02 1.015150769D+01-6.048367310D-05  
 1.333942001D-08  
 -1.526772528D-12 7.063339180D-17 -9.101110590D+04-  
 2.417825980D+01  
 PF2CL3 Gurvich,1989 pt1 p442 pt2 p294.  
 2 tpris89 P 1.00F 2.00CL 3.00 0.00 0.00 0 175.32867 -  
 878744.962  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 20165.238  
 1.842099543D+05-3.334402390D+03 2.388510873D+01-1.030943175D-02  
 7.356504220D-06  
 -2.498621785D-09 2.513997646D-13 -9.279549890D+04-  
 1.027991579D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 20165.238  
 -3.655272540D+05-2.029694160D+02 1.615238015D+01-6.118796570D-05  
 1.355610375D-08  
 -1.557129640D-12 7.224359970D-17 -1.104941533D+05-  
 5.387308961D+01  
 PF3 Gurvich,1989 pt1 p427 pt2 p279.  
 2 tpris89 P 1.00F 3.00 0.00 0.00 0.00 0 87.96897 -  
 957400.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12936.493  
 8.480984480D+04-1.102340691D+03 7.160715110D+00 1.438278338D-02-  
 2.318137222D-05  
 1.702244315D-08-4.810991950D-12 -1.111837495D+05-  
 1.457652362D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12936.493  
 -2.957040675D+05-2.997689931D+02 1.022297023D+01-8.890263450D-05  
 1.958901359D-08  
 -2.240491075D-12 1.035952523D-16 -1.173743464D+05-  
 2.777419177D+01  
 PF3CL2 Gurvich,1989 pt1 p441 pt2 p293.  
 2 tpris89 P 1.00F 3.00CL 2.00 0.00 0.00 0 158.87437 -  
 1122022.916  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19047.184  
 1.822497206D+05-3.089610245D+03 2.067710388D+01-1.168732391D-03-  
 5.020540740D-06  
 5.804573350D-09-1.965367906D-12 -1.228120667D+05-  
 8.627977921D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19047.184  
 -4.223838050D+05-3.207965220D+02 1.624013000D+01-9.623655310D-05  
 2.129279712D-08  
 -2.443515401D-12 1.132904350D-16 -1.392642151D+05-  
 5.531286311D+01  
 PF4CL Gurvich,1989 pt1 p439 pt2 p291.  
 2 tpris89 P 1.00F 4.00CL 1.00 0.00 0.00 0 142.42007 -  
 1364909.395  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18320.605  
 1.804240323D+05-2.741096618D+03 1.680192838D+01 9.919315250D-03-  
 2.025636171D-05  
 1.617979147D-08-4.772611520D-12 -1.532382587D+05-  
 6.679120281D+01

1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18320.605  
 -4.781140040D+05-4.264812830D+02 1.631812121D+01-1.271374903D-04  
 2.806715254D-08  
 -3.215166300D-12 1.488512118D-16 -1.680488362D+05-  
 5.735845121D+01  
 PF5 Gurvich,1989 pt1 p429 pt2 p280.  
 2 tpis89 P 1.00F 5.00 0.00 0.00 0.00 0 125.96578 -  
 1593300.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16537.609  
 1.855778473D+05-2.436979828D+03 1.201012406D+01 2.339343049D-02-  
 3.813944410D-05  
 2.796136412D-08-7.870704880D-12 -1.814566568D+05-  
 4.486488740D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16537.609  
 -5.668727840D+05-6.677917910D+02 1.649789569D+01-1.990099440D-04  
 4.395007100D-08  
 -5.036849540D-12 2.332945909D-16 -1.944321623D+05-  
 6.261721040D+01  
 PH Gurvich,1989 pt1 p420 pt2 p272.  
 2 tpis89 P 1.00H 1.00 0.00 0.00 0.00 0 31.98170  
 230752.104  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8648.104  
 2.273633198D+04-3.972674060D+02 6.233697660D+00-9.181784600D-03  
 1.523328123D-05  
 -1.085888585D-08 2.929760547D-12 2.852768404D+04-  
 1.095191197D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8648.104  
 7.814730650D+05-3.038451204D+03 7.467481020D+00-1.837522255D-03  
 7.165947700D-07  
 -1.142128853D-10 6.175410560D-15 4.536260180D+04-  
 2.467298140D+01  
 PH2 Gurvich,1989 pt1 p422 pt2 p273.  
 2 tpis89 P 1.00H 2.00 0.00 0.00 0.00 0 32.98964  
 119553.470  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9981.571  
 1.555268372D+04-1.841602025D+02 4.895896040D+00-3.495436600D-03  
 1.053418945D-05  
 -8.377562920D-09 2.270766150D-12 1.409839468D+04-  
 2.210564792D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9981.571  
 1.127884913D+06-4.715238250D+03 1.021498300D+01-1.167573820D-03  
 2.150542671D-07  
 -1.624213739D-11 3.766225240D-16 4.183074630D+04-  
 4.231623250D+01  
 PH2- Gurvich,1989 pt1 p423 pt2 p274.  
 2 tpis89 P 1.00H 2.00E 1.00 0.00 0.00 0 32.99019 -  
 9265.418  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9960.082  
 6.950684490D+04-7.719162910D+02 7.383537620D+00-8.522947210D-03  
 1.474476507D-05  
 -9.847160810D-09 2.413107871D-12 1.582295850D+03-  
 1.761306419D+01

1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9960.082  
 1.382525815D+06-5.213400670D+03 1.021694832D+01-1.116316349D-03  
 2.215004171D-07  
 -2.338005187D-11 1.015580932D-15 2.990683733D+04-  
 4.378711585D+01  
 PH3 Chase,1998 p1348.  
 2 j 6/62 P 1.00H 3.00 0.00 0.00 0.00 0 33.99758  
 5439.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10136.622  
 -6.384325340D+03 4.057567410D+02-1.565680086D-01 1.338380613D-02-  
 8.275391430D-06  
 3.024360831D-09-6.421764630D-13 -2.159842124D+03  
 2.385561888D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10136.622  
 1.334801106D+06-6.725463520D+03 1.445857073D+01-1.639736883D-03  
 3.409218570D-07  
 -3.736272080D-11 1.672947506D-15 3.910325710D+04-  
 7.198781190D+01  
 PN Gurvich,1989 pt1 p446 pt2 p299.  
 2 tpi89 P 1.00N 1.00 0.00 0.00 0.00 0 44.98050  
 171487.305  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8702.105  
 -5.103203840D+04 8.202926680D+02-1.392772765D+00 1.287989789D-02-  
 1.401425371D-05  
 7.775633460D-09-1.751539330D-12 1.573226520D+04  
 3.251070766D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8702.105  
 -2.495625593D+05 1.760438830D+02 4.144121960D+00 2.478018097D-04-  
 5.674896300D-08  
 4.263645120D-12 3.063920924D-16 1.770317267D+04  
 1.325518731D+00  
 PO Gurvich,1989 pt1 p404 pt2 p258.  
 2 tpi89 P 1.00O 1.00 0.00 0.00 0.00 0 46.97316 -  
 27857.687  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9390.113  
 -6.845754060D+04 1.141295708D+03-2.779556060D+00 1.678458047D-02-  
 1.974879516D-05  
 1.192602320D-08-2.927460912D-12 -9.847745040D+03  
 4.184328297D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9390.113  
 -3.366667440D+05 6.229355840D+02 3.565605460D+00 6.516620720D-04-  
 2.061770841D-07  
 3.184413230D-11-1.573691908D-15 -8.939790390D+03  
 6.954859188D+00  
 PO- Gurvich,1989 pt1 p407 pt2 p259.  
 2 tpi89 P 1.00O 1.00E 1.00 0.00 0.00 0 46.97371 -  
 140067.094  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8778.106  
 5.434346320D+04-4.123623550D+02 3.746483880D+00 3.858636470D-03-  
 5.963343040D-06  
 4.278286360D-09-1.139722989D-12 -1.555810937D+04  
 3.404436468D+00

1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8778.106  
 -8.480294780D+02 3.470544870D+02 2.877890167D+00 1.622182445D-03-  
 4.870190990D-07  
 6.645752270D-11-3.395703760D-15 -1.987209540D+04  
 1.075444355D+01  
 POCL3 Gurvich,1989 pt1 p436 pt2 p287.  
 2 tpris89 P 1.000 1.00CL 3.00 0.00 0.00 0 153.33126 -  
 568400.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17715.956  
 4.793788160D+04-1.270388280D+03 1.367716460D+01 1.082672100D-03-  
 1.736104060D-06  
 8.460890640D-10-1.174661330D-13 -6.507571880D+04-  
 4.314706821D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17715.956  
 -2.185937970D+05-5.080269680D+02 1.337784650D+01-1.510731050D-04  
 3.340986780D-08  
 -3.835329760D-12 1.779329880D-16 -7.009315090D+04-  
 3.984747181D+01  
 POFCL2 Gurvich,1989 pt1 p444 pt2 p297.  
 2 tpris89 P 1.000 1.00F 1.00CL 2.00 0.00 0 136.87696 -  
 793889.312  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16454.188  
 4.694061560D+04-1.069242600D+03 1.071284279D+01 9.491183300D-03-  
 1.306412424D-05  
 8.426906020D-09-2.140294969D-12 -9.274894990D+04-  
 2.815078377D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16454.188  
 -2.707647503D+05-6.556502270D+02 1.348668421D+01-1.942765035D-04  
 4.291184490D-08  
 -4.921844800D-12 2.282079808D-16 -9.654392140D+04-  
 4.164964152D+01  
 POF2CL Gurvich,1989 pt1 p443 pt2 p296.  
 2 tpris89 P 1.000 1.00F 2.00CL 1.00 0.00 0 120.42267 -  
 1022607.040  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14896.360  
 5.226438160D+04-9.691037700D+02 7.963635980D+00 1.755599796D-02-  
 2.398693997D-05  
 1.572376747D-08-4.079746000D-12 -1.202656893D+05-  
 1.593967449D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14896.360  
 -3.347086590D+05-8.176104810D+02 1.360664320D+01-2.420426112D-04  
 5.343712720D-08  
 -6.126461350D-12 2.839570116D-16 -1.233401194D+05-  
 4.496103811D+01  
 POF3 Gurvich,1989 pt1 p430 pt2 p281.  
 2 tpris89 P 1.000 1.00F 3.00 0.00 0.00 0 103.96837 -  
 1252000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14166.349  
 2.966030710D+04-4.276705750D+02 3.669146100D+00 2.839493780D-02-  
 3.768318000D-05  
 2.449104540D-08-6.341972870D-12 -1.501124530D+05  
 5.160417996D+00

1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14166.349  
 -3.690602420D+05-1.005552540D+03 1.374529940D+01-2.971037110D-04  
 6.554526640D-08  
 -7.509987330D-12 3.478969910D-16 -1.499761730D+05-  
 4.882214181D+01  
 PO2 Gurvich,1989 pt1 p408 pt2 p260.  
 2 tpris89 P 1.000 2.00 0.00 0.00 0.00 0 62.97256 -  
 281527.237  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10512.866  
 -6.372698220D+04 1.036741044D+03-2.877797967D+00 2.278134083D-02-  
 2.567920328D-05  
 1.465060412D-08-3.387996700D-12 -3.993544720D+04  
 4.425309380D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10512.866  
 4.926210990D+05-2.605465745D+03 9.517605610D+00-1.180371565D-03  
 2.532912819D-07  
 -1.789964539D-11 1.800381054D-16 -2.028884763D+04-  
 2.969743125D+01  
 PO2- Gurvich,1989 pt1 p409 pt2 p261.  
 2 tpris89 P 1.000 2.00E 1.00 0.00 0.00 0 62.97311 -  
 597623.751  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10613.749  
 2.702423135D+04 2.939956284D+01 1.162686114D+00 1.599897972D-02-  
 1.979229263D-05  
 1.208847527D-08-2.956640480D-12 -7.285946270D+04  
 1.963118182D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10613.749  
 1.628679152D+06-5.989199980D+03 1.369318836D+01-3.623843790D-03  
 9.488198340D-07  
 -1.040308759D-10 4.019033660D-15 -3.685959500D+04-  
 5.956796220D+01  
 PS Gurvich,1989 pt1 p444 pt2 p298.  
 2 tpris89 P 1.00S 1.00 0.00 0.00 0.00 0 63.03976  
 150431.316  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9616.116  
 -7.689786800D+02-4.637824070D+01 4.104649170D+00 1.555262273D-03-  
 2.315757288D-06  
 1.661425178D-09-4.631238400D-13 1.707875808D+04  
 4.230675966D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9616.116  
 -2.702729081D+05 8.883548220D+02 3.169190120D+00 1.022480817D-03-  
 3.803740480D-07  
 7.019861880D-11-4.269122310D-15 1.121510462D+04  
 1.147336428D+01  
 P2 Gurvich,1989 pt1 p398 pt2 p255.  
 2 tpris89 P 2.00 0.00 0.00 0.00 0.00 0 61.94752  
 144000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8904.107  
 3.053922510D+04-3.246177590D+02 4.022463810D+00 3.232094790D-03-  
 5.511052450D-06  
 4.195572930D-09-1.215032180D-12 1.796910870D+04  
 1.645350331D+00



1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8904.107  
 -7.806936490D+05 2.307910870D+03 1.411743130D+00 2.108237420D-03-  
 7.360856620D-07  
 1.259360120D-10-7.079752490D-15 1.329824740D+03  
 2.169741365D+01  
 P203 Gurvich,1989 pt1 p410 pt2 p262.  
 2 tpris89 P 2.000 3.00 0.00 0.00 0.00 0 109.94572 -  
 684645.274  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16094.881  
 -6.645753890D+04 7.580900550D+02 9.888436770D-01 2.859878730D-02-  
 3.231142110D-05  
 1.834525170D-08-4.212489300D-12 -8.820036740D+04  
 2.689914458D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16094.881  
 -2.175344110D+05-1.369902000D+03 1.401142960D+01-4.023856960D-04  
 8.868345780D-08  
 -1.015657280D-11 4.704356060D-16 -7.922757000D+04-  
 4.739487232D+01  
 P204 Gurvich,1989 pt1 p411 pt2 p263.  
 2 tpris89 P 2.000 4.00 0.00 0.00 0.00 0 125.94512 -  
 933754.627  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17325.580  
 -4.376091260D+04 4.905102830D+02 9.643649370D-01 3.886073580D-02-  
 4.675509220D-05  
 2.812625630D-08-6.824406100D-12 -1.168997790D+05  
 2.379582767D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17325.580  
 -3.670114860D+05-1.638423730D+03 1.721188610D+01-4.826580150D-04  
 1.064461900D-07  
 -1.219610070D-11 5.650654580D-16 -1.090435930D+05-  
 6.714276593D+01  
 P205 Gurvich,1989 pt1 p411 pt2 p264.  
 2 tpris89 P 2.000 5.00 0.00 0.00 0.00 0 141.94452 -  
 1124370.354  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22049.905  
 -2.999159220D+04-4.594506590D+01 6.987486830D+00 2.883302970D-02-  
 3.104509530D-05  
 1.643868680D-08-3.467942300D-12 -1.381901400D+05-  
 3.400572711D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22049.905  
 -3.247080160D+05-2.016975080D+03 2.048699340D+01-5.910641150D-04  
 1.301993020D-07  
 -1.490682940D-11 6.903573410D-16 -1.306290160D+05-  
 8.031642952D+01  
 P3 Gurvich,1989 pt1 p402 pt2 p256.  
 2 tpris89 P 3.00 0.00 0.00 0.00 0.00 0 92.92128  
 210000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12005.602  
 4.693358950D+04-8.643589320D+02 8.734247530D+00 1.094534560D-05-  
 1.998573320D-06  
 2.096750510D-09-6.922889710D-13 2.774847340D+04-  
 2.063587261D+01

1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12005.602  
 -1.253513060D+05-8.306734620D+01 7.561956770D+00-2.474403950D-05  
 5.457276930D-09  
 -6.244660570D-13 2.887724220D-17 2.308722280D+04-  
 1.228310621D+01  
 P306 Gurvich,1989 pt1 p412 pt2 p265.  
 2 tpris89 P 3.000 6.00 0.00 0.00 0.00 0 188.91768 -  
 1575681.029  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 23439.282  
 2.014493813D+05-3.053488073D+03 1.602114098D+01 4.316889900D-02-  
 6.376544260D-05  
 4.422867920D-08-1.200020334D-11 -1.776503811D+05-  
 6.556267890D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 23439.282  
 -8.787968100D+05-1.651988071D+03 2.772258397D+01-4.859326700D-04  
 1.067867708D-07  
 -1.218015776D-11 5.614911960D-16 -1.909165548D+05-  
 1.220665277D+02  
 P4 Gurvich,1989 pt1 p402 pt2 p257.  
 2 tpris89 P 4.00 0.00 0.00 0.00 0.00 0 123.89504  
 58900.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14108.648  
 1.205141850D+05-2.345711790D+03 1.773946550D+01-1.456314970D-02  
 1.587594090D-05  
 -9.314710310D-09 2.271491670D-12 1.608846480D+04-  
 7.088590647D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14108.648  
 -1.858705860D+05-6.284546890D+01 1.004844880D+01-1.987668850D-05  
 4.482408440D-09  
 -5.226103670D-13 2.455791290D-17 3.848210920D+03-  
 2.477297797D+01  
 P406 Gurvich,1989 pt1 p413 pt2 p266.  
 2 tpris89 P 4.000 6.00 0.00 0.00 0.00 0 219.89144 -  
 1606000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 24797.523  
 3.760894750D+05-5.685832620D+03 2.914225450D+01 2.251532120D-02-  
 4.510269630D-05  
 3.588312690D-08-1.057572060D-11 -1.688562480D+05-  
 1.451359851D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 24797.523  
 -1.008997240D+06-8.872753990D+02 2.866064830D+01-2.636018940D-04  
 5.810940720D-08  
 -6.648086960D-12 3.074391930D-16 -1.997138900D+05-  
 1.281853821D+02  
 P407 Gurvich,1989 pt1 p414 pt2 p267.  
 2 tpris89 P 4.000 7.00 0.00 0.00 0.00 0 235.89084 -  
 1984448.045  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 26372.317  
 3.218586960D+05-4.871444730D+03 2.454417068D+01 4.015509550D-02-  
 6.524197150D-05  
 4.756554180D-08-1.332975491D-11 -2.184517427D+05-  
 1.181504792D+02

1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 26372.317  
 -1.102947375D+06-1.511077128D+03 3.210979500D+01-4.371803760D-04  
 9.516639610D-08  
 -1.075204176D-11 4.911025680D-16 -2.429096540D+05-  
 1.473140859D+02  
 P408 Gurvich,1989 pt1 p415 pt2 p268.  
 2 tpris89 P 4.000 8.00 0.00 0.00 0.00 0 251.89024 -  
 2302214.078  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 27946.336  
 2.719326942D+05-4.118600390D+03 2.028714235D+01 5.685416990D-02-  
 8.400739630D-05  
 5.823389060D-08-1.578647160D-11 -2.604539703D+05-  
 9.407162070D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 27946.336  
 -1.173177311D+06-2.200632995D+03 3.563010130D+01-6.489849740D-04  
 1.429623989D-07  
 -1.635821725D-11 7.571070760D-16 -2.783843144D+05-  
 1.679636960D+02  
 P409 Gurvich,1989 pt1 p416 pt2 p269.  
 2 tpris89 P 4.000 9.00 0.00 0.00 0.00 0 267.88964 -  
 2613979.111  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 29521.355  
 2.199916395D+05-3.336464940D+03 1.586413106D+01 7.402452330D-02-  
 1.034835052D-04  
 6.944438320D-08-1.840733450D-11 -3.018742692D+05-  
 6.997967670D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 29521.355  
 -1.233696783D+06-2.917032808D+03 3.917757110D+01-8.736402980D-04  
 1.937914895D-07  
 -2.230510118D-11 1.037248818D-15 -3.129637516D+05-  
 1.897176420D+02  
 P4010 Gurvich,1989 pt1 p419 pt2 p271.  
 2 tpris89 P 4.000 10.00 0.00 0.00 0.00 0 283.88905 -  
 2906223.447  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 31096.553  
 1.670142268D+05-2.540243300D+03 1.136853403D+01 9.137812160D-02-  
 1.231990626D-04  
 8.081032230D-08-2.106787011D-11 -3.410151910D+05-  
 4.643431340D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 31096.553  
 -1.337201132D+06-3.516382330D+03 4.260403310D+01-1.037406404D-03  
 2.287613089D-07  
 -2.620219946D-11 1.213529528D-15 -3.459515050D+05-  
 2.115498906D+02  
 Pb Hf:Gurvich,1991. Moore,1971. Moore,1970a. Gordon,1999.  
 3 g 8/97 PB 1.00 0.00 0.00 0.00 0.00 0 207.20000  
 195200.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 1.213382285D+03-1.906116019D+01 2.619299546D+00-3.829519610D-04  
 6.688180450D-07  
 -6.061231080D-10 2.240022429D-13 2.282096238D+04  
 6.201369200D+00

1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 -9.084313070D+06 2.672673180D+04-2.626244039D+01 1.358282305D-02-  
 2.685523566D-06  
 2.352432800D-10-7.324114532D-15 -1.481650666D+05  
 2.154011624D+02  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 5.325474970D+08-2.751419152D+05 6.303031930D+01-6.813672740D-03  
 4.447489610D-07  
 -1.519361678D-11 2.043475665D-16 2.243651683D+06-  
 5.225649900D+02  
 Pb+ Moore1971. Moore,1970a. Gordon,1999.  
 3 g10/97 PB 1.00E -1.00 0.00 0.00 0.00 0 207.19945  
 916996.528  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 9.486689040D+00-1.134955793D-01 2.500549799D+00-1.382464681D-06  
 1.906022991D-09  
 -1.368396828D-12 4.003528117D-16 1.095438901D+05  
 7.538855900D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 1.320690183D+06-4.096048010D+03 7.389101510D+00-2.807751909D-03  
 7.830991650D-07  
 -9.310600910D-11 4.016371727D-15 1.354347306D+05-  
 2.722020908D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 4.101539500D+08-2.538072503D+05 6.239804790D+01-6.542962120D-03  
 3.507316530D-07  
 -8.114133770D-12 5.908352630D-17 2.122867468D+06-  
 5.163550210D+02  
 Pb- Hotop,1985. Gordon,1999.  
 3 g 9/97 PB 1.00E 1.00 0.00 0.00 0.00 0 207.20055  
 153881.928  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 1.776226140D+04  
 8.235132100D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 1.776226140D+04  
 8.235132100D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 1.776226140D+04  
 8.235132100D+00  
 PbBr Gurvich,1991 pt1 p434 pt2 p360.  
 2 tpi91 PB 1.00BR 1.00 0.00 0.00 0.00 0 287.10400  
 64821.322  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10146.122  
 -2.393487988D+03-4.576591210D+01 4.692608280D+00-3.845290630D-04  
 5.888213500D-07

-4.084792890D-10 1.202515201D-13 6.662434770D+03  
5.991705510D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
10146.122  
-2.581831670D+06 7.143490760D+03-2.658193640D+00 3.107722260D-03-  
4.631381540D-07  
1.095529211D-11 1.508555088D-15 -3.970440980D+04  
5.959238650D+01  
PbBr2 Gurvich,1991 pt1 p437 pt2 p362.  
2 tpis91 PB 1.00BR 2.00 0.00 0.00 0.00 0 367.00800 -  
103908.063  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
15021.937  
-6.172766360D+03-6.783207630D+01 7.273156140D+00-5.990596120D-04  
7.358634610D-07  
-4.743604810D-10 1.246922291D-13 -1.427890796D+04-  
6.987992150D-01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
15021.937  
-1.320421479D+04-1.143074947D+00 7.000972540D+00-4.284471610D-07  
1.018044861D-10  
-1.234016791D-14 5.971337650D-19 -1.462213750D+04  
8.868582650D-01  
PbBr3 Gurvich,1991 pt1 p438 pt2 p363.  
2 tpis91 PB 1.00BR 3.00 0.00 0.00 0.00 0 446.91200 -  
104010.957  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
19968.643  
-1.164424250D+04-1.555151665D+02 1.062317321D+01-1.361947117D-03  
1.668738791D-06  
-1.073686019D-09 2.818250340D-13 -1.478208304D+04-  
1.443758579D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
19968.643  
-2.787930766D+04-2.633265111D+00 1.000223199D+01-9.807761410D-07  
2.326232632D-10  
-2.815994460D-14 1.361283735D-18 -1.556981182D+04-  
1.081765474D+01  
PbBr4 Gurvich,1991 pt1 p439 pt2 p364.  
2 tpis91 PB 1.00BR 4.00 0.00 0.00 0.00 0 526.81600 -  
182435.511  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
25871.489  
-1.176458199D+04-2.567166983D+02 1.402223292D+01-2.224117068D-03  
2.716201994D-06  
-1.743340164D-09 4.567359750D-13 -2.462125551D+04-  
2.882020750D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
25871.489  
-3.880216030D+04-4.382933770D+00 1.300369823D+01-1.620061335D-06  
3.834130880D-10  
-4.633967180D-14 2.237427066D-18 -2.592327065D+04-  
2.287710636D+01  
PbCL Gurvich,1991 pt1 p427 pt2 p355.  
2 tpis91 PB 1.00CL 1.00 0.00 0.00 0.00 0 242.65270  
8819.118  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
9787.118  
-2.902700749D+03-8.293459710D+01 4.714824480D+00-1.931473228D-04  
9.105579020D-08

5.419385230D-11-3.284969700D-14 1.254460217D+02  
 4.323192600D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9787.118  
 -3.854285530D+05 6.922197500D+02 4.509971240D+00-6.853421300D-04  
 5.087395500D-07  
 -9.772753810D-11 5.807471580D-15 -5.269684720D+03  
 6.646489160D+00  
**PbCL2** Gurvich,1991 pt1 p430 pt2 p357.  
 2 tpis91 PB 1.00CL 2.00 0.00 0.00 0.00 0 278.10540 -  
 175547.471  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14002.529  
 2.830580143D+03-3.134256659D+02 8.212827290D+00-2.585096173D-03  
 3.109456077D-06  
 -1.972978208D-09 5.123542480D-13 -2.167569042D+04-  
 9.219415480D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14002.529  
 -3.149192744D+04-5.565477580D+00 7.004599540D+00-1.986025455D-06  
 4.651719590D-10  
 -5.579137010D-14 2.678143570D-18 -2.327439309D+04-  
 2.140742521D+00  
**PbCL3** Gurvich,1991 pt1 p432 pt2 p358.  
 2 tpis91 PB 1.00CL 3.00 0.00 0.00 0.00 0 313.55810 -  
 177653.507  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18255.693  
 8.623588970D+02-5.253152750D+02 1.203336337D+01-4.335184980D-03  
 5.215698350D-06  
 -3.310022380D-09 8.596970610D-13 -2.180576379D+04-  
 2.694207393D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18255.693  
 -5.664412790D+04-9.329514790D+00 1.000771099D+01-3.329727570D-06  
 7.799330810D-10  
 -9.354606100D-14 4.490589700D-18 -2.448508643D+04-  
 1.507491301D+01  
**PbCL4** Gurvich,1991 pt1 p433 pt2 p359.  
 2 tpis91 PB 1.00CL 4.00 0.00 0.00 0.00 0 349.01080 -  
 327430.362  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 23449.438  
 1.739405796D+04-8.902139320D+02 1.637565058D+01-7.088992260D-03  
 8.432567340D-06  
 -5.305309390D-09 1.368671294D-12 -3.888215620D+04-  
 4.850134300D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 23449.438  
 -8.266679560D+04-1.639486405D+01 1.301336711D+01-5.716141400D-06  
 1.329368390D-09  
 -1.585922492D-13 7.581763610D-18 -4.343984220D+04-  
 2.874559779D+01  
**PbF** Gurvich,1991 pt1 p419 pt2 p350.  
 2 tpis91 PB 1.00F 1.00 0.00 0.00 0.00 0 226.19840 -  
 98867.789  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9268.111  
 2.684864255D+04-4.751725640D+02 6.019644370D+00-2.718531008D-03  
 2.942882954D-06

-1.687543009D-09 4.086122080D-13 -1.079038653D+04-  
 4.983048840D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9268.111  
 -4.734202750D+05 1.027785283D+03 3.888658730D+00-1.649813448D-04  
 2.931163260D-07  
 -5.766459650D-11 3.247486190D-15 -2.026165076D+04  
 9.319483890D+00  
**PbF2** Gurvich,1991 pt1 p424 pt2 p352.  
 2 tpis91 PB 1.00F 2.00 0.00 0.00 0.00 0 245.19681 -  
 443427.390  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12572.610  
 5.920552280D+04-1.052529292D+03 1.028969284D+01-5.876346270D-03  
 6.102333130D-06  
 -3.424792640D-09 8.024025420D-13 -4.999050000D+04-  
 2.525115478D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12572.610  
 -8.505899770D+04-3.074244334D+01 7.023346040D+00-9.455183590D-06  
 2.108489027D-09  
 -2.434212002D-13 1.133872429D-17 -5.552236770D+04-  
 5.496073220D+00  
**PbF3** Gurvich,1991 pt1 p425 pt2 p353.  
 2 tpis91 PB 1.00F 3.00 0.00 0.00 0.00 0 264.19521 -  
 489572.613  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15535.047  
 8.553090870D+04-1.731036694D+03 1.556596150D+01-1.022225919D-02  
 1.089984998D-05  
 -6.269998820D-09 1.502616508D-12 -5.300335670D+04-  
 5.335733480D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15535.047  
 -1.459704258D+05-4.820396430D+01 1.003685845D+01-1.501095764D-05  
 3.362474990D-09  
 -3.896020710D-13 1.820152103D-17 -6.206869590D+04-  
 2.006978661D+01  
**PbF4** Gurvich,1991 pt1 p426 pt2 p354.  
 2 tpis91 PB 1.00F 4.00 0.00 0.00 0.00 0 283.19361 -  
 799925.173  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19626.227  
 1.309963563D+05-2.307299499D+03 1.945201440D+01-1.024522729D-02  
 9.395874960D-06  
 -4.626894150D-09 9.450881430D-13 -8.804147460D+04-  
 7.524645820D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19626.227  
 -2.132616322D+05-8.578621950D+01 1.306428551D+01-2.575563598D-05  
 5.693324590D-09  
 -6.526219550D-13 3.022341960D-17 -1.002908979D+05-  
 3.590240280D+01  
**PbI** Gurvich,1991 pt1 p440 pt2 p365.  
 2 tpis91 PB 1.00I 1.00 0.00 0.00 0.00 0 334.10447  
 108904.324  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10339.124  
 -2.717334060D+03-1.542541996D+01 4.565327900D+00-1.061215818D-04  
 2.414841342D-07

-1.876070301D-10 6.460614270D-14 1.181864978D+04  
 7.669802670D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10339.124  
 -3.901070250D+06 1.147976718D+04-8.176109020D+00 6.523454700D-03-  
 1.522611682D-06  
 1.626692202D-10-6.553328880D-15 -6.154433690D+04  
 9.938404970D+01  
**PbI2** Gurvich,1991 pt1 p443 pt2 p367.  
 2 tpris91 PB 1.00I 2.00 0.00 0.00 0.00 0 461.00894 -  
 10252.630  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15247.370  
 -5.904986720D+03-4.833307030D+01 7.195438030D+00-4.298600090D-04  
 5.291412070D-07  
 -3.416402820D-10 8.991341920D-14 -3.107780155D+03  
 1.324773678D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15247.370  
 -1.088339477D+04-8.164418370D-01 7.000697300D+00-3.079876763D-07  
 7.331718140D-11  
 -8.899193880D-15 4.310712500D-19 -3.352096380D+03  
 2.458605463D+00  
**PbI3** Gurvich,1991 pt1 p444 pt2 p368.  
 2 tpris91 PB 1.00I 3.00 0.00 0.00 0.00 0 587.91341  
 21755.412  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 21065.012  
 -1.014996331D+04-5.938078200D+01 1.024073798D+01-5.304694530D-04  
 6.538623030D-07  
 -4.225895720D-10 1.113029818D-13 -1.138482403D+02-  
 8.975540500D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 21065.012  
 -1.624229573D+04-1.002945584D+00 1.000085839D+01-3.796679740D-07  
 9.046751720D-11  
 -1.098840054D-14 5.325388290D-19 -4.138258930D+02-  
 7.579417110D+00  
**PbI4** Gurvich,1991 pt1 p445 pt2 p369.  
 2 tpris91 PB 1.00I 4.00 0.00 0.00 0.00 0 714.81788 -  
 41226.459  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 27520.541  
 -1.217096972D+04-7.226317440D+01 1.329294204D+01-6.454660900D-04  
 7.955761850D-07  
 -5.141632830D-10 1.354188031D-13 -8.528148680D+03-  
 2.010457498D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 27520.541  
 -1.958477744D+04-1.223385179D+00 1.300104732D+01-4.633295690D-07  
 1.104213978D-10  
 -1.341397771D-14 6.501706110D-19 -8.893193200D+03-  
 1.840570345D+01  
**PbO** Gurvich,1991 pt1 p413 pt2 p345.  
 2 tpris91 PB 1.00O 1.00 0.00 0.00 0.00 0 223.19940  
 68137.108  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8962.108  
 3.424025000D+04-4.198050110D+02 4.720306410D+00 1.451061751D-03-  
 3.206035460D-06



2.713956273D-09-8.333275610D-13 9.253186470D+03  
 4.482891210D-01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8962.108  
 2.426996850D+05-1.107731354D+02 3.180684490D+00 1.991815065D-03-  
 1.079782025D-06  
 2.540990941D-10-1.834652493D-14 8.339391540D+03  
 1.050920926D+01  
**PbO2** Gurvich,1991 pt1 p416 pt2 p347.  
 2 tpris91 PB 1.000 2.00 0.00 0.00 0.00 0 239.19880  
 136152.734  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12250.934  
 7.071058290D+04-1.076757462D+03 9.401711730D+00-1.003861584D-03-  
 1.233815617D-06  
 1.858386979D-09-6.834621210D-13 1.999645981D+04-  
 2.503976748D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12250.934  
 -1.307796670D+05-7.314361450D+01 7.554083410D+00-2.143421561D-05  
 4.696464000D-09  
 -5.344972180D-13 2.460760535D-17 1.413386101D+04-  
 1.252684909D+01  
**PbS** Gurvich,1991 pt1 p448 pt2 p371.  
 2 tpris91 PB 1.00S 1.00 0.00 0.00 0.00 0 239.26600  
 127945.313  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9430.113  
 1.529840503D+04-3.439746350D+02 5.680630640D+00-2.232931917D-03  
 2.504608209D-06  
 -1.470427328D-09 3.577527190D-13 1.578551202D+04-  
 2.628894657D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9430.113  
 2.105441649D+06-5.520413580D+03 9.369249260D+00-1.410262019D-03-  
 1.642683362D-07  
 1.451447577D-10-1.393564925D-14 5.009334530D+04-  
 3.217417030D+01  
**PbS2** Gurvich,1991 pt1 p450 pt2 p372.  
 2 tpris91 PB 1.00S 2.00 0.00 0.00 0.00 0 271.33200  
 244049.005  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14021.205  
 2.446375880D+04-6.654855460D+02 9.920201180D+00-4.924194380D-03  
 5.716906290D-06  
 -3.529488830D-09 8.971138350D-13 3.044310130D+04-  
 2.295764446D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14021.205  
 -5.416700300D+04-1.343600342D+01 7.510700360D+00-4.497318630D-06  
 1.032444494D-09  
 -1.219580043D-13 5.785804650D-18 2.701229533D+04-  
 8.714607040D+00  
**Rb** Hf:Cox,1989. Moore,1971. Moore,1970a. Gordon,1999.  
 3 g 1/98 RB 1.00 0.00 0.00 0.00 0.00 0 85.46780  
 80900.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 1.352856616D+01-2.042232679D-01 2.501213823D+00-3.650619900D-06  
 5.884722670D-09

-4.842274720D-12 1.596211946D-15 8.985569210D+03  
 6.207005480D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 -1.138274064D+06 3.804041940D+03-2.750899258D+00 3.891460700D-03-  
 1.632296823D-06  
 3.511893140D-10-2.521064422D-14 -1.466454849D+04  
 4.253442370D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 3.245192200D+08-3.493850870D+05 1.159097652D+02-1.492843123D-02  
 9.582385060D-07  
 -2.996233671D-11 3.657332046D-16 2.636178014D+06-  
 9.586517230D+02  
 Rb+ Moore,1971. IP:Moore,1970a. Gordon,1999.  
 3 g 1/98 RB 1.00E -1.00 0.00 0.00 0.00 0 85.46725  
 490129.128  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 5.820327360D+04  
 5.520506920D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 5.820327360D+04  
 5.520506920D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 4.120352830D+07-2.920376515D+04 1.102096776D+01-1.311457972D-03  
 1.124752629D-07  
 -5.107819770D-12 9.622794537D-17 2.850166118D+05-  
 6.672202250D+01  
 Rb- Hotop,1985. Gordon,1999.  
 3 g 9/97 RB 1.00E 1.00 0.00 0.00 0.00 0 85.46835  
 27818.528  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 2.600405796D+03  
 5.520526170D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 2.600405796D+03  
 5.520526170D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 2.600405796D+03  
 5.520526170D+00  
 RbBO2 Gurvich,1982 pt1 p459 pt2 p483.  
 2 tps82 RB 1.00B 1.000 2.00 0.00 0.00 0 128.27760 -  
 678977.302  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14332.698

4.198657750D+04-6.799448330D+02 8.185151010D+00 2.772536733D-03-  
 6.175770470D-07  
 -9.426136250D-10 4.722414240D-13 -8.020339590D+04-  
 1.239198887D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14332.698  
 9.154463400D+04-1.668328341D+03 1.117268757D+01-4.505533530D-04  
 9.681330590D-08  
 -1.088037652D-11 4.967733660D-16 -7.507903250D+04-  
 3.131951149D+01  
**RbBr** Gurvich,1982 pt1 p446 pt2 p470.  
 2 tpris82 RB 1.00BR 1.00 0.00 0.00 0.00 0 165.37180 -  
 191510.876  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10319.124  
 -5.703859700D+03 2.092281597D+01 4.370607370D+00 4.494604780D-04-  
 4.835438840D-07  
 3.526068600D-10-9.886538320D-14 -2.449112515D+04  
 6.427431700D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10319.124  
 1.609092474D+06-4.466774590D+03 9.064092060D+00-1.995333358D-03  
 4.016633520D-07  
 -4.163091400D-12-3.092443341D-15 4.427467690D+03-  
 2.757714089D+01  
**RbCl** Gurvich,1982 pt1 p443 pt2 p467.  
 2 tpris82 RB 1.00CL 1.00 0.00 0.00 0.00 0 120.92050 -  
 223322.879  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10057.121  
 -5.740809580D+03-1.528835285D+01 4.515200900D+00 1.067270745D-04-  
 6.385945590D-09  
 -1.301381692D-11 1.641459742D-14 -2.814243986D+04  
 4.190111420D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10057.121  
 -1.143043004D+06 4.003861880D+03-1.096156782D+00 4.033581280D-03-  
 1.454151464D-06  
 2.719263762D-10-1.810463980D-14 -5.297686040D+04  
 4.311317450D+01  
**RbF** Gurvich,1982 pt1 p440 pt2 p464.  
 2 tpris82 RB 1.00F 1.00 0.00 0.00 0.00 0 104.46620 -  
 333511.885  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9588.115  
 3.287360190D+04-6.080907460D+02 7.406622360D+00-7.277864720D-03  
 1.013930727D-05  
 -7.141372500D-09 2.014332982D-12 -3.849834130D+04-  
 1.375750778D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9588.115  
 -8.544811150D+05 2.633756505D+03 1.216216506D+00 2.136494067D-03-  
 6.728426080D-07  
 1.134905135D-10-6.825624440D-15 -5.810179110D+04  
 2.588118896D+01  
**RbH** Gurvich,1982 pt1 p435 pt2 p459.  
 2 tpris82 RB 1.00H 1.00 0.00 0.00 0.00 0 86.47574  
 119324.106  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8820.106

8.908270610D+03 4.649870400D+01 1.833967623D+00 8.444279140D-03-  
 1.167538647D-05  
 8.010389420D-09-2.162578321D-12 1.328248009D+04  
 1.279544976D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8820.106  
 -2.937703530D+06 9.379817260D+03-7.542563460D+00 7.493226800D-03-  
 2.159228887D-06  
 2.871300173D-10-1.459981256D-14 -4.595518830D+04  
 8.365664320D+01  
**RbI** Gurvich,1982 pt1 p449 pt2 p473.  
 2 tpris82 RB 1.00I 1.00 0.00 0.00 0.00 0 212.37227 -  
 138480.874  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10459.126  
 -7.693052800D+02-2.968608844D+01 4.648745840D+00-2.962415236D-04  
 5.978135340D-07  
 -4.351255250D-10 1.313617336D-13 -1.786610717D+04  
 5.812409830D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10459.126  
 4.297424850D+06-1.296911161D+04 1.958730402D+01-8.458425590D-03  
 2.463480035D-06  
 -3.191575730D-10 1.458455589D-14 6.432948040D+04-  
 1.009499336D+02  
**RbK** Gurvich,1982 pt1 p462 pt2 p486.  
 2 tpris82 RB 1.00K 1.00 0.00 0.00 0.00 0 124.56610  
 120013.330  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10808.130  
 2.494695429D+04-4.553060660D+02 7.686189950D+00-1.108112244D-02  
 2.093398586D-05  
 -1.824445366D-08 5.617645360D-12 1.516136160D+04-  
 1.063563675D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10808.130  
 -4.175391070D+06 5.918588510D+03 9.202649420D+00-1.060933600D-02  
 4.964826060D-06  
 -8.716698790D-10 5.221887960D-14 -3.272769040D+04-  
 1.372401997D+01  
**RbLi** Gurvich,1982 pt1 p460 pt2 p484.  
 2 tpris82 RB 1.00LI 1.00 0.00 0.00 0.00 0 92.40880  
 164181.324  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10276.124  
 -2.263413044D+03-2.888496910D+01 4.555826540D+00 3.625667530D-04-  
 9.598002220D-07  
 1.631010244D-09-8.159825980D-13 1.853455250D+04  
 2.831743182D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10276.124  
 1.085515194D+07-3.805106970D+04 5.516555040D+01-3.128845612D-02  
 9.261650250D-06  
 -1.264671408D-09 6.431662050D-14 2.543964131D+05-  
 3.520758710D+02  
**RbNO2** Gurvich,1982 pt1 p454 pt2 p478.  
 2 tpris82 RB 1.00N 1.000 2.00 0.00 0.00 0 131.47334 -  
 187629.777  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15770.223

-7.199420030D+04 1.265802595D+03-2.415715742D+00 3.054641420D-02-  
 3.684004050D-05  
 2.247716481D-08-5.547527430D-12 -3.037381667D+04  
 4.814256950D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15770.223  
 -1.644994453D+05-8.499443440D+02 1.063080575D+01-2.517893988D-04  
 5.561420120D-08  
 -6.378805600D-12 2.957679896D-16 -2.128590982D+04-  
 2.568367279D+01  
**RbNO3** Gurvich,1982 pt1 p456 pt2 p480.  
 2 tps82 RB 1.00N 1.000 3.00 0.00 0.00 0 147.47274 -  
 314972.483  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16367.517  
 -2.664669172D+04 8.807634790D+02-3.159459457D+00 4.271229020D-02-  
 5.351029210D-05  
 3.360969750D-08-8.503290510D-12 -4.353595460D+04  
 4.943052940D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16367.517  
 -3.147413867D+05-1.371457846D+03 1.401319759D+01-4.030275020D-04  
 8.878332290D-08  
 -1.016221214D-11 4.704254090D-16 -3.504339940D+04-  
 4.619379200D+01  
**RbNa** Gurvich,1982 pt1 p461 pt2 p485.  
 2 tps82 RB 1.00NA 1.00 0.00 0.00 0.00 0 108.45757  
 131470.328  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10665.128  
 2.974455567D+04-5.082790590D+02 7.734033520D+00-1.013006840D-02  
 1.745455325D-05  
 -1.398725470D-08 3.968106770D-12 1.682379436D+04-  
 1.240085290D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10665.128  
 4.297114270D+06-1.831013588D+04 3.454394200D+01-2.230134993D-02  
 7.339874530D-06  
 -1.064784996D-09 5.617598460D-14 1.242610951D+05-  
 1.993661980D+02  
**RbO** Gurvich,1982 pt1 p429 pt2 p452.  
 2 tps82 RB 1.00O 1.00 0.00 0.00 0.00 0 101.46720  
 52489.324  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10337.124  
 1.900081316D+05-3.428228990D+03 2.480251273D+01-5.051654580D-02  
 6.476338760D-05  
 -4.198012420D-08 1.093889043D-11 2.083898450D+04-  
 1.097559150D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10337.124  
 6.170756880D+05-2.175089620D+03 8.290412210D+00-2.996487663D-03  
 1.233144275D-06  
 -2.115810631D-10 1.242607430D-14 1.828164827D+04-  
 2.117386042D+01  
**RbOH** Gurvich,1997.  
 2 g 9/97 RB 1.00O 1.00H 1.00 0.00 0.00 0 102.47514 -  
 238000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11761.202

1.213832721D+04-5.441411590D+02 8.459814640D+00-3.561526560D-03  
2.992872390D-06  
-7.280267400D-10-4.553847180D-14 -2.787262486D+04-  
1.913421991D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
11761.202  
8.958583130D+05-2.332339000D+03 7.971192480D+00 1.044439355D-04-  
6.328257750D-08  
1.029358824D-11-5.743277790D-16 -1.515568947D+04-  
1.950051629D+01  
Rb2Br2 Gurvich,1982 pt1 p447 pt2 p471.  
2 tpris82 RB 2.00BR 2.00 0.00 0.00 0.00 0 330.74360 -  
551801.433  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
21696.566  
-8.005525400D+03-2.111968088D+01 1.008629404D+01-1.911936090D-04  
2.366059490D-07  
-1.533722380D-10 4.048725060D-14 -6.927313600D+04-  
9.622434630D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
21696.566  
-1.014535336D+04-3.601550320D-01 1.000031058D+01-1.380745805D-07  
3.302067950D-11  
-4.021581820D-15 1.953006729D-19 -6.937960880D+04-  
9.122562360D+00  
Rb2CL2 Gurvich,1982 pt1 p444 pt2 p468.  
2 tpris82 RB 2.00CL 2.00 0.00 0.00 0.00 0 241.84100 -  
618373.536  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
20785.574  
-1.125039522D+04-6.756953990D+01 1.027381915D+01-6.031848990D-04  
7.433324780D-07  
-4.803372160D-10 1.264973638D-13 -7.706757500D+04-  
1.363652947D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
20785.574  
-1.818875133D+04-1.137903580D+00 1.000097318D+01-4.302156400D-07  
1.024725787D-10  
-1.244291058D-14 6.028912390D-19 -7.740897670D+04-  
1.204843757D+01  
Rb2F2 Gurvich,1982 pt1 p441 pt2 p465.  
2 tpris82 RB 2.00F 2.00 0.00 0.00 0.00 0 208.93241 -  
854913.348  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
18889.758  
-8.178347100D+03-3.334733540D+02 1.131540799D+01-2.842914926D-03  
3.454959580D-06  
-2.209373419D-09 5.772073270D-13 -1.042230504D+05-  
2.368991587D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
18889.758  
-4.376574390D+04-5.761452040D+00 1.000482691D+01-2.104159548D-06  
4.962416270D-10  
-5.982174970D-14 2.882751742D-18 -1.059176154D+05-  
1.603254014D+01  
Rb2I2 Gurvich,1982 pt1 p450 pt2 p474.  
2 tpris82 RB 2.00I 2.00 0.00 0.00 0.00 0 424.74454 -  
432956.482  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
22217.518

-5.839663550D+03-9.527537900D+00 1.003904495D+01-8.668754000D-05  
 1.074384368D-07  
 -6.972122230D-11 1.842065721D-14 -5.502780960D+04-  
 7.174113320D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22217.518  
 -6.799834640D+03-1.642527699D-01 1.000014200D+01-6.321420730D-08  
 1.512811170D-11  
 -1.843027189D-15 8.951244180D-20 -5.507579620D+04-  
 6.948045390D+00  
 Rb20 Gurvich,1982 pt1 p431 pt2 p455.  
 2 tps82 RB 2.000 1.00 0.00 0.00 0.00 0 186.93500 -  
 108929.421  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14215.779  
 1.971276138D+04-4.627508860D+02 8.588293130D+00-3.085559728D-03  
 3.451980140D-06  
 -2.068570368D-09 5.132480500D-13 -1.284854711D+04-  
 1.264891828D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14215.779  
 -3.846360090D+04-1.082831019D+01 7.008421890D+00-3.476228120D-06  
 7.869785060D-10  
 -9.195683850D-14 4.325201520D-18 -1.525373768D+04-  
 3.230388780D+00  
 Rb202 Gurvich,1982 pt1 p434 pt2 p457.  
 2 tps82 RB 2.000 2.00 0.00 0.00 0.00 0 202.93440 -  
 215848.468  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16847.132  
 3.260553230D+04-7.578164720D+02 1.070815124D+01 1.148004329D-03-  
 3.291243670D-06  
 2.853106637D-09-8.721590680D-13 -2.475317258D+04-  
 2.434276460D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16847.132  
 -1.318567396D+05-9.647737790D+01 1.007222726D+01-2.894921706D-05  
 6.405639100D-09  
 -7.351419390D-13 3.408561710D-17 -2.882179733D+04-  
 1.910948823D+01  
 Rb202H2 Gurvich,1997. .  
 2 g 9/97 RB 2.000 2.00H 2.00 0.00 0.00 0 204.95028 -  
 639000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 23407.379  
 -4.577076530D+03-8.417631000D+02 1.704083828D+01-5.357882540D-03  
 3.951778770D-06  
 -2.051775094D-10-4.085416910D-13 -7.694982170D+04-  
 5.435412780D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 23407.379  
 1.792711652D+06-4.659406600D+03 1.693822422D+01 2.106246492D-04-  
 1.269617470D-07  
 2.063382927D-11-1.150861507D-15 -5.024117630D+04-  
 6.027054920D+01  
 Rb2SO4 Gurvich,1982 pt1 p452 pt2 p476.  
 2 g10/99 RB 2.00S 1.000 4.00 0.00 0.00 0 266.99920 -  
 1096592.052  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 23321.948

6.094854930D+04-6.889705900D+02 7.034242180D+00 3.933945470D-02-  
 5.498920510D-05  
 3.716341080D-08-9.919863380D-12 -1.311877657D+05-  
 4.450162870D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 23321.948  
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 6.289142940D-08  
 -7.219324300D-12 3.348718190D-16 -1.338713151D+05-  
 7.056246320D+01  
 Rn Ref-Elm. Moore, 1971. Gordon, 1999.  
 3 g 5/97 RN 1.00 0.00 0.00 0.00 0.00 0 222.01760  
 0.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 3.389432090D-06-1.311675533D-07 2.500000001D+00-2.978593139D-12  
 4.337050730D-15  
 -3.182040220D-18 9.247787030D-22 -7.453749990D+02  
 6.952441980D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 2.730190029D+04-8.284672620D+01 2.598178483D+00-5.813729850D-05  
 1.819136527D-08  
 -2.866656182D-12 1.789322176D-16 -2.202809340D+02  
 6.255005710D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 9.180866680D+08-6.245854600D+05 1.724946531D+02-2.325758595D-02  
 1.636222413D-06  
 -5.369173150D-11 6.507189926D-16 4.883105900D+06-  
 1.449516146D+03  
 Rn+ Moore, 1971. Gordon, 1999.  
 3 g 1/97 RN 1.00E -1.00 0.00 0.00 0.00 0 222.01705  
 1043270.264  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 -9.697148970D-02 1.106742047D-03 2.499994937D+00 1.189388239D-08-  
 1.515895754D-11  
 9.958934810D-15-2.640751817D-18 1.247304760D+05  
 8.338761700D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 -1.998285319D+04 5.930675660D+01 2.432476003D+00 3.716025920D-05-  
 1.012057848D-08  
 1.192256661D-12-3.184521980D-17 1.243528478D+05  
 8.821997790D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 -2.408821471D+07 1.571151698D+04-1.411683762D+00 4.495267600D-04-  
 2.324033616D-08  
 5.830243350D-13-5.821682810D-18 9.187457500D+02  
 4.233613280D+01  
 S Hf: Cox, 1989 p22. Martin, 1990. Gordon, 1999.  
 3 g 5/97 S 1.00 0.00 0.00 0.00 0.00 0 32.06600  
 277170.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6657.425  
 -3.174841820D+02-1.924704923D+02 4.686825930D+00-5.841365600D-03  
 7.538533520D-06  
 -4.863586040D-09 1.256976992D-12 3.323592180D+04-  
 5.718477190D+00



1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6657.425  
 -4.854244790D+05 1.438830408D+03 1.258504116D+00 3.797990430D-04  
 1.630685864D-09  
 -9.547095850D-12 8.041466646D-16 2.334995270D+04  
 1.559559533D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6657.425  
 -1.302005414D+08 6.909362020D+04-1.176228025D+01 1.601540850D-03-  
 1.050533340D-07  
 4.341829020D-12-7.675621927D-17 -5.261485030D+05  
 1.322195719D+02  
 S+ Martin,1990. Gordon,1999.  
 3 g 1/98 S 1.00E -1.00 0.00 0.00 0.00 0 32.06545  
 1282496.428  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 1.535026117D+05  
 5.436270120D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 1.346218684D+06-4.056871510D+03 7.153436550D+00-2.523562352D-03  
 6.429539610D-07  
 -6.431672160D-11 2.141387919D-15 1.792823835D+05-  
 2.786930401D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 1.542254583D+08-1.023073546D+05 2.591796942D+01-2.111469141D-03  
 9.215571560D-08  
 -1.964168821D-12 2.096218597D-17 9.622418410D+05-  
 2.017239489D+02  
 S- Hotop,1985. Gordon,1999.  
 3 g 4/97 S 1.00E 1.00 0.00 0.00 0.00 0 32.06655  
 70368.505  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6464.905  
 -2.596051473D+03-1.422398653D+02 4.007825670D+00-3.608855910D-03  
 4.236230000D-06  
 -2.520987604D-09 6.079479760D-13 8.197793070D+03-  
 2.582330567D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6464.905  
 2.730311692D+03 1.414072078D+02 2.403340775D+00 3.693577530D-05-  
 7.944080440D-09  
 8.952208380D-13-4.099662820D-17 6.931195700D+03  
 6.575033680D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6464.905  
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 1.808577869D-10  
 5.778854260D-15-7.490337240D-20 6.947841220D+03  
 6.070626550D+00  
 SCL Chase,1998 p803.  
 2 j 6/78 S 1.00CL 1.00 0.00 0.00 0.00 0 67.51870  
 156465.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9819.151  
 1.613051454D+04-5.606249550D+02 8.064931130D+00-9.186326400D-03  
 1.224205395D-05

-8.209562020D-09 2.205087197D-12 1.997739280D+04-  
 1.693352855D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9819.151  
 -9.405123450D+04 3.629760850D+02 4.069959360D+00 3.034029742D-04-  
 8.248301390D-08  
 1.252700734D-11-6.417463650D-16 1.523111069D+04  
 6.014543960D+00  
 SCL2 Chase,1998 p856.  
 2 j 6/78 S 1.00CL 2.00 0.00 0.00 0.00 0 102.97140 -  
 17573.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12445.325  
 5.792311830D+04-1.062447681D+03 1.037694738D+01-6.130229020D-03  
 6.463486000D-06  
 -3.679038050D-09 8.731931650D-13 1.262475821D+03-  
 2.691768909D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12445.325  
 -2.341039963D+05 4.287569580D+02 6.471415390D+00 3.179476740D-04-  
 9.747483080D-08  
 1.393318570D-11-6.394795170D-16 -7.210473700D+03-  
 2.774267324D+00  
 SCL2+ Chase,1998 p857.  
 3 j 6/78 S 1.00CL 2.00E -1.00 0.00 0.00 0 102.97085  
 901383.347  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12453.247  
 4.934876870D+04-9.601641020D+02 9.884792780D+00-4.950257170D-03  
 4.946286970D-06  
 -2.678720604D-09 6.076844030D-13 1.112812037D+05-  
 2.342664359D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12453.247  
 -2.339403605D+05 5.516283260D+02 6.125212160D+00 6.771056320D-04-  
 2.674382769D-07  
 4.935938880D-11-2.955831247D-15 1.026787381D+05  
 1.365670223D-01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12453.247  
 1.159729818D+08-4.231290230D+04 7.753324790D+00 1.215229138D-03-  
 1.338847939D-07  
 5.496166430D-12-8.098916920D-17 4.756171550D+05-  
 2.296332675D+01  
 SD Chase,1998 p1039.  
 2 j 6/77 S 1.00D 1.00 0.00 0.00 0.00 0 34.08010  
 138490.892  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9294.443  
 -3.295574990D+04 1.647104687D+02 4.978984550D+00-8.031585710D-03  
 1.653766397D-05  
 -1.345197981D-08 4.000431530D-12 1.435862329D+04-  
 1.997290002D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9294.443  
 2.456732490D+05-1.180034105D+03 5.284690050D+00-2.384319882D-04  
 6.009960290D-08  
 -7.131163640D-12 4.035858700D-16 2.265545124D+04-  
 8.350439640D+00  
 SF Gurvich,1989 pt1 p302 pt2 p183.

2 tpi89 S 1.00F 1.00 0.00 0.00 0.00 0 51.06440  
 15445.561  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9470.114  
 1.206456774D+04-2.910270770D+02 5.480101570D+00-1.975880235D-03  
 2.473685990D-06  
 -1.610904623D-09 4.310038540D-13 1.991337574D+03-  
 4.544109600D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9470.114  
 7.634580750D+05-2.423638430D+03 7.352198710D+00-1.598026079D-03  
 4.868515020D-07  
 -6.478000530D-11 2.980297310D-15 1.577461591D+04-  
 1.902581898D+01  
 SF+ Chase,1998 p1091 6/76.  
 3 g 1/01 S 1.00F 1.00E -1.00 0.00 0.00 0 51.06385  
 994570.218  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8864.318  
 6.578303670D+04-6.986699970D+02 5.621292240D+00-6.909274110D-04-  
 1.282392780D-07  
 4.021320420D-10-1.424033453D-13 1.221751247D+05-  
 6.682348340D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8864.318  
 -9.374943900D+05 2.377214240D+03 2.052929113D+00 1.081609837D-03-  
 1.535468024D-07  
 8.222691900D-12 3.259746880D-17 1.026849122D+05  
 1.887708706D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8864.318  
 -4.833080340D+07 3.315103280D+04-4.246678200D+00 1.269355284D-03-  
 7.864010490D-08  
 2.406680266D-12-2.892795916D-17 -1.419262455D+05  
 7.611523700D+01  
 SF- Gurvich,1989 pt1 p304 pt2 p184.  
 2 tpi89 S 1.00F 1.00E 1.00 0.00 0.00 0 51.06495 -  
 231346.893  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8875.107  
 5.019879280D+04-5.321549310D+02 4.904849010D+00 9.915307420D-04-  
 2.270841545D-06  
 1.844749756D-09-5.357057200D-13 -2.611388646D+04-  
 3.637438690D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8875.107  
 2.068923125D+05-1.324372811D+03 6.646211240D+00-1.641781588D-03  
 6.783883120D-07  
 -1.198331099D-10 7.121739540D-15 -2.150994816D+04-  
 1.470236246D+01  
 SF2 Gurvich,1989 pt1 p305 pt2 p185.  
 2 tpi89 S 1.00F 2.00 0.00 0.00 0.00 0 70.06281 -  
 293188.734  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11048.373  
 6.870871130D+04-8.432418250D+02 6.269496400D+00 6.484142450D-03-  
 1.145126533D-05  
 8.770291560D-09-2.542611601D-12 -3.229980700D+04-  
 8.800004370D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11048.373

-1.702612287D+05-1.497038204D+02 7.110934140D+00-4.407741600D-05  
 9.682208310D-09  
 -1.104468959D-12 5.095308780D-17 -3.704289490D+04-  
 1.095251819D+01  
 SF2+ Chase,1998 p1144 12/76.  
 3 g 1/01 S 1.00F 2.00E -1.00 0.00 0.00 0 70.06226  
 706015.901  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11234.180  
 1.311648923D+05-1.552127914D+03 9.803424720D+00-2.488118587D-03  
 7.501565130D-07  
 3.135384495D-10-1.986281446D-13 9.137758390D+04-  
 2.792298425D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11234.180  
 -3.847531020D+05 5.327893020D+02 6.281908900D+00 4.522790120D-04-  
 1.426421096D-07  
 2.079708115D-11-9.691709890D-16 7.884213810D+04-  
 4.216089120D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11234.180  
 -1.635869714D+08 1.203460697D+05-2.737707929D+01 4.676205400D-03-  
 3.035589058D-07  
 9.547077170D-12-1.181291324D-16 -8.508449070D+05  
 2.843901644D+02  
 SF2- Chase,1998 p1145 12/76.  
 3 g 1/01 S 1.00F 2.00E 1.00 0.00 0.00 0 70.06336 -  
 394794.960  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12124.875  
 5.284572480D+04-1.032342905D+03 1.006404631D+01-5.209503250D-03  
 5.168381370D-06  
 -2.783420867D-09 6.286410080D-13 -4.423303780D+04-  
 2.699264829D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12124.875  
 -9.376618950D+04-3.638995270D+01 7.027942820D+00-1.142143365D-05  
 2.566295898D-09  
 -2.981125977D-13 1.395700722D-17 -4.967050330D+04-  
 8.483066490D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12124.875  
 -2.168882121D+04-5.051042570D+01 7.011106220D+00-1.262936151D-06  
 7.835542760D-11  
 -2.517641418D-15 3.278401810D-20 -4.951246860D+04-  
 8.370888040D+00  
 SF3 Gurvich,1989 pt1 p306 pt2 p186.  
 2 tpris89 S 1.00F 3.00 0.00 0.00 0.00 0 89.06121 -  
 504101.395  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13548.265  
 1.284008253D+05-2.084871223D+03 1.423421102D+01-4.015032190D-03  
 9.152258040D-07  
 1.109809721D-09-5.988602720D-13 -5.239517340D+04-  
 5.187193040D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13548.265  
 -2.411283460D+05-1.418950375D+02 1.010590548D+01-4.231526910D-05  
 9.336120600D-09  
 -1.068727665D-12 4.944342600D-17 -6.358445860D+04-  
 2.489560112D+01

SF3+ Chase,1998 p1170.

3 j12/76 S 1.00F 3.00E -1.00 0.00 0.00 0 89.06066  
393583.476  
298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
12409.148  
2.157633857D+05-2.564488498D+03 1.323216044D+01-1.749580869D-04-  
3.712958710D-06  
3.580688420D-09-1.084376153D-12 5.876088420D+04-  
5.024128500D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
12409.148  
-3.778260750D+05-1.621770252D+02 9.960265970D+00 1.237729568D-04-  
6.442207890D-08  
1.300856025D-11-7.915106980D-16 4.415426810D+04-  
2.673899086D+01  
6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
12409.148  
8.358347800D+06 2.002176210D+03 7.115714750D+00 6.563028420D-04-  
5.120344380D-08  
1.781530495D-12-2.365386482D-17 3.575488850D+04-  
4.384268480D+00

SF3- Gurvich,1989 pt1 p307 pt2 p187.

2 tpis89 S 1.00F 3.00E 1.00 0.00 0.00 0 89.06176 -  
790124.207  
298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
13722.893  
1.546500675D+05-2.469768526D+03 1.657548496D+01-1.020137434D-02  
9.368008460D-06  
-4.725672600D-09 1.009661431D-12 -8.500157900D+04-  
6.532164790D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
13722.893  
-2.253860964D+05-1.308890242D+02 1.009972380D+01-4.052345530D-05  
9.064565220D-09  
-1.049320641D-12 4.899201260D-17 -9.800227200D+04-  
2.524366339D+01

SF4 Gurvich,1989 pt1 p307 pt2 p188.

2 tpis89 S 1.00F 4.00 0.00 0.00 0.00 0 108.05961 -  
760000.000  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
15382.882  
1.636183265D+05-2.531316261D+03 1.559106568D+01 3.326704310D-03-  
1.054935525D-05  
9.391363050D-09-2.914816694D-12 -8.115558920D+04-  
6.131531570D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
15382.882  
-3.777125160D+05-2.937595659D+02 1.321902007D+01-8.747669450D-05  
1.929905265D-08  
-2.209423506D-12 1.022335559D-16 -9.483175340D+04-  
4.243059890D+01

SF4+ Chase,1998 p1188.

3 j12/76 S 1.00F 4.00E -1.00 0.00 0.00 0 108.05906  
416111.962  
298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
16505.547  
2.309587324D+05-3.383777670D+03 2.101756367D+01-1.106529555D-02  
9.038097280D-06  
-4.055912640D-09 7.712575180D-13 6.425375150D+04-  
8.938223520D+01

1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16505.547  
 -4.189172750D+05 4.002889640D+01 1.283873264D+01 1.340235036D-04-  
 4.818135180D-08  
 7.574595960D-12-3.696670780D-16 4.469944230D+04-  
 3.760377210D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16505.547  
 -3.761690270D+07 2.881726011D+04 4.470948840D+00 1.170801362D-03-  
 7.325658000D-08  
 2.214151827D-12-2.649348632D-17 -1.772949712D+05  
 3.397690370D+01  
 SF4- Chase,1998 p1189.  
 3 j12/76 S 1.00F 4.00E 1.00 0.00 0.00 0 108.06016 -  
 887464.320  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18480.321  
 1.005523355D+05-2.267351994D+03 1.979284560D+01-1.163761842D-02  
 1.161792139D-05  
 -6.288895470D-09 1.426371272D-12 -9.895597430D+04-  
 7.916364690D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18480.321  
 3.208822080D+05-1.710416599D+03 1.494425485D+01-1.057207329D-03  
 2.742846920D-07  
 -2.905761211D-11 1.084482543D-15 -1.005231225D+05-  
 5.164255190D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18480.321  
 5.436095670D+07-3.546125020D+04 2.105391090D+01-7.366819310D-04  
 3.537247530D-08  
 -8.825254090D-13 9.049180280D-18 1.694175033D+05-  
 1.089710755D+02  
 SF5 Gurvich,1989 pt1 p308 pt2 p189.  
 2 tpis89 S 1.00F 5.00 0.00 0.00 0.00 0 127.05802 -  
 902663.287  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18811.479  
 2.224176850D+05-4.043991750D+03 2.707196786D+01-1.744176604D-02  
 1.604198715D-05  
 -7.997243020D-09 1.667968061D-12 -9.220078270D+04-  
 1.232426161D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18811.479  
 -3.892426370D+05-1.825826536D+02 1.613765057D+01-5.544834230D-05  
 1.231433706D-08  
 -1.417173409D-12 6.584889400D-17 -1.135671054D+05-  
 5.577523020D+01  
 SF5+ Chase,1998 p1200.  
 3 j12/77 S 1.00F 5.00E -1.00 0.00 0.00 0 127.05747  
 172644.006  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16347.344  
 3.777135620D+05-5.646075120D+03 3.049404270D+01-2.176488368D-02  
 1.941993792D-05  
 -9.556201140D-09 2.000077302D-12 4.592204810D+04-  
 1.489889509D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16347.344  
 -9.814342320D+05 7.208817390D+02 1.564386818D+01-2.452519972D-04  
 2.241690996D-07

-3.990035890D-11 2.279087545D-15 9.090953190D+03-  
 5.531459450D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16347.344  
 9.063623020D+06-8.079630910D+03 1.805068495D+01-2.624346278D-05-  
 4.739171840D-09  
 2.144486076D-13-2.737984333D-18 7.597515770D+04-  
 7.692262690D+01  
 SF5- Gurvich,1989 pt1 p309 pt2 p190.  
 2 tpris89 S 1.00F 5.00E 1.00 0.00 0.00 0 127.05856 -  
 1204622.287  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19049.913  
 2.095031134D+05-3.930081140D+03 2.702127215D+01-1.792973203D-02  
 1.718122152D-05  
 -9.000560190D-09 1.988018147D-12 -1.291816581D+05-  
 1.231672739D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19049.913  
 -3.733219200D+05-1.793729521D+02 1.613699748D+01-5.577539970D-05  
 1.249477046D-08  
 -1.448104799D-12 6.767462300D-17 -1.498554401D+05-  
 5.631438210D+01  
 SF6 Gurvich,1989 pt1 p311 pt2 p191.  
 2 tpris89 S 1.00F 6.00 0.00 0.00 0.00 0 146.05642 -  
 121940.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16940.067  
 3.309526740D+05-4.737685050D+03 2.247738068D+01 1.046954309D-02-  
 2.560641961D-05  
 2.153716967D-08-6.516098960D-12 -1.255360583D+05-  
 1.091760042D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16940.067  
 -7.306726500D+05-6.367056550D+02 1.947442853D+01-1.894325671D-04  
 4.178722830D-08  
 -4.783744950D-12 2.213516129D-16 -1.510609837D+05-  
 8.147573560D+01  
 SF6- Chase,1998 p1206.  
 3 j 6/77 S 1.00F 6.00E 1.00 0.00 0.00 0 146.05697 -  
 1341876.033  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17490.714  
 4.985809210D+05-6.934445740D+03 3.441318330D+01-1.984032360D-02  
 1.497871222D-05  
 -6.133234650D-09 1.045159581D-12 -1.297069066D+05-  
 1.747984392D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17490.714  
 -6.818073510D+05-5.947429960D+02 1.945009842D+01-1.820212649D-04  
 4.057079570D-08  
 -4.683820930D-12 2.182263999D-16 -1.658902452D+05-  
 7.965844860D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17490.714  
 1.777074958D+05-6.533730340D+02 1.914322537D+01-1.624883879D-05  
 1.006454127D-09  
 -3.230395820D-14 4.203897370D-19 -1.646993323D+05-  
 7.753345240D+01  
 SH D0:Continetti,1991. Gurvich,1989 pt1 p296 pt2 p179.

2 g10/01 S 1.00H 1.00 0.00 0.00 0.00 0 33.07394  
 142135.309  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9098.109  
 6.389434680D+03-3.747960920D+02 7.548145770D+00-1.288875477D-02  
 1.907786343D-05  
 -1.265033728D-08 3.235158690D-12 1.742902395D+04-  
 1.760757308D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9098.109  
 1.682631601D+06-5.177152210D+03 9.198168520D+00-2.323550224D-03  
 6.543914780D-07  
 -8.468470420D-11 3.864741550D-15 4.899214490D+04-  
 3.770395740D+01  
 SH- Gurvich,1989 pt1 p297 pt2 p180.  
 2 g10/01 S 1.00H 1.00E 1.00 0.00 0.00 0 33.07449 -  
 86574.096  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8646.104  
 3.878070760D+04-5.742590600D+02 6.898544460D+00-1.001352412D-02  
 1.486460572D-05  
 -9.750368900D-09 2.446909813D-12 -8.735388980D+03-  
 1.615961954D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8646.104  
 1.198715402D+06-3.894846820D+03 7.660422330D+00-1.355237590D-03  
 3.342370240D-07  
 -3.350722310D-11 9.055084780D-16 1.317477387D+04-  
 2.818366081D+01  
 SN Gurvich,1989 pt1 p392 pt2 p252.  
 2 tpis89 S 1.00N 1.00 0.00 0.00 0.00 0 46.07274  
 267388.313  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9393.113  
 -6.835412350D+04 1.147567483D+03-2.877802574D+00 1.724864320D-02-  
 2.058999904D-05  
 1.261369640D-08-3.139030141D-12 2.564143612D+04  
 4.224010350D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9393.113  
 -4.837284460D+05 1.058075590D+03 3.086198804D+00 9.111360780D-04-  
 2.764061722D-07  
 4.157370110D-11-2.128351755D-15 2.379345477D+04  
 1.033225525D+01  
 SO Gurvich,1989 pt1 p286 pt2 p173.  
 2 tpis89 S 1.00O 1.00 0.00 0.00 0.00 0 48.06540  
 4760.306  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8798.106  
 -3.342757000D+04 6.403862500D+02-1.006641228D+00 1.381512705D-02-  
 1.704486364D-05  
 1.061294930D-08-2.645796205D-12 -3.371292190D+03  
 3.093865084D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8798.106  
 -1.443410557D+06 4.113874360D+03-5.383695780D-01 2.794153269D-03-  
 6.633352260D-07  
 7.838221190D-11-3.560509070D-15 -2.708838059D+04  
 3.615361450D+01  
 SO- Gurvich,1989 pt1 p288 pt2 p174.



2 tpis89 S 1.000 1.00E 1.00 0.00 0.00 0 48.06595 -  
 105968.086  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9467.114  
 8.420196970D+03-6.916586680D+01 3.837666610D+00 2.166482062D-03-  
 2.811222562D-06  
 1.793426453D-09-4.521795950D-13 -1.354162531D+04  
 4.316172810D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9467.114  
 1.767156147D+05-6.633987360D+02 5.177279810D+00-2.853461125D-04  
 7.214421530D-08  
 -3.676469490D-12-2.910092894D-16 -9.984438010D+03-  
 3.951425550D+00  
 SOF2 Gurvich,1989 pt1 p312 pt2 p192.  
 2 tpis89 S 1.000 1.00F 2.00 0.00 0.00 0 86.06221 -  
 584952.313  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12624.845  
 6.114579650D+04-9.081119670D+02 6.883623260D+00 1.192459695D-02-  
 1.671006410D-05  
 1.110723646D-08-2.910788226D-12 -6.742935840D+04-  
 1.125457002D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12624.845  
 -2.510555779D+05-6.074439610D+02 1.045046709D+01-1.796384979D-04  
 3.964169730D-08  
 -4.543055240D-12 2.104969923D-16 -7.072071710D+04-  
 2.904332761D+01  
 SO2 Gurvich,1989 pt1 p288 pt2 p175.  
 2 tpis89 S 1.000 2.00 0.00 0.00 0.00 0 64.06480 -  
 296810.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10548.127  
 -5.310842140D+04 9.090311670D+02-2.356891244D+00 2.204449885D-02-  
 2.510781471D-05  
 1.446300484D-08-3.369070940D-12 -4.113752080D+04  
 4.045514860D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10548.127  
 -1.127640116D+05-8.252261380D+02 7.616178630D+00-1.999327610D-04  
 5.655631430D-08  
 -5.454316610D-12 2.918294102D-16 -3.351308690D+04-  
 1.655773744D+01  
 SO2- Gurvich,1989 pt1 p290 pt2 p176.  
 2 tpis89 S 1.000 2.00E 1.00 0.00 0.00 0 64.06535 -  
 408606.069  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10749.431  
 9.460901660D+04-8.562691050D+02 5.360074220D+00 7.609576740D-03-  
 1.092005659D-05  
 7.202547730D-09-1.850138220D-12 -4.580094810D+04-  
 3.929933190D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10749.431  
 -1.793400005D+05-3.663168760D+02 7.274441050D+00-1.101944663D-04  
 2.443328132D-08  
 -2.809735019D-12 1.305160431D-16 -4.973072610D+04-  
 1.261418815D+01  
 SO2CL2 Chase,1998 p847.

2 j 6/71 S 1.000 2.00CL 2.00 0.00 0.00 0 134.97020 -  
 354803.200  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16028.704  
 6.821592390D+03-5.849569200D+02 8.596756910D+00 1.197228675D-02-  
 1.333760700D-05  
 7.126129000D-09-1.496150016D-12 -4.230783810D+04-  
 1.652457918D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16028.704  
 -2.376639109D+05-9.647740410D+02 1.371469904D+01-2.850327057D-04  
 6.293509620D-08  
 -7.217844260D-12 3.346840220D-16 -4.190072990D+04-  
 4.481942130D+01  
 SO2FCL Chase,1998 p754.  
 2 j 6/71 S 1.000 2.00F 1.00CL 1.00 0.00 0 118.51590 -  
 556472.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14700.981  
 3.684561300D+04-8.038358950D+02 7.526186880D+00 1.620141782D-02-  
 1.970595270D-05  
 1.166250330D-08-2.759241465D-12 -6.503598190D+04-  
 1.299744760D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14700.981  
 -2.915402438D+05-1.107134423D+03 1.381845158D+01-3.258514460D-04  
 7.184741000D-08  
 -8.230625200D-12 3.812925620D-16 -6.552472690D+04-  
 4.709165560D+01  
 SO2F2 Gurvich,1989 pt1 p313 pt2 p193.  
 2 tpis89 S 1.000 2.00F 2.00 0.00 0.00 0 102.06161 -  
 760000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13490.451  
 5.533153530D+04-8.074639680D+02 5.287172160D+00 2.294547775D-02-  
 2.891025299D-05  
 1.785631907D-08-4.418919500D-12 -8.899428820D+04-  
 4.124241910D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13490.451  
 -3.403904450D+05-1.309288764D+03 1.396601541D+01-3.840088150D-04  
 8.456688780D-08  
 -9.678246870D-12 4.480014280D-16 -8.901994140D+04-  
 5.109268580D+01  
 SO3 Gurvich,1989 pt1 p292 pt2 p177.  
 2 tpis89 S 1.000 3.00 0.00 0.00 0.00 0 80.06420 -  
 395900.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11688.499  
 -3.952855290D+04 6.208572570D+02-1.437731716D+00 2.764126467D-02-  
 3.144958662D-05  
 1.792798000D-08-4.126386660D-12 -5.184106170D+04  
 3.391333090D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11688.499  
 -2.166923781D+05-1.301022399D+03 1.096287985D+01-3.837100020D-04  
 8.466889040D-08  
 -9.705399290D-12 4.498397540D-16 -4.398283990D+04-  
 3.655215440D+01  
 S2 Gurvich,1989 pt1 p270 pt2 p165.

2 tpi89 S 2.00 0.00 0.00 0.00 0.00 0 64.13200  
 128600.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9132.110  
 3.528091780D+04-4.222156580D+02 4.677433490D+00 1.724046361D-03-  
 3.862208210D-06  
 3.336156340D-09-9.930661540D-13 1.654767715D+04-  
 7.956811240D-01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9132.110  
 -1.588128788D+04 6.315480880D+02 2.449628069D+00 1.986240565D-03-  
 6.507927240D-07  
 1.002813651D-10-5.596990050D-15 1.085508427D+04  
 1.458549193D+01  
 S2- Gurvich,1989 pt1 p274 pt2 p166.  
 2 tpi89 S 2.00E 1.00 0.00 0.00 0.00 0 64.13255 -  
 37132.385  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9597.115  
 1.025558251D+04-6.166128250D+02 8.182052840D+00-8.311203580D-03  
 9.720274160D-06  
 -5.775476780D-09 1.393690695D-12 -3.063559874D+03-  
 1.906063363D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9597.115  
 4.830204030D+05-1.319171302D+03 6.031778480D+00-7.965560690D-04  
 2.282241690D-07  
 -2.504364698D-11 7.280550780D-16 2.660258490D+03-  
 9.010433540D+00  
 S2CL2 Chase,1998 p859 6/78.  
 2 g12/00 S 2.00CL 2.00 0.00 0.00 0.00 0 135.03740 -  
 16736.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16520.761  
 7.974974740D+04-1.636770024D+03 1.583744686D+01-1.186906072D-02  
 1.413008027D-05  
 -8.484903930D-09 1.981743887D-12 3.276872420D+03-  
 5.293743650D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16520.761  
 6.328816000D+05-3.442705800D+03 1.519637350D+01-2.960877176D-03  
 6.888284370D-07  
 -7.990692530D-11 3.692466060D-15 1.526672656D+04-  
 5.453313890D+01  
 S2F2 Thiiothionyl fluoride. Chase,1998 p1147.  
 2 j 6/76 S 2.00F 2.00 0.00 0.00 0.00 0 102.12881 -  
 401413.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13717.892  
 1.252904041D+05-1.941243874D+03 1.325382183D+01-1.341525124D-03-  
 2.772465632D-06  
 3.658169290D-09-1.299531209D-12 -4.067208250D+04-  
 4.560825680D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13717.892  
 -2.591757719D+05-1.059653069D+02 1.006588551D+01-2.274618148D-05  
 5.412343140D-09  
 -9.911387140D-13 9.621861440D-17 -5.147675180D+04-  
 2.375663203D+01  
 S2O Gurvich,1989 pt1 p293 pt2 p178.

2 tpis89 S 2.000 1.00 0.00 0.00 0.00 0 80.13140 -  
 56035.495  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11128.557  
 1.092703310D+04-9.523099870D+01 3.144525430D+00 1.176854200D-02-  
 1.580266840D-05  
 1.037645040D-08-2.708622260D-12 -7.500471900D+03  
 1.104173640D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11128.557  
 -1.442139790D+05-3.276430130D+02 7.244286110D+00-9.776538300D-05  
 2.162712700D-08  
 -2.482782220D-12 1.151778750D-16 -7.438553930D+03-  
 1.085177000D+01  
 S3 Gurvich,1989 pt1 p275 pt2 p167.  
 2 tpis89 S 3.00 0.00 0.00 0.00 0.00 0 96.19800  
 144738.328  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11974.328  
 7.245395740D+04-1.162146759D+03 9.955413680D+00-4.158026220D-03  
 3.241778390D-06  
 -1.264648239D-09 1.777450535D-13 2.146275475D+04-  
 2.587521187D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11974.328  
 -1.117805401D+05-5.197908390D+01 7.038760840D+00-1.546804022D-05  
 3.408340410D-09  
 -3.896862360D-13 1.800860389D-17 1.525406485D+04-  
 7.609998320D+00  
 S4 Gurvich,1989 pt1 p280 pt2 p168.  
 2 tpis89 S 4.00 0.00 0.00 0.00 0.00 0 128.26400  
 135632.333  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14280.333  
 1.198664135D+05-2.040786521D+03 1.510235054D+01-7.041104300D-03  
 5.350405000D-06  
 -2.002348038D-09 2.569940995D-13 2.410909409D+04-  
 5.503148560D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14280.333  
 -2.068333537D+05-9.696151430D+01 1.007243210D+01-2.895047053D-05  
 6.387806190D-09  
 -7.311767430D-13 3.382265290D-17 1.321109530D+04-  
 2.344867559D+01  
 S5 Gurvich,1989 pt1 p281 pt2 p169.  
 2 tpis89 S 5.00 0.00 0.00 0.00 0.00 0 160.33000  
 132993.354  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19053.354  
 1.361370439D+05-2.955476536D+03 2.633358816D+01-4.125806530D-02  
 7.056814030D-05  
 -5.611095330D-08 1.659457200D-11 2.675307046D+04-  
 1.069710599D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19053.354  
 -4.038495160D+06 8.601803880D+03 7.443780900D+00 1.533393812D-03-  
 2.532718676D-07  
 2.145210795D-11-7.213102680D-16 -4.686925420D+04  
 1.104233874D+01  
 S6 Gurvich,1989 pt1 p282 pt2 p170.

2 tpis89 S 6.00 0.00 0.00 0.00 0.00 0 192.39600  
 101315.180  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22787.179  
 9.780307210D+04-2.568470130D+03 2.467025557D+01-1.619983175D-02  
 1.712334526D-05  
 -9.746296740D-09 2.486964867D-12 2.037888389D+04-  
 1.014409841D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22787.179  
 3.686845060D+06-7.695017900D+03 1.860721995D+01 2.290382548D-03-  
 1.219834021D-06  
 2.060780798D-10-1.190354318D-14 6.032486480D+04-  
 7.490241040D+01  
 S7 Gurvich,1989 pt1 p283 pt2 p171.  
 2 tpis89 S 7.00 0.00 0.00 0.00 0.00 0 224.46200  
 111890.369  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 26274.368  
 1.233655613D+05-3.200543640D+03 3.015678887D+01-2.197472483D-02  
 2.487892075D-05  
 -1.506049557D-08 3.768925990D-12 2.390005896D+04-  
 1.275977703D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 26274.368  
 -2.726396041D+05-7.373215220D+01 1.905771987D+01-2.394575885D-05  
 5.442671300D-09  
 -6.379663480D-13 3.008212993D-17 7.308458830D+03-  
 6.159107750D+01  
 S8 Gurvich,1989 pt1 p284 pt2 p172.  
 2 tpis89 S 8.00 0.00 0.00 0.00 0.00 0 256.52800  
 101277.122  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 31573.122  
 3.145625719D+05-6.116510160D+03 4.875327540D+01-6.241794650D-02  
 7.421831750D-05  
 -3.726449310D-08 5.799429880D-12 3.573890840D+04-  
 2.288701509D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 31573.122  
 -8.727921130D+06 1.221627968D+04 2.209959617D+01-3.494064830D-03  
 1.397604162D-06  
 -2.169815281D-10 1.212304364D-14 -8.658110820D+04-  
 6.435737830D+01  
 Sc Hf:Gurvich,1982. Sugar,1985. Gordon,1999.  
 3 g 1/99 SC 1.00 0.00 0.00 0.00 0.00 0 44.95591  
 377700.259  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7002.259  
 -3.700805940D+03 1.692506026D+02 1.842242597D+00 1.364835821D-03-  
 1.580085847D-06  
 9.613111150D-10-2.392381918D-13 4.385215240D+04  
 1.072781921D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7002.259  
 8.810382650D+06-2.711232975D+04 3.476588660D+01-1.861104581D-02  
 5.290283900D-06  
 -6.585408060D-10 2.997850429D-14 2.162460097D+05-  
 2.225618519D+02  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7002.259

2.283130511D+09-1.367701232D+06 3.213593060D+02-3.563171100D-02  
 2.093254715D-06  
 -6.238650020D-11 7.425605615D-16 1.092708359D+07-  
 2.781409383D+03  
 Sc+ Sugar,1985. Gordon,1999.  
 3 g 7/97 SC 1.00E -1.00 0.00 0.00 0.00 0 44.95536  
 1017145.222  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7161.922  
 -5.884930160D+03 1.479044408D+02 2.009576456D+00 7.389566970D-04-  
 6.617964820D-07  
 6.841073760D-10-2.164125532D-13 1.208439139D+05  
 1.026570620D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7161.922  
 1.973658531D+06-4.954384100D+03 6.360627350D+00-7.168785920D-04  
 2.464991123D-08  
 9.632373790D-12-8.544709642D-16 1.543423764D+05-  
 2.261925782D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7161.922  
 2.219151811D+08-1.287881370D+05 3.265593870D+01-3.379963200D-03  
 1.981741972D-07  
 -5.190207160D-12 4.635586113D-17 1.149364313D+06-  
 2.553294937D+02  
 Sc- Hotop,1985. Used J from isoelectronic Ti. Gordon,1999.  
 3 g 9/97 SC 1.00E 1.00 0.00 0.00 0.00 0 44.95646  
 352558.828  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 4.165746390D+04  
 8.270420720D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 4.165746390D+04  
 8.270420720D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 4.165746390D+04  
 8.270420720D+00  
 ScO D0,Props(extrap):Gurvich,1982 pt1 p140 pt2 p143.  
 3 tpris9 SC 1.000 1.00 0.00 0.00 0.00 0 60.95531 -  
 55065.294  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8787.106  
 -3.136784613D+03 2.271981685D+02 8.850757320D-01 1.052430774D-02-  
 1.431954596D-05  
 9.652351070D-09-2.586210633D-12 -8.550798770D+03  
 2.012706847D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8787.106  
 1.224192443D+06-3.918915720D+03 8.679848810D+00-1.995893306D-03  
 4.066989850D-07  
 -1.504459913D-11-8.472998900D-16 1.677322594D+04-  
 2.951656272D+01

6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8787.106  
 5.435720930D+08-2.629571561D+05 4.324788690D+01-8.590816240D-04-  
 1.205059380D-07  
 6.918221540D-12-1.109417319D-16 2.162498313D+06-  
 3.650332350D+02  
 ScO+ D0, Estim.cons:Gurvich,1982 pt1 p142 pt2 p145.  
 3 g10/99 SC 1.000 1.00E -1.00 0.00 0.00 0 60.95476  
 561209.966  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8777.066  
 4.588560270D+04-3.367114370D+02 3.527206400D+00 3.988850300D-03-  
 5.568985430D-06  
 3.650281190D-09-9.356491500D-13 6.838350790D+04  
 4.339812700D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8777.066  
 -1.814357141D+06 5.853425320D+03-3.657101210D+00 5.734364510D-03-  
 2.092878161D-06  
 3.695645020D-10-2.214038347D-14 2.955364078D+04  
 5.660889410D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8777.066  
 4.395803280D+09-2.670232109D+06 6.250769670D+02-6.991767580D-02  
 4.175372710D-06  
 -1.274326266D-10 1.571603736D-15 2.130530393D+07-  
 5.428823800D+03  
 ScO2 Gurvich,1982 pt1 p143 pt2 p147.  
 2 tpis82 SC 1.000 2.00 0.00 0.00 0.00 0 76.95471 -  
 413650.667  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10752.133  
 4.794700960D+04-4.298358590D+02 3.417206500D+00 1.361338544D-02-  
 2.047465023D-05  
 1.455906041D-08-4.038087690D-12 -4.861049530D+04  
 7.670013330D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10752.133  
 -1.903902542D+05-2.315588820D+02 7.172104910D+00-6.859209640D-05  
 1.510998557D-08  
 -1.727951588D-12 7.988980500D-17 -5.112974750D+04-  
 1.090764597D+01  
 Sc2O Gurvich,1982 pt1 p144 pt2 p148.  
 2 tpis82 SC 2.000 1.00 0.00 0.00 0.00 0 105.91122 -  
 23044.208  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11709.844  
 2.550002615D+04-3.077608607D+02 4.671215040D+00 8.696142250D-03-  
 1.283873116D-05  
 8.988966810D-09-2.461994147D-12 -2.614951944D+03  
 2.920017180D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11709.844  
 -1.350880396D+05-1.854540692D+02 7.138294080D+00-5.529432140D-05  
 1.221589315D-08  
 -1.400490463D-12 6.488858110D-17 -4.240235140D+03-  
 9.372710950D+00  
 Sc2O2 Gurvich,1982 pt1 p145 pt2 p149.  
 2 tpis82 SC 2.000 2.00 0.00 0.00 0.00 0 121.91062 -  
 490571.020

200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13133.780  
 3.468445490D+03 2.617988314D+02-3.052099624D-01 3.076104070D-02-  
 4.183478360D-05  
 2.794218425D-08-7.412672050D-12 -6.144013210D+04  
 2.915248555D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13133.780  
 -2.977348677D+05-5.803677920D+02 1.043318377D+01-1.734165462D-04  
 3.836089790D-08  
 -4.403078030D-12 2.042208922D-16 -5.964866280D+04-  
 2.855828369D+01  
 Si Hf:Cox,1989. NIST data version1.1 [Online]1997.  
 Gordon,1999.  
 3 g 8/97 SI 1.00 0.00 0.00 0.00 0.00 0 28.08550  
 450000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7550.258  
 9.836140810D+01 1.546544523D+02 1.876436670D+00 1.320637995D-03-  
 1.529720059D-06  
 8.950562770D-10-1.952873490D-13 5.263510310D+04  
 9.698288880D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7550.258  
 -6.169298850D+05 2.240683927D+03-4.448619320D-01 1.710056321D-03-  
 4.107714160D-07  
 4.558884780D-11-1.889515353D-15 3.953558760D+04  
 2.679668061D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7550.258  
 -9.286548940D+08 5.443989890D+05-1.206739736D+02 1.359662698D-02-  
 7.606498660D-07  
 2.149746065D-11-2.474116774D-16 -4.293792120D+06  
 1.086382839D+03  
 Si+ Martin,1983. Gordon,1999.  
 3 g 4/97 SI 1.00E -1.00 0.00 0.00 0.00 0 28.08495  
 1242508.045  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7342.945  
 -4.329791880D+04 6.795894490D+02 2.257046144D-01 4.118600490D-03-  
 4.234881600D-06  
 2.327995626D-09-5.318388059D-13 1.452039813D+05  
 1.934650510D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7342.945  
 5.919390230D+04-4.856730950D+01 2.556312024D+00-3.503397160D-05  
 1.190298787D-08  
 -2.082923821D-12 1.471452049D-16 1.491431392D+05  
 5.244267140D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7342.945  
 -4.364077210D+07 2.434350601D+04-2.763336522D+00 5.924483200D-04-  
 4.454048310D-08  
 2.509351585D-12-5.090212919D-17 -4.683214410D+04  
 5.196564190D+01  
 Si- Chase,1998 p1887 3/83. EA:Hotop,1985. Gordon,1999.  
 3 g 4/97 SI 1.00E 1.00 0.00 0.00 0.00 0 28.08605  
 308817.528  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428



-7.940146670D+02 5.567418420D+00 2.499837183D+00-9.481394460D-05  
3.171246930D-07  
-4.191323180D-10 2.035924380D-13 3.636443380D+04  
5.270119840D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428  
-6.162070100D+06 1.883310402D+04-1.899302450D+01 1.111021657D-02-  
2.535790208D-06  
2.699962923D-10-1.105062911D-14 -8.314089310D+04  
1.595298253D+02  
6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428  
-5.429517960D+07 3.297105700D+04-2.470579690D+00 3.966577600D-04-  
1.764141255D-08  
4.115769760D-13-3.904369380D-18 -2.315881505D+05  
5.226601830D+01  
SiBr Gurvich,1991 pt1 p280 pt2 p249.  
2 tpris91 SI 1.00BR 1.00 0.00 0.00 0.00 0 107.98950  
175157.421  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
10035.121  
7.370283350D+03-5.051062960D+02 8.280591040D+00-1.005383920D-02  
1.357050920D-05  
-9.115449900D-09 2.447477685D-12 2.184405475D+04-  
1.662032657D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
10035.121  
1.317799940D+06-3.669795020D+03 8.511686120D+00-1.987602041D-03  
5.035414890D-07  
-4.490120190D-11 8.235670070D-16 4.332851550D+04-  
2.467075472D+01  
SiBr2 Gurvich,1991 pt1 p281 pt2 p250.  
2 tpris91 SI 1.00BR 2.00 0.00 0.00 0.00 0 187.89350 -  
51000.000  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
13317.161  
2.386616151D+04-6.415693470D+02 9.345879110D+00-4.792904140D-03  
5.582538470D-06  
-3.455312380D-09 8.800338940D-13 -5.014757020D+03-  
1.740767596D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
13317.161  
-5.147343940D+04-1.277719997D+01 7.010202240D+00-4.296331860D-06  
9.877651970D-10  
-1.168133105D-13 5.546681380D-18 -8.319542250D+03-  
3.611826610D+00  
SiBr3 Gurvich,1991 pt1 p282 pt2 p251.  
2 tpris91 SI 1.00BR 3.00 0.00 0.00 0.00 0 267.79750 -  
157000.000  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
17461.440  
3.972806860D+04-1.066475023D+03 1.380836232D+01-7.641114720D-03  
8.775865830D-06  
-5.372430850D-09 1.356453455D-12 -1.651795623D+04-  
3.784055370D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
17461.440  
-8.888024740D+04-2.267879074D+01 1.001791167D+01-7.481150750D-06  
1.709242690D-09  
-2.011596627D-13 9.515534150D-18 -2.203026938D+04-  
1.537574366D+01

SiBr4 Gurvich,1991 pt1 p283 pt2 p252.

2 tpris91 SI 1.00BR 4.00 0.00 0.00 0.00 0 347.70150 -  
415800.000  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
22313.721  
6.821086740D+04-1.520370776D+03 1.810453360D+01-9.734688420D-03  
1.072367466D-05  
-6.343858290D-09 1.557228200D-12 -4.616585210D+04-  
5.976120630D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
22313.721  
-1.271409281D+05-3.768087950D+01 1.302910642D+01-1.194958251D-05  
2.693843051D-09  
-3.137193207D-13 1.471642663D-17 -5.408998830D+04-  
2.940384330D+01

SiC Gurvich,1991 pt1 p301 pt2 p265.

2 tpris91 SI 1.00C 1.00 0.00 0.00 0.00 0 40.09620  
734946.140  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
9217.111  
-6.223330890D+03 3.141790457D+02 3.893130830D-01 1.187507540D-02-  
1.639277197D-05  
1.131808223D-08-3.045324231D-12 8.606227730D+04  
2.310166717D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
9217.111  
-6.268806030D+04 7.209836920D+02 2.162879732D+00 2.201299585D-03-  
6.569466590D-07  
9.177110260D-11-4.969166740D-15 8.321225850D+04  
1.601675317D+01

SiC2 Gurvich,1991 pt1 p302 pt2 p266.

2 tpris91 SI 1.00C 2.00 0.00 0.00 0.00 0 52.10690  
631360.938  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
11685.409  
-4.119628990D+04 6.869747180D+02 2.361343691D-02 1.532939217D-02-  
1.435588838D-05  
6.375228740D-09-1.059204957D-12 7.130890710D+04  
2.828850316D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
11685.409  
7.026893090D+06-2.466148437D+04 3.915453030D+01-2.002884068D-02  
6.307353690D-06  
-8.848383510D-10 4.530549850D-14 2.267325155D+05-  
2.366622024D+02

SiCL Gurvich,1991 pt1 p271 pt2 p243.

2 tpris91 SI 1.00CL 1.00 0.00 0.00 0.00 0 63.53820  
142363.219  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
9884.119  
1.248508319D+04-2.044170347D+02 4.977070850D+00-5.160756260D-04  
2.931980374D-07  
-3.666615230D-12-3.393037130D-14 1.686528019D+04-  
2.264028063D-01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
9884.119  
3.767294560D+05-1.147956509D+03 5.735408430D+00-5.784890810D-04  
1.517304648D-07  
-1.291391394D-11 1.554628420D-16 2.306278401D+04-  
6.098522310D+00

SiCL2 Gurvich,1991 pt1 p273 pt2 p244.

2 tpis91 SI 1.00CL 2.00 0.00 0.00 0.00 0 98.99090 -  
 163069.287  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12529.294  
 5.305550970D+04-1.015842786D+03 1.032848185D+01-6.212267520D-03  
 6.715825400D-06  
 -3.908801640D-09 9.461732150D-13 -1.650218093D+04-  
 2.649926665D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12529.294  
 -8.050871570D+04-2.661025523D+01 7.020414720D+00-8.335824720D-06  
 1.871092411D-09  
 -2.171552767D-13 1.015849895D-17 -2.181294885D+04-  
 6.638773330D+00  
 SiCL3 Gurvich,1991 pt1 p275 pt2 p245.  
 2 tpis91 SI 1.00CL 3.00 0.00 0.00 0.00 0 134.44360 -  
 336271.670  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15717.467  
 8.691708460D+04-1.677556857D+03 1.511519060D+01-8.937031000D-03  
 9.097353530D-06  
 -5.014579960D-09 1.155962016D-12 -3.477477300D+04-  
 5.087216510D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15717.467  
 -1.477180114D+05-5.335200980D+01 1.004043521D+01-1.635121060D-05  
 3.641940110D-09  
 -4.200600590D-13 1.955201587D-17 -4.360571650D+04-  
 2.006633448D+01  
 SiCL4 Gurvich,1991 pt1 p276 pt2 p246.  
 2 tpis91 SI 1.00CL 4.00 0.00 0.00 0.00 0 169.89630 -  
 662200.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19455.438  
 1.171646285D+05-2.185821461D+03 1.908250496D+01-9.636335720D-03  
 8.836847690D-06  
 -4.360042400D-09 8.940232430D-13 -7.212802110D+04-  
 7.301533280D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19455.438  
 -2.100330761D+05-8.476107710D+01 1.306364027D+01-2.554020420D-05  
 5.653818470D-09  
 -6.488752670D-13 3.008025543D-17 -8.372268130D+04-  
 3.592585840D+01  
 SiF Gurvich,1991 pt1 p264 pt2 p238.  
 2 tpis91 SI 1.00F 1.00 0.00 0.00 0.00 0 47.08390 -  
 25232.686  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9456.114  
 1.478223768D+04 1.357998649D+01 2.324182643D+00 7.132851180D-03-  
 1.022951215D-05  
 7.148396470D-09-1.964689785D-12 -3.995380650D+03  
 1.231128121D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9456.114  
 -3.653637880D+05 8.722860040D+02 3.377218270D+00 7.508152430D-04-  
 2.308898619D-07  
 3.766781800D-11-2.143080403D-15 -1.011697664D+04  
 8.968132820D+00  
 SiFCL Gurvich,1991 pt1 p279 pt2 p248.

2 t<sub>pis91</sub> SI 1.00F 1.00CL 1.00 0.00 0.00 0 82.53660 -  
 377826.516  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11832.884  
 4.176954640D+04-5.926575380D+02 6.409770710D+00 4.641682610D-03-  
 7.978461910D-06  
 6.008728370D-09-1.720953157D-12 -4.398296070D+04-  
 6.259742900D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11832.884  
 -1.284698945D+05-1.247550173D+02 7.092893850D+00-3.707311770D-05  
 8.175173010D-09  
 -9.356435210D-13 4.328544340D-17 -4.723309720D+04-  
 8.337398160D+00  
 SiF2 Gurvich,1991 pt1 p266 pt2 p239.  
 2 t<sub>pis91</sub> SI 1.00F 2.00 0.00 0.00 0.00 0 66.08231 -  
 592838.108  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11204.470  
 4.053236650D+04-3.997637560D+02 4.055303880D+00 1.153423049D-02-  
 1.757586754D-05  
 1.260369111D-08-3.517105220D-12 -7.047770460D+04  
 3.879854420D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11204.470  
 -1.675200202D+05-1.846212090D+02 7.136986350D+00-5.450769860D-05  
 1.199012961D-08  
 -1.369470187D-12 6.324889990D-17 -7.287401020D+04-  
 1.117933348D+01  
 SiF3 Gurvich,1991 pt1 p268 pt2 p240  
 2 t<sub>pis91</sub> SI 1.00F 3.00 0.00 0.00 0.00 0 85.08071 -  
 996436.577  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13018.554  
 5.755369980D+04-7.179595770D+02 5.379396940D+00 1.813065142D-02-  
 2.738373356D-05  
 1.946519470D-08-5.390790560D-12 -1.177631169D+05-  
 3.442902040D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13018.554  
 -2.903283702D+05-3.427876940D+02 1.025536335D+01-1.019796690D-04  
 2.250326132D-08  
 -2.577117181D-12 1.192923177D-16 -1.218088967D+05-  
 2.725261142D+01  
 SiF4 Johnson,1986. McDowell,1982. Chase,1998 p1190 (6/76).  
 2 g 6/01 SI 1.00F 4.00 0.00 0.00 0.00 0 104.07911 -  
 1615780.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15365.713  
 1.069670784D+04-9.569638640D+01 2.513988593D+00 3.309781030D-02-  
 4.573044080D-05  
 3.091834452D-08-8.269304050D-12 -1.956252529D+05  
 1.133722022D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15365.713  
 -3.845892320D+05-6.569979910D+02 1.348925720D+01-5.100471360D-05  
 5.346329580D-08  
 -4.959598110D-12 2.299314375D-16 -1.957284479D+05-  
 4.673894650D+01  
 SiH Gurvich,1991 pt1 p257 pt2 p234.

2 tpi91 SI 1.00H 1.00 0.00 0.00 0.00 0 29.09344  
 368636.210  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9145.110  
 -6.426676300D+03 7.417251210D+01 3.973491600D+00-4.149408880D-03  
 1.022918384D-05  
 -8.592386360D-09 2.567093743D-12 4.281745800D+04  
 2.246937150D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9145.110  
 4.042086490D+05-2.364796524D+03 7.627499140D+00-2.496591233D-03  
 1.108436410D-06  
 -1.943991955D-10 1.136251507D-14 5.704737680D+04-  
 2.448054429D+01  
 SiH+ Chase,1998 p1308.  
 2 j12/71 SI 1.00H 1.00E -1.00 0.00 0.00 0 29.09289  
 1147671.167  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8654.261  
 -4.307157170D+04 3.884958240D+02 2.546166863D+00-6.686325980D-04  
 5.186277020D-06  
 -4.818569740D-09 1.445702640D-12 1.349079707D+05  
 9.027950090D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8654.261  
 1.711692033D+05-1.045807287D+03 4.838648240D+00 1.277940891D-04-  
 6.883872450D-08  
 1.418843480D-11-7.855316960D-16 1.431721450D+05-  
 7.553299140D+00  
 SiHBr3 Chase,1998 p514.  
 2 j12/76 SI 1.00H 1.00BR 3.00 0.00 0.00 0 268.80544 -  
 302922.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17823.429  
 1.322811122D+05-2.205365507D+03 1.775084194D+01-1.047794569D-02  
 1.286821723D-05  
 -7.743124260D-09 1.819060891D-12 -2.834992682D+04-  
 6.331199540D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17823.429  
 2.199973526D+05-2.024458552D+03 1.435781007D+01-5.037015840D-04  
 1.054049755D-07  
 -1.160828765D-11 5.217257680D-16 -2.842086214D+04-  
 4.536437170D+01  
 SiHCL Gurvich,1991 pt1 p277 pt2 p247.  
 2 tpi91 SI 1.00H 1.00CL 1.00 0.00 0.00 0 64.54614  
 54945.913  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10665.413  
 5.909673050D+04-8.780064030D+02 7.999687930D+00-4.663141270D-03  
 8.594986000D-06  
 -6.608073550D-09 1.868076396D-12 9.567570340D+03-  
 1.690015008D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10665.413  
 1.012152890D+05-1.163239598D+03 7.376366550D+00 1.874151313D-04-  
 1.661351093D-07  
 3.964414040D-11-2.640580080D-15 1.141064087D+04-  
 1.507679495D+01  
 SiHCL3 Chase,1998 880.

2 j12/76 SI 1.00H 1.00CL 3.00 0.00 0.00 0 135.45154 -  
 496222.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16151.608  
 1.659565586D+05-2.552498122D+03 1.750117375D+01-7.885728660D-03  
 8.092567490D-06  
 -3.980420600D-09 7.059173320D-13 -4.951316600D+04-  
 6.758520050D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16151.608  
 1.728644072D+05-2.116727327D+03 1.441802307D+01-5.255249620D-04  
 1.098826178D-07  
 -1.209327059D-11 5.432187050D-16 -5.130351940D+04-  
 5.036361890D+01  
 SiHF Gurvich,1991 pt1 p270 pt2 p242.  
 2 tpi91 SI 1.00H 1.00F 1.00 0.00 0.00 0 48.09184 -  
 162657.169  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10230.231  
 2.192598671D+04-6.175229080D+01 2.127372739D+00 1.123538312D-02-  
 1.322503985D-05  
 8.307307390D-09-2.010545971D-12 -2.016994845D+04  
 1.367184876D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10230.231  
 4.049752240D+06-9.295526820D+03 1.071754366D+01 1.868124220D-03-  
 1.129820372D-06  
 1.960250100D-10-1.144682011D-14 4.133225200D+04-  
 4.736317600D+01  
 SiHF3 Chase,1998 p1160.  
 2 j 6/76 SI 1.00H 1.00F 3.00 0.00 0.00 0 86.08865 -  
 1200808.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13544.634  
 8.325879390D+04-8.178594460D+02 4.041717240D+00 2.726104628D-02-  
 3.787831480D-05  
 2.630589305D-08-7.289582500D-12 -1.416146961D+05  
 1.382806532D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13544.634  
 7.820100800D+04-2.592742261D+03 1.475104214D+01-6.531047200D-04  
 1.372428937D-07  
 -1.516371051D-11 6.832497150D-16 -1.336611887D+05-  
 5.851450950D+01  
 SiHI3 Chase,1998 p1266.  
 2 j12/76 SI 1.00H 1.00I 3.00 0.00 0.00 0 409.80685 -  
 74475.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19135.424  
 1.113840054D+05-1.974457175D+03 1.791396249D+01-1.219208519D-02  
 1.613169233D-05  
 -1.038096942D-08 2.613287761D-12 -2.256377425D+03-  
 5.995455130D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19135.424  
 2.279424252D+05-1.898603142D+03 1.428134804D+01-4.776026950D-04  
 1.003097496D-07  
 -1.107859145D-11 4.990338200D-16 -1.614547674D+03-  
 4.122943070D+01  
 SiH2 Gurvich,1991 pt1 p260. Fredin,1985. Dubois,1968.

2 g 3/01 SI 1.00H 2.00 0.00 0.00 0.00 0 30.10138  
 273332.530  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10018.102  
 -2.063863564D+04 3.305862200D+02 2.099271145D+00 3.542539370D-03  
 3.378876670D-06  
 -5.383845620D-09 2.081191273D-12 3.011784298D+04  
 1.282333570D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10018.102  
 4.624039370D+06-1.143436110D+04 1.264880870D+01 9.114899500D-04-  
 8.766611540D-07  
 1.646297357D-10-9.965090370D-15 1.072475101D+05-  
 6.606078070D+01  
 SiH2Br2 Chase,1998 p481.  
 2 j12/76 SI 1.00H 2.00BR 2.00 0.00 0.00 0 189.90938 -  
 190372.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14272.222  
 1.651528003D+05-2.468145554D+03 1.608639427D+01-9.413840900D-03  
 1.407423872D-05  
 -9.240751450D-09 2.255641666D-12 -1.276482614D+04-  
 5.945374320D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14272.222  
 5.665851440D+05-3.973919620D+03 1.567387912D+01-9.943802290D-04  
 2.084856022D-07  
 -2.299521351D-11 1.034736283D-15 -2.990690180D+03-  
 6.190476520D+01  
 SiH2CL2 Chase,1998 p823.  
 2 j12/76 SI 1.00H 2.00CL 2.00 0.00 0.00 0 101.00678 -  
 320494.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13384.948  
 1.894281754D+05-2.650960252D+03 1.549874174D+01-6.533130750D-03  
 9.306098260D-06  
 -5.639698670D-09 1.213664264D-12 -2.720912007D+04-  
 6.006332540D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13384.948  
 5.400204580D+05-4.062337290D+03 1.573118788D+01-1.015038389D-03  
 2.127060243D-07  
 -2.345079226D-11 1.054871984D-15 -1.823098225D+04-  
 6.544541390D+01  
 SiH2F2 Chase,1998 p1108.  
 2 j 6/76 SI 1.00H 2.00F 2.00 0.00 0.00 0 68.09819 -  
 790776.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11988.206  
 1.272188427D+05-1.241724310D+03 4.899435890D+00 2.123882008D-02-  
 2.725708700D-05  
 1.860857446D-08-5.226604330D-12 -8.980466920D+04-  
 5.111815500D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11988.206  
 4.726534080D+05-4.388517690D+03 1.596032597D+01-1.102993658D-03  
 2.315838331D-07  
 -2.556974559D-11 1.151499711D-15 -7.316184460D+04-  
 7.098989270D+01  
 SiH2I2 Chase,1998 p1313.

2 j12/76 SI 1.00H 2.00I 2.00 0.00 0.00 0 283.91032 -  
 38074.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14917.266  
 1.539963319D+05-2.414436989D+03 1.684409354D+01-1.212037580D-02  
 1.808453226D-05  
 -1.207740133D-08 3.040799276D-12 5.073073250D+03-  
 6.098720820D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14917.266  
 5.942390830D+05-3.924814480D+03 1.563850289D+01-9.805706340D-04  
 2.054871384D-07  
 -2.265587199D-11 1.019168663D-15 1.513627352D+04-  
 5.940812520D+01  
 SiH3 Gurvich,1991 pt1 p261 pt2 p236.  
 2 g 3/99 SI 1.00H 3.00 0.00 0.00 0.00 0 31.10932  
 204357.366  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10276.989  
 4.341142820D+03 2.277185085D+02 6.508250350D-01 1.221438558D-02-  
 4.347604270D-06  
 -1.774916828D-09 1.184191367D-12 2.259993826D+04  
 1.968347482D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10276.989  
 6.056321220D+05-4.721254060D+03 1.329129523D+01-1.256824868D-03  
 2.688285940D-07  
 -3.010741582D-11 1.370945857D-15 4.974420640D+04-  
 6.140503100D+01  
 SiH3Br Chase,1998 p439.  
 2 j12/76 SI 1.00H 3.00BR 1.00 0.00 0.00 0 111.01332 -  
 78241.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11769.378  
 1.521065525D+05-1.987744479D+03 1.131460743D+01-1.806099407D-03  
 7.769262470D-06  
 -6.233478170D-09 1.585331846D-12 -9.248868880D+02-  
 3.846463690D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11769.378  
 9.279285780D+05-5.917935790D+03 1.699209298D+01-1.487507364D-03  
 3.123451161D-07  
 -3.449071470D-11 1.553431675D-15 2.241560128D+04-  
 7.948611590D+01  
 SiH3CL Chase,1998 p764.  
 2 j12/76 SI 1.00H 3.00CL 1.00 0.00 0.00 0 66.56202 -  
 141838.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11440.706  
 1.633388301D+05-2.030302118D+03 1.068016138D+01 4.942370140D-04  
 4.305174760D-06  
 -3.748327270D-09 8.893504210D-13 -8.180714980D+03-  
 3.688957500D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11440.706  
 9.087780940D+05-5.958949560D+03 1.702076016D+01-1.498450667D-03  
 3.146813781D-07  
 -3.475168460D-11 1.565281681D-15 1.493793206D+04-  
 8.127278540D+01  
 SiH3F Chase,1998 p1058.



2 j 6/76 SI 1.00H 3.00F 1.00 0.00 0.00 0 50.10772 -  
 376560.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10931.622  
 1.267836290D+05-1.177593516D+03 4.499188960D+00 1.658543011D-02-  
 1.678598921D-05  
 1.019153931D-08-2.803920232D-12 -4.010392970D+04-  
 4.481080920D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10931.622  
 8.624313170D+05-6.103370570D+03 1.712733597D+01-1.540724131D-03  
 3.239628720D-07  
 -3.581056890D-11 1.614151380D-15 -1.261487616D+04-  
 8.399227210D+01  
 SiH3I Chase,1998 p1342.  
 2 j12/76 SI 1.00H 3.00I 1.00 0.00 0.00 0 158.01379 -  
 2092.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12078.229  
 1.459384799D+05-1.982982746D+03 1.196516737D+01-3.937505950D-03  
 1.087991733D-05  
 -8.433135920D-09 2.196078188D-12 8.063208310D+03-  
 4.064553320D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12078.229  
 9.361149180D+05-5.859720290D+03 1.695376698D+01-1.473497130D-03  
 3.094475885D-07  
 -3.417462470D-11 1.539334807D-15 3.127499231D+04-  
 7.801700080D+01  
 SiH4 Silane. Gurvich,1991 pt1 p263 pt 2 p237.  
 2 tpi91 SI 1.00H 4.00 0.00 0.00 0.00 0 32.11726  
 34700.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10535.001  
 7.872993290D+04-5.526087050D+02 2.498944303D+00 1.442118274D-02-  
 8.467107310D-06  
 2.726164641D-09-5.436754370D-13 6.269669060D+03  
 4.965461830D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10535.001  
 1.290378740D+06-7.813399780D+03 1.828851664D+01-1.975620946D-03  
 4.156502150D-07  
 -4.596745610D-11 2.072777131D-15 4.766887950D+04-  
 9.801697460D+01  
 SiI Gurvich,1991 pt1 p284 pt2 p253.  
 2 tpi91 SI 1.00I 1.00 0.00 0.00 0.00 0 154.98997  
 262953.420  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9941.120  
 9.492081340D+04-1.573960062D+03 1.237908109D+01-1.593864820D-02  
 1.692049005D-05  
 -9.215558320D-09 2.046186848D-12 3.779735670D+04-  
 4.066407850D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9941.120  
 8.529402790D+05-2.442039471D+03 7.722977520D+00-1.985601243D-03  
 6.542866630D-07  
 -9.494158290D-11 4.890041370D-15 4.578160940D+04-  
 1.733975081D+01  
 SiI2 Chase,1998 p1432.

2 j12/76 SI 1.00I 2.00 0.00 0.00 0.00 0 281.89444  
 92466.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13792.515  
 1.163352403D+04-4.514482170D+02 8.707978130D+00-3.580664930D-03  
 4.253714430D-06  
 -2.673478266D-09 6.891558980D-13 1.126247142D+04-  
 1.155818335D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13792.515  
 1.002168907D+04 1.433017148D+01 6.701330550D+00 3.960769900D-04-  
 2.073866165D-07  
 4.553457100D-11-3.016798280D-15 9.007368100D+03  
 2.887336913D-01  
 SiN Gurvich,1991 pt1 p295 pt2 p261.  
 2 g 5/99 SI 1.00N 1.00 0.00 0.00 0.00 0 42.09224  
 403668.437  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8736.137  
 -1.464672152D+04 1.374993497D+02 3.678508580D+00-6.158499200D-03  
 2.309417067D-05  
 -2.294461481D-08 7.395665680D-12 4.673212990D+04  
 6.494565540D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8736.137  
 -2.932685132D+06 5.853688590D+03 1.321451677D+00 1.258329284D-03-  
 3.773886360D-07  
 6.887761040D-11-4.189842590D-15 6.527148810D+03  
 2.553145875D+01  
 SiO Gurvich,1991 pt1 p247 pt2 p227  
 2 tpi91 SI 1.00O 1.00 0.00 0.00 0.00 0 44.08490 -  
 98842.418  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8715.105  
 -4.722771050D+04 8.063137640D+02-1.636976133D+00 1.454275546D-02-  
 1.723202046D-05  
 1.042397340D-08-2.559365273D-12 -1.666585903D+04  
 3.355795700D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8715.105  
 -1.765134162D+05-3.199177090D+01 4.477441930D+00 4.591764710D-06  
 3.558143150D-08  
 -1.327012559D-11 1.613253297D-15 -1.350842360D+04-  
 8.386957330D-01  
 SiO2 Gurvich,1991 pt1 p256 pt2 p233.  
 2 tpi91 SI 1.00O 2.00 0.00 0.00 0.00 0 60.08430 -  
 322073.477  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10542.523  
 -3.362948780D+04 4.734078920D+02 2.309770671D-01 1.850230806D-02-  
 2.242786671D-05  
 1.364981554D-08-3.351935030D-12 -4.226487490D+04  
 2.295803206D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10542.523  
 -1.464031193D+05-6.261441060D+02 7.964563710D+00-1.854119096D-04  
 4.095214670D-08  
 -4.697206760D-12 2.178054280D-16 -3.791834770D+04-  
 2.045285414D+01  
 SiS Gurvich,1991 pt1 p290 pt2 p258.

2 tpis91 SI 1.00S 1.00 0.00 0.00 0.00 0 60.15150  
 108194.407  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8932.107  
 3.599449290D+04-4.239723300D+02 4.654014420D+00 1.588470782D-03-  
 3.310254360D-06  
 2.706096479D-09-8.113517820D-13 1.411515571D+04-  
 1.183176921D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8932.107  
 -2.102323897D+06 6.228836180D+03-3.004120882D+00 4.495499930D-03-  
 1.368821364D-06  
 1.998097253D-10-9.882035800D-15 -2.795538166D+04  
 5.405831280D+01  
 SiS2 Gurvich,1991 pt1 p294 pt2 p260.  
 2 tpis91 SI 1.00S 2.00 0.00 0.00 0.00 0 92.21750  
 7022.717  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12203.217  
 4.397745660D+04-7.430013120D+02 7.941588360D+00 2.038083730D-03-  
 4.646337600D-06  
 3.848014360D-09-1.157260149D-12 2.801077853D+03-  
 1.736885072D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12203.217  
 -1.266489071D+05-9.774235220D+01 7.572803680D+00-2.905413928D-05  
 6.405587840D-09  
 -7.329273340D-13 3.389819780D-17 -1.244672263D+03-  
 1.352707210D+01  
 Si2 Gurvich,1991 pt1 p240 pt2 p225.  
 2 tpis91 SI 2.00 0.00 0.00 0.00 0.00 0 56.17100  
 580195.524  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10296.124  
 1.237596221D+04-1.024904376D+02 4.354848520D+00 1.281063335D-03-  
 2.531991623D-06  
 2.265694244D-09-7.001290140D-13 6.906942850D+04  
 3.251125200D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10296.124  
 1.370060657D+06-4.207060040D+03 9.337432890D+00-2.749217168D-03  
 9.586345960D-07  
 -1.372449748D-10 6.765028100D-15 9.510884540D+04-  
 3.168385190D+01  
 Si2C Gurvich,1991 pt1 p304 pt2 p267.  
 2 tpis91 SI 2.00C 1.00 0.00 0.00 0.00 0 68.18170  
 554093.904  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11582.346  
 -4.553366200D+03 1.314796415D+02 2.469106923D+00 1.276520680D-02-  
 1.656910776D-05  
 1.065289663D-08-2.739192976D-12 6.470049920D+04  
 1.468838980D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11582.346  
 -1.253829442D+05-3.414277790D+02 7.254365330D+00-1.017635503D-04  
 2.250902158D-08  
 -2.584074852D-12 1.198884876D-16 6.608009380D+04-  
 1.146216579D+01  
 Si2F6 Lyman,2001.

2 g 6/01 SI 2.00F 6.00 0.00 0.00 0.00 0 170.16142 -  
 2383290.080  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 26694.292  
 1.580767450D+04-2.975292881D+02 7.512591500D+00 4.552796230D-02-  
 6.421876840D-05  
 4.357408730D-08-1.166762282D-11 -2.886707444D+05-  
 7.721784770D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 26694.292  
 -9.186303140D+05 1.573948683D+02 2.141256129D+01-2.681898667D-04  
 7.212280110D-08  
 -9.184252660D-12 4.537238360D-16 -2.966176753D+05-  
 7.849022470D+01  
 Si2N Chase,1998 p1611.  
 2 j 3/67 SI 2.00N 1.00 0.00 0.00 0.00 0 70.17774  
 397480.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11822.188  
 2.318271938D+04-3.674843790D+02 5.409658600D+00 8.176389400D-03-  
 1.220312934D-05  
 8.580609100D-09-2.354927059D-12 4.809278030D+04-  
 3.042204799D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11822.188  
 -2.805026986D+05 2.502366876D+02 7.092456100D+00 2.853120795D-04-  
 9.792101810D-08  
 1.552154244D-11-8.036260450D-16 4.342014790D+04-  
 1.009570825D+01  
 Si3 Gurvich,1991 pt1 p246 pt2 p226.  
 2 g 7/95 SI 3.00 0.00 0.00 0.00 0.00 0 84.25650  
 627867.381  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12519.793  
 -1.114208177D+04 1.575785843D+02 2.486135003D+00 1.631637255D-02-  
 2.208240021D-05  
 1.372008287D-08-3.262330700D-12 7.328253850D+04  
 1.588081347D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12519.793  
 -1.699395561D+06 4.697815380D+03 2.618198124D+00 1.959082075D-03-  
 2.581160603D-07  
 6.103444860D-12 6.086309240D-16 4.277916810D+04  
 2.586540384D+01  
 Sn Hf:Cox,1989 Moore,1971. Gordon,1999.  
 3 g 7/97 SN 1.00 0.00 0.00 0.00 0.00 0 118.71000  
 301200.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6214.713  
 -1.248692263D+05 1.618841190D+03-4.602397350D+00 1.045433308D-02  
 2.998265550D-06  
 -1.068699386D-08 4.323421310D-12 2.748364008D+04  
 4.805067230D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6214.713  
 -5.145695640D+06 1.140575108D+04-4.179632060D+00 2.236390679D-03-  
 3.603219770D-07  
 2.440237836D-11-2.937628285D-16 -4.215013570D+04  
 5.981450930D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6214.713

-1.119787114D+09 6.427046040D+05-1.378615913D+02 1.453867222D-02-  
 7.109586030D-07  
 1.501409263D-11-8.940758657D-17 -5.111296870D+06  
 1.245625545D+03  
 Sn+ Moore,1971. Gordon,1999.  
 3 g 7/97 SN 1.00E -1.00 0.00 0.00 0.00 0 118.70945  
 1015949.928  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 -5.571297780D+03 1.222323189D+02 1.566361415D+00 3.397061410D-03-  
 6.312922290D-06  
 5.585452080D-09-1.689021340D-12 1.209024120D+05  
 1.162634765D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 4.622916850D+06-1.185958712D+04 1.237026473D+01-2.773624217D-03  
 3.098513490D-07  
 -5.362951440D-12-8.663474691D-16 1.994322977D+05-  
 6.837108280D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 1.913728057D+08-1.145730242D+05 3.070294184D+01-3.387878800D-03  
 1.966377351D-07  
 -4.388396290D-12 2.057062343D-17 1.031631149D+06-  
 2.370157923D+02  
 Sn- Hotop,1985. Gordon,1999.  
 3 g 9/97 SN 1.00E 1.00 0.00 0.00 0.00 0 118.71055  
 179495.949  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6490.449  
 2.722796000D+05-3.369935800D+03 1.743906405D+01-2.810527618D-02  
 2.790684767D-05  
 -1.442400675D-08 3.070159757D-12 3.753227750D+04-  
 8.007856970D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6490.449  
 -6.447713220D+04 7.430555100D+02 1.921380256D+00 2.361623997D-04-  
 5.280668360D-08  
 6.102339380D-12-2.843422486D-16 1.645739414D+04  
 1.265436865D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6490.449  
 -1.314284778D+06 8.972354270D+02 2.302354538D+00 2.246840970D-05-  
 1.392571963D-09  
 4.468904450D-14-5.811846560D-19 1.428800599D+04  
 1.004933765D+01  
 SnBr Gurvich,1991 pt1 p378 pt2 p321.  
 2 tpris91 SN 1.00BR 1.00 0.00 0.00 0.00 0 198.61400  
 75644.020  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9986.120  
 2.564193542D+04-5.259122330D+02 7.687410690D+00-9.654205420D-03  
 1.482863248D-05  
 -9.942236980D-09 2.475051091D-12 1.020483889D+04-  
 1.126550396D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9986.120  
 1.815578541D+06-6.728264580D+03 1.332464516D+01-4.608102300D-03  
 1.236439537D-06  
 -1.528863587D-10 6.971513500D-15 4.925583090D+04-  
 5.640962780D+01

SnBr2 Gurvich,1991 pt1 p380 pt2 p323.  
 2 tpris91 SN 1.00BR 2.00 0.00 0.00 0.00 0 278.51800 -  
 118974.592  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14595.408  
 -4.995753060D+03-1.366498896D+02 7.543563850D+00-1.181772507D-03  
 1.442445852D-06  
 -9.254217260D-10 2.423731634D-13 -1.575506969D+04-  
 3.595584020D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14595.408  
 -1.940894091D+04-2.335607932D+00 7.001969260D+00-8.622241870D-07  
 2.039869794D-10  
 -2.464780359D-14 1.189850894D-18 -1.644828122D+04-  
 4.349354750D-01

SnBr3 Gurvich,1991 pt1 p381 pt2 p324.  
 2 tpris91 SN 1.00BR 3.00 0.00 0.00 0.00 0 358.42200 -  
 158716.446  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19280.454  
 -8.050416470D+03-2.897962523D+02 1.114443355D+01-2.475383807D-03  
 3.010051350D-06  
 -1.925695320D-09 5.032605090D-13 -2.070066649D+04-  
 1.895965383D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19280.454  
 -3.893004530D+04-4.990844170D+00 1.000418437D+01-1.824996910D-06  
 4.305646660D-10  
 -5.191887930D-14 2.502455595D-18 -2.217299473D+04-  
 1.229854098D+01

SnBr4 Gurvich,1991 pt1 p384 pt2 p326.  
 2 tpris91 SN 1.00BR 4.00 0.00 0.00 0.00 0 438.32600 -  
 324216.982  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 25043.018  
 -5.832840920D+03-4.270198470D+02 1.467466525D+01-3.604263230D-03  
 4.36686290D-06  
 -2.785875130D-09 7.265087870D-13 -4.082916450D+04-  
 3.447104360D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 25043.018  
 -5.176812920D+04-7.426126950D+00 1.300619502D+01-2.692587978D-06  
 6.336759800D-10  
 -7.627087190D-14 3.671112000D-18 -4.300166340D+04-  
 2.471455118D+01

SnCL Gurvich,1991 pt1 p370 pt2 p315.  
 2 tpris91 SN 1.00CL 1.00 0.00 0.00 0.00 0 154.16270  
 34658.816  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9644.116  
 3.351549730D+04-6.832208620D+02 8.393917730D+00-1.164434373D-02  
 1.812159499D-05  
 -1.261999170D-08 3.295213470D-12 6.051790890D+03-  
 1.667834870D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9644.116  
 7.741605680D+05-3.602048480D+03 9.749059820D+00-2.596198909D-03  
 6.367712160D-07  
 -6.754295570D-11 2.484167602D-15 2.442447662D+04-  
 3.225454390D+01

SnCL2 Gurvich,1991 pt1 p373 pt2 p317.

2 tpis91 SN 1.00CL 2.00 0.00 0.00 0.00 0 189.61540 -  
 202648.283  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13681.717  
 9.524665900D+03-4.329845640D+02 8.644720280D+00-3.458409610D-03  
 4.117852030D-06  
 -2.592639269D-09 6.692363600D-13 -2.432921127D+04-  
 1.299144326D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13681.717  
 -3.903588490D+04-7.947962680D+00 7.006487620D+00-2.776594714D-06  
 6.461341420D-10  
 -7.119067400D-15 3.688131180D-18 -2.654529653D+04-  
 3.368085920D+00  
 SnCL3 Gurvich,1991 pt1 p374 pt2 p318.  
 2 tpis91 SN 1.00CL 3.00 0.00 0.00 0.00 0 225.06810 -  
 292372.455  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17554.045  
 1.760076813D+04-8.142805480D+02 1.306326984D+01-6.395596190D-03  
 7.574624570D-06  
 -4.749711460D-09 1.222182656D-12 -3.413430960D+04-  
 3.457680270D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17554.045  
 -7.482966400D+04-1.528523914D+01 1.001240305D+01-5.285581240D-06  
 1.226095111D-09  
 -1.459895108D-13 6.968879780D-18 -3.830878270D+04-  
 1.663063737D+01  
 SnCL4 Gurvich,1991 pt1 p376 pt2 p320.  
 2 tpis91 SN 1.00CL 4.00 0.00 0.00 0.00 0 260.52080 -  
 478465.969  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22474.031  
 4.245967870D+04-1.280574318D+03 1.768445328D+01-9.574779520D-03  
 1.115620323D-05  
 -6.907229270D-09 1.759652856D-12 -5.504009040D+04-  
 5.827353690D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22474.031  
 -1.078336862D+05-2.554305872D+01 1.302040391D+01-8.595125900D-06  
 1.976570888D-09  
 -2.337929994D-13 1.110287624D-17 -6.163562030D+04-  
 3.072703313D+01  
 SnF Gurvich,1991 pt1 p365 pt2 p310.  
 2 tpis91 SN 1.00F 1.00 0.00 0.00 0.00 0 137.70840 -  
 95017.090  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9136.110  
 6.098503520D+04-9.860306290D+02 8.994731210D+00-1.223012156D-02  
 1.840583578D-05  
 -1.267926607D-08 3.291331020D-12 -7.882614480D+03-  
 2.221921734D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9136.110  
 2.589715476D+04-1.484478214D+03 7.378518930D+00-1.324244440D-03  
 2.847634043D-07  
 -2.360371345D-11 6.116783710D-16 -4.776688970D+03-  
 1.681202516D+01  
 SnF2 Gurvich,1991 pt1 p368 pt2 p312.

2 tpis91 SN 1.00F 2.00 0.00 0.00 0.00 0 156.70681 -  
 510956.951  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12243.049  
 7.042391850D+04-1.137505955D+03 1.008659352D+01-4.722855930D-03  
 4.135702920D-06  
 -1.921143972D-09 3.640760280D-13 -5.756670820D+04-  
 2.571566624D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12243.049  
 -1.027758772D+05-4.451751620D+01 7.033268760D+00-1.329882797D-05  
 2.934271938D-09  
 -3.358415920D-13 1.553358669D-17 -6.362125880D+04-  
 6.810084520D+00  
 SnF3 Gurvich,1991 pt1 p369 pt2 p313.  
 2 tpis91 SN 1.00F 3.00 0.00 0.00 0.00 0 175.70521 -  
 646630.479  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14799.721  
 1.095555529D+05-1.950557979D+03 1.541407832D+01-8.546518770D-03  
 7.800551820D-06  
 -3.825942220D-09 7.787747760D-13 -7.056794920D+04-  
 5.494639480D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14799.721  
 -1.829319689D+05-7.557358680D+01 1.005671455D+01-2.275132668D-05  
 5.034695820D-09  
 -5.776530960D-13 2.677214170D-17 -8.091897590D+04-  
 2.191673972D+01  
 SnF4 Gurvich,1991 pt1 p369 pt2 p314.  
 2 tpis91 SN 1.00F 4.00 0.00 0.00 0.00 0 194.70361 -  
 1024766.717  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18801.983  
 1.390441119D+05-2.168784371D+03 1.691802917D+01-2.318608529D-03-  
 2.045847976D-06  
 3.430087900D-09-1.289228860D-12 -1.153563396D+05-  
 6.370604750D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18801.983  
 -2.635692764D+05-1.445469969D+02 1.310690681D+01-4.237755790D-05  
 9.286871950D-09  
 -1.057062694D-12 4.867108680D-17 -1.271539967D+05-  
 3.803921900D+01  
 SnI Gurvich,1991 pt1 p384 pt2 p327.  
 2 tpis91 SN 1.00I 1.00 0.00 0.00 0.00 0 245.61447  
 172725.022  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10177.122  
 2.670212235D+04-5.006026350D+02 7.490673150D+00-8.746346550D-03  
 1.289688397D-05  
 -8.211344930D-09 1.936120475D-12 2.177249172D+04-  
 9.354806850D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10177.122  
 -5.554991850D+04-1.530457453D+03 7.932601390D+00-2.108885464D-03  
 7.809803600D-07  
 -1.348104887D-10 8.207184700D-15 2.744864953D+04-  
 1.626822892D+01  
 SnI2 Gurvich,1991 pt1 p387 pt2 p329.



2 tpis91 SN 1.00I 2.00 0.00 0.00 0.00 0 372.51894 -  
 8066.737  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14883.263  
 -5.739254890D+03-9.435024450D+01 7.377956660D+00-8.258348940D-04  
 1.011687040D-06  
 -6.508451600D-10 1.708186600D-13 -2.622644500D+03-  
 9.605814960D-01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14883.263  
 -1.559453390D+04-1.594789414D+00 7.001351160D+00-5.935324240D-07  
 1.407432564D-10  
 -1.703457321D-14 8.233611710D-19 -3.100608319D+03  
 1.235038509D+00  
 SnI3 Gurvich,1991 pt1 p388 pt2 p330.  
 2 tpis91 SN 1.00I 3.00 0.00 0.00 0.00 0 499.42341 -  
 8017.540  
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 20309.360  
 -1.069978099D+04-1.387693540D+02 1.055637633D+01-1.216435658D-03  
 1.490873499D-06  
 -9.594499630D-10 2.518810438D-13 -3.314229880D+03-  
 1.249558209D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 20309.360  
 -2.517534870D+04-2.348282890D+00 1.000199130D+01-8.752764840D-07  
 2.076464980D-10  
 -2.514060336D-14 1.215482266D-18 -4.017055610D+03-  
 9.263908460D+00  
 SnI4 Gurvich,1991 pt1 p391 pt2 p332.  
 2 tpis91 SN 1.00I 4.00 0.00 0.00 0.00 0 626.32788 -  
 118854.043  
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 26745.957  
 -1.283146793D+04-1.459885093D+02 1.358634885D+01-1.283554646D-03  
 1.574557147D-06  
 -1.013990168D-09 2.663370430D-13 -1.751178045D+04-  
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 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 26745.957  
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 2.196515817D-10  
 -2.661071614D-14 1.287167546D-18 -1.825083832D+04-  
 2.027484281D+01  
 SnO Gurvich,1991 pt1 p359 pt2 p307.  
 2 tpis91 SN 1.000 1.00 0.00 0.00 0.00 0 134.70940  
 21911.054  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8874.107  
 2.547788022D+04-2.293583066D+02 3.421593530D+00 4.713300040D-03-  
 7.365971320D-06  
 5.379738870D-09-1.519277855D-12 2.853047679D+03  
 6.673965270D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8874.107  
 -2.555955548D+06 7.870053500D+03-5.439768730D+00 6.307819180D-03-  
 2.068871370D-06  
 3.307074880D-10-1.848169716D-14 -4.841663910D+04  
 7.175952460D+01  
 SnO2 Gurvich,1991 pt1 p364 pt2 p309.

2 tpis91 SN 1.000 2.00 0.00 0.00 0.00 0 150.70880  
 11680.180  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11795.680  
 4.707674080D+04-6.114568670D+02 6.117433910D+00 7.514014660D-03-  
 1.238371787D-05  
 9.220915990D-09-2.632417597D-12 2.981068066D+03-  
 8.144926410D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11795.680  
 -1.573558926D+05-1.427316788D+02 7.605700760D+00-4.198008530D-05  
 9.218742430D-09  
 -1.051372983D-12 4.849579270D-17 -5.234531870D+02-  
 1.428360169D+01

SnS Gurvich,1991 pt1 p394 pt2 p334.  
 2 tpis91 SN 1.00S 1.00 0.00 0.00 0.00 0 150.77600  
 111099.012  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9301.112  
 2.724877813D+04-4.924126380D+02 6.221654730D+00-3.409406960D-03  
 3.984913680D-06  
 -2.470702874D-09 6.339341460D-13 1.452495307D+04-  
 6.791275280D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9301.112  
 -1.797985129D+06 6.141736320D+03-4.019504880D+00 5.993829180D-03-  
 2.188735204D-06  
 3.899542000D-10-2.406563630D-14 -2.611349815D+04  
 6.256821700D+01

SnS2 Gurvich,1991 pt1 p397 pt2 p336.  
 2 tpis91 SN 1.00S 2.00 0.00 0.00 0.00 0 182.84200  
 149645.595  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13635.095  
 3.877145410D+04-8.486953940D+02 1.042083990D+01-5.686902670D-03  
 6.373829770D-06  
 -3.825158100D-09 9.502480960D-13 2.006027952D+04-  
 2.723723128D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13635.095  
 -6.764084050D+04-1.970189679D+01 7.515333870D+00-6.332559180D-06  
 1.434207625D-09  
 -1.676383081D-13 7.886911900D-18 1.565053629D+04-  
 9.922728430D+00

Sn2 Gurvich,1991 pt1 p354 pt2 p305.  
 2 tpis91 SN 2.00 0.00 0.00 0.00 0.00 0 237.42000  
 421343.737  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11373.137  
 -1.329666654D+05 1.639179787D+03-1.902868972D+00 1.290431677D-02-  
 1.120542242D-05  
 4.502993860D-09-6.056237770D-13 4.097452710D+04  
 4.435408030D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11373.137  
 -4.275783040D+06 1.236421656D+04-8.438336170D+00 7.088056290D-03-  
 1.712012737D-06  
 1.805262952D-10-7.058656810D-15 -3.001418720D+04  
 1.005138538D+02

Sr Hf:Gurvich,1996a. Moore,1971. Moore,1970a. Gordon,1999.

3 g 1/98 SR 1.00 0.00 0.00 0.00 0.00 0 87.62000  
 160500.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 4.190649840D+00-6.304437580D-02 2.500373027D+00-1.115455943D-06  
 1.785248643D-09  
 -1.456209589D-12 4.750132981D-16 1.855852648D+04  
 5.555772840D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 1.489414410D+07-4.375335050D+04 5.137266280D+01-2.592566025D-02  
 6.582990000D-06  
 -6.949611800D-10 2.417779662D-14 2.977545522D+05-  
 3.454890770D+02  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 5.562233720D+08-6.093193220D+05 2.109096848D+02-3.010063957D-02  
 2.178021676D-06  
 -7.824003460D-11 1.109909620D-15 4.579268340D+06-  
 1.752716908D+03  
 Sr+ Moore,1971. Gordon,1999.  
 3 g 1/98 SR 1.00E -1.00 0.00 0.00 0.00 0 87.61945  
 716166.328  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
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 2.249493149D-09  
 -1.610827539D-12 4.698612333D-16 8.538981180D+04  
 6.247259240D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 3.145095058D+06-9.514756890D+03 1.350086948D+01-6.059717120D-03  
 1.594068746D-06  
 -1.718800946D-10 6.322256169D-15 1.457991907D+05-  
 7.236416930D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 9.016769220D+08-6.244641660D+05 1.695763594D+02-2.154835606D-02  
 1.462482744D-06  
 -4.930465390D-11 6.505705019D-16 4.966238870D+06-  
 1.431844579D+03  
 SrBr Gurvich,1996a pt1 p522 pt2 p402.  
 3 tpis96 SR 1.00BR 1.00 0.00 0.00 0.00 0 167.52400 -  
 63917.678  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10107.122  
 -7.549812420D+02-7.359532010D+01 4.828035810D+00-7.160584650D-04  
 1.028527433D-06  
 -6.888370720D-10 1.880257878D-13 -8.686168450D+03  
 4.151153090D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10107.122  
 3.009976114D+06-9.193192240D+03 1.526033745D+01-6.009253950D-03  
 1.692611858D-06  
 -2.039438429D-10 8.807775840D-15 4.922806130D+04-  
 7.068253830D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10107.122  
 2.274974243D+08-1.566004653D+05 4.234598410D+01-3.477076740D-03  
 1.358747452D-07

-2.623018618D-12 1.969298231D-17 1.221445664D+06-  
 3.265840740D+02  
 SrBr2 Gurvich,1996a pt1 p524 pt2 p404.  
 2 tpris96 SR 1.00BR 2.00 0.00 0.00 0.00 0 247.42800 -  
 406725.851  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16334.649  
 -4.632458660D+03-7.244938640D+01 7.800217160D+00-6.772125310D-04  
 8.537780240D-07  
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 5.285074760D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16334.649  
 -1.186173059D+04-1.404383013D+00 7.501215570D+00-5.415983190D-07  
 1.296969275D-10  
 -1.580911652D-14 7.681582270D-19 -5.118575210D+04-  
 3.552037110D+00  
 SrCL Gurvich,1996a pt1 p515 pt2 p398.  
 3 tpris96 SR 1.00CL 1.00 0.00 0.00 0.00 0 123.07270 -  
 127867.882  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9800.118  
 3.555346320D+03-1.729385697D+02 5.213451020D+00-1.542910668D-03  
 2.025835568D-06  
 -1.327076633D-09 3.547175960D-13 -1.588288066D+04  
 4.818108220D-01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9800.118  
 2.070217324D+06-6.199891730D+03 1.150315072D+01-3.675685460D-03  
 9.461732350D-07  
 -9.203765750D-11 2.707242192D-15 2.271471632D+04-  
 4.561058880D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9800.118  
 1.382269500D+08-9.659524410D+04 2.600419230D+01-1.405193291D-03  
 2.007238545D-08  
 7.119698480D-13-2.001316762D-17 7.447979070D+05-  
 1.876849204D+02  
 SrCL+ Gurvich,1996a pt1 p516 pt2 p399.  
 3 g 8/98 SR 1.00CL 1.00E -1.00 0.00 0.00 0 123.07215  
 408112.162  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9582.762  
 1.689043529D+03-1.749284676D+02 5.065328640D+00-9.857327840D-04  
 1.071655138D-06  
 -5.988127130D-10 1.395650932D-13 4.861190260D+04  
 2.491965147D-01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9582.762  
 -2.132475783D+04-4.057948270D+00 4.503149390D+00 3.826202380D-05  
 2.676951510D-09  
 5.667610500D-14 1.613288103D-18 4.769326030D+04  
 3.637718840D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9582.762  
 -1.041313813D+04-7.208302400D+00 4.501589780D+00 3.937923600D-05  
 2.394465390D-09  
 9.062292570D-14 4.723672450D-21 4.772357520D+04  
 3.647371680D+00  
 SrCL2 Gurvich,1996a pt1 p520 pt2 p401.

2 tpis96 SR 1.00CL 2.00 0.00 0.00 0.00 0 158.52540 -  
 484813.902  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14416.098  
 1.913170011D+03-2.681156951D+02 8.081334300D+00-2.393329295D-03  
 2.976397494D-06  
 -1.943902862D-09 5.174307710D-13 -5.910111850D+04-  
 8.457833220D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14416.098  
 -2.592716099D+04-5.263785850D+00 7.004475240D+00-1.970397814D-06  
 4.679671200D-10  
 -5.670215880D-14 2.742892387D-18 -6.045399530D+04-  
 2.192208452D+00  
 SrF Gurvich,1996a pt1 p507 pt2 p394.  
 3 tpis96 SR 1.00F 1.00 0.00 0.00 0.00 0 106.61840 -  
 303552.788  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9283.112  
 2.725008615D+04-4.850019720D+02 6.112697200D+00-3.008469209D-03  
 3.368465800D-06  
 -1.987813072D-09 4.884161090D-13 -3.536890390D+04-  
 6.683739180D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9283.112  
 8.702340490D+05-2.589818770D+03 7.200264220D+00-1.173446296D-03  
 1.996165066D-07  
 1.103842667D-11-2.343183859D-15 -2.133671699D+04-  
 1.667390309D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9283.112  
 -3.448093370D+07 2.208058158D+04-5.125719860D+00 2.209099383D-03-  
 1.551627196D-07  
 5.125524390D-12-6.680071600D-17 -2.048593542D+05  
 7.995585500D+01  
 SrF+ Gurvich,1996a pt1 p511 pt2 p395.  
 3 g 8/98 SR 1.00F 1.00E -1.00 0.00 0.00 0 106.61785  
 209468.312  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9106.812  
 4.009624200D+04-5.944946080D+02 6.182330330D+00-2.716159750D-03  
 2.641369127D-06  
 -1.383123292D-09 3.052935853D-13 2.697149351D+04-  
 8.313659450D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9106.812  
 -4.752082060D+04-2.526802345D+01 4.519295280D+00 2.556426750D-05  
 3.382541830D-09  
 -1.511394636D-13 9.537491180D-18 2.383861417D+04  
 1.892197325D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9106.812  
 -2.403608095D+03-3.242568700D+01 4.507124800D+00 3.261116540D-05  
 1.672393446D-09  
 5.130259820D-14 2.102366585D-20 2.392692006D+04  
 1.974517090D+00  
 SrF2 Gurvich,1996a pt1 p514 pt2 p397.  
 2 tpis96 SR 1.00F 2.00 0.00 0.00 0.00 0 125.61681 -  
 784793.795  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13269.601

4.170759650D+04-8.500132410D+02 1.002806064D+01-6.098485190D-03  
 7.056261330D-06  
 -4.359374310D-09 1.111308310D-12 -9.217859850D+04-  
 2.325100053D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13269.601  
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 1.490473613D-09  
 -1.756437040D-13 8.317093850D-18 -9.656701250D+04-  
 5.402308760D+00  
 SrH Gurvich,1996a pt1 p499 pt2 p388.  
 2 tpris96 SR 1.00H 1.00 0.00 0.00 0.00 0 88.62794  
 219227.105  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8723.105  
 -4.317796890D+04 7.676429700D+02-1.594398638D+00 1.500711077D-02-  
 1.826296898D-05  
 1.136757659D-08-2.855588359D-12 2.179685693D+04  
 3.324674230D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8723.105  
 -2.269825428D+05 1.345209458D+03 1.152194421D+00 3.109555289D-03-  
 1.188080968D-06  
 2.073091147D-10-1.300839287D-14 1.735547062D+04  
 2.112916944D+01  
 SrI Gurvich,1996a pt1 p526 pt2 p405.  
 3 tpris96 SR 1.00I 1.00 0.00 0.00 0.00 0 214.52447 -  
 7851.676  
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 10283.124  
 -2.467498501D+03-2.535495809D+01 4.603298480D+00-1.613676212D-04  
 2.694294049D-07  
 -1.564795762D-10 3.826482280D-14 -2.175538291D+03  
 6.411481880D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10283.124  
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 1.636071150D-06  
 -2.205540591D-10 1.078496824D-14 4.219077170D+04-  
 5.530833200D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10283.124  
 1.557303348D+08-1.150787674D+05 3.550520760D+01-3.375329300D-03  
 1.695651221D-07  
 -4.438653930D-12 4.852777450D-17 8.917357880D+05-  
 2.613917335D+02  
 SrI2 Gurvich,1996a pt1 p528 pt2 p407.  
 2 tpris96 SR 1.00I 2.00 0.00 0.00 0.00 0 341.42894 -  
 278218.842  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16701.658  
 -4.391849690D+03-3.757267350D+01 7.656993500D+00-3.561721300D-04  
 4.508689010D-07  
 -2.983230473D-10 8.018658660D-14 -3.553303460D+04-  
 2.598281578D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16701.658  
 -8.090381920D+03-7.348263230D-01 7.500640060D+00-2.863515042D-07  
 6.876556970D-11  
 -8.398807360D-15 4.086968160D-19 -3.572106420D+04-  
 1.693119087D+00

SrO Gurvich,1996a pt1 p495 pt2 p384.  
 3 tpi96 SR 1.000 1.00 0.00 0.00 0.00 0 103.61940 -  
 14207.691  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9040.109  
 4.224891670D+04-5.913517870D+02 5.964363000D+00-2.105712736D-03  
 2.028373972D-06  
 -1.197885492D-09 3.466289920D-13 1.018053721D+02-  
 7.511427470D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9040.109  
 -5.172933050D+07 1.510821000D+05-1.614513515D+02 8.516051790D-02-  
 2.091669402D-05  
 2.452307103D-09-1.108841292D-13 -9.687829520D+05  
 1.197846971D+03  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9040.109  
 1.988729112D+08-9.438733680D+04 2.862378041D+01-2.923338947D-03  
 1.808436182D-07  
 -5.719087480D-12 7.320935570D-17 7.583246290D+05-  
 2.033702568D+02  
 SrO+ Gurvich,1996a pt1 p497 pt2 p386. Partridge,1986.  
 3 g 8/98 SR 1.000 1.00E -1.00 0.00 0.00 0 103.61885  
 630053.722  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10104.122  
 4.618674160D+04-4.604560920D+02 5.605360720D+00-1.511707524D-03  
 1.328692506D-06  
 -6.244610540D-10 1.274632229D-13 7.694140460D+04-  
 3.377441410D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10104.122  
 1.035147885D+06-3.339081120D+03 8.520055290D+00-2.340803237D-03  
 7.338594440D-07  
 -1.031868417D-10 5.087079240D-15 9.540749060D+04-  
 2.491223445D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10104.122  
 -6.910421610D+07 1.253686165D+04 9.522159370D+00-1.279343636D-03  
 8.998760920D-08  
 -2.931863956D-12 3.752244570D-17 -5.778506890D+04-  
 3.231958760D+01  
 SrOH Gurvich,1996a pt1 p502 pt2 p390.  
 2 tpi96 SR 1.000 1.00H 1.00 0.00 0.00 0 104.62734 -  
 194085.726  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11046.666  
 4.640006560D+04-9.938685540D+02 9.784948960D+00-5.774377620D-03  
 5.126164110D-06  
 -1.833418356D-09 1.926013410D-13 -2.022721196D+04-  
 2.740670981D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11046.666  
 2.545648379D+06-7.416195980D+03 1.381956204D+01-3.096481934D-03  
 7.723894210D-07  
 -7.921280320D-11 2.740829111D-15 2.231302058D+04-  
 6.148781130D+01  
 SrOH+ Gurvich,1996a pt1 p503 pt2 p391.  
 2 tpi96 SR 1.000 1.00H 1.00E -1.00 0.00 0 104.62679  
 310169.605

298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11104.569  
 3.857366940D+04-9.030242330D+02 9.451103250D+00-5.042516280D-03  
 4.190101890D-06  
 -1.196920603D-09 1.606318743D-14 3.995067720D+04-  
 2.601486110D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11104.569  
 8.679695660D+05-2.340609538D+03 7.976829750D+00 1.023752569D-04-  
 6.286032330D-08  
 1.024851502D-11-5.723683920D-16 5.073157720D+04-  
 2.027046917D+01  
 Sr(OH)2 Gurvich,1996a pt1 p506 pt2 p393.  
 2 tpis96 SR 1.000 2.00H 2.00 0.00 0.00 0 121.63468 -  
 596694.573  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17011.921  
 7.205090300D+04-1.789465226D+03 1.729429139D+01-1.169280781D-02  
 1.106702894D-05  
 -4.490146090D-09 6.603997460D-13 -6.605394040D+04-  
 6.388681220D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17011.921  
 1.750013518D+06-4.681601500D+03 1.395548402D+01 2.035019560D-04-  
 1.253496115D-07  
 2.044549432D-11-1.142004855D-15 -4.427170240D+04-  
 5.051456850D+01  
 SrS Gurvich,1996a pt1 p529 pt2 p409.  
 2 tpis96 SR 1.00S 1.00 0.00 0.00 0.00 0 119.68600  
 104351.315  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9536.115  
 1.256440807D+04-3.150436559D+02 5.721722510D+00-2.630479718D-03  
 3.384699750D-06  
 -2.296256846D-09 6.512086680D-13 1.277295160D+04-  
 3.693862410D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9536.115  
 -1.379432947D+07 3.921331580D+04-3.602866380D+01 1.818513386D-02-  
 3.275858160D-06  
 2.324312746D-10-3.614555700D-15 -2.410246179D+05  
 2.991679767D+02  
 Sr2 Gurvich,1996a pt1 p491 pt2 p382.  
 2 tpis96 SR 2.00 0.00 0.00 0.00 0.00 0 175.24000  
 307570.337  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11365.137  
 -1.108859753D+05 5.927604010D+02 8.439688550D+00-2.652801112D-02  
 4.435825970D-05  
 -3.399915490D-08 9.965546680D-12 3.157615033D+04-  
 7.033966650D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11365.137  
 2.098445682D+05 1.038650130D+02 2.309332330D+00 1.330517507D-04-  
 4.426433390D-08  
 6.711419150D-12-3.374128000D-16 3.636642690D+04  
 2.168088517D+01  
 Ta Hf:Gurvich,1982 p85. Moore,1971. Gordon,1999.  
 3 g 7/97 TA 1.00 0.00 0.00 0.00 0.00 0 180.94790  
 782518.638



200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6199.638  
 -1.150907339D+04 4.780730430D+01 3.185588390D+00-5.366528160D-03  
 1.288379705D-05  
 -1.045798666D-08 3.050617695D-12 9.299797630D+04  
 5.336056610D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6199.638  
 1.689726898D+06-5.986854660D+03 9.565039670D+00-2.511649459D-03  
 6.443031170D-07  
 -7.189237250D-11 3.113352070D-15 1.306710983D+05-  
 4.335096270D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6199.638  
 -8.413419560D+08 6.381509040D+05-1.856031850D+02 2.797353600D-02-  
 2.073321805D-06  
 7.397299170D-11-1.017863944D-15 -4.836410620D+06  
 1.607007750D+03  
 Ta+ Moore,1971. Gordon,1999.  
 3 g 7/97 TA 1.00E -1.00 0.00 0.00 0.00 0 180.94735  
 1549679.335  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6337.835  
 2.869712865D+05-3.084920994D+03 1.430679704D+01-1.984772164D-02  
 1.951445133D-05  
 -8.970946030D-09 1.501974665D-12 2.013828712D+05-  
 6.306427830D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6337.835  
 3.656142130D+06-1.254073524D+04 1.865022579D+01-7.943274660D-03  
 2.151786937D-06  
 -2.816764844D-10 1.413722944D-14 2.636876455D+05-  
 1.065864286D+02  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6337.835  
 3.724273560D+07-3.405709310D+04 1.630056321D+01-2.064987830D-03  
 1.616826024D-07  
 -5.752060330D-12 7.636581870D-17 4.405115500D+05-  
 1.040237652D+02  
 Ta- Hotop,1985. Gordon,1999.  
 3 g 9/97 TA 1.00E 1.00 0.00 0.00 0.00 0 180.94845  
 745469.429  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6416.129  
 1.873982301D+05-1.681268679D+03 6.480040150D+00-2.254355782D-04  
 2.028434876D-06  
 -4.679801430D-09 1.997027996D-12 9.793496020D+04-  
 2.049618155D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6416.129  
 -4.235467480D+06 1.101056361D+04-4.736911070D+00 2.503562129D-03-  
 4.821851690D-07  
 4.886408030D-11-2.030547835D-15 1.574699408D+04  
 6.491802700D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6416.129  
 4.149884030D+05 1.227972146D+03 2.209211582D+00 3.401090760D-05-  
 2.136872502D-09  
 6.906775410D-14-9.017779200D-19 8.249065600D+04  
 1.195636187D+01  
 TaCL5 Chase,1998 p923.

2 j12/74 TA 1.00CL 5.00 0.00 0.00 0.00 0 358.21140 -  
 764835.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 26869.100  
 6.306483290D+04-1.771221442D+03 2.255083356D+01-1.360238041D-02  
 1.613009806D-05  
 -1.016307761D-08 2.631917453D-12 -8.792737110D+04-  
 8.097864910D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 26869.100  
 -1.426444545D+05-3.894340320D+01 1.603142370D+01-1.333676355D-05  
 3.084307611D-09  
 -3.663930060D-13 1.745841795D-17 -9.701297170D+04-  
 4.256987000D+01  
 TaO Gurvich,1982 pt1 p86 pt2 p89.  
 3 tpris89 TA 1.000 1.00 0.00 0.00 0.00 0 196.94730  
 242534.705  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8766.105  
 -1.395738049D+04 3.945236990D+02-6.301696410D-02 1.308595441D-02-  
 1.862339730D-05  
 1.366155583D-08-3.924551230D-12 2.645195419D+04  
 2.741671469D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8766.105  
 6.106591120D+06-1.984135246D+04 2.815797433D+01-1.330045882D-02  
 3.876807490D-06  
 -5.068872770D-10 2.443666035D-14 1.525814433D+05-  
 1.658307106D+02  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8766.105  
 -1.076924766D+08 1.287348862D+04 1.361132509D+01-1.443306356D-03  
 9.697469230D-08  
 -3.170023830D-12 4.113579900D-17 -1.302536682D+05-  
 6.687940680D+01  
 TaO2 Gurvich,1982 pt1 p89 pt2 p91.  
 2 tpris82 TA 1.000 2.00 0.00 0.00 0.00 0 212.94670 -  
 173662.006  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10699.099  
 1.516356303D+04 7.058414760D+01 6.918516990D-01 2.020605733D-02-  
 2.928317413D-05  
 2.081417374D-08-5.751106690D-12 -2.212199468D+04  
 2.484662500D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10699.099  
 1.297565964D+06-4.149217430D+03 1.041680373D+01-1.045478838D-03  
 2.754904271D-07  
 -3.297043130D-11 1.356249074D-15 3.418985670D+03-  
 3.392642790D+01  
 Ti Hf:Cox,1989. Sugar,1985. Gordon,1999.  
 3 g 7/97 TI 1.00 0.00 0.00 0.00 0.00 0 47.86700  
 473000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7539.141  
 -4.570179400D+04 6.608092020D+02 4.295257490D-01 3.615029910D-03-  
 3.549792810D-06  
 1.759952494D-09-3.052720871D-13 5.270947930D+04  
 2.026149738D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7539.141

-1.704786714D+05 1.073852803D+03 1.181955014D+00 2.245246352D-04  
 3.091697848D-07  
 -5.740027280D-11 2.927371014D-15 4.978069910D+04  
 1.740431368D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7539.141  
 1.152797766D+09-7.222408380D+05 1.777167465D+02-2.008059096D-02  
 1.221052354D-06  
 -3.811452080D-11 4.798092423D-16 5.772614540D+06-  
 1.518080466D+03  
 Ti+ Sugar,1985. Gordon,1999.  
 3 g 7/97 TI 1.00E -1.00 0.00 0.00 0.00 0 47.86645  
 1137624.029  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7899.829  
 1.707457044D+05-1.727524602D+03 9.615885330D+00-1.089655060D-02  
 8.201809650D-06  
 -2.871464413D-09 3.420382976D-13 1.447897558D+05-  
 3.463143660D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7899.829  
 -7.685463080D+05 2.545868100D+03 3.423862780D-01 7.099901360D-04  
 2.706231875D-08  
 -2.371660100D-11 1.895443077D-15 1.198821489D+05  
 2.484799150D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7899.829  
 3.918035620D+07-2.534581605D+04 9.586759720D+00-7.584155410D-04  
 4.432999350D-08  
 -8.442571760D-13-4.517128089D-19 3.344440620D+05-  
 5.220026270D+01  
 Ti- Hotop,1985. Gordon,1999.  
 3 g 9/97 TI 1.00E 1.00 0.00 0.00 0.00 0 47.86755  
 459203.814  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7562.614  
 -3.006484990D+03 2.040911689D+02 1.822638976D+00 1.245254812D-03-  
 1.309239865D-06  
 7.372143220D-10-1.724319779D-13 5.346772050D+04  
 1.205926588D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7562.614  
 2.341117640D+04 2.580413872D+00 2.497754577D+00 9.769072040D-07-  
 2.280024955D-10  
 2.717202291D-14-1.295670294D-18 5.454662180D+04  
 7.999823950D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7562.614  
 1.417514172D+04 5.638799640D+00 2.498751709D+00 1.426579908D-07-  
 8.889194940D-12  
 2.867172222D-16-3.746329300D-21 5.451843520D+04  
 7.994109450D+00  
 TiCL Chase,1998 p808.  
 2 j12/68 TI 1.00CL 1.00 0.00 0.00 0.00 0 83.31970  
 150850.926  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9680.626  
 -1.714177839D+04 3.103259047D+02 8.920935980D-01 1.383436793D-02-  
 1.885370354D-05  
 1.212085912D-08-3.032162427D-12 1.558066453D+04  
 2.244777844D+01

1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9680.626  
 -9.633225420D+05 2.868829781D+03 1.973820676D+00 1.752668011D-03-  
 4.255434360D-07  
 5.049103400D-11-2.304720715D-15 -1.811011561D+03  
 2.319449747D+01  
 TiCL2 Chase,1998 p866.  
 2 j12/68 TI 1.00CL 2.00 0.00 0.00 0.00 0 118.77240 -  
 237230.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13545.270  
 1.324354656D+04-5.762829320D+02 9.640047290D+00-4.475120950D-03  
 5.398794870D-06  
 -3.525800490D-09 9.746004550D-13 -2.792066683D+04-  
 2.218348383D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13545.270  
 -3.190012950D+06 1.015763826D+04-4.840794770D+00 6.822006340D-03-  
 1.700753270D-06  
 2.118106588D-10-1.041245457D-14 -9.480982980D+04  
 7.823195190D+01  
 TiCL3 Chase,1998 p887.  
 2 j12/68 TI 1.00CL 3.00 0.00 0.00 0.00 0 154.22510 -  
 539320.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15374.947  
 1.243282268D+05-2.320728253D+03 1.779895274D+01-1.160889348D-02  
 1.006643154D-05  
 -4.811940690D-09 1.006186828D-12 -5.609602510D+04-  
 6.732754940D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15374.947  
 -9.408792310D+04-1.255351109D+02 1.066923972D+01-2.637456897D-04  
 7.959169350D-08  
 -1.176740054D-11 6.416223480D-16 -6.769114680D+04-  
 2.369165091D+01  
 TiCL4 Chase,1998 p906.  
 2 j12/67 TI 1.00CL 4.00 0.00 0.00 0.00 0 189.67780 -  
 763160.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 21613.541  
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 2.702903947D+01

1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
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 UF+ Gurvich,1982 pt1 p203 pt2 p226.

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18643.063

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 4.008173850D-06  
 5.140230790D-10-2.511687821D-14 -3.125140933D+05  
 1.274038784D+02  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 21876.775  
 -1.308421305D+08 8.061319300D+04-3.939161520D+00 1.853747295D-03-  
 1.116700599D-07  
 3.508474880D-12-4.490622440D-17 -8.552752700D+05  
 1.210372085D+02  
 UF5 Gurvich,1982 pt1 p219 pt2 p251.  
 3 tpris82 U 1.00F 5.00 0.00 0.00 0.00 0 333.02092 -  
 1949823.884  
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 23602.882  
 1.615769193D+05-2.976611537D+03 2.537542420D+01-1.930105670D-02  
 2.561852107D-05  
 -1.747402896D-08 4.732059380D-12 -2.239089616D+05-  
 1.024264836D+02  
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 23602.882  
 -1.695373880D+06 3.735425350D+03 1.218748040D+01 2.418608203D-03-  
 5.678526160D-07

6.002765610D-11-2.430740809D-15 -2.645107342D+05-  
 1.883137480D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 23602.882  
 -2.820007103D+07 1.475725044D+04 1.466020135D+01 5.538728810D-05-  
 3.572588510D-10  
 -4.414506670D-14 1.011890437D-18 -3.622893270D+05-  
 3.137230623D+01  
 UF5+ Gurvich,1982 pt1 p220 pt2 p253.  
 3 tpris82 U 1.00F 5.00E -1.00 0.00 0.00 0 333.02037 -  
 853617.242  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 23612.158  
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 1.339849041D-05  
 -7.078572690D-09 1.573404040D-12 -9.226404850D+04-  
 9.830243940D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 23612.158  
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 -9.537160520D-13 4.460145080D-17 -1.076293931D+05-  
 4.763374170D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 23612.158  
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 4.725516370D+01  
 UF5- Gurvich,1982 pt1 p221 pt2 p255.  
 3 tpris82 U 1.00F 5.00E 1.00 0.00 0.00 0 333.02146 -  
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 25192.963  
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 1.562795472D-05  
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 4.690020530D+00  
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 25192.963  
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 25192.963  
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 5.100027930D-09  
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 2.232978311D+01  
 UF6 Gurvich,1982 pt1 p223 pt2 p257.  
 3 tpris82 U 1.00F 6.00 0.00 0.00 0.00 0 352.01932 -  
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 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 26623.352  
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 -4.821754110D-09 8.325132450D-13 -2.461045194D+05-  
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 26623.352

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 -4.136090060D-15 5.365237680D-20 -2.646640074D+05-  
 6.513581540D+01  
 UF6- Gurvich,1982 pt1 p224 pt2 p258.  
 3 tpis82 U 1.00F 6.00E 1.00 0.00 0.00 0 352.01987 -  
 2691306.150  
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 27730.597  
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 8.298576160D-06  
 -2.582889593D-09 2.790817248D-13 -3.135307376D+05-  
 1.128934794D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 27730.597  
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 4.517491710D-07  
 7.821820470D-11-4.560334720D-15 -2.855667984D+05-  
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 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 27730.597  
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 4.049760430D-08  
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 1.746878630D+00  
 UO Gurvich,1982 pt1 p186 pt2 p205.  
 3 tpis82 U 1.00O 1.00 0.00 0.00 0.00 0 254.02830  
 30488.589  
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 9538.289  
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 3.226786780D+02  
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 9538.289  
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 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9538.289  
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 8.455141670D-08  
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 7.355640190D+01  
 UO+ Gurvich,1982 pt1 p189 pt2 p207.  
 3 tpis82 U 1.00O 1.00E -1.00 0.00 0.00 0 254.02775  
 580971.927  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8824.227  
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 6.851856740D-07  
 5.552073190D-11-5.893012030D-14 6.952999740D+04  
 9.583869820D+00

1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8824.227  
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 5.066033910D-07  
 -7.373977470D-11 4.074766430D-15 7.789085840D+04-  
 2.115284256D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8824.227  
 -4.623486280D+07 4.390299020D+04-9.206507600D+00 2.335209239D-03-  
 1.678226513D-07  
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 1.200887990D+02  
 UOF Gurvich,1982 pt1 p225 pt2 p259.  
 2 tpris82 U 1.000 1.00F 1.00 0.00 0.00 0 273.02670 -  
 542182.744  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14005.456  
 3.861248470D+02 5.162286900D+01 4.888962520D+00 7.265633560D-03-  
 1.134176875D-05  
 8.509041750D-09-2.354655485D-12 -6.719813380D+04  
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 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14005.456  
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 2.648894949D-06  
 3.114551623D-10-1.416111895D-14 -1.478976701D+05  
 1.184570600D+02  
 UOF2 Gurvich,1982 pt1 p226 pt2 p261.  
 2 tpris82 U 1.000 1.00F 2.00 0.00 0.00 0 292.02511 -  
 1115510.264  
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 17816.436  
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 -2.490530206D-08 7.580617640D-12 -1.374686016D+05-  
 3.470029670D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17816.436  
 -1.198944060D+06 3.852173410D+03 4.639109750D+00 4.087738440D-03-  
 1.087067018D-06  
 1.306398384D-10-6.036901520D-15 -1.612637583D+05  
 2.018237184D+01  
 UOF3 Gurvich,1982 pt1 p229 pt2 p264.  
 2 tpris82 U 1.000 1.00F 3.00 0.00 0.00 0 311.02351 -  
 1510638.039  
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 19827.161  
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 -1.049770051D-08 2.922353602D-12 -1.743844024D+05-  
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 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19827.161  
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 5.666241720D-07  
 5.989062110D-11-2.424534810D-15 -2.105491714D+05-  
 5.670532850D+00  
 UOF4 Gurvich,1982 pt1 p230 pt2 p265.  
 2 tpris82 U 1.000 1.00F 4.00 0.00 0.00 0 330.02191 -  
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 22742.734  
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 1.517555623D-09-7.768799740D-13 -2.061284178D+05-  
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 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22742.734  
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 UO2 Gurvich,1982 pt1 p193 pt2 p211.  
 3 tpris82 U 1.000 2.00 0.00 0.00 0.00 0 270.02770 -  
 477819.903  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13460.097  
 -1.129650727D+05 4.270730270D+02 8.413694010D+00-9.764280000D-03  
 2.199903691D-05  
 -1.907665954D-08 6.029889910D-12 -6.251443300D+04-  
 1.300704869D+01  
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 13460.097  
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 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13460.097  
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 4.527223330D-09  
 1.134573678D-13-1.350744532D-18 -2.459740375D+05  
 1.133700234D+01  
 UO2+ Gurvich,1982 pt1 p194 pt2 p213.  
 3 tpris82 U 1.000 2.00E -1.00 0.00 0.00 0 270.02715  
 51493.919  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11576.519  
 4.488023380D+04-6.489236420D+02 6.874243560D+00 2.281949316D-03  
 1.859218752D-07  
 -1.849509036D-09 8.149965330D-13 7.891740230D+03-  
 1.028257239D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11576.519  
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 5.624101440D-07  
 5.939451640D-11-2.401047056D-15 -2.048558817D+04  
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 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11576.519  
 -2.778324150D+07 1.456161876D+04 6.203516610D+00 5.043474040D-05-  
 4.877674180D-11  
 -5.408292310D-14 1.141506994D-18 -1.172230791D+05  
 2.164589039D+00  
 UO2- Gurvich,1982 pt1 p195 pt2 p215.  
 3 tpris82 U 1.000 2.00E 1.00 0.00 0.00 0 270.02825 -  
 573700.021  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
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 4.145760310D+01  
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 13777.379  
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 U02F Gurvich,1982 pt1 p226 pt2 p260.  
 2 tpris82 U 1.000 2.00F 1.00 0.00 0.00 0 289.02610 -  
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 15803.758  
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 15803.758  
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 5.988823520D-11-2.424485602D-15 -1.478357384D+05  
 8.736139080D+00  
 U02F2 Gurvich,1982 pt1 p228 pt2 p263.  
 2 tpris82 U 1.000 2.00F 2.00 0.00 0.00 0 308.02451 -  
 1354232.027  
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 19067.973  
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 9.301197040D-09-2.781220538D-12 -1.580310734D+05-  
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 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19067.973  
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 U03 Gurvich,1982 pt1 p197 pt2 p218.  
 3 tpris82 U 1.000 3.00 0.00 0.00 0.00 0 286.02710 -  
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 2.106191042D-05  
 1.545856318D-08-4.378566290D-12 -9.413369350D+04-  
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 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
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 1.052843810D-06  
 1.849985929D-10-1.102849619D-14 -1.173360017D+05  
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 15144.745

1.632929098D+09-9.419553920D+05 2.142384145D+02-2.094922993D-02  
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-3.129107183D-11 3.504914590D-16 7.448065370D+06-  
1.824526663D+03  
UO3- Gurvich,1982 pt1 p198 pt2 p220.  
3 tpris82 U 1.000 3.00E 1.00 0.00 0.00 0 286.02765 -  
1305154.518  
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15427.082  
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5.675228000D-06  
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1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
15427.082  
-1.632938634D+06 3.667495410D+03 6.240030650D+00 2.396952522D-03-  
5.629490230D-07  
5.945413130D-11-2.403730982D-15 -1.845927385D+05  
7.032058960D+00  
6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
15427.082  
-2.781940595D+07 1.456116475D+04 8.703650860D+00 5.041649230D-05-  
4.751131470D-11  
-5.412647410D-14 1.142098108D-18 -2.812591514D+05-  
5.495926150D+00  
V Hf:Gurvich,1982 p59. Sugar,1985. Gordon,1999.  
3 g 7/97 V 1.00 0.00 0.00 0.00 0.00 0 50.94150  
517267.064  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
7907.064  
-5.535376020D+04 5.593338510D+02 2.675543482D+00-6.243049630D-03  
1.565902337D-05  
-1.372845314D-08 4.168388810D-12 5.820664360D+04  
9.524567490D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
7907.064  
1.200390300D+06-5.027005300D+03 1.058830594D+01-5.044326100D-03  
1.488547375D-06  
-1.785922508D-10 8.113013866D-15 9.170740910D+04-  
4.768336320D+01  
6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
7907.064  
2.456040166D+09-1.339992028D+06 2.781039851D+02-2.638937359D-02  
1.303527149D-06  
-3.214680330D-11 3.099999094D-16 1.087152043D+07-  
2.439954380D+03  
V+ Sugar,1985. Gordon,1999.  
3 g 7/97 V 1.00E -1.00 0.00 0.00 0.00 0 50.94095  
1173745.411  
298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
7897.811  
7.568834460D+04-8.415273820D+02 7.559232710D+00-1.441722656D-02  
2.038356397D-05  
-1.289073883D-08 3.065656561D-12 1.444478191D+05-  
1.991067645D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
7897.811  
2.347072054D+06-9.021197190D+03 1.477349798D+01-6.891896880D-03  
1.968884877D-06  
-2.539798544D-10 1.226783122D-14 1.958351444D+05-  
7.855592930D+01



6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7897.811  
 2.516527258D+08-1.866476656D+05 5.633587110D+01-7.198536950D-03  
 5.074401490D-07  
 -1.699749225D-11 2.157800037D-16 1.585980536D+06-  
 4.512822600D+02  
 V- Hotop,1985. Gordon,1999.  
 3 g 9/97 V 1.00E 1.00 0.00 0.00 0.00 0 50.94205  
 460386.063  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7878.263  
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 1.506038188D-06  
 8.491815170D-10-1.987980413D-13 5.347402920D+04  
 1.261900982D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7878.263  
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 2.139749508D-10  
 2.581021334D-14-1.240812796D-18 5.470007080D+04  
 7.977900240D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7878.263  
 1.601102910D+04 5.820974900D+00 2.498705489D+00 1.484212570D-07-  
 9.272956840D-12  
 2.997799727D-16-3.924862230D-21 5.466692550D+04  
 7.974557420D+00  
 VCL4 Nagarajan,1963. Creighton,1966. Blankenship,1962.  
 2 g10/00 V 1.00CL 4.00 0.00 0.00 0.00 0 192.75230 -  
 527058.480  
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 21783.098  
 7.719834710D+04-1.702854040D+03 1.882697965D+01-1.130896832D-02  
 1.266950765D-05  
 -7.625019340D-09 1.907582465D-12 -5.863748540D+04-  
 6.559172040D+01  
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 21783.098  
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 4.094111780D-07  
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 4.348283760D+00  
 VN Chase,1998 p1616.  
 2 j12/73 V 1.00N 1.00 0.00 0.00 0.00 0 64.94824  
 523000.000  
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 8799.744  
 -1.581737285D+04 4.868165420D+02-1.045200388D+00 1.685261043D-02-  
 2.334616543D-05  
 1.588710050D-08-4.279080880D-12 5.981481400D+04  
 3.144995355D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8799.744  
 1.018619667D+06-3.932305570D+03 9.856823610D+00-3.289221710D-03  
 1.005181767D-06  
 -1.243211436D-10 5.486776560D-15 8.557318340D+04-  
 3.552830670D+01  
 VO Gurvich,1982 pt1 p62 pt2 p64.  
 3 tpis89 V 1.00O 1.00 0.00 0.00 0.00 0 66.94090  
 148582.706

200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8773.106  
 -1.311619784D+04 3.747816970D+02 9.300834860D-02 1.244977714D-02-  
 1.688540028D-05  
 1.142443381D-08-3.040589320D-12 1.523789920D+04  
 2.536811755D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8773.106  
 2.986190283D+06-1.011344974D+04 1.718161749D+01-7.876705030D-03  
 2.562279547D-06  
 -3.547400350D-10 1.770268056D-14 7.961254880D+04-  
 8.789993010D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8773.106  
 1.004530292D+08-9.008780230D+04 3.186107720D+01-2.862639937D-03  
 1.440482244D-07  
 -3.802861470D-12 4.195092660D-17 7.011401290D+05-  
 2.336810859D+02  
 V02 Gurvich,1982 pt1 p64 pt2 p66.  
 2 tpi82 V 1.000 2.00 0.00 0.00 0.00 0 82.94030 -  
 232697.655  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10622.449  
 -6.678585860D+03 3.911597580D+02-1.028549847D+00 2.401523419D-02-  
 3.337378810D-05  
 2.283623543D-08-6.199143100D-12 -3.074609276D+04  
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 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10622.449  
 1.210632401D+05-1.627832993D+03 9.252713100D+00-1.572703139D-03  
 5.231430160D-07  
 -6.476071140D-11 2.847226026D-15 -2.097306345D+04-  
 2.547380687D+01  
 V4010 Gurvich,1982 pt1 p69 pt2 p70.  
 2 g10/99 V 4.000 10.00 0.00 0.00 0.00 0 363.76000 -  
 2825164.486  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 36796.033  
 3.385739160D+05-5.353929260D+03 2.993220131D+01 5.818836520D-02-  
 9.696340160D-05  
 7.274756990D-08-2.091628357D-11 -3.189349370D+05-  
 1.466398396D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 36796.033  
 -1.360273270D+06-1.341692860D+03 4.099138590D+01-3.932265530D-04  
 8.628494120D-08  
 -9.835944090D-12 4.535637290D-16 -3.484616120D+05-  
 1.907911348D+02  
 W Hf:Gurvich,1982 p42. Moore,1971. Moore,1970a.  
 Gordon,1999.  
 3 g 4/98 W 1.00 0.00 0.00 0.00 0.00 0 183.84000  
 851243.526  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6216.526  
 1.595223922D+05-2.673843928D+03 2.060469727D+01-6.252315230D-02  
 1.105654838D-04  
 -8.453511610D-08 2.336187771D-11 1.139648616D+05-  
 9.011836900D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6216.526

-8.048745960D+06 1.465700424D+04-2.508531501D-01-2.596486992D-03  
 1.409225475D-06  
 -2.233011706D-10 1.262640862D-14 -3.091130919D+03  
 3.955822190D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6216.526  
 1.421636486D+09-4.325365550D+05-8.841615070D+00 1.645538940D-02-  
 1.908373835D-06  
 8.530482890D-11-1.360501851D-15 3.994798750D+06-  
 1.266418236D+01  
 W+ Moore,1971. Gordon,1999.  
 3 g 7/97 W 1.00E -1.00 0.00 0.00 0.00 0 183.83945  
 1627840.965  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6221.265  
 -1.969284929D+05 2.670137332D+03-1.131686913D+01 3.308183730D-02-  
 3.629035500D-05  
 2.066142971D-08-4.808285562D-12 1.820950862D+05  
 8.552104480D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6221.265  
 6.387743400D+06-2.061811463D+04 2.759291576D+01-1.244535845D-02  
 3.271200490D-06  
 -4.065463720D-10 1.912595872D-14 3.245174430D+05-  
 1.716919194D+02  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6221.265  
 6.839559150D+07-8.981711810D+04 3.845720800D+01-5.465752290D-03  
 4.024981150D-07  
 -1.342970538D-11 1.667637540D-16 8.546932820D+05-  
 2.892805521D+02  
 W- Hotop,1985. Gordon,1999.  
 3 g 1/99 W 1.00E 1.00 0.00 0.00 0.00 0 183.84055  
 766391.528  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 9.142981370D+04  
 8.461169670D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 9.142981370D+04  
 8.461169670D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 9.142981370D+04  
 8.461169670D+00  
 WCL6 Chase,1998 p935.  
 2 j12/66 W 1.00CL 6.00 0.00 0.00 0.00 0 396.55620 -  
 493712.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 30790.955  
 3.339391670D+04-1.697366080D+03 2.560612352D+01-1.425247881D-02  
 1.739682668D-05  
 -1.120537864D-08 2.951522890D-12 -5.673059240D+04-  
 9.741466980D+01

1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 30790.955  
 -1.516735473D+05-3.451379250D+01 1.902867176D+01-1.242486969D-05  
 2.917675103D-09  
 -3.505981440D-13 1.685355887D-17 -6.535779790D+04-  
 5.894915640D+01  
 WO Gurvich,1982 pt1 p43 pt2 p47.  
 3 tpris82 W 1.000 1.00 0.00 0.00 0.00 0 199.83940  
 401735.711  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9259.111  
 -1.933758411D+04 4.936690840D+02-4.116148220D-01 1.307976507D-02-  
 1.689145619D-05  
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 3.002592661D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9259.111  
 1.262156956D+06-4.177263120D+03 9.358286470D+00-2.887612220D-03  
 8.893933960D-07  
 -8.955318700D-11 2.504359614D-15 7.313380640D+04-  
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 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9259.111  
 1.942009403D+08-1.501316158D+05 4.237023540D+01-3.309676390D-03  
 1.396809578D-07  
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 3.296819210D+02  
 WOCL4 Chase,1998 p900.  
 2 j 3/67 W 1.000 1.00CL 4.00 0.00 0.00 0 341.65020 -  
 573493.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22271.379  
 2.658812693D+04-9.336913240D+02 1.321377385D+01 1.270930811D-02-  
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 1.405106974D-08-3.899382140D-12 -6.792290790D+04-  
 3.594870210D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22271.379  
 -3.049028285D+05-3.539425860D+02 1.626432703D+01-1.058245461D-04  
 2.340548846D-08  
 -2.685852021D-12 1.245412684D-16 -7.272546740D+04-  
 4.991761780D+01  
 WO2 Gurvich,1982 pt1 p47 pt2 p50.  
 2 tpris82 W 1.000 2.00 0.00 0.00 0.00 0 215.83880  
 29061.744  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10714.848  
 3.120918919D+03 2.413883468D+02-3.024119184D-01 2.324333417D-02-  
 3.378812680D-05  
 2.380934019D-08-6.421592880D-12 1.442005265D+03  
 2.957655179D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10714.848  
 -7.537406680D+05 3.204643050D+03 6.701965600D-01 4.488238870D-03-  
 8.858328460D-07  
 6.245171750D-11-9.046613900D-16 -1.769420230D+04  
 3.405724010D+01  
 WO2CL2 Chase,1998 p849.  
 2 j 3/67 W 1.000 2.00CL 2.00 0.00 0.00 0 286.74420 -  
 671532.000

200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19503.817  
 4.300154480D+02-2.438547856D+02 7.976306990D+00 1.715005722D-02-  
 2.487975176D-05  
 1.737644163D-08-4.771928400D-12 -8.232812400D+04-  
 7.844774560D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19503.817  
 -2.404791730D+05-3.068379644D+02 1.322814502D+01-9.100220710D-05  
 2.006581020D-08  
 -2.296837607D-12 1.062829386D-16 -8.367493060D+04-  
 3.491556940D+01  
 W03 Gurvich,1982 pt1 p50 pt2 p52.  
 2 tpris82 W 1.000 3.00 0.00 0.00 0.00 0 231.83820 -  
 319725.213  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13267.943  
 7.262461460D+03 3.429391090D+01 1.573061955D+00 2.754971099D-02-  
 3.994827310D-05  
 2.809371537D-08-7.777545730D-12 -4.001733270D+04  
 1.857409963D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13267.943  
 1.732203640D+06-6.284719780D+03 1.681358864D+01-3.472089360D-03  
 8.079935800D-07  
 -6.589378720D-11 1.142928957D-15 -2.473075565D+03-  
 7.407474090D+01  
 W03- Gurvich,1982 pt1 p51 pt2 p53.  
 2 tpris82 W 1.000 3.00E 1.00 0.00 0.00 0 231.83875 -  
 650475.961  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13714.639  
 1.630999684D+05-1.967609682D+03 1.201970914D+01 1.681260779D-03-  
 5.859360060D-06  
 5.028616330D-09-1.434012198D-12 -7.009203990D+04-  
 3.936901040D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13714.639  
 4.637832510D+05-1.347089334D+03 9.773637560D+00 1.071395459D-03-  
 3.842403660D-07  
 5.737531900D-11-3.157605982D-15 -7.239515570D+04-  
 2.391116343D+01  
 (W03)2 Gurvich,1982 pt1 p52 pt2 p54.  
 2 tpris82 W 2.000 6.00 0.00 0.00 0.00 0 463.67640 -  
 1210443.298  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 25543.014  
 8.088414510D+04-9.060340790D+02 7.601575390D+00 5.241008510D-02-  
 7.922356390D-05  
 5.708640180D-08-1.606775042D-11 -1.441496996D+05-  
 1.093524051D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 25543.014  
 -6.674072430D+05-7.032518360D+02 2.251617461D+01-2.035473339D-04  
 4.444320340D-08  
 -5.045188080D-12 2.318375739D-16 -1.502699479D+05-  
 8.613988980D+01  
 (W03)3 Gurvich,1982 pt1 p53 pt2 p55.  
 2 tpris82 W 3.000 9.00 0.00 0.00 0.00 0 695.51460 -  
 2013291.101

200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 40688.367  
 3.485390010D+04-1.933496319D+02 8.206544780D+00 8.599515510D-02-  
 1.257565252D-04  
 8.891567220D-08-2.471213564D-11 -2.462453469D+05-  
 5.657325260D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 40688.367  
 -9.450263310D+05-1.133837222D+03 3.483479230D+01-3.301361100D-04  
 7.226602130D-08  
 -8.221581630D-12 3.785050840D-16 -2.488486308D+05-  
 1.441551053D+02  
 (W03)4 Gurvich,1982 pt1 p54 pt2 p56.  
 2 tpris82 W 4.000 12.00 0.00 0.00 0.00 0 927.35280 -  
 2817433.885  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 54538.739  
 1.388606167D+04 2.287518563D+02 8.662370000D+00 1.219700696D-01-  
 1.770499494D-04  
 1.246790033D-07-3.456182860D-11 -3.467839600D+05-  
 3.603937290D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 54538.739  
 -1.277530217D+06-1.566538532D+03 4.715363520D+01-4.563263220D-04  
 9.990758360D-08  
 -1.136816181D-11 5.234399340D-16 -3.477418470D+05-  
 2.051588395D+02  
 (W03)5 Gurvich,1982 pt1 p56 pt2 p57.  
 2 tpris82 W 5.000 15.00 0.00 0.00 0.00 0 1159.19100 -  
 3551492.326  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 68473.453  
 1.497576743D+04 2.719999782D+02 1.138626896D+01 1.523302100D-01-  
 2.211447753D-04  
 1.557377753D-07-4.317244680D-11 -4.371424320D+05-  
 1.441643481D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 68473.453  
 -1.600667953D+06-1.958437864D+03 5.944227390D+01-5.705105630D-04  
 1.249090916D-07  
 -1.421320416D-11 6.544458260D-16 -4.384095860D+05-  
 2.660238838D+02  
 Xe Ref-Elm. Moore,1971. Moore,1970a. Gordon,1999.  
 3 g 1/99 XE 1.00 0.00 0.00 0.00 0.00 0 131.29000  
 0.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -7.453750000D+02  
 6.164419930D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 4.025226680D+03-1.209507521D+01 2.514153347D+00-8.248102080D-06  
 2.530232618D-09  
 -3.892333230D-13 2.360439138D-17 -6.685800730D+02  
 6.063676440D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6197.428  
 2.540397456D+08-1.105373774D+05 1.382644099D+01 1.500614606D-03-  
 3.935359030D-07

2.765790584D-11-5.943990574D-16 9.285443830D+05-  
1.109834899D+02  
Xe+ Moore,1971. Moore,1970a. Gordon,1999.  
3 g 3/97 XE 1.00E -1.00 0.00 0.00 0.00 0 131.28945  
1176552.232  
298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428  
1.002923620D+02-1.218753648D+00 2.506016493D+00-1.547411334D-05  
2.191372741D-08  
-1.623684074D-11 4.929132670D-15 1.407665368D+05  
7.516678190D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428  
-1.241683887D+04-1.500654643D+02 2.964678293D+00-4.693396660D-04  
1.959138719D-07  
-3.037761925D-11 1.637361082D-15 1.414966808D+05  
4.565651460D+00  
6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428  
-2.562275878D+08 1.570476914D+05-3.635537230D+01 5.019392580D-03-  
3.438107240D-07  
1.140544651D-11-1.295661530D-16 -1.103556546D+06  
3.436188470D+02  
Zn Hf:Cox,1989. Sugar,1995. Gordon,1999.  
3 g 6/97 ZN 1.00 0.00 0.00 0.00 0.00 0 65.39000  
130400.000  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428  
0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 1.493805072D+04  
5.118861010D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428  
-1.755591489D+05 4.984139240D+02 1.969386292D+00 2.608808787D-04-  
5.627195080D-08  
2.723336049D-12 4.266685808D-16 1.173773458D+04  
8.961085650D+00  
6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428  
-2.087287962D+08 1.578178131D+05-3.622033110D+01 3.345230020D-03-  
8.567422720D-09  
-7.122544740D-12 1.691187274D-16 -1.217847671D+06  
3.459439960D+02  
Zn+ Sugar,1995. Gordon,1999.  
3 g 6/97 ZN 1.00E -1.00 0.00 0.00 0.00 0 65.38945  
1043000.128  
298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428  
4.098344940D-04-4.343581620D-06 2.500000019D+00-4.389036810D-11  
5.563969200D-14  
-3.638228260D-17 9.607881995D-21 1.246979918D+05  
5.811995500D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428  
-3.436179460D+05 9.567355240D+02 1.511478952D+00 4.613467960D-04-  
8.786800980D-08  
7.558567780D-13 1.168827311D-15 1.185321933D+05  
1.300742670D+01  
6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6197.428

-3.011747676D+09 2.074729347D+06-5.589526960D+02 7.501396440D-02-  
 5.136763100D-06  
 1.741662147D-10-2.323920111D-15 -1.609057856D+07  
 4.824788010D+03  
 Zr Hf:Gurvich,1982. Moore,1971. Hackett,1986. Gordon,1999.  
 3 g 1/98 ZR 1.00 0.00 0.00 0.00 0.00 0 91.22400  
 599318.611  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6815.611  
 6.715899960D+04-9.435981740D+02 6.359756180D+00-9.790119730D-04-  
 7.608224150D-06  
 9.308717430D-09-3.124675586D-12 7.588019470D+04-  
 1.665770522D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6815.611  
 6.006771840D+06-1.566960605D+04 1.796982350D+01-6.763409650D-03  
 1.733678968D-06  
 -2.064699786D-10 9.334092610D-15 1.734636249D+05-  
 1.051117377D+02  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6815.611  
 5.207701380D+08-2.825652444D+05 6.077054350D+01-5.081211410D-03  
 2.345845819D-07  
 -6.237212120D-12 8.010718759D-17 2.351487351D+06-  
 5.093183060D+02  
 Zr+ Moore,1971. Moore,1970a. Gordon,1999.  
 3 g 1/98 ZR 1.00E -1.00 0.00 0.00 0.00 0 91.22345  
 1246246.292  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7471.892  
 1.739842193D+05-2.224598466D+03 1.400787829D+01-2.378785396D-02  
 2.641058912D-05  
 -1.442565487D-08 3.135982142D-12 1.598210714D+05-  
 5.816728810D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7471.892  
 7.298137160D+05-2.017117556D+03 5.037498300D+00-5.503371950D-04  
 1.023753499D-07  
 -1.261537793D-11 7.092401042D-16 1.620884945D+05-  
 9.820640860D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7471.892  
 -2.294818875D+07 1.860972745D+04-1.661509984D+00 6.020341290D-04-  
 3.930742580D-08  
 1.543806931D-12-2.618341088D-17 4.907298890D+03  
 4.642130480D+01  
 Zr- Hotop,1985. Gordon,1999.  
 3 g 2/98 ZR 1.00E 1.00 0.00 0.00 0.00 0 91.22455  
 552952.398  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7749.498  
 3.046662367D+04-8.074277210D+02 9.213006110D+00-1.614342054D-02  
 1.908653551D-05  
 -1.138888914D-08 2.745019116D-12 6.903034030D+04-  
 2.862644371D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7749.498  
 8.471861160D+04 3.175439340D+02 2.251491246D+00 1.018645389D-04-  
 2.285208242D-08  
 2.647293502D-12-1.235813604D-16 6.422337600D+04  
 1.081261057D+01



6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7749.498  
 -4.386641560D+05 3.768748730D+02 2.417088403D+00 9.411538660D-06-  
 5.824251210D-10  
 1.866281342D-14-2.423724320D-19 6.334701050D+04  
 9.677778690D+00  
 ZrN Chase,1998 p1620.  
 2 j 6/63 ZR 1.00N 1.00 0.00 0.00 0.00 0 105.23074  
 713372.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8862.870  
 2.259109156D+04-1.802590198D+02 3.130058377D+00 5.427709280D-03-  
 8.264614840D-06  
 5.958438220D-09-1.670274535D-12 8.578881490D+04  
 8.470725350D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8862.870  
 -7.255790890D+04-8.126796600D+01 4.559924400D+00 1.291161650D-05  
 5.203830770D-09  
 -5.927436670D-13 2.731548854D-17 8.468648390D+04  
 1.493633834D+00  
 ZrO Gurvich,1982 pt1 p118 pt2 p118.  
 3 tpi82 ZR 1.00O 1.00 0.00 0.00 0.00 0 107.22340  
 83922.708  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8970.108  
 -5.091761400D+05 8.652770090D+03-5.294740150D+01 1.728961761D-01-  
 2.457230895D-04  
 1.672135156D-07-4.423012380D-11 -3.095129818D+04  
 3.132576719D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8970.108  
 4.648098310D+05 3.442314470D+02 4.815779180D+00-4.660633140D-04  
 2.140489079D-07  
 -2.054364483D-11 4.084667760D-16 7.317340700D+03  
 1.502933548D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8970.108  
 1.343456923D+08-7.851088360D+04 1.981614195D+01-8.027211020D-04  
 2.522081797D-09  
 7.959625600D-13-1.684162816D-17 6.406670590D+05-  
 1.358472283D+02  
 ZrO+ Gurvich,1982 pt1 p122 pt2 p120.  
 3 tpi82 ZR 1.00O 1.00E -1.00 0.00 0.00 0 107.22285  
 720614.114  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9464.114  
 1.032911549D+04 7.304661220D+01 2.606345299D+00 5.099300290D-03-  
 6.250338760D-06  
 3.797460020D-09-9.198416900D-13 8.533233780D+04  
 1.267311019D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9464.114  
 -4.937166560D+05 6.699900760D+02 4.575353470D+00-6.923237900D-04  
 4.280600940D-07  
 -7.547660220D-11 4.414279860D-15 8.018880660D+04  
 2.928943704D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9464.114  
 4.389941590D+07-2.084044161D+04 8.167126240D+00-5.668596640D-05-  
 8.861355220D-09

4.773106180D-13-7.435660480D-18 2.554517908D+05-  
3.127152387D+01  
ZrO2 Gurvich,1982 pt1 p125. Chase,1998 p1772 12/65. -  
2 g10/99 ZR 1.000 2.00 0.00 0.00 0.00 0 123.22280  
317042.737  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
12008.263  
3.637649000D+04-2.620658297D+02 3.692866870D+00 1.214524156D-02-  
1.822445342D-05  
1.299215204D-08-3.615900110D-12 -3.801990880D+04  
8.290857600D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
12008.263  
2.854363887D+06-8.738589890D+03 1.621315114D+01-4.417922830D-03  
8.959096920D-07  
-4.054667110D-11-2.147732083D-15 1.527510023D+04-  
7.481995490D+01  
Ag(cr) Cubic. Ref-Elm. Cox,1989 p228.  
1 coda89 AG 1.00 0.00 0.00 0.00 0.00 1 107.86820  
0.000  
200.000 1235.0807 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
5745.000  
-7.099236470D+04 7.254788020D+02 1.066518380D-01 5.529541550D-03-  
4.425590850D-06  
2.091668120D-09-3.888924460D-13 -4.614014260D+03  
5.074216040D+00  
Ag(L) Liquid. Ref-Elm. Cox,1989 p228.  
1 coda89 AG 1.00 0.00 0.00 0.00 0.00 2 107.86820  
0.000  
1235.080 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
5745.000  
0.000000000D+00 0.000000000D+00 4.017073770D+00 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -4.672269970D+02-  
1.771527070D+01  
AL(cr) Cubic. Ref-Elm. Cox,1989 p217.  
1 coda89 AL 1.00 0.00 0.00 0.00 0.00 1 26.98154  
0.000  
200.000 933.6107 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
4540.000  
-6.251811430D+04 6.343934350D+02-7.131883820D-01 1.088725280D-02-  
1.458741820D-05  
9.961160880D-09-1.774928010D-12 -3.985439320D+03  
6.561100200D+00  
AL(L) Liquid. Ref-Elm. Cox,1989 p217.  
1 coda89 AL 1.00 0.00 0.00 0.00 0.00 2 26.98154  
0.000  
933.610 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
4540.000  
0.000000000D+00 0.000000000D+00 3.818625510D+00 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -9.576323160D+01-  
1.752553420D+01  
ALBr3(cr) Monoclinic. Gurvich,1996a pt1 p187 pt2 p150. -  
1 tpis96 AL 1.00BR 3.00 0.00 0.00 0.00 1 266.69354  
511500.000  
200.000 371.1607 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
21920.000  
-1.907292099D+05 0.000000000D+00 2.665662652D+01-8.326099820D-02  
1.395828123D-04

0.000000000D+00 0.000000000D+00 -6.763881140D+04-  
 1.126522667D+02  
 ALBr3(L) Liquid. Gurvich,1996a pt1 p187 pt2 p150.  
 1 tpris96 AL 1.00BR 3.00 0.00 0.00 0.00 2 266.69354 -  
 511500.000  
 371.160 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 21920.000  
 0.000000000D+00 0.000000000D+00 1.503395871D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.481402080D+04-  
 6.083617689D+01  
 ALCL3(cr) Monoclinic. Gurvich,1996a pt1 p172 pt2 p133.  
 1 tpris96 AL 1.00CL 3.00 0.00 0.00 0.00 1 133.33964 -  
 705100.000  
 200.000 465.7007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16980.000  
 -2.605551108D+05 2.535762396D+03-1.248379067D+00 2.465425813D-02-  
 8.048550150D-06  
 0.000000000D+00 0.000000000D+00 -1.007777032D+05  
 2.030375677D+01  
 ALCL3(L) Liquid. Gurvich,1996a pt1 p172 pt2 p133.  
 1 tpris96 AL 1.00CL 3.00 0.00 0.00 0.00 2 133.33964 -  
 705100.000  
 465.700 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16980.000  
 0.000000000D+00 0.000000000D+00 1.509409454D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -8.559022460D+04-  
 6.519014639D+01  
 ALF3(II) Hexagonal. Gurvich,1996a pt1 p156 pt2 p119.  
 2 tpris96 AL 1.00F 3.00 0.00 0.00 0.00 1 83.97675 -  
 1510400.000  
 100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11620.400  
 0.000000000D+00 0.000000000D+00-2.444621150D+00 6.248607440D-02-  
 8.043962500D-05  
 0.000000000D+00 0.000000000D+00 -1.829961207D+05  
 6.871585170D+00  
 298.150 728.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11620.400  
 0.000000000D+00 0.000000000D+00-3.158574588D+00 7.101368571D-02-  
 1.246540085D-04  
 7.930377136D-08 0.000000000D+00 -1.829283321D+05  
 9.661469435D+00  
 ALF3(I) Cubic. Gurvich,1996a pt1 p156 pt2 p119.  
 1 tpris96 AL 1.00F 3.00 0.00 0.00 0.00 2 83.97675 -  
 1510400.000  
 728.000 2100.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11620.400  
 -1.060675855D+05 0.000000000D+00 1.114052422D+01 1.092668119D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.853502219D+05-  
 5.651122021D+01  
 ALH3(a) Alpha,hexagonal. Gurvich,1996a pt1 p144 pt2 p108.  
 1 tpris96 AL 1.00H 3.00 0.00 0.00 0.00 1 30.00536 -  
 11400.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 5440.000  
 5.744612990D+05-7.649579650D+03 3.481355430D+01-4.495737990D-02  
 2.948551342D-05

0.000000000D+00 0.000000000D+00 3.549793150D+04-  
2.050727589D+02  
ALI3(cr) Hexagonal. Gurvich,1996a pt1 p193 pt2 p155.  
1 tpris96 AL 1.00I 3.00 0.00 0.00 0.00 1 407.69495 -  
302900.000  
298.150 461.4707 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
22300.000  
-3.486280460D+03 0.000000000D+00 8.644374370D+00 1.088065032D-02  
5.040262220D-07  
0.000000000D+00 0.000000000D+00 -3.950736400D+04-  
2.968661932D+01  
ALI3(L) Liquid. Gurvich,1996a pt1 p193 pt2 p155.  
1 tpris96 AL 1.00I 3.00 0.00 0.00 0.00 2 407.69495 -  
302900.000  
461.470 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
22300.000  
0.000000000D+00 0.000000000D+00 1.455287203D+01 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -3.913903150D+04-  
5.670488781D+01  
ALN(cr) Hexagonal. Gurvich,1996a pt1 p202 pt2 p163.  
2 tpris96 AL 1.00N 1.00 0.00 0.00 0.00 1 40.98828 -  
319000.000  
100.000 300.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
3870.000  
3.654741530D+03 0.000000000D+00 -2.148600451D+00 2.744441314D-02-  
2.763366825D-05  
0.000000000D+00 0.000000000D+00 -3.868948290D+04  
7.733969220D+00  
300.000 1800.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
3870.000  
-1.801549340D+05 0.000000000D+00 5.525280504D+00 4.025492783D-04  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -4.063616530D+04-  
3.018829926D+01  
ALN(L) Liquid. Gurvich,1996a pt1 p202 pt2 p163.  
2 tpris96 AL 1.00N 1.00 0.00 0.00 0.00 3 40.98828 -  
319000.000  
1800.000 2700.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
3870.000  
0.000000000D+00 0.000000000D+00 4.491184688D+00 9.460569534D-04  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -3.955518910D+04-  
2.338770283D+01  
2700.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
3870.000  
0.000000000D+00 0.000000000D+00 8.058201866D+00 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -3.755928440D+04-  
4.598731266D+01  
AL(OH)3(a) Gibbsite. Gurvich,1996a pt1 p150 pt2 p114.  
1 tpris96 AL 1.00O 3.00H 3.00 0.00 0.00 1 78.00356 -  
1293500.000  
100.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
12460.000  
-2.376748819D+04 9.289791210D+02 -1.532337335D+01 1.307578268D-01-  
2.205157141D-04  
1.567014467D-07 0.000000000D+00 -1.605485750D+05  
6.795129010D+01  
AL2O3(a) Alpha,corundum. Gurvich,1996a pt1 p134 pt2 p103.

3 tpis96 AL 2.000 3.00 0.00 0.00 0.00 1 101.96128 -  
 1675700.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10016.000  
 -5.391549970D+06 1.036676983D+05-8.173229150D+02 3.388258720D+00-  
 7.512400360D-03  
 8.659248820D-06-4.066085670D-09 -6.660134650D+05  
 4.235502230D+03  
 500.000 1200.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10016.000  
 -6.042087868D+05 0.000000000D+00 1.475480816D+01 8.272285438D-04  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.079235447D+05-  
 8.136029480D+01  
 1200.000 2327.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10016.000  
 0.000000000D+00 0.000000000D+00 1.293774378D+01 1.992781294D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.060787581D+05-  
 6.966603728D+01  
 AL2O3(L) Liquid. Gurvich,1996a pt1 p134 pt2 p103.  
 1 tpis96 AL 2.000 3.00 0.00 0.00 0.00 3 101.96128 -  
 1675700.000  
 2327.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10016.000  
 0.000000000D+00 0.000000000D+00 1.959225499D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.027701571D+05-  
 1.108590952D+02  
 AL2S3(a) Hexagonal alpha. Gurvich,1996a pt1 p201 pt2 p162.  
 2 tpis96 AL 2.00S 3.00 0.00 0.00 0.00 1 150.16108 -  
 648500.000  
 100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18630.440  
 0.000000000D+00 0.000000000D+00-1.347810098D+00 8.478152110D-02-  
 1.270516814D-04  
 0.000000000D+00 0.000000000D+00 -8.024014680D+04  
 2.103644584D+00  
 298.150 1273.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18630.440  
 -1.943109095D+05 0.000000000D+00 1.417618116D+01 2.164890054D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -8.297075040D+04-  
 6.845362098D+01  
 AL2S3(b) Rhombohedral gamma. Gurvich,1996a pt1 p201 pt2 p162.  
 1 tpis96 AL 2.00S 3.00 0.00 0.00 0.00 3 150.16108 -  
 648500.000  
 1273.000 1373.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18630.440  
 0.000000000D+00 0.000000000D+00 1.683803375D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -8.445251510D+04-  
 8.466769750D+01  
 AL2S3(L) Liquid. Gurvich,1996a pt1 p201 pt2 p162.  
 1 tpis96 AL 2.00S 3.00 0.00 0.00 0.00 4 150.16108 -  
 648500.000  
 1373.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18630.440  
 0.000000000D+00 0.000000000D+00 1.924346714D+01 0.000000000D+00  
 0.000000000D+00

0.000000000D+00 0.000000000D+00 -8.114023330D+04-  
 9.722848599D+01  
 AL2SiO5(an) Andalusite. Chase,1998 p160.  
 3 j 9/67 AL 2.00SI 1.000 5.00 0.00 0.00 1 162.04558 -  
 2592072.000  
 200.000 600.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17093.000  
 -5.435020350D+05 8.364904470D+03-5.479541870D+01 2.421451459D-01-  
 3.247828060D-04  
 1.619746222D-07 0.000000000D+00 -3.531115760D+05  
 2.892220103D+02  
 600.000 1500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17093.000  
 9.635670330D+06-6.505315100D+04 1.886717981D+02-2.227599181D-01  
 1.677460173D-04  
 -6.532301110D-08 1.041420443D-11 4.284683500D+04-  
 1.170130476D+03  
 1500.000 3000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17093.000  
 5.600590290D+07-1.591905491D+05 2.058003747D+02-1.103017260D-01  
 3.860284650D-05  
 -6.943079960D-09 5.126291370D-13 6.964365160D+05-  
 1.424396263D+03  
 AL4C3(cr) Hexagonal. Gurvich,1996a pt1 p207 pt2 p168.  
 2 tpis96 AL 4.00C 3.00 0.00 0.00 0.00 1 143.95825 -  
 206900.000  
 100.000 300.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16470.000  
 4.384127580D+03 0.000000000D+00-5.803779650D+00 1.009595640D-01-  
 1.158851541D-04  
 0.000000000D+00 0.000000000D+00 -2.660263745D+04  
 1.884004031D+01  
 300.000 2500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16470.000  
 -4.483607573D+05 0.000000000D+00 1.788920814D+01 4.024290066D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.190056250D+04-  
 9.494910735D+01  
 B(b) Beta. Ref-Elm. Chase,1998 p177-180. McBride,1993a.  
 2 j 6/83 B 1.00 0.00 0.00 0.00 0.00 1 10.81100  
 0.000  
 200.000 600.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 1214.000  
 2.598259342D+05-4.770773050D+03 3.464124480D+01-1.287342209D-01  
 2.897864235D-04  
 -3.307265950D-07 1.500151011D-10 2.146946846D+04-  
 1.830824723D+02  
 600.000 2350.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 1214.000  
 -8.697700220D+02-8.050405960D+02 4.079712880D+00-6.423381350D-04  
 4.846017800D-07  
 -1.252780673D-10 1.335923595D-14 3.397919930D+03-  
 2.505906587D+01  
 B(L) Liquid. Ref-Elm. Chase,1998 p177-180. McBride,1993a.  
 1 j 6/83 B 1.00 0.00 0.00 0.00 0.00 2 10.81100  
 0.000  
 2350.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 1214.000  
 0.000000000D+00 0.000000000D+00 3.818625511D+00 0.000000000D+00  
 0.000000000D+00

0.000000000D+00 0.000000000D+00 3.360603140D+03-  
 2.073167308D+01  
 BN(cr) Hexagonal. Gurvich,1996a pt1 p103 pt2 p82.  
 2 tpris96 B 1.00N 1.00 0.00 0.00 0.00 1 24.81774 -  
 251000.000  
 200.000 1200.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 2628.425  
 4.927312430D+05-6.086406850D+03 2.678226753D+01-4.529686640D-02  
 5.305526030D-05  
 -3.041114432D-08 6.795343860D-12 -2.413474891D+02-  
 1.570534002D+02  
 1200.000 3240.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 2628.425  
 -8.394039490D+05 0.000000000D+00 6.231256640D+00-1.258688680D-05  
 2.018144787D-09  
 0.000000000D+00 0.000000000D+00 -3.427269230D+04-  
 3.687260910D+01  
 BN(L) Liquid. Gurvich,1996a pt1 p103 pt2 p82.  
 1 tpris96 B 1.00N 1.00 0.00 0.00 0.00 2 24.81774 -  
 251000.000  
 3240.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 2628.425  
 0.000000000D+00 0.000000000D+00 8.058201866D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.023409980D+04-  
 4.862382389D+01  
 B203(cr) Hexagonal. Gurvich,1996a pt1 p21 pt2 p16.  
 1 tpris96 B 2.00O 3.00 0.00 0.00 0.00 1 69.62020 -  
 1273500.000  
 100.000 723.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9301.499  
 -5.595297380D+04 1.311214190D+03-1.178535942D+01 7.702795250D-02-  
 9.740126500D-05  
 4.692119720D-08 1.804813810D-12 -1.599672923D+05  
 5.866759160D+01  
 B203(L) Liquid. Gurvich,1996a pt1 p21 pt2 p16.  
 1 tpris96 B 2.00O 3.00 0.00 0.00 0.00 2 69.62020 -  
 1273500.000  
 723.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9301.499  
 3.774124994D+05 0.000000000D+00 1.528015481D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.562115789D+05-  
 8.056094941D+01  
 B2S3(cr) Monoclinic. Gurvich,1996a pt1 p101 pt2 p80.  
 1 tpris96 B 2.00S 3.00 0.00 0.00 0.00 1 117.82000 -  
 243000.000  
 298.150 840.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17200.400  
 -9.430501617D+04 0.000000000D+00 1.190088171D+01 8.711277033D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.347775180D+04-  
 5.890696350D+01  
 B2S3(L) Liquid. Gurvich,1996a pt1 p101 pt2 p80.  
 1 tpris96 B 2.00S 3.00 0.00 0.00 0.00 2 117.82000 -  
 243000.000  
 840.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17200.400  
 0.000000000D+00 0.000000000D+00 1.755966377D+01 0.000000000D+00  
 0.000000000D+00

0.000000000D+00 0.000000000D+00 -2.921234633D+04-  
 8.268126136D+01  
 B303H3(cr) Chase,1998 p287.  
 3 j 3/65 B 3.00H 3.000 3.00 0.00 0.00 1 83.45502 -  
 1262313.000  
 298.150 700.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 -5.328545240D+05 3.767360370D+03 6.890276350D-01-4.217091030D-03  
 8.303566290D-05  
 -6.146021890D-08 0.000000000D+00 -1.757027581D+05  
 2.395113516D+01  
 700.000 1400.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 5.084004120D+07-3.177180280D+05 8.113753320D+02-1.045412717D+00  
 7.976442970D-04  
 -3.265400500D-07 5.554759650D-11 1.623716865D+06-  
 5.113032450D+03  
 1400.000 2000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 -3.234845810D+08 1.232060747D+06-1.920881017D+03 1.628142178D+00-  
 7.579315580D-04  
 1.870131216D-07-1.915685535D-11 -7.655560210D+06  
 1.307505171D+04  
 B4C(cr) Hexagonal. Gurvich,1996a pt1 p111 pt2 p89  
 2 tpis96 B 4.00C 1.00 0.00 0.00 0.00 1 55.25470 -  
 62000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 5611.469  
 -3.582115390D+07 6.748884130D+05-5.160630080D+03 2.049973510D+01-  
 4.453648770D-02  
 5.049831300D-05-2.340979136D-08 -3.040618105D+06  
 2.693617477D+04  
 500.000 2743.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 5611.469  
 -5.772904970D+05 0.000000000D+00 1.274373364D+01 5.718209610D-05  
 1.287030822D-06  
 0.000000000D+00 0.000000000D+00 -1.320621763D+04-  
 7.266962500D+01  
 B4C(L) Liquid. Chase,1998 pp556-8.  
 1 j 6/83 B 4.00C 1.00 0.00 0.00 0.00 2 55.25470 -  
 62000.000  
 2743.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 5611.469  
 0.000000000D+00 0.000000000D+00 1.635454164D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.250553215D+03-  
 9.163227046D+01  
 Ba(cr) Crystal. Ref-Elm. Alcock,1993.  
 2 srd 93 BA 1.00 0.00 0.00 0.00 0.00 1 137.32700  
 0.000  
 80.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6906.992  
 -1.121413048D+03 0.000000000D+00 2.794031158D+00 3.089779193D-03-  
 8.812305235D-06  
 1.741533776D-08 0.000000000D+00 -9.306838000D+02-  
 9.109787138D+00  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6906.992  
 0.000000000D+00 0.000000000D+00 2.773344430D+00 2.037522355D-03  
 0.000000000D+00



0.000000000D+00 0.000000000D+00 -9.174338100D+02-  
8.909706262D+00

Ba(L) Liquid. Ref-Elm. Alcock,1993.  
1 srd 93 BA 1.00 0.00 0.00 0.00 0.00 2 137.32700  
0.000  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6906.992  
0.000000000D+00 0.000000000D+00 4.810866786D+00 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -9.920623810D+02-  
2.000275711D+01

BaBr2(cr) Rhombic. Gurvich,1996a pt1 p578 pt2 p438.  
1 tpis96 BA 1.00BR 2.00 0.00 0.00 0.00 1 297.13500 -  
752000.000  
298.000 1130.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
19000.460  
-7.817658527D+03 0.000000000D+00 8.433088661D+00 2.644894287D-03  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -9.310239840D+04-  
3.084013513D+01

BaBr2(L) Liquid. Gurvich,1996a pt1 p578 pt2 p438.  
1 tpis96 BA 1.00BR 2.00 0.00 0.00 0.00 2 297.13500 -  
752000.000  
1130.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
19000.460  
0.000000000D+00 0.000000000D+00 1.262852531D+01 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -9.227494300D+04-  
5.391493900D+01

BaCO3(a) CrIII,rhombic. Gurvich,1996a pt1 p588 pt2 p446.  
2 tpis96 BA 1.00C 1.00O 3.00 0.00 0.00 1 197.33590 -  
1214000.000  
200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
16510.460  
-2.877181104D+07 5.413510470D+05-4.125297560D+03 1.638620098D+01-  
3.558188760D-02  
4.031953330D-05-1.867325900D-08 -2.581769925D+06  
2.154826876D+04  
500.000 1083.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
16510.460  
-4.578261377D+05 0.000000000D+00 1.897622349D+01-1.614166078D-02  
1.493894409D-05  
0.000000000D+00 0.000000000D+00 -1.526176829D+05-  
9.306389650D+01

BaCO3(b) CrII,hexagonal. Gurvich,1996a pt1 p588 pt2 p446.  
1 tpis96 BA 1.00C 1.00O 3.00 0.00 0.00 3 197.33590 -  
1214000.000  
1083.000 1233.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
16510.460  
0.000000000D+00 0.000000000D+00 1.900292380D+01 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -1.534042929D+05-  
9.996568172D+01

BaCO3(c) CrI,cubic. Gurvich,1996a pt1 p588 pt2 p446.  
1 tpis96 BA 1.00C 1.00O 3.00 0.00 0.00 4 197.33590 -  
1214000.000  
1233.000 1828.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
16510.460  
0.000000000D+00 0.000000000D+00 1.924346714D+01 0.000000000D+00  
0.000000000D+00

0.000000000D+00 0.000000000D+00 -1.533520950D+05-  
 1.013948007D+02  
 BaCO<sub>3</sub>(L) Liquid. Gurvich,1996a pt1 p588 pt2 p446.  
 1 tpris96 BA 1.00C 1.000 3.00 0.00 0.00 5 197.33590 -  
 1214000.000  
 1828.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16510.460  
 0.000000000D+00 0.000000000D+00 1.984482549D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.496405113D+05-  
 1.032798247D+02  
 BaCl<sub>2</sub>(a) CrII,rhombic. Gurvich,1996a pt1 p574 pt2 p435.  
 2 tpris96 BA 1.00CL 2.00 0.00 0.00 0.00 1 208.23240 -  
 855200.000  
 100.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16700.460  
 -7.376444120D+04 1.806760784D+03-1.415837573D+01 1.391571933D-01-  
 4.179089240D-04  
 6.207438290D-07-3.577305500D-10 -1.127273901D+05  
 7.349900590D+01  
 500.000 1198.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16700.460  
 7.096028509D+02 0.000000000D+00 8.343245723D+00 2.300676769D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.054434434D+05-  
 3.333989736D+01  
 BaCl<sub>2</sub>(b) CrI,cubic. Gurvich,1996a pt1 p574 pt2 p435.  
 1 tpris96 BA 1.00CL 2.00 0.00 0.00 0.00 3 208.23240 -  
 855200.000  
 1198.000 1234.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16700.460  
 0.000000000D+00 0.000000000D+00 1.575558872D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.105803253D+05-  
 8.137880037D+01  
 BaCl<sub>2</sub>(L) Liquid. Gurvich,1996a pt1 p574 pt2 p435.  
 1 tpris96 BA 1.00CL 2.00 0.00 0.00 0.00 4 208.23240 -  
 855200.000  
 1234.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16700.460  
 0.000000000D+00 0.000000000D+00 1.310961199D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.054088841D+05-  
 6.099987667D+01  
 BaF<sub>2</sub>(a) CrIII,cubic. Gurvich,1996a pt1 p567 pt2 p431.  
 2 tpris96 BA 1.00F 2.00 0.00 0.00 0.00 1 175.32381 -  
 1206000.000  
 100.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14440.460  
 1.441693954D+05-4.606283760D+03 5.412180390D+01-2.221460987D-01  
 5.733095130D-04  
 -7.321844990D-07 3.715051400D-10 -1.283756240D+05-  
 2.649277473D+02  
 500.000 1240.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14440.460  
 -2.180525371D+04 0.000000000D+00 7.730461567D+00 3.587703906D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.475854552D+05-  
 3.364924914D+01  
 BaF<sub>2</sub>(b) CrII. Gurvich,1996a pt1 p567 pt2 p431.

1 tpis96 BA 1.00F 2.00 0.00 0.00 0.00 3 175.32381 -  
 1206000.000  
 1240.000 1480.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14440.460  
 0.000000000D+00 0.000000000D+00 1.515423038D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.533548254D+05-  
 8.153942783D+01  
 BaF2 (c) CrI. Gurvich,1996a pt1 p567 pt2 p431.  
 1 tpis96 BA 1.00F 2.00 0.00 0.00 0.00 4 175.32381 -  
 1206000.000  
 1480.000 1641.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14440.460  
 0.000000000D+00 0.000000000D+00 1.551504538D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.535821388D+05-  
 8.396607945D+01  
 BaF2 (L) Liquid. Gurvich,1996a pt1 p567 pt2 p431.  
 1 tpis96 BA 1.00F 2.00 0.00 0.00 0.00 5 175.32381 -  
 1206000.000  
 1641.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14440.460  
 0.000000000D+00 0.000000000D+00 1.262852531D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.467045237D+05-  
 6.129240287D+01  
 BaH2 (a) CrII, rhombic Gurvich,1996a pt1 p556 pt2 p424. -  
 1 tpis96 BA 1.00H 2.00 0.00 0.00 0.00 1 139.34288 -  
 190000.000  
 298.150 871.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9100.474  
 0.000000000D+00 0.000000000D+00 4.530874339D+00 3.359308005D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.435180761D+04-  
 1.923955725D+01  
 BaH2 (b) CrI, rhombic Gurvich,1996a pt1 p556 pt2 p424. -  
 1 tpis96 BA 1.00H 2.00 0.00 0.00 0.00 2 139.34288 -  
 190000.000  
 871.000 1473.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9100.474  
 0.000000000D+00 0.000000000D+00 8.539288545D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.589536064D+04-  
 4.267585539D+01  
 BaH2 (L) Liquid Gurvich,1996a pt1 p556 pt2 p424. -  
 1 tpis96 BA 1.00H 2.00 0.00 0.00 0.00 3 139.34288 -  
 190000.000  
 1473.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9100.474  
 0.000000000D+00 0.000000000D+00 9.020375224D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.359720958D+04-  
 4.414413915D+01  
 BaI2 (cr) Rhombic. Gurvich,1996a pt1 p582 pt2 p441. -  
 2 tpis96 BA 1.00I 2.00 0.00 0.00 0.00 1 391.13594 -  
 606000.000  
 100.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19230.400  
 1.510332529D+04-6.224807000D+02 1.545037842D+01-3.239437030D-02  
 9.253598890D-05

```

-1.251913725D-07 6.804559110D-11 -7.305629580D+04-
6.364696150D+01
  500.000 984.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
19230.400
-3.247335080D+02 0.000000000D+00 8.607723125D+00 2.399780624D-03
0.000000000D+00
  0.000000000D+00 0.000000000D+00 -7.555873070D+04-
2.989160688D+01
BaI2(L) Liquid. Gurvich,1996a pt1 p582 pt2 p441.
  1 tpris96 BA 1.00I 2.00 0.00 0.00 0.00 3 391.13594 -
606000.000
  984.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
19230.400
  0.000000000D+00 0.000000000D+00 1.359069867D+01 0.000000000D+00
0.000000000D+00
  0.000000000D+00 0.000000000D+00 -7.611264840D+04-
5.863183475D+01
BaO(cr) Cubic Gurvich,1996a pt1 p547 pt2 p418.
  3 tpris96 BA 1.00O 1.00 0.00 0.00 0.00 1 153.32640 -
548000.000
  200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
9962.459
-3.734308680D+06 7.030482670D+04-5.334141930D+02 2.143135900D+00-
4.664219600D-03
  5.294704440D-06-2.456512761D-09 -3.833163320D+05
2.789047565D+03
  500.000 1400.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
9962.459
-7.551858137D+04 0.000000000D+00 6.798957485D+00-1.205482945D-03
7.325747398D-07
  0.000000000D+00 0.000000000D+00 -6.814216420D+04-
3.017618534D+01
  1400.000 2246.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
9962.459
  1.380021192D+07 0.000000000D+00-1.685992319D+01 1.166250326D-02
0.000000000D+00
  0.000000000D+00 0.000000000D+00 -3.704906000D+04
1.274565988D+02
BaO(L) Liquid Gurvich,1996a pt1 p547 pt2 p418.
  1 tpris96 BA 1.00O 1.00 0.00 0.00 0.00 3 153.32640 -
548000.000
  2246.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
9962.459
  0.000000000D+00 0.000000000D+00 1.001863008D+01 0.000000000D+00
0.000000000D+00
  0.000000000D+00 0.000000000D+00 -6.861430250D+04-
5.267326797D+01
Ba(OH)2(b) CrII,rhombic Gurvich,1996a pt1 p558 pt2 p427.
  1 tpris96 BA 1.00O 2.00H 2.00 0.00 0.00 1 171.34168 -
940600.000
  100.000 519.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
16148.440
  5.078717800D+04-1.641996937D+03 1.964278489D+01-3.730614630D-02
1.039952734D-04
-8.659369050D-08 2.282290989D-11 -1.085585521D+05-
9.701503650D+01
Ba(OH)2(a) CrI,rhombic Gurvich,1996a pt1 p558 pt2 p427.
  1 tpris96 BA 1.00O 2.00H 2.00 0.00 0.00 2 171.34168 -
940600.000
  519.000 681.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
16148.440

```

0.000000000D+00 0.000000000D+00 1.491368704D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.176117467D+05-  
 7.252241184D+01  
 Ba(OH)2(L) Liquid Gurvich,1996a pt1 p558 pt2 p427.  
 1 tpris96 BA 1.000 2.00H 2.00 0.00 0.00 3 171.34168 -  
 940600.000  
 681.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16148.440  
 0.000000000D+00 0.000000000D+00 1.659749041D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.168340700D+05-  
 8.068104197D+01  
 BaS(cr) Cubic. Gurvich,1996a pt1 p584 pt2 p443.  
 2 tpris96 BA 1.00S 1.00 0.00 0.00 0.00 1 169.39300 -  
 470000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10820.450  
 3.369786470D+05-6.138740230D+03 4.922553770D+01-1.599274620D-01  
 3.314481350D-04  
 -3.600847800D-07 1.611281388D-10 -3.028248993D+04-  
 2.539125160D+02  
 500.000 2500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10820.450  
 -2.050631967D+04 0.000000000D+00 5.920852822D+00 8.307164223D-04  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.839868930D+04-  
 2.466233780D+01  
 BaS(L) Liquid. Gurvich,1996a pt1 p584 pt2 p443.  
 1 tpris96 BA 1.00S 1.00 0.00 0.00 0.00 3 169.39300 -  
 470000.000  
 2500.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10820.450  
 0.000000000D+00 0.000000000D+00 8.058201866D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.356075540D+04-  
 3.627577743D+01  
 BaSO4(a) CrII,rhombic. Gurvich,1996a pt1 p587 pt2 p445.  
 2 tpris96 BA 1.00S 1.000 4.00 0.00 0.00 1 233.39060 -  
 1470000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19180.440  
 -1.712286968D+07 3.212789860D+05-2.441820133D+03 9.713067900D+00-  
 2.105021811D-02  
 2.383101570D-05-1.103328957D-08 -1.624343960D+06  
 1.276058048D+04  
 500.000 1423.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19180.440  
 -2.747004935D+05 0.000000000D+00 1.352094110D+01 6.200004570D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.820275447D+05-  
 6.454315519D+01  
 BaSO4(b) CrI,cubic. Gurvich,1996a pt1 p587 pt2 p445.  
 1 tpris96 BA 1.00S 1.000 4.00 0.00 0.00 3 233.39060 -  
 1470000.000  
 1423.000 1853.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19180.440  
 0.000000000D+00 0.000000000D+00 2.044618384D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.842091207D+05-  
 1.050884025D+02

BaSO4(L) Liquid. Gurvich,1996a pt1 p587 pt2 p435.

1 tps96 BA 1.00S 1.000 4.00 0.00 0.00 4 233.39060 -  
1470000.000  
1853.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
19180.440  
0.000000000D+00 0.000000000D+00 2.044618384D+01 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -1.793982539D+05-  
1.024921441D+02

Be(a) Alpha. Ref-Elm. Alcock,1993.

2 srd 93 BE 1.00 0.00 0.00 0.00 0.00 1 9.01218  
0.000  
100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
1942.068  
3.532378938D+03 0.000000000D+00-1.827528020D+00 1.895481514D-02-  
2.121592253D-05  
0.000000000D+00 0.000000000D+00 -9.832146860D+01  
6.866894114D+00  
298.150 1543.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
1942.068  
-7.064757875D+04 0.000000000D+00 2.550360755D+00 6.848268870D-04  
1.157013462D-07  
0.000000000D+00 0.000000000D+00 -1.028803669D+03-  
1.399471510D+01

Be(b) Beta. Ref-Elm. Alcock,1993.

1 srd 93 BE 1.00 0.00 0.00 0.00 0.00 2 9.01218  
0.000  
1543.000 1563.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
1942.068  
0.000000000D+00 0.000000000D+00 3.608150089D+00 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -8.524497790D+02-  
2.002895768D+01

Be(L) Liquid. Ref-Elm. Alcock,1993.

1 srd 93 BE 1.00 0.00 0.00 0.00 0.00 3 9.01218  
0.000  
1563.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
1942.068  
0.000000000D+00 0.000000000D+00 3.545608821D+00 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 2.074755804D+02-  
1.895341257D+01

BeAL2O4(cr) Chase,1998 pp139-41.

3 j12/79 BE 1.00AL 2.000 4.00 0.00 0.00 1 126.97286 -  
2300782.000  
200.000 600.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
13088.000  
5.671733300D+05-8.864346630D+03 4.407635150D+01-3.612460380D-02  
3.491655240D-05  
-1.451255323D-08 0.000000000D+00 -2.361266575D+05-  
2.603504873D+02  
600.000 1200.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
13088.000  
3.035781649D+07-2.195328809D+05 6.571002230D+02-9.751675120D-01  
8.342636270D-04  
-3.757959390D-07 6.972665420D-11 9.154378130D+05-  
4.048262870D+03  
1200.000 2146.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
13088.000  
5.346540420D+06-2.333165977D+04 6.465121650D+01-5.623102150D-02  
4.944443190D-05

-2.347465372D-08 4.584679740D-12 -1.453507980D+05-  
3.997587750D+02

BeAL2O4 (L) Chase,1998 pp139-41.  
1 j12/79 BE 1.00AL 2.000 4.00 0.00 0.00 2 126.97286 -  
2300782.000  
2146.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
13088.000  
0.000000000D+00 0.000000000D+00 2.963602185D+01 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -2.805665995D+05-  
1.711673740D+02

BeBr2 (cr) Cr, rhombic. Gurvich,1996a pt1 p376 pt2 p301.  
1 tpi96 BE 1.00BR 2.00 0.00 0.00 0.00 1 168.82018 -  
358000.000  
298.150 781.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
14900.000  
-1.296528599D+05 0.000000000D+00 9.544519160D+00 8.967455689D-04  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -4.637767130D+04-  
4.238810553D+01

BeBr2 (L) Liquid.Gurvich,1996a pt1 p376 pt2 p301.  
1 tpi96 BE 1.00BR 2.00 0.00 0.00 0.00 2 168.82018 -  
358000.000  
781.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
14900.000  
0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -4.571223050D+04-  
5.534538359D+01

BeCO3 (cr) Gurvich,1996a pt1 p385 pt2 p310.  
1 tpi96 BE 1.00C 1.000 3.00 0.00 0.00 1 69.02108 -  
1045000.000  
298.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
9200.480  
-3.688732108D+05 0.000000000D+00 1.057428520D+01 4.670148932D-03  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -1.302813975D+05-  
5.746109667D+01

BeCL2 (a) Cr, rhombic. Gurvich,1996a pt1 p370 pt2 p296.  
1 tpi96 BE 1.00CL 2.00 0.00 0.00 0.00 1 79.91758 -  
496200.000  
200.000 676.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
11420.000  
-9.696336540D+05 1.653841300D+04-1.120322868D+02 4.343457410D-01-  
8.234422230D-04  
7.967601960D-07-3.089202126D-10 -1.372167152D+05  
5.981191760D+02

BeCL2 (b) CrI. Gurvich,1996a pt1 p370 pt2 p296.  
1 tpi96 BE 1.00CL 2.00 0.00 0.00 0.00 2 79.91758 -  
496200.000  
676.000 688.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
11420.000  
0.000000000D+00 0.000000000D+00 8.056999150D+00 2.516083329D-03  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -6.169505530D+04-  
3.701517264D+01

BeCL2 (L) Liquid.Gurvich,1996a pt1 p370 pt2 p296.  
1 tpi96 BE 1.00CL 2.00 0.00 0.00 0.00 3 79.91758 -  
496200.000  
688.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
11420.000

0.000000000D+00 0.000000000D+00 1.106499361D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.212751630D+04-  
 5.342382325D+01  
 BeF2 (a) CrII,hexagonal.Gurvich,1996a pt1 p364 pt2 p292.  
 1 tpris96 BE 1.00F 2.00 0.00 0.00 0.00 1 47.00899 -  
 1027000.000  
 200.000 493.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8468.000  
 3.082582728D+05-5.000745390D+03 3.049066381D+01-5.416146720D-02  
 5.846680620D-05  
 0.000000000D+00 0.000000000D+00 -1.011928897D+05-  
 1.687961461D+02  
 BeF2 (b) CrI,hexagonal.Gurvich,1996a pt1 p364 pt2 p292.  
 1 tpris96 BE 1.00F 2.00 0.00 0.00 0.00 2 47.00899 -  
 1027000.000  
 493.000 823.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8468.000  
 0.000000000D+00 0.000000000D+00 5.652527930D+00 3.986885577D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.252903029D+05-  
 2.679700109D+01  
 BeF2 (L) Liquid.Gurvich,1996a pt1 p364 pt2 p292.  
 1 tpris96 BE 1.00F 2.00 0.00 0.00 0.00 3 47.00899 -  
 1027000.000  
 823.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8468.000  
 -1.882035141D+06 0.000000000D+00 1.234468417D+01-1.836548396D-04  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.310986361D+05-  
 6.898102574D+01  
 BeI2 (cr) Cr,rhombic. Gurvich,1996a pt1 p379 pt2 p304.  
 1 tpris96 BE 1.00I 2.00 0.00 0.00 0.00 1 262.82112 -  
 191000.000  
 298.150 763.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15200.000  
 -1.443741122D+05 0.000000000D+00 1.007828483D+01 3.371214900D-04  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.647594661D+04-  
 4.378170625D+01  
 BeI2 (L) Liquid.Gurvich,1996a pt1 p379 pt2 p304.  
 1 tpris96 BE 1.00I 2.00 0.00 0.00 0.00 2 262.82112 -  
 191000.000  
 763.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15200.000  
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.551070377D+04-  
 5.349837990D+01  
 BeO (a) CrII,hexagonal. Gurvich,1996a pt1 p348 pt2 p278.  
 2 tpris96 BE 1.00O 1.00 0.00 0.00 0.00 1 25.01158 -  
 609400.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 2837.000  
 2.047701543D+05-2.981173217D+03 1.385643338D+01-1.581697711D-02  
 2.353849388D-05  
 -1.941029834D-08 6.520569610D-12 -5.922219190D+04-  
 8.231113660D+01  
 1000.000 2373.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 2837.000



1.024057237D+06 1.937465590D+03-2.170213872D+00 6.700940070D-03-  
 1.829092628D-06  
 2.757893870D-10-2.712743027D-14 -8.276808970D+04  
 1.896607400D+01  
 BeO(b) CrI,tetragonal. Gurvich,1996a pt1 p348 pt2 p278.  
 1 tpris96 BE 1.000 1.00 0.00 0.00 0.00 2 25.01158 -  
 609400.000  
 2373.000 2851.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 2837.000  
 0.000000000D+00 0.000000000D+00 6.735213500D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -7.674474850D+04-  
 3.937528813D+01  
 BeO(L) Liquid. Gurvich,1996a pt1 p348 pt2 p278.  
 1 tpris96 BE 1.000 1.00 0.00 0.00 0.00 3 25.01158 -  
 609400.000  
 2851.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 2837.000  
 0.000000000D+00 0.000000000D+00 1.010282025D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -7.600243170D+04-  
 6.253805395D+01  
 Be(OH)2(b) Rhombic,beta.Gurvich,1996a pt1 p359 pt2 p289.  
 2 tpris96 BE 1.000 2.00H 2.00 0.00 0.00 1 43.02686 -  
 905700.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8293.440  
 -2.821507074D+07 5.306026240D+05-4.050124700D+03 1.608285663D+01-  
 3.491136410D-02  
 3.956008990D-05-1.833019806D-08 -2.495097922D+06  
 2.114570392D+04  
 500.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8293.440  
 -4.549275904D+05 0.000000000D+00 1.198362862D+01 2.034996650D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.141192354D+05-  
 6.597431876D+01  
 BeS(cr) Cr,cubic. Gurvich,1996a pt1 p381 pt2 p306.  
 1 tpris96 BE 1.00S 1.00 0.00 0.00 0.00 1 41.07818 -  
 236000.000  
 298.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 5500.480  
 -1.061156941D+05 0.000000000D+00 4.876054031D+00 1.363880734D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.025444334D+04-  
 2.469606404D+01  
 BeSO4(a) CrIII,tetr. Gurvich,1996a pt1 p383 pt2 p308.  
 1 tpris96 BE 1.00S 1.000 4.00 0.00 0.00 1 105.07578 -  
 1200000.000  
 200.000 861.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12970.000  
 9.674052850D+05-1.525976877D+04 9.078019340D+01-2.151323890D-01  
 3.405813330D-04  
 -2.623119799D-07 8.137303080D-11 -7.417050650D+04-  
 5.024380540D+02  
 BeSO4(b) CrII,rhombic. Gurvich,1996a pt1 p383 pt2 p308.  
 1 tpris96 BE 1.00S 1.000 4.00 0.00 0.00 2 105.07578 -  
 1200000.000  
 861.000 912.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12970.000

0.000000000D+00 0.000000000D+00 1.804075045D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.508085273D+05-  
 9.670719282D+01  
 BeSO4(c) CrI,cubic. Gurvich,1996a pt1 p383 pt2 p308.  
 1 tpi96 BE 1.00S 1.000 4.00 0.00 0.00 3 105.07578 -  
 120000.000  
 912.000 1400.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12970.000  
 0.000000000D+00 0.000000000D+00 1.804075045D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.505559568D+05-  
 9.643025148D+01  
 BeSO4(L) Liquid. Gurvich,1996a pt1 p383 pt2 p308.  
 1 tpi96 BE 1.00S 1.000 4.00 0.00 0.00 4 105.07578 -  
 120000.000  
 1400.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12970.000  
 0.000000000D+00 0.000000000D+00 1.804075045D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.498343268D+05-  
 9.591480146D+01  
 Be2C(cr) Barin,1989. Barin,1973.  
 1 bar 89 BE 2.00C 1.00 0.00 0.00 0.00 1 30.03506 -  
 116984.640  
 298.150 2400.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 0.000000000D+00 0.000000000D+00 4.437364559D+00 2.569424296D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.550714068D+04-  
 2.408584259D+01  
 Be2C(L) Barin,1989. Barin,1973.  
 1 bar 89 BE 2.00C 1.00 0.00 0.00 0.00 2 30.03506 -  
 116984.640  
 2400.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 0.000000000D+00 0.000000000D+00 1.107076665D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.496946374D+04-  
 6.577435374D+01  
 Be3N2(a) CrII,cubic. Gurvich,1996a pt1 p384 pt2 p309.  
 2 tpi96 BE 3.00N 2.00 0.00 0.00 0.00 1 55.05003 -  
 58800.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7124.000  
 6.443341310D+05-9.239880870D+03 4.211333200D+01-4.513325350D-02  
 3.232975930D-05  
 0.000000000D+00 0.000000000D+00 -2.674920290D+04-  
 2.511544265D+02  
 500.000 1673.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7124.000  
 -2.278465381D+05 4.432191420D+02 1.376274664D+00 3.225384830D-02-  
 2.704770612D-05  
 8.116575420D-09-6.682374890D-14 -7.562743780D+04-  
 1.197625563D+01  
 Be3N2(b) CrI,hexagonal. Gurvich,1996a pt1 p384 pt2 p309.  
 1 tpi96 BE 3.00N 2.00 0.00 0.00 0.00 2 55.05003 -  
 58800.000  
 1673.000 2473.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7124.000

0.000000000D+00 0.000000000D+00 1.743939210D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -7.850942150D+04-  
 1.016302777D+02  
 Be3N2(L) Liquid. Gurvich,1996a pt1 p384 pt2 p309.  
 1 tpris96 BE 3.00N 2.00 0.00 0.00 0.00 3 55.05003 -  
 588000.000  
 2473.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7124.000  
 0.000000000D+00 0.000000000D+00 2.008536883D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -7.182303830D+04-  
 1.169540588D+02  
 Br2(cr) Rhombic. Gurvich,1989 pt2 p314. Chase,1998 p471 (6/82).  
 1 g 8/01 BR 2.00 0.00 0.00 0.00 0.00 1 159.80800  
 0.000  
 200.000 265.9007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 24520.000  
 -5.550117110D+06 1.610953162D+05-1.913542203D+03 1.201711944D+01-  
 4.170621540D-02  
 7.615296370D-05-5.694588430D-08 -6.565415920D+05  
 9.135571000D+03  
 Br2(L) Liq.Ref-Elm.Gurvich,1989 pt2 p314.Chase,1998  
 p471(6/82).  
 2 g 8/01 BR 2.00 0.00 0.00 0.00 0.00 2 159.80800  
 0.000  
 265.900 332.5037 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 24520.000  
 5.661619720D+06-6.002788720D+04 3.963572800D+01 2.194289283D+00-  
 1.209616100D-02  
 2.608732123D-05-2.065978604D-08 3.167204530D+05-  
 6.832596160D+02  
 332.503 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 24520.000  
 0.000000000D+00 0.000000000D+00 9.056697268D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.699852754D+03-  
 3.329354185D+01  
 C(gr) Graphite. Ref-Elm. TRC(4/83) vc,uc,tc1000-1002.  
 3 n 4/83 C 1.00 0.00 0.00 0.00 0.00 1 12.01070  
 0.000  
 200.000 600.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 1053.500  
 1.132856760D+05-1.980421677D+03 1.365384188D+01-4.636096440D-02  
 1.021333011D-04  
 -1.082893179D-07 4.472258860D-11 8.943859760D+03-  
 7.295824740D+01  
 600.000 2000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 1053.500  
 3.356004410D+05-2.596528368D+03 6.948841910D+00-3.484836090D-03  
 1.844192445D-06  
 -5.055205960D-10 5.750639010D-14 1.398412456D+04-  
 4.477183040D+01  
 2000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 1053.500  
 2.023105106D+05-1.138235908D+03 3.700279500D+00-1.833807727D-04  
 6.343683250D-08  
 -7.068589480D-12 3.335435980D-16 5.848134850D+03-  
 2.350925275D+01  
 Ca(a) Alpha. Ref-Elm. Alcock,1993.

2 srd 93 CA 1.00 0.00 0.00 0.00 0.00 1 40.07800  
 0.000  
 200.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 5782.945  
 2.209214594D+04 0.000000000D+00 -2.387095323D+00 4.674833430D-02-  
 1.481690580D-04  
 1.686114356D-07 0.000000000D+00 -3.160902334D+02  
 9.998907900D+00  
 298.150 716.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 5782.945  
 8.959632100D+03 0.000000000D+00 2.440591375D+00 1.722094077D-03  
 4.744000490D-07  
 0.000000000D+00 0.000000000D+00 -7.783440840D+02-  
 9.273708050D+00  
 Ca(b) Beta. Ref-Elm. Alcock,1993.  
 1 srd 93 CA 1.00 0.00 0.00 0.00 0.00 2 40.07800  
 0.000  
 716.000 1115.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 5782.945  
 0.000000000D+00 0.000000000D+00 5.701117685D+00 -5.810564904D-03  
 4.022125176D-06  
 0.000000000D+00 0.000000000D+00 -1.516788311D+03-  
 2.607588230D+01  
 Ca(L) Liquid. Ref-Elm. Alcock,1993.  
 1 srd 93 CA 1.00 0.00 0.00 0.00 0.00 3 40.07800  
 0.000  
 1115.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 5782.945  
 0.000000000D+00 0.000000000D+00 4.570323447D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -9.822680100D+02-  
 2.119893317D+01  
 CaBr2(cr) Rhombic Gurvich,1996a pt1 p473 pt2 p368.  
 1 tpris96 CA 1.00BR 2.00 0.00 0.00 0.00 1 199.88600 -  
 683800.000  
 298.150 1015.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17000.490  
 -2.826384237D+04 0.000000000D+00 8.872561342D+00 1.586623866D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -8.505243950D+04-  
 3.554898721D+01  
 CaBr2(L) Liquid Gurvich,1996a pt1 p473 pt2 p368.  
 1 tpris96 CA 1.00BR 2.00 0.00 0.00 0.00 2 199.88600 -  
 683800.000  
 1015.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17000.490  
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -8.390932270D+04-  
 5.231487518D+01  
 CaCO3(cr) Hexagonal Gurvich,1996a pt1 p483 pt2 p376.  
 2 tpris96 CA 1.00C 1.000 3.00 0.00 0.00 1 100.08690 -  
 1206600.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14480.499  
 -1.329862425D+07 2.500517168D+05 -1.907177167D+03 7.616666270D+00-  
 1.655870860D-02  
 1.879382277D-05 -8.720713270D-09 -1.271058215D+06  
 9.957497560D+03  
 500.000 1603.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14480.499

-2.583555736D+05 0.000000000D+00 1.197256363D+01 3.263812299D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.497009803D+05-  
 5.961133653D+01  
 CaCO<sub>3</sub>(L) Liquid Gurvich,1996a pt1 p483 pt2 p376.  
 1 tpris96 CA 1.00C 1.000 3.00 0.00 0.00 3 100.08690 -  
 1206600.000  
 1603.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14480.499  
 0.000000000D+00 0.000000000D+00 1.924346714D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.526719277D+05-  
 1.052847193D+02  
 CaCl<sub>2</sub>(cr) Rhombic. Gurvich,1996a pt1 p467 pt2 p365.  
 2 tpris96 CA 1.00CL 2.00 0.00 0.00 0.00 1 110.98340 -  
 795800.000  
 100.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15300.460  
 6.000206010D+03-4.466152170D+02 8.199988600D+00 2.374917562D-02-  
 1.002337283D-04  
 1.782027609D-07-1.141389034D-10 -9.606057780D+04-  
 3.912159570D+01  
 500.000 1048.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15300.460  
 -3.018818908D+04 0.000000000D+00 8.644766799D+00 1.529735366D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -9.845880750D+04-  
 3.684266549D+01  
 CaCl<sub>2</sub>(L) Liquid. Gurvich,1996a pt1 p467 pt2 p365.  
 1 tpris96 CA 1.00CL 2.00 0.00 0.00 0.00 2 110.98340 -  
 795800.000  
 1048.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15300.460  
 2.661491778D+06 0.000000000D+00 1.078355790D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -9.391818610D+04-  
 4.566953897D+01  
 CaF<sub>2</sub>(a) CrII,cubic.Gurvich,1996a pt1 p461 pt2 p361.  
 3 tpris96 CA 1.00F 2.00 0.00 0.00 0.00 1 78.07481 -  
 1228000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11640.000  
 -9.875281260D+05 1.337426670D+04-6.261903110D+01 1.617894422D-01-  
 1.271795719D-04  
 0.000000000D+00 0.000000000D+00 -2.146045473D+05  
 3.617287210D+02  
 500.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11640.000  
 -6.961842180D+06 4.692065010D+04-1.157708151D+02 1.655025287D-01-  
 1.108459197D-04  
 3.213053720D-08 0.000000000D+00 -4.101016540D+05  
 7.419533450D+02  
 1000.000 1424.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11640.000  
 1.438558077D+09 7.852955040D+05-1.342916213D+04 2.192783112D+01-  
 1.383442475D-02  
 3.122877330D-06 0.000000000D+00 2.168972069D+06  
 7.823794920D+04  
 CaF<sub>2</sub>(b) CrI,cubic.Gurvich,1996a pt1 p461 pt2 p361.  
 1 tpris96 CA 1.00F 2.00 0.00 0.00 0.00 2 78.07481 -  
 1228000.000

1424.000 1691.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11640.000  
 1.535768139D+08 0.000000000D+00-1.699774473D+02 7.733123360D-02  
 3.585714680D-07  
 0.000000000D+00 0.000000000D+00 1.356828739D+05  
 1.185723820D+03  
 CaF2 (L) Liquid.Gurvich,1996a pt1 p461 pt2 p361.  
 1 tpris96 CA 1.00F 2.00 0.00 0.00 0.00 3 78.07481 -  
 1228000.000  
 1691.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11640.000  
 0.000000000D+00 0.000000000D+00 1.190689530D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.479539740D+05-  
 5.967665213D+01  
 CaH2 (a) CrII,rhombic Gurvich,1996a pt1 p449 pt2 p354.  
 1 tpris96 CA 1.00H 2.00 0.00 0.00 0.00 1 42.09388 -  
 177000.000  
 298.150 1053.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6770.474  
 0.000000000D+00 0.000000000D+00 3.599731073D+00 4.465566822D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.255982511D+04-  
 1.686197756D+01  
 CaH2 (b) CrI,cubic Gurvich,1996a pt1 p449 pt2 p354.  
 1 tpris96 CA 1.00H 2.00 0.00 0.00 0.00 2 42.09388 -  
 177000.000  
 1053.000 1273.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6770.474  
 0.000000000D+00 0.000000000D+00 8.298745206D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.422633646D+04-  
 4.409678633D+01  
 CaH2 (L) Liquid Gurvich,1996a pt1 p449 pt2 p354.  
 1 tpris96 CA 1.00H 2.00 0.00 0.00 0.00 3 42.09388 -  
 177000.000  
 1273.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6770.474  
 0.000000000D+00 0.000000000D+00 9.020375224D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.249899474D+04-  
 4.717727797D+01  
 CaI2 (cr) Hexagonal Gurvich,1996a pt1 p476 pt2 p371.  
 2 tpris96 CA 1.00I 2.00 0.00 0.00 0.00 1 293.88694 -  
 536400.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17970.499  
 -1.811328452D+06 3.127451814D+04-2.136599007D+02 8.328705880D-01-  
 1.721725832D-03  
 1.878967812D-06-8.440013400D-10 -2.101977983D+05  
 1.142802698D+03  
 500.000 1056.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17970.499  
 -6.638996165D+03 0.000000000D+00 8.652825001D+00 2.284560365D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.721736780D+04-  
 3.254333551D+01  
 CaI2 (L) Liquid Gurvich,1996a pt1 p476 pt2 p371.  
 1 tpris96 CA 1.00I 2.00 0.00 0.00 0.00 3 293.88694 -  
 536400.000

1056.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17970.499  
 0.000000000D+00 0.000000000D+00 1.238798197D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.485425310D+04-  
 5.137218163D+01  
 CaO(cr) Cubic Gurrvich,1996a pt1 p442 pt2 p348.  
 2 tpis96 CA 1.000 1.00 0.00 0.00 0.00 1 56.07740 -  
 634920.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6750.499  
 -4.775526940D+06 9.037711420D+04-6.944320810D+02 2.802477174D+00-  
 6.129403220D-03  
 6.982167800D-06-3.247543840D-09 -4.829411430D+05  
 3.619046320D+03  
 500.000 3172.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6750.499  
 -1.459376440D+05 0.000000000D+00 7.174205094D+00-1.959947129D-03  
 1.291116374D-06  
 -2.077091735D-10 0.000000000D+00 -7.891525080D+04-  
 3.658562837D+01  
 CaO(L) Liquid Gurrvich,1996a pt1 p442 pt2 p348.  
 1 tpis96 CA 1.000 1.00 0.00 0.00 0.00 3 56.07740 -  
 634920.000  
 3172.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6750.499  
 0.000000000D+00 0.000000000D+00 1.010282025D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -7.991857230D+04-  
 5.908720013D+01  
 Ca(OH)2(cr) Hexagonal Gurrvich,1996a pt1 p454 pt2 p357.  
 2 tpis96 CA 1.000 2.00H 2.00 0.00 0.00 1 74.09268 -  
 985900.000  
 100.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14160.490  
 -2.058838935D+05 6.172554490D+03-7.499750990D+01 5.012182400D-01-  
 1.423348682D-03  
 1.994984415D-06-1.095038067D-09 -1.452026205D+05  
 3.552445040D+02  
 500.000 1023.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14160.490  
 -1.245413139D+05 0.000000000D+00 1.073593032D+01 3.982435525D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.223707243D+05-  
 5.302395390D+01  
 Ca(OH)2(L) Liquid Gurrvich,1996a pt1 p454 pt2 p357.  
 1 tpis96 CA 1.000 2.00H 2.00 0.00 0.00 3 74.09268 -  
 985900.000  
 1023.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14160.490  
 0.000000000D+00 0.000000000D+00 1.840156546D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.245191822D+05-  
 9.860760364D+01  
 CaS(cr) Cubic Gurrvich,1996a pt1 p478 pt2 p373.  
 2 tpis96 CA 1.00S 1.00 0.00 0.00 0.00 1 72.14400 -  
 475000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9010.499  
 4.758681130D+06-8.840702110D+04 6.675047510D+02-2.576855161D+00  
 5.527281760D-03

-6.202901900D-06 2.852128154D-09 3.401344700D+05-  
 3.494344760D+03  
 500.000 2800.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9010.499  
 -1.428827435D+04 0.000000000D+00 5.567375588D+00 1.006673875D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.888163400D+04-  
 2.530572359D+01  
 CaS(L) Liquid Gurvich,1996a pt1 p478 pt2 p373.  
 1 tpis96 CA 1.00S 1.00 0.00 0.00 0.00 3 72.14400 -  
 475000.000  
 2800.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9010.499  
 0.000000000D+00 0.000000000D+00 8.058201866D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.348566620D+04-  
 3.924995523D+01  
 CaSO4(II) Rhombic Gurvich,1996a pt1 p481 pt2 p375.  
 2 tpis96 CA 1.00S 1.000 4.00 0.00 0.00 1 136.14160 -  
 1434000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17200.499  
 -1.361977472D+07 2.584929291D+05-1.984800641D+03 7.969448170D+00-  
 1.736805219D-02  
 1.974370111D-05-9.168768090D-09 -1.334631522D+06  
 1.035139350D+04  
 500.000 1473.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17200.499  
 -2.983940124D+05 0.000000000D+00 1.359671225D+01 5.857230312D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.777846313D+05-  
 6.802481458D+01  
 CaSO4(I) Cubic Gurvich,1996a pt1 p481 pt2 p375.  
 1 tpis96 CA 1.00S 1.000 4.00 0.00 0.00 3 136.14160 -  
 1434000.000  
 1473.000 1733.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17200.499  
 0.000000000D+00 0.000000000D+00 1.984482549D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.798298668D+05-  
 1.045004358D+02  
 CaSO4(L) Liquid Gurvich,1996a pt1 p481 pt2 p375.  
 1 tpis96 CA 1.00S 1.000 4.00 0.00 0.00 4 136.14160 -  
 1434000.000  
 1733.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17200.499  
 0.000000000D+00 0.000000000D+00 1.984482549D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.764622601D+05-  
 1.025572120D+02  
 Cd(cr) Crystal. Ref-Elm. Cox,1989 p223.  
 1 coda89 CD 1.00 0.00 0.00 0.00 0.00 1 112.41100 -  
 0.000  
 100.000 594.2587 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6247.000  
 1.375273221D+05-3.221590070D+03 3.121905502D+01-1.226136798D-01  
 2.838880568D-04  
 -3.286884020D-07 1.520469817D-10 1.302807037D+04-  
 1.551324136D+02  
 Cd(L) Liquid. Ref-Elm. Cox,1989 p223.



1 coda89 CD 1.00 0.00 0.00 0.00 0.00 2 112.41100  
0.000  
594.258 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6247.000  
0.000000000D+00 0.000000000D+00 3.596122922D+00 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -4.220394750D+02-  
1.323298164D+01

Co (a) Alpha. Ref-Elm. Chase,1998 pp943-6.  
2 j 9/67 CO 1.00 0.00 0.00 0.00 0.00 1 58.93320  
0.000  
200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
4771.000  
-8.651834510D+05 1.462135206D+04-9.971089110D+01 3.794338600D-01-  
7.800106350D-04  
8.553583960D-07-3.890151670D-10 -6.795963460D+04  
5.306550210D+02  
500.000 700.1007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
4771.000  
-9.877560740D+05 6.820602200D+03-1.521637485D+01 2.234541680D-02-  
9.019246600D-06  
0.000000000D+00 0.000000000D+00 -3.852839040D+04  
1.014399403D+02

Co (b) Beta. Ref-Elm. Below Lambda trans. Chase,1998 pp943-6.  
2 j 9/67 CO 1.00 0.00 0.00 0.00 0.00 2 58.93320  
0.000  
700.100 800.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
4771.000  
0.000000000D+00 0.000000000D+00 2.125113886D+00 2.218475342D-03  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -6.197709420D+02-  
8.944546990D+00  
800.000 1394.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
4771.000  
-1.576349295D+09 9.154318170D+06-2.197967504D+04 2.793356668D+01-  
1.980310380D-02  
7.425124740D-06-1.149433030D-09 -5.182198410D+07  
1.399846247D+05

Co (b) Beta. Ref-Elm. Above Lambda trans. Chase,1998 pp943-6.  
2 j 9/67 CO 1.00 0.00 0.00 0.00 0.00 3 58.93320  
0.000  
1394.000 1400.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
4771.000  
0.000000000D+00 0.000000000D+00 3.070872109D+02-2.155487195D-01  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -2.139292950D+05-  
1.913104819D+03  
1400.000 1768.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
4771.000  
1.648338062D+09-4.036220190D+06 3.722685700D+03-1.526326566D+00  
2.354674115D-04  
0.000000000D+00 0.000000000D+00 2.649010262D+07-  
2.751466647D+04

Co (L) Liquid. Ref-Elm. Chase,1998 pp943-6.  
1 j 9/67 CO 1.00 0.00 0.00 0.00 0.00 4 58.93320  
0.000  
1768.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
4771.000  
0.000000000D+00 0.000000000D+00 4.871122892D+00 0.000000000D+00  
0.000000000D+00

0.000000000D+00 0.000000000D+00 -1.761381676D+02-  
2.448402276D+01  
Cr(cr) Below lambda trans. Ref-Elm. Chase,1998 pp959-62.  
1 j 6/73 CR 1.00 0.00 0.00 0.00 0.00 1 51.99610  
0.000  
200.000 311.5007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
4057.000  
8.051084050D+05-1.339842819D+04 8.273507290D+01-2.075857041D-01  
2.008764131D-04  
0.000000000D+00 0.000000000D+00 6.182357950D+04-  
4.559971660D+02  
Cr(cr) Above lambda trans. Ref-Elm. Chase,1998 pp959-62.  
2 j 6/73 CR 1.00 0.00 0.00 0.00 0.00 2 51.99610  
0.000  
311.500 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
4057.000  
-2.534425357D+05 3.119404093D+03-1.358439770D+01 4.323570220D-02-  
5.624102820D-05  
3.652910710D-08-8.973298370D-12 -1.606559079D+04  
7.858043710D+01  
1000.000 2130.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
4057.000  
-3.005006418D+07 1.264410306D+05-2.139399408D+02 1.937684814D-01-  
9.423205780D-05  
2.445139082D-08-2.606793685D-12 -7.582388710D+05  
1.441907828D+03  
Cr(L) Liquid. Ref-Elm. Chase,1998 pp959-62.  
1 j 6/73 CR 1.00 0.00 0.00 0.00 0.00 3 51.99610  
0.000  
2130.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
4057.000  
0.000000000D+00 0.000000000D+00 4.730284767D+00 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 5.755633080D+02-  
2.453179007D+01  
CrN(cr) Chase,1998 p966.  
3 j12/73 CR 1.00N 1.00 0.00 0.00 0.00 1 66.00284 -  
117152.000  
200.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
7705.000  
0.000000000D+00 0.000000000D+00-1.314063090D+00 2.565693051D-02  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -1.483864491D+04  
4.372952650D+00  
298.150 400.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
7705.000  
1.223200207D+06 0.000000000D+00-2.407090178D+01 5.583146740D-02  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -5.292218790D+03  
1.319158541D+02  
400.000 2500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
7705.000  
-2.661907798D+05 1.615547039D+03 1.892576742D+00 4.987173370D-03-  
2.514705667D-06  
7.617792270D-10-9.124276740D-14 -2.496407842D+04-  
3.735659490D+00  
Cr2N(cr) JPCRD 1998 Mono.9 p971.  
3 j12/73 CR 2.00N 1.00 0.00 0.00 0.00 1 117.99894 -  
125520.000  
298.150 700.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
0.000

5.676714650D+06-6.561919460D+04 2.971622148D+02-6.132148300D-01  
 6.373067250D-04  
 -2.569754132D-07 0.000000000D+00 3.113488256D+05-  
 1.716694497D+03  
 700.000 1500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 8.246680410D+05-1.965549089D+03 5.659967790D+00 1.366241998D-02-  
 1.241835551D-05  
 6.313550760D-09-1.192405400D-12 -3.594772610D+03-  
 3.071970867D+01  
 1500.000 2500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 4.325258320D+09-1.355254539D+07 1.757503878D+04-1.205560629D+01  
 4.623646210D-03  
 -9.389890050D-07 7.891119490D-11 8.506076540D+07-  
 1.227417790D+05  
 Cr2O3 (I') Hexagonal. Gurvich, 1982 pt1 p18 pt2 p22.  
 1 tpris82 CR 2.000 3.00 0.00 0.00 0.00 1 151.99040 -  
 1140600.000  
 200.000 306.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15300.000  
 -2.112979833D+06 0.000000000D+00 2.207431906D+02-1.164973854D+00  
 1.853971249D-03  
 0.000000000D+00 0.000000000D+00 -1.746831159D+05-  
 9.949025210D+02  
 Cr2O3 (I) Hexagonal. Gurvich, 1982 pt1 p18 pt2 p22.  
 1 tpris82 CR 2.000 3.00 0.00 0.00 0.00 2 151.99040 -  
 1140600.000  
 306.000 310.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15300.000  
 0.000000000D+00 0.000000000D+00 6.705915562D+03-4.303760534D+01  
 6.919229155D-02  
 0.000000000D+00 0.000000000D+00 -8.349875160D+05-  
 2.844167579D+04  
 Cr2O3 (I) Hexagonal. Gurvich, 1982 pt1 p18 pt2 p22.  
 1 tpris82 CR 2.000 3.00 0.00 0.00 0.00 3 151.99040 -  
 1140600.000  
 310.000 335.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15300.000  
 0.000000000D+00 0.000000000D+00 2.443570337D+02-1.399445548D+00  
 2.113509996D-03  
 0.000000000D+00 0.000000000D+00 -1.665032895D+05-  
 1.059172219D+03  
 Cr2O3 (I) Hexagonal. Gurvich, 1982 pt1 p18 pt2 p22.  
 1 tpris82 CR 2.000 3.00 0.00 0.00 0.00 4 151.99040 -  
 1140600.000  
 335.000 2705.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15300.000  
 -3.415474875D+05 0.000000000D+00 1.616932327D+01-1.517828471D-03  
 1.014852348D-06  
 0.000000000D+00 0.000000000D+00 -1.430478214D+05-  
 8.374919535D+01  
 Cr2O3 (L) Liquid. Gurvich, 1982 pt1 p18 pt2 p22.  
 1 tpris82 CR 2.000 3.00 0.00 0.00 0.00 5 151.99040 -  
 1140600.000  
 2705.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15300.000  
 0.000000000D+00 0.000000000D+00 2.044618384D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.383139935D+05-  
 1.123603099D+02

Cs(cr) Crystal. Ref-Elm. Cox,1989 p263.

1 coda89 CS 1.00 0.00 0.00 0.00 0.00 1 132.90545  
0.000  
100.000 301.5907 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
7711.000  
6.519841350D+04-1.756639077D+03 1.999681093D+01-6.938328820D-02  
1.093682552D-04  
0.000000000D+00 0.000000000D+00 6.382890840D+03-  
9.338251570D+01

Cs(L) Liquid. Ref-Elm. Cox,1989 p263.

2 coda89 CS 1.00 0.00 0.00 0.00 0.00 2 132.90545  
0.000  
301.590 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
7711.000  
-4.218078030D+04-1.745861711D+01 5.702246950D+00-5.113948550D-03  
3.201752440D-06  
-1.767959558D-10 4.827862700D-14 -1.290810964D+03-  
2.031478114D+01  
1000.000 2000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
7711.000  
-7.255372990D+05 3.001930225D+03 1.782289032D-01 2.832281079D-04  
1.810515176D-07  
7.718855550D-10-8.889289510D-14 -1.920877274D+04  
1.635273378D+01

CsBO2(cr) Cubic. Gurvich,1982 pt1 p504 pt2 p525.

2 tpis82 CS 1.00B 1.000 2.00 0.00 0.00 1 175.71525 -  
962000.000  
200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
14368.000  
1.241529552D+07-2.256720327D+05 1.662515290D+03-6.320716230D+00  
1.337407484D-02  
-1.484168930D-05 6.761667750D-09 9.049643320D+05-  
8.739017110D+03  
500.000 1005.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
14368.000  
-1.344267330D+05 0.000000000D+00 1.014162565D+01 3.564309650D-03  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -1.193344436D+05-  
4.705131010D+01

CsBO2(L) Liquid. Gurvich,1982 pt1 p504 pt2 p525.

1 tpis82 CS 1.00B 1.000 2.00 0.00 0.00 2 175.71525 -  
962000.000  
1005.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
14368.000  
0.000000000D+00 0.000000000D+00 1.743939210D+01 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -1.214875849D+05-  
9.061903610D+01

CsBr(cr) Cubic. Gurvich,1982 pt1 p488 pt2 p511.

2 tpis82 CS 1.00BR 1.00 0.00 0.00 0.00 1 212.80945 -  
405600.000  
200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
13135.000  
8.214717410D+05-1.533809444D+04 1.213999610D+02-4.502622350D-01  
9.722874060D-04  
-1.094185412D-06 5.042592550D-10 1.851486523D+04-  
6.252270680D+02  
500.000 910.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
13135.000  
0.000000000D+00 0.000000000D+00 5.882254010D+00 1.622332026D-03  
0.000000000D+00

0.000000000D+00 0.000000000D+00 -5.060809300D+04-  
2.041491096D+01  
CsBr(L) Liquid. Gurvich,1982 pt1 p488 pt2 p511.  
1 tpris82 CS 1.00BR 1.00 0.00 0.00 0.00 2 212.80945 -  
405600.000  
910.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
13135.000  
0.000000000D+00 0.000000000D+00 9.020375224D+00 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -4.995364530D+04-  
3.720087044D+01  
CsCl(a) Cubic. Gurvich,1982 pt1 p485 pt2 p508.  
2 tpris82 CS 1.00CL 1.00 0.00 0.00 0.00 1 168.35815 -  
442310.000  
200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
12450.000  
-1.703772998D+06 3.247452440D+04-2.455466631D+02 1.009178034D+00-  
2.207551915D-03  
2.517334138D-06-1.172381667D-09 -2.005014179D+05  
1.287839193D+03  
500.000 743.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
12450.000  
-3.937950690D+04 0.000000000D+00 6.626999920D+00 4.235262420D-04  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -5.532407590D+04-  
2.593783387D+01  
CsCl(b) Cubic. Gurvich,1982 pt1 p485 pt2 p508.  
1 tpris82 CS 1.00CL 1.00 0.00 0.00 0.00 2 168.35815 -  
442310.000  
743.000 919.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
12450.000  
0.000000000D+00 0.000000000D+00 7.841712861D+00 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -5.570430740D+04-  
3.314329722D+01  
CsCl(L) Liquid. Gurvich,1982 pt1 p485 pt2 p508.  
1 tpris82 CS 1.00CL 1.00 0.00 0.00 0.00 3 168.35815 -  
442310.000  
919.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
12450.000  
0.000000000D+00 0.000000000D+00 8.839967719D+00 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -5.417056700D+04-  
3.728749769D+01  
CsF(cr) Cubic. Gurvich,1982 pt1 p481 pt2 p505.  
2 tpris82 CS 1.00F 1.00 0.00 0.00 0.00 1 151.90385 -  
557100.000  
200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
11760.000  
-2.453746682D+06 4.440981600D+04-3.216355300D+02 1.258524529D+00-  
2.661147803D-03  
2.959315715D-06-1.350383298D-09 -2.700040022D+05  
1.698453355D+03  
500.000 976.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
11760.000  
0.000000000D+00 0.000000000D+00 5.088206230D+00 3.543462080D-03  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -6.867788740D+04-  
1.886662026D+01  
CsF(L) Liquid. Gurvich,1982 pt1 p481 pt2 p505.

1 tps82 CS 1.00F 1.00 0.00 0.00 0.00 2 151.90385 -  
 557100.000  
 976.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11760.000  
 0.000000000D+00 0.000000000D+00 8.659560215D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.786592520D+04-  
 3.731740982D+01  
 CsH(cr) Cubic. Gurvich,1982 pt1 p476 pt2 p500.  
 1 tps82 CS 1.00H 1.00 0.00 0.00 0.00 1 133.91339 -  
 54040.000  
 298.150 801.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10500.000  
 -5.041788392D+04 0.000000000D+00 4.142517118D+00 4.385946977D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -8.098615840D+03-  
 1.641381626D+01  
 CsH(L) Liquid. Gurvich,1982 pt1 p476 pt2 p500.  
 1 tps82 CS 1.00H 1.00 0.00 0.00 0.00 2 133.91339 -  
 54040.000  
 801.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10500.000  
 0.000000000D+00 0.000000000D+00 6.735213500D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.901332940D+03-  
 2.794351109D+01  
 CsI(cr) Cubic. Gurvich,1982 pt1 p492 pt2 p514.  
 2 tps82 CS 1.00I 1.00 0.00 0.00 0.00 1 259.80992 -  
 348100.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13470.000  
 1.754014150D+06-3.232916500D+04 2.467159187D+02-9.287377130D-01  
 1.973235969D-03  
 -2.193580686D-06 1.003390730D-09 1.023639971D+05-  
 1.282961001D+03  
 500.000 905.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13470.000  
 -1.690343843D+04 0.000000000D+00 7.346625000D+00-4.804073480D-03  
 6.604565720D-06  
 0.000000000D+00 0.000000000D+00 -4.395851780D+04-  
 2.611726446D+01  
 CsI(L) Liquid. Gurvich,1982 pt1 p492 pt2 p514.  
 1 tps82 CS 1.00I 1.00 0.00 0.00 0.00 2 259.80992 -  
 348100.000  
 905.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13470.000  
 0.000000000D+00 0.000000000D+00 8.539288545D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.226975350D+04-  
 3.246075054D+01  
 CsNO2(I) Cubic. Gurvich,1982 pt1 p498 pt2 p519.  
 1 tps82 CS 1.00N 1.000 2.00 0.00 0.00 1 178.91099 -  
 379900.000  
 298.150 679.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 23420.000  
 0.000000000D+00 0.000000000D+00 1.151300558D+01-3.537430348D-03  
 5.931437932D-06  
 0.000000000D+00 0.000000000D+00 -4.901898420D+04-  
 4.387814029D+01  
 CsNO2(L) Liquid. Gurvich,1982 pt1 p498 pt2 p519.

1 tpis82 CS 1.00N 1.000 2.00 0.00 0.00 2 178.91099 -  
 379900.000  
 679.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 23420.000  
 0.000000000D+00 0.000000000D+00 1.274879698D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.874363630D+04-  
 5.104014160D+01  
 CsNO3(a) Hexagonal. Gurvich,1982 pt1 p500 pt2 p521.  
 1 tpis82 CS 1.00N 1.000 3.00 0.00 0.00 1 194.91039 -  
 505000.000  
 200.000 427.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 20050.000  
 -3.246405120D+06 5.377946540D+04-3.399293910D+02 1.103526542D+00-  
 1.665374892D-03  
 1.005891643D-06 0.000000000D+00 -3.130119262D+05  
 1.853516509D+03  
 CsNO3(b) Cubic. Gurvich,1982 pt1 p500 pt2 p521.  
 1 tpis82 CS 1.00N 1.000 3.00 0.00 0.00 2 194.91039 -  
 505000.000  
 427.000 682.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 20050.000  
 -8.675315803D+05 0.000000000D+00 2.211459244D+01-4.596061584D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.970758310D+04-  
 1.102656798D+02  
 CsNO3(L) Cubic. Gurvich,1982 pt1 p500 pt2 p521.  
 1 tpis82 CS 1.00N 1.000 3.00 0.00 0.00 3 194.91039 -  
 505000.000  
 682.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 20050.000  
 0.000000000D+00 0.000000000D+00 1.804075045D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.506630270D+04-  
 8.345202339D+01  
 CsOH(b) Beta. Gurvich,1997.  
 2 g 8/97 CS 1.00O 1.00H 1.00 0.00 0.00 1 149.91279 -  
 416200.000  
 100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14103.000  
 -1.070491244D+06 2.726790967D+04-2.447999195D+02 9.717566950D-01-  
 1.304183626D-03  
 0.000000000D+00 0.000000000D+00 -1.676915176D+05  
 1.260979156D+03  
 298.150 498.2007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14103.000  
 2.988510447D+05 0.000000000D+00-5.599488124D+00 4.758933479D-02-  
 3.982976748D-05  
 0.000000000D+00 0.000000000D+00 -4.914854260D+04  
 3.370083195D+01  
 CsOH(c) Gamma. Gurvich,1997.  
 1 g 8/97 CS 1.00O 1.00H 1.00 0.00 0.00 3 149.91279 -  
 416200.000  
 498.200 615.5007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14103.000  
 0.000000000D+00 0.000000000D+00 8.743750383D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.198053970D+04-  
 3.591737929D+01  
 CsOH(L) Liquid. Gurvich,1997.

1 g 8/97 CS 1.000 1.00H 1.00 0.00 0.00 4 149.91279 -  
 416200.000  
 615.500 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14103.000  
 0.000000000D+00 0.000000000D+00 1.022309192D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.195536080D+04-  
 4.389810453D+01  
 CsO2 (a) Tetragonal. Gurvich,1982 pt1 p472 pt2 p494.  
 1 tpis82 CS 1.000 2.00 0.00 0.00 0.00 1 164.90425 -  
 286100.000  
 298.150 403.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18000.000  
 0.000000000D+00 0.000000000D+00 6.423469330D+00 1.032375931D-02  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.678373920D+04-  
 2.259778952D+01  
 CsO2 (c) Cubic. Gurvich,1982 pt1 p472 pt2 p494.  
 1 tpis82 CS 1.000 2.00 0.00 0.00 0.00 2 164.90425 -  
 286100.000  
 403.000 723.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18000.000  
 0.000000000D+00 0.000000000D+00 1.058390693D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.762205990D+04-  
 4.339551574D+01  
 CsO2 (L) Liquid. Gurvich,1982 pt1 p472 pt2 p494.  
 1 tpis82 CS 1.000 2.00 0.00 0.00 0.00 3 164.90425 -  
 286100.000  
 723.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18000.000  
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.645253810D+04-  
 4.983623140D+01  
 Cs2CO3 (cr) Gurvich,1982 pt1 p502 pt2 p523.  
 2 tpis82 CS 2.00C 1.000 3.00 0.00 0.00 1 325.81980 -  
 1134900.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 25727.000  
 -2.861109977D+06 6.041289230D+04-5.002404530D+02 2.198717904D+00-  
 5.002265900D-03  
 5.885981300D-06-2.807201102D-09 -4.049923380D+05  
 2.581625553D+03  
 500.000 1066.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 25727.000  
 -2.194678436D+05 0.000000000D+00 1.478581229D+01 8.646042770D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.420250493D+05-  
 6.346394980D+01  
 Cs2CO3 (L) Liquid. Gurvich,1982 pt1 502 pt2 p523.  
 1 tpis82 CS 2.00C 1.000 3.00 0.00 0.00 2 325.81980 -  
 1134900.000  
 1066.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 25727.000  
 0.000000000D+00 0.000000000D+00 2.465569228D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.436995486D+05-  
 1.194626528D+02  
 Cs2O (cr) Hexagonal. Gurvich,1982 pt1 p472 pt2 p495.



2 tpis82 CS 2.000 1.00 0.00 0.00 0.00 1 281.81030 -  
 346400.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17680.000  
 -5.627068090D+05 9.379197410D+03-5.661406600D+01 2.388479040D-01-  
 4.761089540D-04  
 5.101511920D-07-2.256975084D-10 -8.742010290D+04  
 3.144128417D+02  
 500.000 768.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17680.000  
 0.000000000D+00 0.000000000D+00 7.940814720D+00 4.024410190D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.420852680D+04-  
 2.877552024D+01  
 Cs2O(L) Liquid. Gurvich,1982 pt1 p472 pt2 p495.  
 1 tpis82 CS 2.000 1.00 0.00 0.00 0.00 2 281.81030 -  
 346400.000  
 768.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17680.000  
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.375456510D+04-  
 4.970156357D+01  
 Cs2O2(cr) Rhombic Gurvich,1982 pt1 p475 pt2 p498.  
 1 tpis82 CS 2.000 2.00 0.00 0.00 0.00 1 297.80970 -  
 440000.000  
 298.150 867.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 21300.000  
 0.000000000D+00 0.000000000D+00 1.003895599D+01 4.651506824D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.611939360D+04-  
 3.693586892D+01  
 Cs2O2(L) Liquid. Gurvich,1982 pt1 p475 pt2 p498.  
 1 tpis82 CS 2.000 2.00 0.00 0.00 0.00 2 297.80970 -  
 440000.000  
 867.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 21300.000  
 0.000000000D+00 0.000000000D+00 1.611640373D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.699432080D+04-  
 7.096530706D+01  
 Cs2SO4(a) Rhombohedral. Gurvich,1982 pt1 p496 pt2 p517.  
 2 tpis82 CS 2.00S 1.000 4.00 0.00 0.00 1 361.87450 -  
 1442900.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 27740.000  
 -9.607719290D+06 1.823999086D+05-1.398882747D+03 5.671901780D+00-  
 1.240281336D-02  
 1.414114808D-05-6.571017390D-09 -9.952928170D+05  
 7.301725680D+03  
 500.000 920.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 27740.000  
 -2.673923999D+05 0.000000000D+00 1.731761674D+01 9.163180750D-03-  
 1.678705593D-05  
 2.444634119D-08 0.000000000D+00 -1.799058942D+05-  
 7.688396220D+01  
 Cs2SO4(b) Gurvich,1982 pt1 p496 pt2 p517.  
 1 tpis82 CS 2.00S 1.000 4.00 0.00 0.00 2 361.87450 -  
 1442900.000  
 920.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 27740.000

0.000000000D+00 0.000000000D+00-2.345297558D+01 5.324523033D-02  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.607408251D+05  
 1.601933430D+02  
 Cs2SO4(c) Hexagonal. Gurvich,1982 pt1 p496 pt2 p517.  
 1 tps82 CS 2.00S 1.000 4.00 0.00 0.00 3 361.87450 -  
 1442900.000  
 1000.000 1288.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 27740.000  
 0.000000000D+00 0.000000000D+00 1.021611616D+01 1.412157782D-02  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.748480906D+05-  
 3.326085070D+01  
 Cs2SO4(L) Liquid. Gurvich,1982 pt1 p496 pt2 p517.  
 1 tps82 CS 2.00S 1.000 4.00 0.00 0.00 4 361.87450 -  
 1442900.000  
 1288.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 27740.000  
 0.000000000D+00 0.000000000D+00 2.489623562D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.778210954D+05-  
 1.169167420D+02  
 Cu(cr) Cubic. Ref-Elm.Cox,1989 p226.  
 1 coda89 CU 1.00 0.00 0.00 0.00 0.00 1 63.54600  
 0.000  
 200.000 1358.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 5004.000  
 -2.455775109D+04 1.648069205D+02 2.080947143D+00 2.639078305D-03-  
 2.714101362D-06  
 1.402864982D-09-9.724321640D-14 -1.737850969D+03-  
 8.133166800D+00  
 Cu(L) Liquid. Ref-Elm.Cox,1989 p226.  
 1 coda89 CU 1.00 0.00 0.00 0.00 0.00 2 63.54600  
 0.000  
 1358.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 5004.000  
 0.000000000D+00 0.000000000D+00 3.944910764D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.111013775D+02-  
 1.836065775D+01  
 CuBr(a) Alpha. Pankratz,1984 p177.  
 1 g10/00 CU 1.00BR 1.00 0.00 0.00 0.00 1 143.45000 -  
 105604.160  
 298.150 657.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 9.282973940D+07-1.403844530D+06 8.783223470D+03-2.905323712D+01  
 5.373393350D-02  
 -5.266133060D-05 2.137926033D-08 6.589039380D+06-  
 4.752115490D+04  
 CuBr(b) Beta. Pankratz,1984 p177.  
 1 g10/00 CU 1.00BR 1.00 0.00 0.00 0.00 2 143.45000 -  
 105604.160  
 657.000 741.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 2.030134717D+04 0.000000000D+00 8.680899310D+00 1.192698187D-04  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.494845171D+04-  
 3.784920540D+01  
 CuBr(c) Gamma. Pankratz,1984 p177.  
 1 g10/00 CU 1.00BR 1.00 0.00 0.00 0.00 3 143.45000 -  
 105604.160

741.000 759.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 0.000000000D+00 0.000000000D+00 6.996549990D+00-2.480878428D-06  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.343768009D+04-  
 2.630094995D+01  
 CuBr(L) Liquid. Pankratz,1984 p177.  
 1 g10/00 CU 1.00BR 1.00 0.00 0.00 0.00 4 143.45000 -  
 105604.160  
 759.000 1500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 5.249558100D+06-2.757081290D+04 7.103036660D+01-7.368389880D-02  
 4.263508020D-05  
 -1.219118967D-08 1.489531692D-12 1.442863364D+05-  
 4.366365590D+02  
 CuBr2(cr) Crystal. Pankratz,1984 p181.  
 1 g10/00 CU 1.00BR 2.00 0.00 0.00 0.00 1 223.35400 -  
 138490.400  
 298.150 800.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 -2.314796663D+04 0.000000000D+00 9.183704151D+00 6.239886656D-04  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.949996594D+04-  
 3.714221219D+01  
 CuCL(a) Alpha. Pankratz,1984 p182.  
 1 g10/00 CU 1.00CL 1.00 0.00 0.00 0.00 1 98.99870 -  
 155644.800  
 298.150 685.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 -3.658126050D+07 4.622460750D+05-2.297616527D+03 5.656465110D+00-  
 6.837763380D-03  
 3.261042890D-06 0.000000000D+00 -2.287516266D+06  
 1.303469843D+04  
 CuCL(b) Beta. Pankratz,1984 p182.  
 1 g10/00 CU 1.00CL 1.00 0.00 0.00 0.00 2 98.99870 -  
 155644.800  
 685.000 696.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 0.000000000D+00 0.000000000D+00 9.573589740D+00-1.820889604D-05  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.177033413D+04-  
 4.503412690D+01  
 CuCL(L) Liquid. Pankratz,1984 p182.  
 1 g10/00 CU 1.00CL 1.00 0.00 0.00 0.00 3 98.99870 -  
 155644.800  
 696.000 1700.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 2.136369978D+07-1.123842012D+05 2.576303311D+02-2.967521373D-01  
 1.937139129D-04  
 -6.602332990D-08 9.216872010D-12 6.263960470D+05-  
 1.640361694D+03  
 CuCL2(cr) Crystal. Pankratz,1984 p185.  
 1 g10/00 CU 1.00CL 2.00 0.00 0.00 0.00 1 134.45140 -  
 217986.400  
 298.150 675.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 -2.119456576D+04-7.996037250D+02 1.293400534D+01-6.531311580D-03  
 7.387791880D-06  
 -2.975231314D-09 0.000000000D+00 -2.535822405D+04-  
 6.185052500D+01  
 CuCL2(L) Liquid. Pankratz,1984 p185.

1 g10/00 CU 1.00CL 2.00 0.00 0.00 0.00 2 134.45140 -  
 217986.400  
 675.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 0.000000000D+00 0.000000000D+00 9.913368316D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.929700009D+04-  
 4.386870689D+01  
 CuF(cr) Crystal. Pankratz,1984 p186.  
 1 g10/00 CU 1.00F 1.00 0.00 0.00 0.00 1 82.54440 -  
 209200.000  
 298.150 1300.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 8.970191630D+04-8.507461080D+02 7.497889560D+00 2.741560003D-03-  
 2.987072214D-06  
 1.372974641D-09-2.449154828D-13 -2.234632002D+04-  
 3.796523780D+01  
 CuF2(cr) Crystal. Pankratz,1984 p188.  
 1 g10/00 CU 1.00F 2.00 0.00 0.00 0.00 1 101.54281 -  
 539819.680  
 298.150 1109.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 2.173703718D+04-4.937180300D+02 7.140314880D+00 9.517087050D-03-  
 7.459164380D-06  
 1.904472482D-09 4.473847180D-13 -6.452906470D+04-  
 3.535501070D+01  
 CuF2(L) Liquid. Pankratz,1984 p188.  
 1 g10/00 CU 1.00F 2.00 0.00 0.00 0.00 2 101.54281 -  
 539819.680  
 1109.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 0.000000000D+00 0.000000000D+00 1.207719998D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.351133500D+04-  
 5.654007188D+01  
 CuI(a) King,1973. Pankratz,1984 p190.  
 1 g11/00 CU 1.00I 1.00 0.00 0.00 0.00 1 190.45047 -  
 67780.800  
 200.000 642.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12179.624  
 3.341893600D+07-6.258598240D+05 4.752824990D+03-1.866377479D+01  
 4.013741700D-02  
 -4.477073620D-05 2.026229192D-08 2.806623546D+06-  
 2.484310642D+04  
 CuI(b) Beta. Pankratz,1984 p190.  
 1 g11/00 CU 1.00I 1.00 0.00 0.00 0.00 2 190.45047 -  
 67780.800  
 642.000 680.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12179.624  
 0.000000000D+00 0.000000000D+00 1.665647164D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.582086031D+04-  
 8.975455543D+01  
 CuI(c) Gamma. Pankratz,1984 p190.  
 1 g11/00 CU 1.00I 1.00 0.00 0.00 0.00 3 190.45047 -  
 67780.800  
 680.000 868.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12179.624  
 0.000000000D+00 0.000000000D+00 8.252753319D+00 0.000000000D+00  
 0.000000000D+00

0.000000000D+00 0.000000000D+00 -9.787795700D+03-  
 3.447628919D+01  
 CuI(L) Liquid. Pankratz,1984 p190.  
 1 g11/00 CU 1.00I 1.00 0.00 0.00 0.00 4 190.45047 -  
 67780.800  
 868.000 1600.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12179.624  
 -1.011252768D+08 4.982205420D+05-1.002812164D+03 1.087833779D+00-  
 6.564648130D-04  
 2.096109501D-07-2.761239948D-11 -2.912510925D+06  
 6.575842050D+03  
 CuO(cr) Crystal. King,1973 p56.  
 2 g11/00 CU 1.00O 1.00 0.00 0.00 0.00 1 79.54540 -  
 155644.800  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7100.248  
 -4.516917320D+05 5.470078090D+03-2.199474390D+01 5.929815860D-02-  
 4.346152590D-05  
 0.000000000D+00 0.000000000D+00 -4.709485370D+04  
 1.305030297D+02  
 500.000 1400.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7100.248  
 1.200465628D+06-7.265787600D+03 2.078520457D+01-1.455522591D-02  
 1.267438982D-05  
 -1.010207859D-08 3.818025500D-12 2.099455971D+04-  
 1.272540351D+02  
 Cu(OH)2(cr) Crystal. King,1973 p62.  
 1 g10/00 CU 1.00O 2.00H 2.00 0.00 0.00 1 97.56068 -  
 443085.600  
 298.150 2000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 -2.719377798D+05 2.064524617D+03 2.639692948D+00 1.680803576D-02-  
 1.185312108D-05  
 4.128854220D-09-5.731701790D-13 -6.740281360D+04-  
 3.697949500D+00  
 CuS(cr) Crystal. Pankratz,1987 p99.  
 1 g10/00 CU 1.00S 1.00 0.00 0.00 0.00 1 95.61200 -  
 55647.200  
 298.150 717.8247 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 -2.883682516D+06 3.709375520D+04-1.908896435D+02 5.441914820D-01-  
 8.255987560D-04  
 6.585650750D-07-2.151268669D-10 -1.888895944D+05  
 1.072934856D+03  
 CuSO4(cr) Crystal. King,1973 p68.  
 2 g10/00 CU 1.00S 1.00O 4.00 0.00 0.00 1 159.60960 -  
 768600.800  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16869.888  
 -6.059594400D+06 1.149925970D+05-8.865821710D+02 3.621436210D+00-  
 7.953212370D-03  
 9.136099910D-06-4.293593660D-09 -6.103352510D+05  
 4.617693800D+03  
 500.000 1500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16869.888  
 4.517267510D+06-3.693547470D+04 1.240090231D+02-1.574474634D-01  
 1.231374136D-04  
 -4.209750670D-08 3.791447690D-12 1.020928632D+05-  
 7.502604750D+02  
 Cu2O(cr) Crystal. King,1973 p60.

2 g10/00 CU 2.000 1.00 0.00 0.00 0.00 1 143.09140 -  
 170707.200  
 200.000 600.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12598.024  
 6.943093940D+05-1.107206812D+04 7.007600820D+01-1.693010736D-01  
 2.296941394D-04  
 -1.193708373D-07 0.000000000D+00 2.971995795D+04-  
 3.800603570D+02  
 600.000 1516.7007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12598.024  
 4.899293250D+06-3.226767710D+04 9.242913240D+01-1.133053506D-01  
 8.886458460D-05  
 -3.911779590D-08 8.170753140D-12 1.562364374D+05-  
 5.668285450D+02  
 Cu2O(L) Liquid. King,1973 p60.  
 1 g10/00 CU 2.000 1.00 0.00 0.00 0.00 2 143.09140 -  
 170707.200  
 1516.700 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12598.024  
 0.000000000D+00 0.000000000D+00 1.199819496D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.922442298D+04-  
 5.674847630D+01  
 Cu2S(a) Alpha. Pankratz,1987 p101.  
 1 g10/00 CU 2.00S 1.00 0.00 0.00 0.00 1 159.15800 -  
 75730.400  
 298.150 376.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 1.219944245D+05 0.000000000D+00 2.442685885D+00 1.822933284D-02  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.023757104D+04-  
 4.696533160D+00  
 Cu2S(b) Beta. Pankratz,1987 p101.  
 1 g10/00 CU 2.00S 1.00 0.00 0.00 0.00 2 159.15800 -  
 75730.400  
 376.000 720.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 -1.211638496D+06 1.256233530D+04-3.683304810D+01 9.547244050D-02-  
 9.864227170D-05  
 3.946755750D-08 0.000000000D+00 -7.698051300D+04  
 2.352740334D+02  
 Cu2S(c) Gamma. Pankratz,1987 p101.  
 1 g10/00 CU 2.00S 1.00 0.00 0.00 0.00 3 159.15800 -  
 75730.400  
 720.000 1400.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 1.585983458D+07-9.420242290D+04 2.398981626D+02-2.943865388D-01  
 2.084368440D-04  
 -7.757369510D-08 1.184191791D-11 5.203074640D+05-  
 1.502163502D+03  
 Cu2S(L) Liquid. Pankratz,1987 p101.  
 1 g10/00 CU 2.00S 1.00 0.00 0.00 0.00 4 159.15800 -  
 75730.400  
 1400.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 0.000000000D+00 0.000000000D+00 1.078393315D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.075259326D+04-  
 4.551698813D+01  
 Fe(a) Alpha. Ref-Elm.Below Lambda trans. Chase,1998 p1221.

3 j 3/78 FE 1.00 0.00 0.00 0.00 0.00 1 55.84500  
 0.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 4507.000  
 1.350490931D+04-7.803806250D+02 9.440171470D+00-2.521767704D-02  
 5.350170510D-05  
 -5.099094730D-08 1.993862728D-11 2.416521408D+03-  
 4.749002850D+01  
 500.000 800.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 4507.000  
 3.543032740D+06-2.447150531D+04 6.561020930D+01-7.043929680D-02  
 3.181052870D-05  
 0.000000000D+00 0.000000000D+00 1.345059978D+05-  
 4.133788690D+02  
 800.000 1042.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 4507.000  
 2.661026334D+09-7.846827970D+06-7.289212280D+02 2.613888297D+01-  
 3.494742140D-02  
 1.763752622D-05-2.907723254D-09 5.234868470D+07-  
 1.529052200D+04  
 Fe(a) Alpha. Ref-Elm. Above Lambda trans. Chase, 1998 pp1221-5.  
 1 j 3/78 FE 1.00 0.00 0.00 0.00 0.00 2 55.84500  
 0.000  
 1042.000 1184.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 4507.000  
 2.481923052D+08 0.000000000D+00-5.594349090D+02 3.271704940D-01  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 6.467503430D+05  
 3.669168720D+03  
 Fe(c) Gamma. Ref-Elm. Chase, 1998 pp1221-5.  
 1 j 3/78 FE 1.00 0.00 0.00 0.00 0.00 3 55.84500  
 0.000  
 1184.000 1665.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 4507.000  
 1.442428576D+09-5.335491340D+06 8.052828000D+03-6.303089630D+00  
 2.677273007D-03  
 -5.750045530D-07 4.718611960D-11 3.264264250D+07-  
 5.508852170D+04  
 Fe(d) Delta. Ref-Elm. Chase, 1998 pp1221-5.  
 1 j 3/78 FE 1.00 0.00 0.00 0.00 0.00 4 55.84500  
 0.000  
 1665.000 1809.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 4507.000  
 -3.450190030D+08 0.000000000D+00 7.057501520D+02-5.442977890D-01  
 1.190040139D-04  
 0.000000000D+00 0.000000000D+00 -8.045725750D+05-  
 4.545180320D+03  
 Fe(L) Liquid. Ref-Elm. Chase, 1998 pp1221-5.  
 1 j 3/78 FE 1.00 0.00 0.00 0.00 0.00 5 55.84500  
 0.000  
 1809.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 4507.000  
 0.000000000D+00 0.000000000D+00 5.535383324D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.270608703D+03-  
 2.948115042D+01  
 Fe(CO)5(L) Liquid. Chase, 1998 p697.  
 1 j 3/78 FE 1.00C 5.000 5.00 0.00 0.00 1 195.89550 -  
 766090.400  
 253.100 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 52934.000

0.000000000D+00 0.000000000D+00 2.811771229D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.005222674D+05-  
 1.196624513D+02  
 FeCL2(cr) Crystal. Chase,1998 pp819-21.  
 1 j12/70 FE 1.00CL 2.00 0.00 0.00 0.00 1 126.75040 -  
 341833.000  
 200.000 950.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16273.000  
 -3.757527240D+04 5.932070220D+00 8.822760280D+00 3.742344220D-03-  
 4.622462850D-06  
 4.041497880D-09-1.447289303D-12 -4.403595790D+04-  
 3.721747350D+01  
 FeCL2(L) Liquid. Chase,1998 pp819-21.  
 1 j12/70 FE 1.00CL 2.00 0.00 0.00 0.00 2 126.75040 -  
 341833.000  
 950.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16273.000  
 0.000000000D+00 0.000000000D+00 1.228851730D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.110842530D+04-  
 5.319067642D+01  
 FeCL3(cr) Pankratz,1984 p228. Stuve,1980.  
 2 g12/00 FE 1.00CL 3.00 0.00 0.00 0.00 1 162.20310 -  
 399237.280  
 200.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19440.538  
 -4.411357940D+06 9.339652130D+04-7.909985950D+02 3.467913380D+00-  
 7.632263650D-03  
 7.316486370D-06-1.314023921D-09 -4.596567330D+05  
 4.056239320D+03  
 298.150 577.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19440.538  
 -1.373170458D+05 1.246888186D+03 4.499842520D+00 1.632234838D-02-  
 3.871665510D-06  
 0.000000000D+00 0.000000000D+00 -5.761466240D+04-  
 9.144353090D+00  
 FeCL3(L) Pankratz,1984 p228. Stuve,1980.  
 1 g12/00 FE 1.00CL 3.00 0.00 0.00 0.00 2 162.20310 -  
 399237.280  
 577.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19440.538  
 0.000000000D+00 0.000000000D+00 1.610293331D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.849183540D+04-  
 6.711333581D+01  
 Fe.9470(cr) Wustite. Pankratz,1983 p155.  
 1 g11/00 FE 0.950 1.00 0.00 0.00 0.00 1 68.88461 -  
 266269.760  
 298.150 1652.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 -1.179193966D+04 1.388393372D+02 2.999841854D+00 1.274527210D-02-  
 1.883886065D-05  
 1.274258345D-08-3.042206479D-12 -3.417350500D+04-  
 1.284759120D+01  
 Fe.9470(L) Wustite Liquid. Pankratz,1983 p155.  
 1 g11/00 FE 0.950 1.00 0.00 0.00 0.00 2 68.88461 -  
 266269.760  
 1652.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000



0.000000000D+00 0.000000000D+00 8.147077819D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.255080650D+04-  
 3.995344357D+01  
 FeOCL(cr) Stuve,1980.  
 2 g12/00 FE 1.000 1.00CL 1.00 0.00 0.00 1 107.29710 -  
 410994.320  
 200.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12940.275  
 7.211593840D+08-1.800235674D+07 1.865368524D+05-1.026861036D+03  
 3.167682830D+00  
 -5.191522260D-03 3.531434870D-06 7.557107690D+07-  
 9.148719350D+05  
 298.150 700.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12940.275  
 -2.937711808D+05 2.628264415D+03-4.552872200D+00 3.806463330D-02-  
 5.536092880D-05  
 4.502460810D-08-1.258510270D-11 -6.531943100D+04  
 3.377057910D+01  
 Fe(OH)2(cr) Crystal. Chase,1998 p1229.  
 2 j 6/66 FE 1.000 2.00H 2.00 0.00 0.00 1 89.85968 -  
 574045.000  
 298.150 800.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 4.240926040D+05-5.246013500D+03 3.564078140D+01-5.777285350D-02  
 8.334162550D-05  
 -5.353404280D-08 1.183994084D-11 -4.642385900D+04-  
 1.937387923D+02  
 800.000 1500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 8.260012740D+06-3.584848620D+04 6.631482130D+01-2.947893247D-02  
 4.572669670D-06  
 1.317544528D-09-2.977356578D-13 1.429652898D+05-  
 4.364616280D+02  
 Fe(OH)3(cr) Crystal. Chase,1998 p1231.  
 1 j 6/66 FE 1.000 3.00H 3.00 0.00 0.00 1 106.86702 -  
 832616.000  
 298.150 1500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 -7.418284690D+04 4.915361510D+01 6.351612700D+00 2.730299149D-02-  
 2.006100982D-05  
 7.511526410D-09-1.262038044D-12 -1.036132609D+05-  
 3.117351481D+01  
 FeS(a) Alpha. Pankratz,1987. Chase,1998 pp1241-3 9/77.  
 1 g11/00 FE 1.00S 1.00 0.00 0.00 0.00 1 87.91100 -  
 99621.040  
 200.000 411.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9414.000  
 6.562987140D+06-1.108882861D+05 7.200477640D+02-2.169002385D+00  
 3.009472055D-03  
 -1.385164934D-06 0.000000000D+00 4.996994470D+05-  
 3.905129920D+03  
 FeS(b) Beta. Pankratz,1987. Chase,1998 pp1241-3 9/77.  
 1 g11/00 FE 1.00S 1.00 0.00 0.00 0.00 2 87.91100 -  
 99621.040  
 411.000 598.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9414.000  
 0.000000000D+00 0.000000000D+00 8.730809152D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.445777846D+04-  
 4.227609187D+01

FeS(c)                      Gamma. Pankratz,1987. Chase,1998 pp1241-3 9/77.                      -  
 1 g11/00 FE    1.00S    1.00    0.00    0.00    0.00    3    87.91100  
 99621.040  
       598.000    1465.0007 -2.0 -1.0    0.0    1.0    2.0    3.0    4.0    0.0  
 9414.000  
 -4.651400530D+05 2.845200913D+03 3.227601660D+00 1.639542844D-03-  
 2.119596921D-06  
       2.366217205D-09-3.529138060D-13                      -3.030024550D+04-  
 3.662233560D+00

FeS(L)                      Liquid. Pankratz,1987. Chase,1998 pp1241-3 9/77.                      -  
 1 g11/00 FE    1.00S    1.00    0.00    0.00    0.00    4    87.91100  
 99621.040  
       1465.000    6000.0007 -2.0 -1.0    0.0    1.0    2.0    3.0    4.0    0.0  
 9414.000  
       0.000000000D+00 0.000000000D+00 7.548249987D+00 0.000000000D+00  
 0.000000000D+00  
       0.000000000D+00 0.000000000D+00                      -9.925935040D+03-  
 3.215631501D+01

FeSO4(cr)                      Chase,1998 p1240.                      -  
 2 j 6/66 FE    1.00S    1.000    4.00    0.00    0.00    1    151.90860  
 928848.000  
       200.000    700.0007 -2.0 -1.0    0.0    1.0    2.0    3.0    4.0    0.0  
 16769.472  
 -6.203392950D+05 8.502519150D+03-4.378024090D+01 1.731987422D-01-  
 2.431424518D-04  
       1.792173046D-07-5.528922570D-11                      -1.550636343D+05  
 2.467116078D+02  
       700.000    2000.0007 -2.0 -1.0    0.0    1.0    2.0    3.0    4.0    0.0  
 16769.472  
 -7.679585180D+06 3.308117000D+04-4.678167570D+01 6.781223220D-02-  
 3.741392130D-05  
       1.099952323D-08-1.320141816D-12                      -3.134827612D+05  
 3.336437670D+02

FeS2(cr)                      Pyrite. Chase,1998 p1246.                      -  
 2 j 9/77 FE    1.00S    2.00    0.00    0.00    0.00    1    119.97700  
 171544.000  
       200.000    600.0007 -2.0 -1.0    0.0    1.0    2.0    3.0    4.0    0.0  
 9641.000  
 -2.506864207D+05 3.294827830D+03-1.713873471D+01 8.733851000D-02-  
 1.306227449D-04  
       7.362001640D-08 0.000000000D+00                      -3.800873290D+04  
 9.277002410D+01  
       600.000    1400.0007 -2.0 -1.0    0.0    1.0    2.0    3.0    4.0    0.0  
 9641.000  
       9.114353860D+05-5.471736420D+03 2.097363178D+01-1.514620285D-02  
 1.275975810D-05  
 -4.881556790D-09 7.710203910D-13                      7.794979850D+03-  
 1.227198763D+02

Fe2O3(cr)                      Hematite below Curie pt. Pankratz,1983 p158.                      -  
 2 g 1/01 FE    2.000    3.00    0.00    0.00    0.00    1    159.68820  
 824248.000  
       298.150    600.0007 -2.0 -1.0    0.0    1.0    2.0    3.0    4.0    0.0  
 0.000  
 -2.713211885D+06 2.323047773D+04-6.765701770D+01 1.306052231D-01-  
 6.970688120D-05  
       0.000000000D+00 0.000000000D+00                      -2.256089397D+05  
 4.228072580D+02  
       600.000    960.0007 -2.0 -1.0    0.0    1.0    2.0    3.0    4.0    0.0  
 0.000  
       3.333492510D+08-1.859961832D+06 3.885138190D+03-3.562599480D+00  
 1.231055904D-03

0.000000000D+00 0.000000000D+00 1.058058870D+07-  
 2.555306055D+04  
 Fe2O3(cr) Hematite above Curie pt. Pankratz,1983 p158.  
 2 g 1/01 FE 2.000 3.00 0.00 0.00 0.00 2 159.68820 -  
 824248.000  
 960.000 1800.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 -2.844009066D+07 1.253786450D+05-2.119080355D+02 2.221481558D-01-  
 1.206765164D-04  
 3.480738050D-08-4.165297860D-12 -8.483926520D+05  
 1.433002161D+03  
 1800.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 0.000000000D+00 0.000000000D+00 1.711439880D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.041599645D+05-  
 8.780613745D+01  
 Fe2(SO4)3(cr) Chase,1998 p1249.  
 2 j 6/66 FE 2.00S 3.000 12.00 0.00 0.00 1 399.88080 -  
 2582992.400  
 298.150 700.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 -3.987499800D+06 4.471584410D+04-1.871627045D+02 5.203843270D-01-  
 5.255167310D-04  
 2.053709591D-07 0.000000000D+00 -5.418976280D+05  
 1.097303717D+03  
 700.000 2000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 -1.749475174D+07 7.308320780D+04-9.392951360D+01 1.468051405D-01-  
 7.963099160D-05  
 2.311696556D-08-2.739014918D-12 -7.607146510D+05  
 6.865330290D+02  
 Fe3O4(cr) Magnetite. Pankratz,1983 p160. Westrum,1969.  
 3 g 1/01 FE 3.000 4.00 0.00 0.00 0.00 1 231.53260 -  
 1118383.200  
 200.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 24762.073  
 -5.182671230D+07 1.293463453D+06-1.341121962D+04 7.401842440D+01-  
 2.285725885D-01  
 3.752884300D-04-2.559338368D-07 -5.570751240D+06  
 6.575689710D+04  
 298.150 800.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 24762.073  
 -4.407671380D+06 5.351760270D+04-2.613667759D+02 7.431931490D-01-  
 9.767843990D-04  
 5.858865440D-07-8.780843180D-11 -4.018075450D+05  
 1.478276107D+03  
 800.000 850.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 24762.073  
 0.000000000D+00 0.000000000D+00-1.070116148D+02 1.738436706D-01  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -9.231022600D+04  
 6.169265720D+02  
 Fe3O4(cr) Magnetite above Curie Pt. Pankratz,1983 p160.  
 1 g 1/01 FE 3.000 4.00 0.00 0.00 0.00 2 231.53260 -  
 1118383.200  
 850.000 1870.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 24762.073  
 5.731691980D+07-1.816105186D+05 2.777813396D+02-1.849830315D-01  
 6.145641150D-05

-3.660350860D-09-1.383713617D-12 9.906992850D+05-  
1.868855147D+03  
Fe3O4(L) Liquid. Chase,1998 p1250 6/65.  
1 g 1/01 FE 3.000 4.00 0.00 0.00 0.00 3 231.53260 -  
1118383.200  
1870.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
24762.073  
0.000000000D+00 0.000000000D+00 2.415439996D+01 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -1.242541349D+05-  
1.109781572D+02  
Ga(cr) Rhombic. Ref-Elm. Gurvich,1996a pt1 p209 pt2 p169.  
1 tpis96 GA 1.00 0.00 0.00 0.00 0.00 1 69.72300  
0.000  
100.000 302.9207 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
5640.000  
1.665524651D+03-1.667535996D+02 3.860876380D+00-1.325442179D-03  
2.405494396D-06  
0.000000000D+00 0.000000000D+00 -1.577791876D+02-  
1.730178030D+01  
Ga(L) Liquid. Ref-Elm. Gurvich,1996a pt1 p209 pt2 p169.  
1 tpis96 GA 1.00 0.00 0.00 0.00 0.00 2 69.72300  
0.000  
302.920 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
5640.000  
2.846830421D+04 0.000000000D+00 3.135362156D+00-3.620177256D-05  
2.898547239D-08  
0.000000000D+00 0.000000000D+00 -1.716496723D+02-  
1.053717280D+01  
GaBr3(cr) Gurvich,1996a pt1 p242 pt2 p195.  
1 tpis96 GA 1.00BR 3.00 0.00 0.00 0.00 1 309.43500 -  
387000.000  
298.150 397.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
25000.000  
0.000000000D+00 0.000000000D+00 3.563409028D+00 2.798433101D-02  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -4.885137800D+04-  
6.997495329D+00  
GaBr3(L) Liquid. Gurvich,1996a pt1 p242 pt2 p195.  
1 tpis96 GA 1.00BR 3.00 0.00 0.00 0.00 2 309.43500 -  
387000.000  
397.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
25000.000  
0.000000000D+00 0.000000000D+00 1.544288238D+01 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -4.990695050D+04-  
6.330801668D+01  
GaCL3(cr) Triclinic. Gurvich,1996a pt1 p234 pt2 p188.  
1 tpis96 GA 1.00CL 3.00 0.00 0.00 0.00 1 176.08110 -  
527000.000  
298.150 351.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
20000.000  
0.000000000D+00 0.000000000D+00 2.725476306D+00 2.958442530D-02  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -6.551070110D+04-  
8.232857519D+00  
GaCL3(L) Liquid. Gurvich,1996a pt1 p234 pt2 p188.  
1 tpis96 GA 1.00CL 3.00 0.00 0.00 0.00 2 176.08110 -  
527000.000  
351.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
20000.000

0.000000000D+00 0.000000000D+00 1.310961199D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.599449360D+04-  
 5.489418092D+01  
 GaF3(cr) Hexagonal. Gurvich,1996a pt1 p226 pt2 p181.  
 1 tpris96 GA 1.00F 3.00 0.00 0.00 0.00 1 126.71821 -  
 1175000.000  
 298.150 2000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16700.000  
 0.000000000D+00 0.000000000D+00 9.361585950D+00 4.503211855D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.443105216D+05-  
 4.313509369D+01  
 GaI3(cr) Rhombic. Gurvich,1996a pt1 p249 pt2 p202.  
 1 tpris96 GA 1.00I 3.00 0.00 0.00 0.00 1 450.43641 -  
 218000.000  
 298.150 485.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 29000.000  
 0.000000000D+00 0.000000000D+00 6.461715723D+00 1.866676449D-02  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.897546082D+04-  
 1.772605384D+01  
 GaI3(L) Liquid. Gurvich,1996a pt1 p249 pt2 p202.  
 1 tpris96 GA 1.00I 3.00 0.00 0.00 0.00 2 450.43641 -  
 218000.000  
 485.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 29000.000  
 0.000000000D+00 0.000000000D+00 1.656140891D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.012686264D+04-  
 6.793170105D+01  
 Ga2O3(cr) Monoclinic. Gurvich,1996a pt1 p219 pt2 p176.  
 2 tpris96 GA 2.00O 3.00 0.00 0.00 0.00 1 187.44420 -  
 1091000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14550.000  
 -1.515635939D+07 2.787922412D+05-2.090093764D+03 8.236854680D+00-  
 1.771414598D-02  
 1.991804320D-05-9.167934200D-09 -1.391968792D+06  
 1.094221304D+04  
 500.000 2080.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14550.000  
 -2.857534599D+05 0.000000000D+00 1.375883846D+01 1.799504721D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.363570445D+05-  
 7.032081677D+01  
 Ga2O3(L) Liquid. Gurvich,1996a pt1 p219 pt2 p176.  
 1 tpris96 GA 2.00O 3.00 0.00 0.00 0.00 3 187.44420 -  
 1091000.000  
 2080.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14550.000  
 0.000000000D+00 0.000000000D+00 1.924346714D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.317078351D+05-  
 1.026657694D+02  
 Ge(cr) Cubic. Ref-Elm. Gurvich,1991 pt1 p308 pt2 p268.  
 2 tpris91 GE 1.00 0.00 0.00 0.00 0.00 1 72.61000  
 0.000  
 200.000 400.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 4636.360

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-2.396506145D+05 3.150572150D+03-1.333941357D+01 3.647997810D-02-
2.942104614D-05
0.000000000D+00 0.000000000D+00 -1.613882957D+04
7.939211600D+01
400.000 1211.4007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
4636.360
-1.888241797D+04 0.000000000D+00 2.898173070D+00 3.591659130D-04
0.000000000D+00
0.000000000D+00 0.000000000D+00 -9.433864080D+02-
1.298669726D+01
Ge(L) Liquid. Ref-Elm. Gurvich,1991 pt1 p308 pt2 p268.
1 tpris91 GE 1.00 0.00 0.00 0.00 0.00 2 72.61000
0.000
1211.400 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
4636.360
0.000000000D+00 0.000000000D+00 3.319498082D+00 0.000000000D+00
0.000000000D+00
0.000000000D+00 0.000000000D+00 3.278996640D+03-
1.185992953D+01
GeO2(II) Tetragonal Rutile, Gurvich,1991 pt1 p319 pt2 p275.
2 tpris91 GE 1.000 2.00 0.00 0.00 0.00 1 104.60880 -
580200.000
100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
7230.400
-1.362061010D+04 0.000000000D+00 1.390091028D+00 1.608814892D-02
0.000000000D+00
0.000000000D+00 0.000000000D+00 -7.095682740D+04-
8.017483700D+00
298.150 1308.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
7230.400
-2.763121338D+05 0.000000000D+00 9.404643208D+00-1.212218158D-03
1.110107511D-06
0.000000000D+00 0.000000000D+00 -7.346830070D+04-
5.004997052D+01
GeO2(I) Hexagonal alpha-quartz,Gurvich,1991 pt1 p319 pt2 p275.
1 tpris91 GE 1.000 2.00 0.00 0.00 0.00 3 104.60880 -
580200.000
1308.000 1388.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
7230.400
-1.535267863D+05 0.000000000D+00 7.481860025D+00 1.711465859D-03
0.000000000D+00
0.000000000D+00 0.000000000D+00 -6.994652970D+04-
3.711331960D+01
GeO2(L) Tetragonal liquid,Gurvich,1991 pt1 p319 pt2 p275.
1 tpris91 GE 1.000 2.00 0.00 0.00 0.00 4 104.60880 -
580200.000
1388.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
7230.400
0.000000000D+00 0.000000000D+00 9.441326067D+00 0.000000000D+00
0.000000000D+00
0.000000000D+00 0.000000000D+00 -6.883837870D+04-
4.738551165D+01
GeS(cr) Crystal(II). Gurvich,1991 pt1 p342 pt2 p296.
2 tpris91 GE 1.00S 1.00 0.00 0.00 0.00 1 104.67600 -
75348.000
100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
9657.400
-1.753890915D+04 0.000000000D+00 4.967049230D+00 3.277123440D-03
0.000000000D+00
0.000000000D+00 0.000000000D+00 -1.074763864D+04-
2.138030847D+01

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298.150 931.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9657.400  
 0.000000000D+00 0.000000000D+00 5.015328624D+00 2.453542061D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.066660187D+04-  
 2.131118286D+01  
 GeS(L) Liquid. Gurvich,1991 pt1 p342 pt2 p296.  
 1 tpis91 GE 1.00S 1.00 0.00 0.00 0.00 3 104.67600 -  
 75348.000  
 931.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9657.400  
 0.000000000D+00 0.000000000D+00 8.058201866D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -9.874413010D+03-  
 3.707715519D+01  
 GeS2(II) Crystal II. Gurvich,1991 pt1 p345 pt2 p298.  
 2 tpis91 GE 1.00S 2.00 0.00 0.00 0.00 1 136.74200 -  
 121500.000  
 100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12750.300  
 -2.239538329D+04 0.000000000D+00 5.754200020D+00 8.048243800D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.676145505D+04-  
 2.405323435D+01  
 298.150 1113.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12750.300  
 -3.367606750D+04 0.000000000D+00 7.889821529D+00 1.310961199D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.713657615D+04-  
 3.427587425D+01  
 GeS2(L) Liquid. Gurvich,1991 pt1 p345 pt2 p298.  
 1 tpis91 GE 1.00S 2.00 0.00 0.00 0.00 2 136.74200 -  
 121500.000  
 1113.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12750.300  
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.893876733D+04-  
 6.006450099D+01  
 HBO2(cr) Crystal,metaboric acid. Gurvich,1996a pt1 p41 pt2 p25.  
 1 tpis96 H 1.00B 1.000 2.00 0.00 0.00 1 43.81774 -  
 804600.000  
 298.150 509.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8460.200  
 0.000000000D+00 0.000000000D+00 4.478916978D+00 7.045514408D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -9.841912440D+04-  
 2.172637097D+01  
 HBO2(L) Liquid, metaboric acid. Gurvich,1996a pt1 p41 pt2 p25.  
 1 tpis96 H 1.00B 1.000 2.00 0.00 0.00 2 43.81774 -  
 804600.000  
 509.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8460.200  
 0.000000000D+00 0.000000000D+00 1.262852531D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -9.993471070D+04-  
 6.555326576D+01  
 H2O(cr) Ice. Gordon,1982.  
 1 g11/99 H 2.000 1.00 0.00 0.00 0.00 1 18.01528 -  
 299108.000

200.000 273.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 -4.026777480D+05 2.747887946D+03 5.738336630D+01-8.267915240D-01  
 4.413087980D-03  
 -1.054251164D-05 9.694495970D-09 -5.530314990D+04-  
 1.902572063D+02  
 H2O(L) Liquid, Cox,1989. Haar,1984. Keenan,1984. Stimson,1969.  
 2 g 8/01 H 2.000 1.00 0.00 0.00 0.00 1 18.01528 -  
 285830.000  
 273.150 373.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13278.000  
 1.326371304D+09-2.448295388D+07 1.879428776D+05-7.678995050D+02  
 1.761556813D+00  
 -2.151167128D-03 1.092570813D-06 1.101760476D+08-  
 9.779700970D+05  
 373.150 600.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13278.000  
 1.263631001D+09-1.680380249D+07 9.278234790D+04-2.722373950D+02  
 4.479243760D-01  
 -3.919397430D-04 1.425743266D-07 8.113176880D+07-  
 5.134418080D+05  
 H2SO4(L) Chase,1998 p1335.  
 1 j 9/77 H 2.00S 1.000 4.00 0.00 0.00 1 98.07948 -  
 813988.832  
 283.456 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 28226.000  
 -7.749933850D+04 1.040538662D+03 4.433804910D+00 3.648845480D-02-  
 1.743440132D-05  
 1.175631937D-08-3.170091690D-12 -1.068997367D+05-  
 1.353966639D+01  
 H3BO3(cr) Triclinic, orthoboric acid. Gurvich,1996a pt1 p48 pt2  
 p31.  
 1 tpi96 H 3.00B 1.000 3.00 0.00 0.00 1 61.83302 -  
 1094800.000  
 200.000 444.1007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13520.430  
 2.370260101D+06-3.116426553D+04 1.488140666D+02-2.710868145D-01  
 2.274904549D-04  
 0.000000000D+00 0.000000000D+00 1.950811769D+04-  
 8.575441950D+02  
 H3BO3(L) Liquid, orthoboric acid. Gurvich,1996a pt1 p48 pt2 p31.  
 1 tpi96 H 3.00B 1.000 3.00 0.00 0.00 2 61.83302 -  
 1094800.000  
 444.100 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13520.430  
 0.000000000D+00 0.000000000D+00 2.164890054D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.367426553D+05-  
 1.100910256D+02  
 H3PO4(cr) Crystal, Phosphoric acid. Chase,1998 p1345-7.  
 1 j12/71 H 3.00P 1.000 4.00 0.00 0.00 1 97.99518 -  
 1284488.000  
 200.000 315.5007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16980.000  
 2.733365471D+03 0.000000000D+00 1.109347863D+00 4.129024570D-02-  
 7.810353320D-06  
 0.000000000D+00 0.000000000D+00 -1.565753156D+05-  
 4.973473130D+00  
 H3PO4(L) Liquid, Phosphoric acid. Chase,1998 pp1345-7.  
 1 j12/71 H 3.00P 1.000 4.00 0.00 0.00 2 97.99518 -  
 1284488.000



315.500 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16980.000  
 4.109081110D+04-4.410343500D+02 8.547791650D+00 3.198261330D-02  
 5.167529530D-06  
 -3.256216600D-09 8.323148740D-13 -1.543175380D+05-  
 4.155398650D+01  
 Hg(cr) Tetragonal. Ref-Elm. Chase,1998 pp1373-4.  
 1 j12/61 HG 1.00 0.00 0.00 0.00 0.00 1 200.59000  
 0.000  
 100.000 234.2907 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9343.000  
 -3.184586610D+03 0.000000000D+00 3.464424870D+00-4.054864610D-03  
 1.766281131D-05  
 0.000000000D+00 0.000000000D+00 -1.282454336D+03-  
 1.132010161D+01  
 Hg(L) Liquid. Ref-Elm. Chase,1998 pp1373-4.  
 2 j12/61 HG 1.00 0.00 0.00 0.00 0.00 2 200.59000  
 0.000  
 234.290 600.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9343.000  
 1.058325418D+05-1.993826150D+03 1.880577074D+01-5.994680920D-02  
 1.228327030D-04  
 -1.293155349D-07 5.530734430D-11 7.916778390D+03-  
 9.064871100D+01  
 600.000 2000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9343.000  
 7.913840080D+05-3.956327060D+03 1.106465862D+01-8.153982650D-03  
 4.970504160D-06  
 -1.510428227D-09 1.872051162D-13 2.213772421D+04-  
 6.072461670D+01  
 HgBr2(cr) Chase,1998 p482 3/62. Pankratz,1984 p302.  
 1 g12/00 HG 1.00BR 2.00 0.00 0.00 0.00 1 360.39800 -  
 175309.600  
 298.150 514.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 -1.853158540D+06 2.003808568D+04-7.235875200D+01 1.451267662D-01-  
 9.240269430D-05  
 0.000000000D+00 0.000000000D+00 -1.255295454D+05  
 4.503769710D+02  
 HgBr2(L) Chase,1998 pp482-4 3/62.  
 1 g12/00 HG 1.00BR 2.00 0.00 0.00 0.00 2 360.39800 -  
 175309.600  
 514.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 0.000000000D+00 0.000000000D+00 1.227853475D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.320342036D+04-  
 4.684603799D+01  
 HgO(cr) Chase,1998 p1382.  
 2 j 6/62 HG 1.000 1.00 0.00 0.00 0.00 1 216.58940 -  
 90789.000  
 200.000 400.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9104.000  
 -1.062935837D+04 0.000000000D+00 3.345782860D+00 8.775373380D-03-  
 6.110417750D-06  
 0.000000000D+00 0.000000000D+00 -1.228859467D+04-  
 1.301600791D+01  
 400.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9104.000  
 1.582008299D+06-1.511620794D+04 6.157172990D+01-1.075963114D-01  
 1.203602940D-04

-7.037671400D-08 1.672097585D-11 6.599870400D+04-  
3.568628600D+02  
I2(cr) Rhombic. Ref-Elm. Gurvich,1989 pt1 p219 pt2 p315.  
1 tps89 I 2.00 0.00 0.00 0.00 0.00 1 253.80894  
0.000  
200.000 386.7507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
13196.000  
-3.901269140D+06 9.143202330D+04-8.900457500D+02 4.671270160D+00-  
1.357161837D-02  
2.073947355D-05-1.292905191D-08 -3.912632630D+05  
4.422603650D+03  
I2(L) Liquid. Ref-Elm. Gurvich,1989 pt1 p219 pt2 p315.  
1 tps89 I 2.00 0.00 0.00 0.00 0.00 2 253.80894  
0.000  
386.750 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
13196.000  
0.000000000D+00 0.000000000D+00 9.568212679D+00 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -1.204453805D+03-  
3.637326088D+01  
In(cr) Tetragonal. Ref-Elm. Gurvich,1996a pt1 255 pt2 p207.  
1 tps96 IN 1.00 0.00 0.00 0.00 0.00 1 114.81800  
0.000  
100.000 429.7847 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6610.080  
8.511616870D+03-3.450470040D+02 6.838785170D+00-1.818530679D-02  
4.122421420D-05  
-2.960008730D-08 0.000000000D+00 4.580589980D+02-  
2.928914154D+01  
In(L) Liquid. Ref-Elm. Gurvich,1996a pt1 255 pt2 p207.  
1 tps96 IN 1.00 0.00 0.00 0.00 0.00 2 114.81800  
0.000  
429.784 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6610.080  
5.092302493D+04 0.000000000D+00 3.302178962D+00-1.313366633D-04  
6.037637816D-08  
0.000000000D+00 0.000000000D+00 -4.511517590D+02-  
1.075015830D+01  
InBr(cr) Rhombic Gurvich,1996a pt1 p289 pt2 p232.  
1 tps96 IN 1.00BR 1.00 0.00 0.00 0.00 1 194.72200 -  
175000.000  
298.150 558.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
12200.000  
0.000000000D+00 0.000000000D+00 4.633586345D+00 4.628534935D-03  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -2.263476911D+04-  
1.455042037D+01  
InBr(L) Liquid Gurvich,1996a pt1 p289 pt2 p232  
1 tps96 IN 1.00BR 1.00 0.00 0.00 0.00 2 194.72200 -  
175000.000  
558.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
12200.000  
0.000000000D+00 0.000000000D+00 8.419016875D+00 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -2.222238473D+04-  
3.267500998D+01  
InBr3(cr) Gurvich,1996a pt1 p292 pt2 p235.  
1 tps96 IN 1.00BR 3.00 0.00 0.00 0.00 1 354.53000 -  
399000.000  
298.150 693.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
24500.000

0.000000000D+00 0.000000000D+00 1.154114915D+01 2.436824299D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.153769860D+04-  
 4.543581045D+01  
 InBr3(L) Liquid Gurchich,1996a pt1 p292 pt2 p235.  
 1 tpris96 IN 1.00BR 3.00 0.00 0.00 0.00 2 354.53000 -  
 399000.000  
 693.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 24500.000  
 0.000000000D+00 0.000000000D+00 1.623667540D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.107949370D+04-  
 6.994831229D+01  
 InCL(crII) Cubic Gurchich,1996a pt1 p280 pt2 p224.  
 1 tpris96 IN 1.00CL 1.00 0.00 0.00 0.00 1 150.27070 -  
 186500.000  
 298.150 387.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12400.000  
 0.000000000D+00 0.000000000D+00 5.163984408D+00 3.438567035D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.412314134D+04-  
 1.842034240D+01  
 InCL(crI) Rhombic Gurchich,1996a pt1 p280 pt2 p224.  
 1 tpris96 IN 1.00CL 1.00 0.00 0.00 0.00 2 150.27070 -  
 186500.000  
 387.000 484.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12400.000  
 0.000000000D+00 0.000000000D+00 6.735213500D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.441117035D+04-  
 2.629006183D+01  
 InCL(L) Liquid Gurchich,1996a pt1 p280 pt2 p224  
 1 tpris96 IN 1.00CL 1.00 0.00 0.00 0.00 3 150.27070 -  
 186500.000  
 484.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12400.000  
 0.000000000D+00 0.000000000D+00 8.058201866D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.248971016D+04-  
 2.917594080D+01  
 InCl3(cr) Monoclinic Gurchich,1996a pt1 p284 pt2 p227.  
 1 tpris96 IN 1.00CL 3.00 0.00 0.00 0.00 1 221.17610 -  
 530000.000  
 298.150 856.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 21000.000  
 0.000000000D+00 0.000000000D+00 1.093437857D+01 3.665158861D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.716697410D+04-  
 4.631386948D+01  
 InCl3(L) Liquid Gurchich,1996a pt1 p284 pt2 p227.  
 1 tpris96 IN 1.00CL 3.00 0.00 0.00 0.00 2 221.17610 -  
 530000.000  
 856.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 21000.000  
 0.000000000D+00 0.000000000D+00 1.407178535D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.526246230D+04-  
 6.056749656D+01  
 InF3(cr) Hexagonal Gurchich,1996a pt1 p274 pt2 p219.  
 1 tpris96 IN 1.00F 3.00 0.00 0.00 0.00 1 171.81321 -  
 1190000.000

298.150 1445.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19400.000  
 0.000000000D+00 0.000000000D+00 9.751747247D+00 4.404348542D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.462265291D+05-  
 4.364479594D+01  
 InF3(L) Liquid Gurvich,1996a pt1 p274 pt2 p219.  
 1 tpi96 IN 1.00F 3.00 0.00 0.00 0.00 2 171.81321 -  
 119000.000  
 1445.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19400.000  
 0.000000000D+00 0.000000000D+00 1.611640373D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.431278760D+05-  
 7.826197980D+01  
 InI(cr) Rhombic Gurvich,1996a pt1 p296 pt2 p240  
 1 tpi96 IN 1.00I 1.00 0.00 0.00 0.00 1 241.72247 -  
 102500.000  
 200.000 637.5007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13354.000  
 -9.253976720D+04 1.215133840D+03-1.038882859D-02 1.368794477D-02-  
 9.117964390D-06  
 1.596277777D-09 1.519819589D-12 -2.009017203D+04  
 1.436598613D+01  
 InI(L) Liquid Gurvich,1996a pt1 p296 pt2 p240  
 1 tpi96 IN 1.00I 1.00 0.00 0.00 0.00 2 241.72247 -  
 102500.000  
 637.500 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13354.000  
 0.000000000D+00 0.000000000D+00 8.443071209D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.331949891D+04-  
 3.168475714D+01  
 InI2(crII) Gurvich,1996a pt1 p299 pt2 p242.  
 1 tpi96 IN 1.00I 2.00 0.00 0.00 0.00 1 368.62694 -  
 176000.000  
 200.000 428.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19197.000  
 2.657410907D+04 0.000000000D+00 6.946210170D+00 6.889884760D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.345592914D+04-  
 2.056620828D+01  
 InI2(crI) Gurvich,1996a pt1 p299 pt2 p242.  
 1 tpi96 IN 1.00I 2.00 0.00 0.00 0.00 2 368.62694 -  
 176000.000  
 428.000 497.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19197.000  
 0.000000000D+00 0.000000000D+00 1.080520680D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.438345996D+04-  
 4.070950647D+01  
 InI2(L) Liquid Gurvich,1996a pt1 p299 pt2 p242.  
 1 tpi96 IN 1.00I 2.00 0.00 0.00 0.00 3 368.62694 -  
 176000.000  
 497.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19197.000  
 0.000000000D+00 0.000000000D+00 1.379516051D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.444424767D+04-  
 5.640525880D+01  
 InI3(cr) Monoclinic Gurvich,1996a pt1 p301 pt2 p244.

1 tpis96 IN 1.00I 3.00 0.00 0.00 0.00 1 495.53141 -  
 224000.000  
 296.000 480.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 29888.000  
 -1.888265213D+03 0.000000000D+00 1.096468704D+01 4.804492387D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.042985260D+04-  
 3.708283570D+01  
 InI3(L) Liquid Gurvich,1996a pt1 p301 pt2 p244.  
 1 tpis96 IN 1.00I 3.00 0.00 0.00 0.00 2 495.53141 -  
 224000.000  
 480.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 29888.000  
 0.000000000D+00 0.000000000D+00 1.652532741D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.031892811D+04-  
 6.447232654D+01  
 In2O3(cr) Cubic. Gurvich,1996a pt1 p267 pt2 p214.  
 2 tpis96 IN 2.00O 3.00 0.00 0.00 0.00 1 277.63420 -  
 923000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16600.000  
 -9.503707350D+06 1.770907496D+05-1.344503703D+03 5.391303710D+00-  
 1.171772659D-02  
 1.329195789D-05-6.163943540D-09 -9.104733670D+05  
 7.021339210D+03  
 500.000 2186.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16600.000  
 -2.719943809D+05 0.000000000D+00 1.461433085D+01 1.210173540D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.163340719D+05-  
 7.291389772D+01  
 In2O3(L) Liquid. Gurvich,1996a pt1 p267 pt2 p214.  
 1 tpis96 IN 2.00O 3.00 0.00 0.00 0.00 2 277.63420 -  
 923000.000  
 2186.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16600.000  
 0.000000000D+00 0.000000000D+00 1.924346714D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.108089477D+05-  
 1.000602622D+02  
 K(cr) Cubic. Ref-Elm. Cox,1989 p257.  
 1 coda89 K 1.00 0.00 0.00 0.00 0.00 1 39.09830  
 0.000  
 200.000 336.8607 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7088.000  
 -1.022031747D+05 0.000000000D+00 1.333752016D+01-5.580990750D-02  
 9.013009100D-05  
 0.000000000D+00 0.000000000D+00 -2.635062430D+03-  
 5.615376520D+01  
 K(L) Liquid. Ref-Elm. Cox,1989 p257.  
 1 coda89 K 1.00 0.00 0.00 0.00 0.00 2 39.09830  
 0.000  
 336.860 2200.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7088.000  
 -3.935722030D+03-4.547278110D+01 4.845244000D+00-3.083546588D-03  
 2.015548866D-06  
 -3.706172930D-11 5.032895480D-15 -8.075609680D+02-  
 1.836641748D+01  
 KALO2(II) Cubic Gurvich,1982 pt1 p416 pt2 p440.

2 tps82 K 1.00AL 1.000 2.00 0.00 0.00 1 98.07864 -  
 1130600.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13355.000  
 -4.112581400D+06 7.776836810D+04-5.971614160D+02 2.439288137D+00-  
 5.340052400D-03  
 6.098541950D-06-2.843205389D-09 -4.867714660D+05  
 3.112191530D+03  
 500.000 810.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13355.000  
 -1.565945988D+05 0.000000000D+00 9.609859180D+00 4.379778490D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.395641536D+05-  
 4.665045360D+01  
 KALO2 (I) Cubic Gurvich,1982 pt1 p416 pt2 p440.  
 1 tps82 K 1.00AL 1.000 2.00 0.00 0.00 2 98.07864 -  
 1130600.000  
 810.000 1986.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13355.000  
 8.202527870D+05 0.000000000D+00 7.962706161D+00 3.725414967D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.366535595D+05-  
 3.415265795D+01  
 KALO2 (L) Liquid. Gurvich,1982 pt1 p416 pt2 p440.  
 1 tps82 K 1.00AL 1.000 2.00 0.00 0.00 3 98.07864 -  
 1130600.000  
 1986.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13355.000  
 0.000000000D+00 0.000000000D+00 1.563531705D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.350952219D+05-  
 8.015693620D+01  
 KBO2 (cr) Hexagonal. Gurvich,1982 pt1 p414 pt2 p438.  
 2 tps82 K 1.00B 1.000 2.00 0.00 0.00 1 81.90810 -  
 983000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12114.000  
 -1.601790683D+07 2.997219831D+05-2.274223151D+03 9.014942220D+00-  
 1.951702277D-02  
 2.207384968D-05-1.021270864D-08 -1.468642542D+06  
 1.188723021D+04  
 500.000 1220.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12114.000  
 -2.328709444D+05 0.000000000D+00 9.862977090D+00 2.740064145D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.220704116D+05-  
 4.870043770D+01  
 KBO2 (L) Liquid. Gurvich,1982 pt1 p414 pt2 p438.  
 1 tps82 K 1.00B 1.000 2.00 0.00 0.00 2 81.90810 -  
 983000.000  
 1220.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12114.000  
 0.000000000D+00 0.000000000D+00 1.743939210D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.250545034D+05-  
 9.581938648D+01  
 KBr (cr) Cubic. Gurvich,1982 pt1 p394 pt2 p422.  
 2 tps82 K 1.00BR 1.00 0.00 0.00 0.00 1 119.00230 -  
 393450.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12210.000

5.931068110D+06-1.101548735D+05 8.346526100D+02-3.241060370D+00  
 6.976184850D-03  
 -7.847251340D-06 3.614707700D-09 4.475606580D+05-  
 4.361638690D+03  
 500.000 1007.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12210.000  
 3.145485337D+04 0.000000000D+00 5.199966220D+00 2.540382104D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.887872000D+04-  
 1.867132005D+01  
 KBr(L) Liquid. Gurvich,1982 pt1 p394 pt2 p422.  
 1 tpris82 K 1.00BR 1.00 0.00 0.00 0.00 2 119.00230 -  
 393450.000  
 1007.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12210.000  
 0.000000000D+00 0.000000000D+00 8.358881040D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.773361440D+04-  
 3.492371367D+01  
 KCN(II) Chase,1998 pp617-9.  
 2 j 3/66 K 1.00C 1.00N 1.00 0.00 0.00 1 65.11574 -  
 113470.000  
 168.300 400.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17343.000  
 4.789226660D+04-6.869399420D+02 1.189656301D+01-9.957932230D-03  
 9.253758250D-06  
 0.000000000D+00 0.000000000D+00 -1.275880363D+04-  
 5.189047360D+01  
 400.000 895.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17343.000  
 -8.550726080D+04 7.115109180D+02 5.642442360D+00 3.733592200D-03-  
 2.880609857D-06  
 8.848387980D-10 0.000000000D+00 -1.981154134D+04-  
 1.586461470D+01  
 KCN(L) Chase,1998 pp617-9.  
 1 j 3/66 K 1.00C 1.00N 1.00 0.00 0.00 2 65.11574 -  
 113470.000  
 895.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17343.000  
 0.000000000D+00 0.000000000D+00 9.057899984D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.522666331D+04-  
 3.545330543D+01  
 KCL(cr) Cubic. Gurvich,1982 pt1 p390 pt2 p419.  
 2 tpris82 K 1.00CL 1.00 0.00 0.00 0.00 1 74.55100 -  
 436490.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11370.000  
 1.179895024D+06-2.217824961D+04 1.730930630D+02-6.545434150D-01  
 1.415897824D-03  
 -1.598259237D-06 7.387534150D-10 4.560782730D+04-  
 8.991527150D+02  
 500.000 1044.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11370.000  
 2.888789664D+02 0.000000000D+00 5.287088550D+00 4.004092160D-03-  
 4.343449010D-06  
 2.753186288D-09 0.000000000D+00 -5.421785640D+04-  
 2.121648362D+01  
 KCL(L) Liquid. Gurvich,1982 pt1 p390 pt2 p419.  
 1 tpris82 K 1.00CL 1.00 0.00 0.00 0.00 2 74.55100 -  
 436490.000

1044.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11370.000  
 0.000000000D+00 0.000000000D+00 8.659560215D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.322113230D+04-  
 3.876839685D+01  
 KF(cr) Cubic. Gurvich,1982 pt1 p387 pt2 p416.  
 2 tpis82 K 1.00F 1.00 0.00 0.00 0.00 1 58.09670 -  
 56990.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10000.000  
 -2.920039956D+06 5.319604560D+04-3.910182930D+02 1.542524798D+00-  
 3.296460120D-03  
 3.692487030D-06-1.695192481D-09 -3.107774664D+05  
 2.055199175D+03  
 500.000 1131.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10000.000  
 -3.379466710D+04 0.000000000D+00 5.806099490D+00 1.562870483D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -7.045670350D+04-  
 2.573881635D+01  
 KF(L) Liquid. Gurvich,1982 pt1 p387 pt2 p416.  
 1 tpis82 K 1.00F 1.00 0.00 0.00 0.00 2 58.09670 -  
 56990.000  
 1131.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10000.000  
 0.000000000D+00 0.000000000D+00 8.455098376D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.905565270D+04-  
 3.960518579D+01  
 KH(cr) Cubic. Gurvich,1982 pt1 p381 pt2 p411.  
 1 tpis82 K 1.00H 1.00 0.00 0.00 0.00 1 40.10624 -  
 57820.000  
 298.150 892.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7800.000  
 -6.457385920D+04 0.000000000D+00 4.092965190D+00 3.996988400D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -8.568660280D+03-  
 1.870503989D+01  
 KH(L) Liquid. Gurvich,1982 pt1 p381 pt2 p411.  
 1 tpis82 K 1.00H 1.00 0.00 0.00 0.00 2 40.10624 -  
 57820.000  
 892.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7800.000  
 0.000000000D+00 0.000000000D+00 6.735213500D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.737318610D+03-  
 3.021766413D+01  
 K(HF2) (a) Alpha. Chase,1998 pp1104-6.  
 1 j 6/71 K 1.00H 1.00F 2.00 0.00 0.00 1 78.10305 -  
 931232.880  
 200.000 469.8507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15294.000  
 2.015718998D+03-3.533789190D+02 8.928247670D+00 2.814397451D-03  
 7.299809050D-06  
 0.000000000D+00 0.000000000D+00 -1.128323001D+05-  
 4.066701520D+01  
 K(HF2) (b) Beta. Chase,1998 pp1104-6.  
 1 j 6/71 K 1.00H 1.00F 2.00 0.00 0.00 2 78.10305 -  
 931232.880



469.850 511.9507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15294.000  
 0.000000000D+00 0.000000000D+00 1.205711461D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.145682138D+05-  
 5.416912090D+01  
 K(HF2) (L) Liquid. Chase,1998 pp1104-6.  
 1 j 6/71 K 1.00H 1.00F 2.00 0.00 0.00 3 78.10305 -  
 931232.880  
 511.950 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15294.000  
 0.000000000D+00 0.000000000D+00 1.258041665D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.140400401D+05-  
 5.587860571D+01  
 KI(cr) Cubic. Gurvich,1982 pt1 p398 pt2 p425.  
 2 tps82 K 1.00I 1.00 0.00 0.00 0.00 1 166.00277 -  
 329300.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12700.000  
 3.849118670D+06-7.198411950D+04 5.507582640D+02-2.141022674D+00  
 4.628312070D-03  
 -5.222322770D-06 2.411694600D-09 2.826852967D+05-  
 2.871024327D+03  
 500.000 954.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12700.000  
 2.770577458D+04 0.000000000D+00 5.235901210D+00 2.694044229D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.119339520D+04-  
 1.772462446D+01  
 KI(L) Liquid. Gurvich,1982 pt1 p398 pt2 p425.  
 1 tps82 K 1.00I 1.00 0.00 0.00 0.00 2 166.00277 -  
 329300.000  
 954.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12700.000  
 0.000000000D+00 0.000000000D+00 8.455098376D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.017867910D+04-  
 3.422733253D+01  
 KNO2 (II) Hexagonal. Gurvich,1982 pt1 p404 pt2 p430.  
 1 tps82 K 1.00N 1.000 2.00 0.00 0.00 1 85.10384 -  
 365900.000  
 200.000 314.7007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22940.000  
 -1.228297484D+07 0.000000000D+00 1.182559906D+03-6.076842320D+00  
 8.778424840D-03  
 0.000000000D+00 0.000000000D+00 -2.452424942D+05-  
 5.366905900D+03  
 KNO2 (I) Cubic. Gurvich,1982 pt1 p404 pt2 p430.  
 1 tps82 K 1.00N 1.000 2.00 0.00 0.00 2 85.10384 -  
 365900.000  
 314.700 711.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22940.000  
 0.000000000D+00 0.000000000D+00 9.827879214D+00 2.012866663D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.687774970D+04-  
 3.782318671D+01  
 KNO2 (L) Liquid. Gurvich,1982 pt1 p404 pt2 p430.  
 1 tps82 K 1.00N 1.000 2.00 0.00 0.00 3 85.10384 -  
 365900.000

711.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22940.000  
 0.000000000D+00 0.000000000D+00 1.226771030D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.609515960D+04-  
 4.958866367D+01  
 KNO3(a) Rhombic. Gurvich,1982 pt1 p407 pt2 p432.  
 1 tpi82 K 1.00N 1.00O 3.00 0.00 0.00 1 101.10324 -  
 494000.000  
 200.000 402.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18750.000  
 3.565624070D+06-6.291319380D+04 4.392599940D+02-1.436497824D+00  
 2.380417773D-03  
 -1.518208824D-06 0.000000000D+00 2.258505778D+05-  
 2.341795728D+03  
 KNO3(b) Hexagonal. Gurvich,1982 pt1 p407 pt2 p432.  
 1 tpi82 K 1.00N 1.00O 3.00 0.00 0.00 2 101.10324 -  
 494000.000  
 402.000 607.7007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18750.000  
 3.211975210D+06 0.000000000D+00-5.032659772D+01 1.462070525D-01-  
 8.159374395D-05  
 0.000000000D+00 0.000000000D+00 -3.934846620D+04  
 2.807123740D+02  
 KNO3(L) Liquid. Gurvich,1982 pt1 p407 pt2 p432.  
 1 tpi82 K 1.00N 1.00O 3.00 0.00 0.00 3 101.10324 -  
 494000.000  
 607.700 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18750.000  
 0.000000000D+00 0.000000000D+00 1.695830542D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.345106350D+04-  
 7.918784042D+01  
 KOH(a) Alpha,beta. Gurvich,1997 p1031.  
 1 g 8/97 K 1.00O 1.00H 1.00 0.00 0.00 1 56.10564 -  
 423400.000  
 100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12600.000  
 -4.380064620D+05 1.125472885D+04-1.023623342D+02 4.375630440D-01-  
 5.920346390D-04  
 0.000000000D+00 0.000000000D+00 -1.002155756D+05  
 5.241308280D+02  
 KOH(b) Beta. Gurvich,1997 p1031.  
 1 g 8/97 K 1.00O 1.00H 1.00 0.00 0.00 2 56.10564 -  
 423400.000  
 298.150 517.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12600.000  
 -2.814357070D+03 0.000000000D+00 6.478313214D+00 6.183767895D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.313882160D+04-  
 2.899826328D+01  
 KOH(c) Gamma. Gurvich,1997 p1031.  
 1 g 8/97 K 1.00O 1.00H 1.00 0.00 0.00 3 56.10564 -  
 423400.000  
 517.000 679.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12600.000  
 0.000000000D+00 0.000000000D+00 9.621733572D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.325857830D+04-  
 4.413346659D+01  
 KOH(L) Liquid. Gurvich,1997 p1031.

1 g 8/97 K 1.000 1.00H 1.00 0.00 0.00 4 56.10564 -  
 423400.000  
 679.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12600.000  
 0.000000000D+00 0.000000000D+00 1.046363526D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.288008340D+04-  
 4.822385687D+01  
 KO2 (b) Tetragonal. Gurvich, 1982 pt1 p375 pt2 p405.  
 1 tpis82 K 1.000 2.00 0.00 0.00 0.00 1 71.09710 -  
 283600.000  
 200.000 422.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16820.000  
 5.149174260D+06-7.614604350D+04 4.537181540D+02-1.295601160D+00  
 1.892822220D-03  
 -1.090404806D-06 0.000000000D+00 3.247518810D+05-  
 2.484666478D+03  
 KO2 (a) Cubic. Gurvich, 1982 pt1 p375 pt2 p405.  
 1 tpis82 K 1.000 2.00 0.00 0.00 0.00 2 71.09710 -  
 283600.000  
 422.000 808.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16820.000  
 0.000000000D+00 0.000000000D+00 1.058390693D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.734259730D+04-  
 4.545206851D+01  
 KO2 (L) Liquid. Gurvich, 1982 pt1 p375 pt2 p405.  
 1 tpis82 K 1.000 2.00 0.00 0.00 0.00 3 71.09710 -  
 283600.000  
 808.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16820.000  
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.603115500D+04-  
 5.204773022D+01  
 K2CO3 (a) Monoclinic. Gurvich, 1982 pt1 p410 pt2 p434.  
 1 tpis82 K 2.00C 1.000 3.00 0.00 0.00 1 138.20550 -  
 1151500.000  
 200.000 693.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22665.000  
 -3.632826430D+05 5.957567840D+03-3.080710797D+01 1.494558714D-01-  
 2.377158989D-04  
 2.231711601D-07-8.466662880D-11 -1.694136603D+05  
 1.763682121D+02  
 K2CO3 (b) Hexagonal. Gurvich, 1982 pt1 p410 pt2 p434.  
 1 tpis82 K 2.00C 1.000 3.00 0.00 0.00 2 138.20550 -  
 1151500.000  
 693.000 1173.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22665.000  
 0.000000000D+00 0.000000000D+00 1.310023080D+01 8.280944999D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.424065852D+05-  
 5.805609552D+01  
 K2CO3 (L) Liquid. Gurvich, 1982 pt1 p410 pt2 p434.  
 1 tpis82 K 2.00C 1.000 3.00 0.00 0.00 3 138.20550 -  
 1151500.000  
 1173.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22665.000  
 0.000000000D+00 0.000000000D+00 2.471582811D+01 0.000000000D+00  
 0.000000000D+00

0.000000000D+00 0.000000000D+00 -1.466663988D+05-  
1.273064200D+02

K20(c) III Cubic. Gurvich,1982 pt1 p377 pt2 p406.  
1 tpis82 K 2.000 1.00 0.00 0.00 0.00 1 94.19600 -  
361700.000  
298.150 590.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
13700.000  
0.000000000D+00 0.000000000D+00 6.140710637D+00 8.448122619D-03  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -4.570860710D+04-  
2.596002023D+01

K20(b) II Cubic. Gurvich,1982 pt1 p377 pt2 p406.  
1 tpis82 K 2.000 1.00 0.00 0.00 0.00 2 94.19600 -  
361700.000  
590.000 645.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
13700.000  
0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -4.762703040D+04-  
5.838924536D+01

K20(a) I Tetragonal. Gurvich,1982 pt1 p377 pt2 p406.  
1 tpis82 K 2.000 1.00 0.00 0.00 0.00 3 94.19600 -  
361700.000  
645.000 1013.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
13700.000  
0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -4.714594370D+04-  
5.764337454D+01

K20(L) Liquid. Gurvich,1982 pt1 p377 pt2 p406.  
1 tpis82 K 2.000 1.00 0.00 0.00 0.00 4 94.19600 -  
361700.000  
1013.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
13700.000  
0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -4.389860860D+04-  
5.443771306D+01

K202(cr) Rhombic. Gurvich,1982 pt1 p379 pt2 p409.  
1 tpis82 K 2.000 2.00 0.00 0.00 0.00 1 110.19540 -  
443000.000  
298.150 818.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
17000.000  
0.000000000D+00 0.000000000D+00 9.151230800D+00 6.015267286D-03  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -5.627614800D+04-  
3.986168914D+01

K202(L) Liquid. Gurvich,1982 pt1 p379 pt2 p409.  
1 tpis82 K 2.000 2.00 0.00 0.00 0.00 2 110.19540 -  
443000.000  
818.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
17000.000  
0.000000000D+00 0.000000000D+00 1.611640373D+01 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -5.749561030D+04-  
7.864151320D+01

K2S(cr) Below lambda. Chase,1998 pp1486-8.  
2 j 3/78 K 2.00S 1.00 0.00 0.00 0.00 1 110.26260 -  
376560.000  
298.150 600.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
0.000

4.724669150D+04-4.465995260D+02 9.600035840D+00 7.836273870D-04  
 1.295338974D-06  
 0.000000000D+00 0.000000000D+00 -4.549501380D+04-  
 4.238203950D+01  
 600.000 1050.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 1.237549376D+09-7.863379810D+06 1.968151557D+04-2.415909047D+01  
 1.451020806D-02  
 -3.388041040D-06 0.000000000D+00 4.392639800D+07-  
 1.251401185D+05  
 K2S(cr) Above lambda. Chase,1998 pp1486-8.  
 2 j 3/78 K 2.00S 1.00 0.00 0.00 0.00 2 110.26260 -  
 376560.000  
 1050.000 1100.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 0.000000000D+00 0.000000000D+00 1.564212060D+02-1.266383838D-01  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.311392922D+05-  
 9.279088390D+02  
 1100.000 1221.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 0.000000000D+00 0.000000000D+00 1.711898382D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.452307000D+04-  
 9.166848070D+01  
 K2S(L) Chase,1998 pp1486-8.  
 1 j 3/78 K 2.00S 1.00 0.00 0.00 0.00 3 110.26260 -  
 376560.000  
 1221.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 0.000000000D+00 0.000000000D+00 1.214261815D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.650451120D+04-  
 5.470849197D+01  
 K2SO4(II) Rhombic. Gurvich,1982 pt1 p402 pt2 p428.  
 2 tpi82 K 2.00S 1.000 4.00 0.00 0.00 1 174.26020 -  
 1437700.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 25435.000  
 7.718871240D+06-1.416712413D+05 1.060181562D+03-4.031007910D+00  
 8.614683760D-03  
 -9.611228510D-06 4.397898620D-09 4.640403120D+05-  
 5.555950140D+03  
 500.000 857.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 25435.000  
 -4.858415070D+04 0.000000000D+00 1.165680854D+01 1.576835485D-02  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.772539211D+05-  
 5.027549500D+01  
 K2SO4(I) Hexagonal. Gurvich,1982 pt1 p402 pt2 p428.  
 1 tpi82 K 2.00S 1.000 4.00 0.00 0.00 2 174.26020 -  
 1437700.000  
 857.000 1342.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 25435.000  
 1.683008379D+07 0.000000000D+00-3.453625048D+01 4.086410384D-02  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.262250083D+05  
 2.527928284D+02  
 K2SO4(L) Liquid. Gurvich,1982 pt1 p402 pt2 p428.  
 1 tpi82 K 2.00S 1.000 4.00 0.00 0.00 3 174.26020 -  
 1437700.000

1342.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 25435.000  
 0.000000000D+00 0.000000000D+00 2.405433393D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.762313671D+05-  
 1.157513010D+02  
 K2SiO3(cr) Rhombic. Gurvich,1982 pt1 p412 pt2 p436.  
 2 tps82 K 2.00SI 1.000 3.00 0.00 0.00 1 154.28030 -  
 1543000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 21860.000  
 2.855673428D+06-5.059971270D+04 3.647712840D+02-1.277216470D+00  
 2.614874944D-03  
 -2.812883261D-06 1.248415754D-09 4.217450990D+04-  
 1.927446205D+03  
 500.000 1249.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 21860.000  
 -1.541934726D+05 0.000000000D+00 1.400996506D+01 6.254878280D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.905514472D+05-  
 6.499565930D+01  
 K2SiO3(L) Liquid. Gurvich,1982 pt1 p412 pt2 p436.  
 1 tps82 K 2.00SI 1.000 3.00 0.00 0.00 2 154.28030 -  
 1543000.000  
 1249.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 21860.000  
 0.000000000D+00 0.000000000D+00 2.285161723D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.941869756D+05-  
 1.182498589D+02  
 K2Si2O5(a) III. Gurvich,1982 pt1 p413 pt2 p437.  
 1 tps82 K 2.00SI 2.000 5.00 0.00 0.00 1 214.36460 -  
 2505000.000  
 200.000 510.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 28820.000  
 -1.332332468D+07 2.509615155D+05-1.911732601D+03 7.658564980D+00-  
 1.652056677D-02  
 1.854450564D-05-8.489711240D-09 -1.432942804D+06  
 9.985815260D+03  
 K2Si2O5(b) II. Gurvich,1982 pt1 p413 pt2 p437.  
 1 tps82 K 2.00SI 2.000 5.00 0.00 0.00 2 214.36460 -  
 2505000.000  
 510.000 867.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 28820.000  
 -1.201153165D+05 0.000000000D+00 1.900352516D+01 1.092379467D-02  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.078422822D+05-  
 8.941094441D+01  
 K2Si2O5(c) I. Gurvich,1982 pt1 p413 pt2 p437.  
 1 tps82 K 2.00SI 2.000 5.00 0.00 0.00 3 214.36460 -  
 2505000.000  
 867.000 1318.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 28820.000  
 0.000000000D+00 0.000000000D+00 2.696791513D+01 5.313602365D-04  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.105104930D+05-  
 1.339782607D+02  
 K2Si2O5(L) Gurvich,1982 pt1 p413 pt2 p437.  
 1 tps82 K 2.00SI 2.000 5.00 0.00 0.00 4 214.36460 -  
 2505000.000

1318.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 28820.000  
 0.000000000D+00 0.000000000D+00 3.307470915D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.138641654D+05-  
 1.739362353D+02  
 K3ALF6(II) Tetragonal. Gurvich,1982 pt1 p418 pt2 p442.  
 1 tpris82 K 3.00AL 1.00F 6.00 0.00 0.00 1 258.26686 -  
 3347000.000  
 298.150 600.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 42600.000  
 0.000000000D+00 0.000000000D+00 1.838593014D+01 2.828982105D-02  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.092884330D+05-  
 7.891279947D+01  
 K3ALF6(I) Cubic. Gurvich,1982 pt1 p418 pt2 p442.  
 1 tpris82 K 3.00AL 1.00F 6.00 0.00 0.00 2 258.26686 -  
 3347000.000  
 600.000 1273.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 42600.000  
 0.000000000D+00 0.000000000D+00 2.893014742D+01 6.707551016D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.109483890D+05-  
 1.321111106D+02  
 K3ALF6(L) Liquid. Gurvich,1982 pt1 p418 pt2 p442.  
 1 tpris82 K 3.00AL 1.00F 6.00 0.00 0.00 3 258.26686 -  
 3347000.000  
 1273.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 42600.000  
 0.000000000D+00 0.000000000D+00 4.726676617D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.141107070D+05-  
 2.430801826D+02  
 Li(cr) Crystal. Ref-Elm. Gurvich,1982 pt1 p245 pt2 p286.  
 2 tpris82 LI 1.00 0.00 0.00 0.00 0.00 1 6.94100  
 0.000  
 200.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 4632.000  
 -9.860652350D+03 0.000000000D+00 2.304323850D+00 2.671663720D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -8.388536120D+02-  
 1.047881686D+01  
 298.150 453.6907 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 4632.000  
 7.238824960D+04 0.000000000D+00 1.570314469D-01 6.770404110D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.049497436D+02  
 9.961763140D-01  
 Li(L) Liquid. Ref-Elm. Gurvich,1982 pt1 p245 pt2 p286.  
 1 tpris82 LI 1.00 0.00 0.00 0.00 0.00 2 6.94100  
 0.000  
 453.690 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 4632.000  
 2.465569228D+04 0.000000000D+00 3.755723428D+00 -6.332303407D-04  
 3.160739478D-07  
 0.000000000D+00 0.000000000D+00 -7.299116690D+02-  
 1.701274654D+01  
 LiAlO2(cr) Chase,1998 pp126-8.  
 2 j12/79 LI 1.00AL 1.00O 2.00 0.00 0.00 1 65.92134 -  
 1188674.400

200.000 700.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9694.328  
 -2.403553110D+06 4.191135380D+04-2.947543676D+02 1.096024513D+00-  
 2.070932308D-03  
 1.989368601D-06-7.643124070D-10 -3.359272460D+05  
 1.562056779D+03  
 700.000 1973.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9694.328  
 -1.440922218D+06 5.833386140D+03-1.030268470D+00 1.461691077D-02-  
 7.831786240D-06  
 2.428705700D-09-3.067767899D-13 -1.811607791D+05  
 2.012864902D+01  
 LiAlO2 (L) Chase,1998 pp126-8.  
 1 j12/79 LI 1.00AL 1.000 2.00 0.00 0.00 2 65.92134 -  
 1188674.400  
 1973.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9694.328  
 0.000000000D+00 0.000000000D+00 1.509649997D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.416553963D+05-  
 8.099434263D+01  
 LiBO2 (cr) Monoclinic. Gurvich,1982 pt1 p298 pt2 p331.  
 2 tpis82 LI 1.00B 1.000 2.00 0.00 0.00 1 49.75080 -  
 1022900.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8880.000  
 -1.298972763D+02 2.476112547D+03-4.025475640D+01 2.755313951D-01-  
 7.202835830D-04  
 9.355885600D-07-4.776147920D-10 -1.326385762D+05  
 1.863684915D+02  
 500.000 1122.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8880.000  
 -1.501059611D+05 0.000000000D+00 7.094387770D+00 5.990864950D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.259108022D+05-  
 3.688511780D+01  
 LiBO2 (L) Liquid. Gurvich,1982 pt1 p298 pt2 p331.  
 1 tpis82 LI 1.00B 1.000 2.00 0.00 0.00 2 49.75080 -  
 1022900.000  
 1122.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8880.000  
 0.000000000D+00 0.000000000D+00 1.736722910D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.294550343D+05-  
 9.861468152D+01  
 LiBr (cr) Cubic. Gurvich,1982 pt1 p284 pt2 p317.  
 2 tpis82 LI 1.00BR 1.00 0.00 0.00 0.00 1 86.84500 -  
 351160.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10476.000  
 3.743262690D+06-7.020131930D+04 5.366833500D+02-2.085864954D+00  
 4.508762520D-03  
 -5.086004120D-06 2.348146084D-09 2.721051038D+05-  
 2.801510974D+03  
 500.000 823.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10476.000  
 1.459008908D+04 0.000000000D+00 4.895008630D+00 3.134322823D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.378446420D+04-  
 1.984092688D+01  
 LiBr (L) Liquid. Gurvich,1982 pt1 p284 pt2 p317.



1 tps82 LI 1.00BR 1.00 0.00 0.00 0.00 2 86.84500 -  
 351160.000  
 823.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10476.000  
 0.000000000D+00 0.000000000D+00 7.853740028D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.305174650D+04-  
 3.455318466D+01  
 LiCl(cr) Cubic. Gurvich,1982 pt1 p279 pt2 p313.  
 2 tps82 LI 1.00CL 1.00 0.00 0.00 0.00 1 42.39370 -  
 408540.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9300.000  
 -2.180497685D+06 3.971320780D+04-2.918258028D+02 1.160079971D+00-  
 2.482284097D-03  
 2.785692272D-06-1.280897066D-09 -2.302427379D+05  
 1.533139994D+03  
 500.000 883.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9300.000  
 -3.595609330D+04 0.000000000D+00 5.480770500D+00 2.332209108D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.099411730D+04-  
 2.499631307D+01  
 LiCl(L) Liquid. Gurvich,1982 pt1 p279 pt2 p313.  
 1 tps82 LI 1.00CL 1.00 0.00 0.00 0.00 2 42.39370 -  
 408540.000  
 883.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9300.000  
 0.000000000D+00 0.000000000D+00 7.601169522D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.954114490D+04-  
 3.460716245D+01  
 LiF(cr) Cubic. Gurvich,1982 pt1 p273 pt2 p309.  
 2 tps82 LI 1.00F 1.00 0.00 0.00 0.00 1 25.93940 -  
 618300.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6473.000  
 9.636751230D+05-1.777983613D+04 1.305502564D+02-4.624287950D-01  
 9.558363610D-04  
 -1.037162482D-06 4.637142460D-10 5.186488570D+03-  
 6.901111630D+02  
 500.000 1122.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6473.000  
 -7.420484740D+04 0.000000000D+00 5.359396170D+00 1.623955670D-03  
 2.090115068D-07  
 0.000000000D+00 0.000000000D+00 -7.628479220D+04-  
 2.715764184D+01  
 LiF(L) Liquid. Gurvich,1982 pt1 p273 pt2 p309.  
 1 tps82 LI 1.00F 1.00 0.00 0.00 0.00 2 25.93940 -  
 618300.000  
 1122.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6473.000  
 0.000000000D+00 0.000000000D+00 7.673332524D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -7.443734250D+04-  
 3.852218670D+01  
 LiH(cr) Cubic. Gurvich,1982 pt1 p263 pt2 p300.  
 1 tps82 LI 1.00H 1.00 0.00 0.00 0.00 1 7.94894 -  
 90650.000  
 200.000 965.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 3883.000

-7.983399540D+03-4.135167420D+02 3.842672410D+00 3.568427660D-03  
 3.560726720D-07  
 9.299007330D-10-5.466520940D-13 -9.882374510D+03-  
 2.193513588D+01  
 LiH(L) Liquid. Gurvich,1982 pt1 p263 pt2 p300.  
 1 tps82 LI 1.00H 1.00 0.00 0.00 0.00 2 7.94894 -  
 90650.000  
 965.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 3883.000  
 0.000000000D+00 0.000000000D+00 6.614941831D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.089088820D+04-  
 3.406734782D+01  
 LiI(cr) Cubic. Gurvich,1982 pt1 p287 pt2 p321.  
 2 tps82 LI 1.00I 1.00 0.00 0.00 0.00 1 133.84547 -  
 273200.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11360.000  
 -6.958662980D+04 4.035715450D+02 7.056546540D+00-1.824255625D-02  
 6.907245220D-05  
 -9.841303530D-08 5.297565590D-11 -3.712485890D+04-  
 2.568066591D+01  
 500.000 742.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11360.000  
 0.000000000D+00 0.000000000D+00 5.248298340D+00 2.986457552D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.455573620D+04-  
 2.036433073D+01  
 LiI(L) Liquid. Gurvich,1982 pt1 p287 pt2 p321.  
 1 tps82 LI 1.00I 1.00 0.00 0.00 0.00 2 133.84547 -  
 273200.000  
 742.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11360.000  
 0.000000000D+00 0.000000000D+00 7.601169522D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.371867140D+04-  
 3.132631144D+01  
 LiNO2(II) Crystal. Gurvich,1982 pt1 p292 pt2 p326.  
 1 tps82 LI 1.00N 1.000 2.00 0.00 0.00 1 52.94654 -  
 368300.000  
 298.150 369.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12100.000  
 0.000000000D+00 0.000000000D+00-1.026999787D+00 2.885846550D-02  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.527251980D+04  
 7.831186054D+00  
 LiNO2(I) Hexagonal. Gurvich,1982 pt1 p292 pt2 p326.  
 1 tps82 LI 1.00N 1.000 2.00 0.00 0.00 2 52.94654 -  
 368300.000  
 369.000 495.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12100.000  
 0.000000000D+00 0.000000000D+00 9.621733572D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.703274180D+04-  
 4.390844045D+01  
 LiNO2(L) Liquid. Gurvich,1982 pt1 p292 pt2 p326.  
 1 tps82 LI 1.00N 1.000 2.00 0.00 0.00 3 52.94654 -  
 368300.000  
 495.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12100.000

0.000000000D+00 0.000000000D+00 1.082445027D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.652158720D+04-  
 4.913541343D+01  
 LiNO3(cr) Hexagonal. Gurvich,1982 pt1 p294 pt2 p328.  
 1 tps82 LI 1.00N 1.00O 3.00 0.00 0.00 1 68.94594 -  
 482700.000  
 298.150 526.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12800.000  
 0.000000000D+00 0.000000000D+00 1.052906305D+01-9.448181552D-03  
 3.365959028D-05  
 0.000000000D+00 0.000000000D+00 -6.107180100D+04-  
 4.616118415D+01  
 LiNO3(L) Liquid. Gurvich,1982 pt1 p294 pt2 p328.  
 1 tps82 LI 1.00N 1.00O 3.00 0.00 0.00 2 68.94594 -  
 482700.000  
 525.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12800.000  
 0.000000000D+00 0.000000000D+00 1.792047878D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.162709200D+04-  
 8.706763908D+01  
 LiOH(cr) Tetragonal. Gurvich,1996b.  
 1 g 9/99 LI 1.00O 1.00H 1.00 0.00 0.00 1 23.94834 -  
 487500.000  
 200.000 746.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7414.000  
 -1.219596094D+06 2.088315832D+04-1.463475951D+02 5.611592820D-01-  
 1.084380003D-03  
 1.071790003D-06-4.218924790D-10 -1.553535026D+05  
 7.744131680D+02  
 LiOH(L) Liquid. Gurvich,1996b.  
 1 g 9/99 LI 1.00O 1.00H 1.00 0.00 0.00 2 23.94834 -  
 487500.000  
 746.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7414.000  
 0.000000000D+00 0.000000000D+00 1.049971676D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.050280710D+04-  
 5.407387960D+01  
 Li2CO3(cr) Monoclinic. Gurvich,1982 pt1 p297 pt2 p330.  
 2 tps82 LI 2.00C 1.00O 3.00 0.00 0.00 1 73.89090 -  
 1214100.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15180.000  
 1.989594337D+07-3.631706770D+05 2.691242782D+03-1.033109020D+01  
 2.201400812D-02  
 -2.454585112D-05 1.122641035D-08 1.495415902D+06-  
 1.413251128D+04  
 500.000 1005.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15180.000  
 -5.276502280D+04 0.000000000D+00 7.025051540D+00 1.809479379D-02  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.490977245D+05-  
 3.487871400D+01  
 Li2CO3(L) Liquid. Gurvich,1982 pt1 p297 pt2 p330.  
 1 tps82 LI 2.00C 1.00O 3.00 0.00 0.00 2 73.89090 -  
 1214100.000  
 1005.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15180.000

0.000000000D+00 0.000000000D+00 2.225025888D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.502292112D+05-  
 1.169607936D+02  
 Li2O(cr) Cubic. Gurvich,1982 pt1 p257 pt2 p295.  
 2 tps82 LI 2.000 1.00 0.00 0.00 0.00 1 29.88140 -  
 597880.000  
 200.000 800.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7251.000  
 3.028110639D+05-4.262752720D+03 1.838105970D+01 8.164277890D-03-  
 6.056855750D-05  
 8.533995130D-08-3.737236310D-11 -5.206402060D+04-  
 1.132207799D+02  
 800.000 1726.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7251.000  
 -5.016824310D+06 2.420062743D+04-4.101266390D+01 5.324367340D-02-  
 2.998210001D-05  
 1.063865942D-08-1.399118443D-12 -2.158188563D+05  
 2.784406390D+02  
 Li2O(L) Liquid. Gurvich,1982 pt1 p257 pt2 p295.  
 1 tps82 LI 2.000 1.00 0.00 0.00 0.00 2 29.88140 -  
 597880.000  
 1726.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7251.000  
 0.000000000D+00 0.000000000D+00 1.250825364D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -7.338860760D+04-  
 6.881025076D+01  
 Li2O2(cr) Hexagonal. Gurvich,1982 pt1 p261 pt2 p298.  
 1 tps82 LI 2.000 2.00 0.00 0.00 0.00 1 45.88080 -  
 632500.000  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10500.000  
 0.000000000D+00 0.000000000D+00 6.874488094D+00 7.197297255D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -7.844135590D+04-  
 3.433817812D+01  
 Li2SO4(a) Alpha. Gurvich,1982 pt1 p291 pt2 p325.  
 2 tps82 LI 2.00S 1.000 4.00 0.00 0.00 1 109.94560 -  
 1436000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18631.000  
 2.307314336D+07-4.440850530D+05 3.473570360D+03-1.406997202D+01  
 3.151077609D-02  
 -3.672532150D-05 1.742494307D-08 1.810572013D+06-  
 1.805254507D+04  
 500.000 848.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18631.000  
 1.379684430D+06 0.000000000D+00-7.865353280D+01 4.280849920D-01-  
 6.782300830D-04  
 3.795553140D-07 0.000000000D+00 -1.584238676D+05  
 3.687429570D+02  
 Li2SO4(b) Beta. Gurvich,1982 pt1 p291 pt2 p325.  
 1 tps82 LI 2.00S 1.000 4.00 0.00 0.00 2 109.94560 -  
 1436000.000  
 848.000 1131.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18631.000  
 0.000000000D+00 0.000000000D+00 2.621922398D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.809832398D+05-  
 1.396630415D+02

Li2SO4(L) Liquid. Gurvich,1982 pt1 p291 pt2 p325. -  
 1 tpris82 LI 2.00S 1.000 4.00 0.00 0.00 3 109.94560 -  
 1436000.000  
 1131.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18631.000  
 0.000000000D+00 0.000000000D+00 2.465569228D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.780963589D+05-  
 1.276811017D+02

Li3AlF6(IV) Rhombic. Gurvich,1982 pt1 p301 pt2 p334. -  
 2 tpris82 LI 3.00AL 1.00F 6.00 0.00 0.00 1 161.79496 -  
 3389600.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 32150.000  
 -9.493305210D+05 1.726015181D+04-1.388395633D+02 7.441178510D-01-  
 1.715868367D-03  
 2.058073373D-06-9.983283300D-10 -4.893133340D+05  
 7.043980840D+02  
 500.000 788.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 32150.000  
 -3.361898910D+05 0.000000000D+00 2.259884943D+01 2.065859808D-02-  
 6.977943650D-06  
 0.000000000D+00 0.000000000D+00 -4.163946960D+05-  
 1.138999049D+02

Li3AlF6(III) Tetragonal. Gurvich,1982 pt1 p301 pt2 p334. -  
 1 tpris82 LI 3.00AL 1.00F 6.00 0.00 0.00 2 161.79496 -  
 3389600.000  
 788.000 873.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 32150.000  
 0.000000000D+00 0.000000000D+00 3.427742585D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.195341580D+05-  
 1.769490331D+02

Li3AlF6(II) Cubic. Gurvich,1982 pt1 p301 pt2 p334. -  
 1 tpris82 LI 3.00AL 1.00F 6.00 0.00 0.00 3 161.79496 -  
 3389600.000  
 873.000 978.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 32150.000  
 0.000000000D+00 0.000000000D+00 3.548014255D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.202233150D+05-  
 1.846804483D+02

Li3AlF6(I) Crystal. Gurvich,1982 pt1 p301 pt2 p334. -  
 1 tpris82 LI 3.00AL 1.00F 6.00 0.00 0.00 4 161.79496 -  
 3389600.000  
 978.000 1058.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 32150.000  
 0.000000000D+00 0.000000000D+00 3.343552416D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.172975860D+05-  
 1.696552845D+02

Li3AlF6(L) Liquid. Gurvich,1982 pt1 p301 pt2 p334. -  
 1 tpris82 LI 3.00AL 1.00F 6.00 0.00 0.00 5 161.79496 -  
 3389600.000  
 1058.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 32150.000  
 0.000000000D+00 0.000000000D+00 4.642486448D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.204684280D+05-  
 2.501224871D+02

Li3N(cr) Chase,1998 p1526.

2 j 3/78 LI 3.00N 1.00 0.00 0.00 0.00 1 34.82974 -  
 164557.000  
 200.000 700.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11213.120  
 1.373485590D+06-2.379184204D+04 1.591917968D+02-4.823554940D-01  
 8.557283860D-04  
 -7.626448860D-07 2.741510774D-10 8.816502990D+04-  
 8.595793090D+02  
 700.000 1300.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11213.120  
 -1.241718958D+08 7.830020910D+05-2.032330783D+03 2.815135927D+00-  
 2.148359487D-03  
 8.689521850D-07-1.452735248D-10 -4.390747670D+06  
 1.278810396D+04  
 Mg(cr) Hexagonal. Ref-Elm. Alcock,1993.  
 2 srd 93 MG 1.00 0.00 0.00 0.00 0.00 1 24.30500  
 0.000  
 100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 4979.161  
 -5.412225134D+03 0.000000000D+00 1.458173723D+00 1.330204666D-02-  
 4.098858502D-05  
 4.754339101D-08 0.000000000D+00 -7.759472010D+02-  
 6.989702348D+00  
 298.150 923.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 4979.161  
 -2.860060304D+04 0.000000000D+00 3.398877384D+00-7.243962663D-04  
 1.405254188D-06  
 0.000000000D+00 0.000000000D+00 -1.089519906D+03-  
 1.545973664D+01  
 Mg(L) Liquid. Ref-Elm. Alcock,1993.  
 1 srd 93 MG 1.00 0.00 0.00 0.00 0.00 2 24.30500  
 0.000  
 923.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 4979.161  
 0.000000000D+00 0.000000000D+00 4.125318269D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.589919480D+02-  
 1.937828582D+01  
 MgAL2O4(cr) Crystal. Chase,1998 pp147-9.  
 2 j12/79 MG 1.00AL 2.000 4.00 0.00 0.00 1 142.26568 -  
 2299110.000  
 200.000 800.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 64479.624  
 9.746254450D+05-1.525021312D+04 8.302860630D+01-1.382241614D-01  
 1.657566530D-04  
 -9.668302460D-08 2.170561037D-11 -2.062543046D+05-  
 4.734083400D+02  
 800.000 2408.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 64479.624  
 -7.339625410D+05 1.248275880D+03 1.548493786D+01 6.232746800D-03-  
 9.669121680D-07  
 2.487422341D-10-2.603898110D-14 -2.909147610D+05-  
 7.914855130D+01  
 MgAL2O4(L) Liquid. Chase,1998 pp147-9.  
 1 j12/79 MG 1.00AL 2.000 4.00 0.00 0.00 2 142.26568 -  
 2299110.000  
 2408.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 64479.624  
 0.000000000D+00 0.000000000D+00 2.641887495D+01 0.000000000D+00  
 0.000000000D+00

0.000000000D+00 0.000000000D+00 -2.688320250D+05-  
 1.419843893D+02  
 MgBr2(cr) Hexagonal. Gurvich,1996a pt1 p418 pt2 p332.  
 1 tpris96 MG 1.00BR 2.00 0.00 0.00 0.00 1 184.11300 -  
 526000.000  
 298.150 984.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15500.499  
 -6.657036915D+04 0.000000000D+00 9.124771033D+00 1.443260036D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.627087500D+04-  
 3.872222733D+01  
 MgBr2(L) Liquid. Gurvich,1996a pt1 p418 pt2 p332.  
 1 tpris96 MG 1.00BR 2.00 0.00 0.00 0.00 2 184.11300 -  
 526000.000  
 984.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15500.499  
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.363378060D+04-  
 5.246637684D+01  
 MgCO3(cr) Hexagonal. Gurvich,1996a pt1 p429 pt2 p341.  
 2 tpris96 MG 1.00C 1.000 3.00 0.00 0.00 1 84.31390 -  
 1096000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11630.499  
 -5.649471920D+06 1.059809340D+05-8.095953810D+02 3.267992680D+00-  
 7.111639940D-03  
 8.088247340D-06-3.758639920D-09 -6.098528470D+05  
 4.221968000D+03  
 500.000 1263.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11630.499  
 -1.743337852D+05 0.000000000D+00 8.820122894D+00 7.696184141D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.353742560D+05-  
 4.570039759D+01  
 MgCO3(L) Liquid. Gurvich,1996a pt1 p429 pt2 p341.  
 1 tpris96 MG 1.00C 1.000 3.00 0.00 0.00 3 84.31390 -  
 1096000.000  
 1263.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11630.499  
 0.000000000D+00 0.000000000D+00 1.804075045D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.336474914D+05-  
 9.615384273D+01  
 MgCL2(cr) Hexagonal. Gurvich,1996a pt1 p413 pt2 p329.  
 2 tpris96 MG 1.00CL 2.00 0.00 0.00 0.00 1 95.21040 -  
 644300.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13770.499  
 3.151271437D+05-4.986561670D+03 3.407490430D+01-6.013327030D-02  
 7.256223640D-05  
 -2.984411528D-08-5.064069590D-12 -5.608909370D+04-  
 1.833415814D+02  
 500.000 987.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13770.499  
 -7.745495525D+04 0.000000000D+00 9.099153167D+00 1.199709905D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -8.051706960D+04-  
 4.185795845D+01  
 MgCL2(L) Liquid. Gurvich,1996a pt1 p413 pt2 p329.

1 tps96 MG 1.00CL 2.00 0.00 0.00 0.00 3 95.21040 -  
 644300.000  
 987.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13770.499  
 7.120082843D+05 0.000000000D+00 1.060122605D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -7.543168500D+04-  
 4.537295861D+01  
 MgF2 (cr) Tetragonal. Gurvich,1996a pt1 p410 pt2 p326.  
 2 tps96 MG 1.00F 2.00 0.00 0.00 0.00 1 62.30181 -  
 1124200.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9920.499  
 -8.758857470D+06 1.630690293D+05-1.234784473D+03 4.913114430D+00-  
 1.064398199D-02  
 1.204196054D-05-5.572295890D-09 -8.710379520D+05  
 6.452721700D+03  
 500.000 1536.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9920.499  
 -1.863609521D+05 0.000000000D+00 9.358338615D+00 4.871002621D-04  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.386463039D+05-  
 4.763420955D+01  
 MgF2 (L) Liquid. Gurvich,1996a pt1 p410 pt2 p326.  
 1 tps96 MG 1.00F 2.00 0.00 0.00 0.00 3 62.30181 -  
 1124200.000  
 1536.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9920.499  
 0.000000000D+00 0.000000000D+00 1.140175428D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.340531621D+05-  
 5.725828106D+01  
 MgH2 (b) Beta,tetragonal. Gurvich,1996a pt1 p402 pt2 p321.  
 1 tps96 MG 1.00H 2.00 0.00 0.00 0.00 1 26.32088 -  
 75700.000  
 200.000 600.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 5310.000  
 4.034912200D+06-6.115400800D+04 3.537084270D+02-9.554057160D-01  
 1.260522797D-03  
 -6.389211330D-07 0.000000000D+00 2.799920215D+05-  
 1.959491159D+03  
 MgH2 (L) Liquid. Gurvich,1996a pt1 p402 pt2 p321.  
 1 tps96 MG 1.00H 2.00 0.00 0.00 0.00 2 26.32088 -  
 75700.000  
 600.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 5310.000  
 0.000000000D+00 0.000000000D+00 9.020375224D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.135051728D+04-  
 4.777194561D+01  
 MgI2 (cr) Hexagonal. Gurvich,1996a pt1 p422 pt2 p335.  
 1 tps96 MG 1.00I 2.00 0.00 0.00 0.00 1 278.11394 -  
 370000.000  
 298.150 906.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17000.499  
 0.000000000D+00 0.000000000D+00 8.291528905D+00 2.232723275D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.707187430D+04-  
 3.179107057D+01  
 MgI2 (L) Liquid. Gurvich,1996a pt1 p422 pt2 p335.



1 tpis96 MG 1.00I 2.00 0.00 0.00 0.00 2 278.11394 -  
 37000.000  
 906.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17000.499  
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.641294920D+04-  
 5.175282479D+01  
 MgO(cr) Cubic Gurvich,1996a pt1 p397 pt2 p317.  
 2 tpis96 MG 1.00O 1.00 0.00 0.00 0.00 1 40.30440 -  
 601600.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 5160.499  
 -8.980784570D+05 1.771245421D+04-1.449325747D+02 6.397591100D-01-  
 1.458346800D-03  
 1.715467374D-06-8.183482370D-10 -1.516290864D+05  
 7.439009690D+02  
 500.000 3100.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 5160.499  
 -1.169521716D+05 0.000000000D+00 5.510366817D+00 1.085932905D-03-  
 4.866191754D-07  
 1.253230798D-10 0.000000000D+00 -7.443482720D+04-  
 2.911564935D+01  
 MgO(L) Liquid Gurvich,1996a pt1 p397 pt2 p317.  
 1 tpis96 MG 1.00O 1.00 0.00 0.00 0.00 3 40.30440 -  
 601600.000  
 3100.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 5160.499  
 0.000000000D+00 0.000000000D+00 1.010282025D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -7.609370840D+04-  
 6.076894048D+01  
 Mg(OH)2(cr) Hexagonal. Gurvich,1996a pt1 p405 pt2 p323.  
 2 tpis96 MG 1.00O 2.00H 2.00 0.00 0.00 1 58.31968 -  
 924350.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11410.000  
 -6.401451840D+05 8.358139990D+03-3.971145400D+01 1.231927219D-01-  
 9.647800650D-05  
 0.000000000D+00 0.000000000D+00 -1.537246903D+05  
 2.258495398D+02  
 500.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11410.000  
 -5.543828430D+06 3.700868610D+04-9.088623340D+01 1.431689186D-01-  
 9.513965240D-05  
 2.532586546D-08 0.000000000D+00 -3.189450890D+05  
 5.801638270D+02  
 Mg(OH)2(L) Liquid. Gurvich,1996a pt1 p405 pt2 p323.  
 1 tpis96 MG 1.00O 2.00H 2.00 0.00 0.00 2 58.31968 -  
 924350.000  
 1100.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11410.000  
 -3.037581289D+05 0.000000000D+00 1.203462381D+01 2.202655358D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.158775486D+05-  
 6.333852645D+01  
 MgS(cr) Cubic. Gurvich,1996a pt1 p424 pt2 p337.  
 2 tpis96 MG 1.00S 1.00 0.00 0.00 0.00 1 56.37100 -  
 348000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8330.499

1.862529340D+06-3.536941040D+04 2.721839670D+02-1.042907730D+00  
 2.246733361D-03  
 -2.528313530D-06 1.164923631D-09 1.157121957D+05-  
 1.421776433D+03  
 500.000 2500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8330.499  
 -2.774667419D+04 0.000000000D+00 5.477652922D+00 1.053219011D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.362757840D+04-  
 2.562621459D+01  
 MgS(L) Liquid. Gurvich,1996a pt1 p424 pt2 p337.  
 1 tps96 MG 1.00S 1.00 0.00 0.00 0.00 3 56.37100 -  
 34800.000  
 2500.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8330.499  
 0.000000000D+00 0.000000000D+00 8.058201866D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.919942750D+04-  
 4.015043492D+01  
 MgSO4(II) CrII,rhombic. Gurvich,1996a pt1 p426 pt2 p339.  
 2 tps96 MG 1.00S 1.000 4.00 0.00 0.00 1 120.36860 -  
 128880.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15400.499  
 7.038799190D+06-1.283866938D+05 9.464955820D+02-3.562117130D+00  
 7.535844540D-03  
 -8.351428640D-06 3.800035070D-09 4.243566150D+05-  
 4.979377480D+03  
 500.000 1283.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15400.499  
 -1.403690656D+05 0.000000000D+00 1.024474082D+01 1.053279147D-02-  
 2.384385851D-06  
 0.000000000D+00 0.000000000D+00 -1.589785092D+05-  
 5.117735953D+01  
 MgSO4(I) CrI,rhombic. Gurvich,1996a pt1 p426 pt2 p339.  
 1 tps96 MG 1.00S 1.000 4.00 0.00 0.00 3 120.36860 -  
 128880.000  
 1283.000 1410.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15400.499  
 0.000000000D+00 0.000000000D+00 1.864210880D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.622917080D+05-  
 9.940197517D+01  
 MgSO4(L) Liquid. Gurvich,1996a pt1 p426 pt2 p339.  
 1 tps96 MG 1.00S 1.000 4.00 0.00 0.00 4 120.36860 -  
 128880.000  
 1410.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15400.499  
 0.000000000D+00 0.000000000D+00 1.864210880D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.605357417D+05-  
 9.815660894D+01  
 MgSiO3(I) Chase,1998 pp1540-2.  
 1 j12/67 MG 1.00SI 1.000 3.00 0.00 0.00 1 100.38870 -  
 1548916.800  
 200.000 903.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12112.680  
 6.634624630D+05-1.098828549D+04 6.661582640D+01-1.408979556D-01  
 2.056144180D-04  
 -1.506280668D-07 4.456006950D-11 -1.365977193D+05-  
 3.704100780D+02

MgSiO<sub>3</sub>(II) Chase,1998 pp1540-2.  
1 j12/67 MG 1.00SI 1.000 3.00 0.00 0.00 2 100.38870 -  
1548916.800  
903.000 1258.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
12112.680  
0.000000000D+00 0.000000000D+00 1.447351774D+01 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -1.916168640D+05-  
7.665690420D+01

MgSiO<sub>3</sub>(III) Chase,1998 pp1540-2.  
1 j12/67 MG 1.00SI 1.000 3.00 0.00 0.00 3 100.38870 -  
1548916.800  
1258.000 1850.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
12112.680  
0.000000000D+00 0.000000000D+00 1.472512607D+01 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -1.917371327D+05-  
7.829669776D+01

MgSiO<sub>3</sub>(L) Chase,1998 pp1540-2.  
1 j12/67 MG 1.00SI 1.000 3.00 0.00 0.00 4 100.38870 -  
1548916.800  
1850.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
12112.680  
0.000000000D+00 0.000000000D+00 1.761258330D+01 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -1.880210286D+05-  
9.512270574D+01

MgTiO<sub>3</sub>(cr) Chase,1998 pp1543-5.  
2 j 6/67 MG 1.00TI 1.000 3.00 0.00 0.00 1 120.17020 -  
1572556.400  
200.000 700.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
13556.160  
7.429774000D+05-1.292212821D+04 8.410507170D+01-2.098263307D-01  
3.615281930D-04  
-3.238214780D-07 1.180955355D-10 -1.313766506D+05-  
4.602729640D+02  
700.000 1953.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
13556.160  
1.601922450D+05-2.633226069D+03 1.883800780D+01-1.678968165D-03  
1.139243183D-06  
-2.244954628D-10 2.663226969D-14 -1.791724552D+05-  
1.059181291D+02

MgTiO<sub>3</sub>(L) Chase,1998 pp1543-5.  
1 j 6/67 MG 1.00TI 1.000 3.00 0.00 0.00 2 120.17020 -  
1572556.400  
1953.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
13556.160  
0.000000000D+00 0.000000000D+00 1.962544997D+01 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -1.909134805D+05-  
1.065587855D+02

MgTi<sub>2</sub>O<sub>5</sub>(cr) Todd,1952. Chase,1998 pp1550-1552 6/67.  
2 g11/00 MG 1.00TI 2.000 5.00 0.00 0.00 1 200.03600 -  
2508218.800  
200.000 800.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
22438.792  
1.244806767D+06-2.122898938D+04 1.352816814D+02-3.207171960D-01  
5.056737150D-04  
-4.075110600D-07 1.330675670D-10 -2.063427950D+05-  
7.421883210D+02

800.000 1963.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22438.792  
 1.206826103D+06-7.504042080D+03 3.472504430D+01-9.398048060D-03  
 7.725115420D-06  
 -2.268307646D-09 2.728749772D-13 -2.651238294D+05-  
 1.981547532D+02  
 MgTi2O5(L) Todd,1952. Chase,1998 pp1550-1552 6/67.  
 1 g11/00 MG 1.00TI 2.000 5.00 0.00 0.00 2 200.03600 -  
 2508218.800  
 1963.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22438.792  
 0.000000000D+00 0.000000000D+00 3.140071995D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.039563022D+05-  
 1.685813857D+02  
 Mg2SiO4(cr) Chase,1998 pp1556-8 12/67.  
 2 g11/00 MG 2.00SI 1.000 4.00 0.00 0.00 1 140.69310 -  
 2177078.400  
 200.000 800.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17279.920  
 9.212035030D+05-1.508156349D+04 9.085102220D+01-1.898897815D-01  
 2.890690717D-04  
 -2.266693109D-07 7.230688250D-11 -1.936097830D+05-  
 5.059650070D+02  
 800.000 2171.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17279.920  
 3.714548590D+06-2.041518891D+04 5.788009140D+01-3.629874490D-02  
 2.183358474D-05  
 -6.504809080D-09 7.908133680D-13 -1.494870518D+05-  
 3.576608370D+02  
 Mg2SiO4(L) Chase,1998 pp1556-8 12/67  
 1 g11/00 MG 2.00SI 1.000 4.00 0.00 0.00 2 140.69310 -  
 2177078.400  
 2170.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17279.920  
 0.000000000D+00 0.000000000D+00 2.465761662D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.669357683D+05-  
 1.346103798D+02  
 Mg2TiO4(cr) Chase,1998 pp1559-61 6/67.  
 2 g11/00 MG 2.00TI 1.000 4.00 0.00 0.00 1 160.47460 -  
 2164354.400  
 200.000 800.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18836.368  
 9.956749990D+05-1.724659186D+04 1.091877188D+02-2.478088109D-01  
 3.830393010D-04  
 -3.022256428D-07 9.684735620D-11 -1.830794683D+05-  
 6.011710070D+02  
 800.000 2013.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18836.368  
 3.251168130D+05-3.023737890D+03 2.335313762D+01-5.057540210D-04  
 2.750958409D-06  
 -9.172292550D-10 1.089453371D-13 -2.490728250D+05-  
 1.278129303D+02  
 Mg2TiO4(L) Chase,1998 pp1559-61 6/67.  
 1 g11/00 MG 2.00TI 1.000 4.00 0.00 0.00 2 160.47460 -  
 2164354.400  
 2013.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18836.368  
 0.000000000D+00 0.000000000D+00 2.747562995D+01 0.000000000D+00  
 0.000000000D+00

0.000000000D+00 0.000000000D+00 -2.615257868D+05-  
1.474539637D+02  
Mg3N2(cr) Cubic. Gurvich,1996a pt1 p427 pt2 p340.  
1 tpris96 MG 3.00N 2.00 0.00 0.00 0.00 1 100.92848 -  
461300.000  
298.150 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
10500.499  
-3.313123684D+05 0.000000000D+00 1.448912804D+01 1.035659347D-03  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -6.095851350D+04-  
7.450243529D+01  
Mn(a) Alpha. Ref-Elm. Chase,1998 pp1571-4.  
1 j 9/67 MN 1.00 0.00 0.00 0.00 0.00 1 54.93805  
0.000  
200.000 980.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
4994.000  
-1.984724642D+04 1.808814126D+02 1.038289801D+00 8.813332010D-03-  
1.298045968D-05  
1.118858744D-08-3.673641300D-12 -1.704143022D+03-  
3.713160980D+00  
Mn(b) Beta. Ref-Elm. Chase,1998 pp1571-4.  
1 j 9/67 MN 1.00 0.00 0.00 0.00 0.00 2 54.93805  
0.000  
980.000 1361.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
4994.000  
-2.033299729D+08 8.595009270D+05-1.444429639D+03 1.217025958D+00-  
5.092264580D-04  
8.499457640D-08 0.000000000D+00 -5.153128480D+06  
9.753553620D+03  
Mn(c) Gamma. Ref-Elm. Chase,1998 pp1571-4.  
1 j 9/67 MN 1.00 0.00 0.00 0.00 0.00 3 54.93805  
0.000  
1361.000 1412.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
4994.000  
-5.539443490D+06 0.000000000D+00 1.249195042D+01-3.172888290D-03  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -1.319440868D+04-  
7.701110710D+01  
Mn(d) Delta. Ref-Elm. Chase,1998 pp1571-4.  
1 j 9/67 MN 1.00 0.00 0.00 0.00 0.00 4 54.93805  
0.000  
1412.000 1519.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
4994.000  
-4.256613510D+06 0.000000000D+00 1.001289188D+01-1.726727732D-03  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -1.000110470D+04-  
6.059129950D+01  
Mn(L) Liquid. Ref-Elm. Chase,1998 pp1571-4.  
1 j 9/67 MN 1.00 0.00 0.00 0.00 0.00 5 54.93805  
0.000  
1519.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
4994.000  
0.000000000D+00 0.000000000D+00 5.535383324D+00 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -9.393783130D+02-  
2.853570386D+01  
Mo(cr) Crystal. Ref-Elm. Chase,1998 pp1577-80.  
3 j 3/78 MO 1.00 0.00 0.00 0.00 0.00 1 95.94000  
0.000  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
4585.000

-4.961689320D+04 4.280941190D+02 7.671984690D-01 5.731518250D-03-  
 6.381641180D-06  
 3.708192420D-09-7.917347080D-13 -3.039584622D+03-  
 1.230467690D+00  
 1000.000 2200.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 4585.000  
 -3.617592720D+06 1.474639904D+04-2.136672658D+01 2.118577261D-02-  
 9.789741690D-06  
 2.496130112D-09-2.422303123D-13 -8.977896080D+04  
 1.507160275D+02  
 2200.000 2896.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 4585.000  
 4.759909590D+09-5.321527320D+06-8.747403120D+02 3.794789480D+00-  
 2.131568725D-03  
 4.974075900D-07-4.325425090D-11 4.096569650D+07  
 1.130483988D+02  
 Mo(L) Liquid. Ref-Elm. Chase,1998 pp1577-80.  
 1 j 3/78 MO 1.00 0.00 0.00 0.00 0.00 2 95.94000  
 0.000  
 2896.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 4585.000  
 0.000000000D+00 0.000000000D+00 4.528949992D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 2.022300696D+03-  
 2.280790783D+01  
 MoO2(cr) Monoclinic. Gurvich,1982 pt1 p27 pt2 p32.  
 2 tpis82 MO 1.000 2.00 0.00 0.00 0.00 1 127.93880 -  
 589300.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8328.000  
 -6.526622370D+06 1.230156278D+05-9.443937510D+02 3.807393330D+00-  
 8.319729080D-03  
 9.477106540D-06-4.408972390D-09 -6.244588120D+05  
 4.921849140D+03  
 500.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8328.000  
 -2.051418601D+05 0.000000000D+00 8.963295880D+00-1.128973209D-04  
 1.146693959D-06  
 0.000000000D+00 0.000000000D+00 -7.424162440D+04-  
 4.664669130D+01  
 MoO3(cr) Rhombic. Gurvich,1982 pt1 p30 pt2 p34.  
 2 tpis82 MO 1.000 3.00 0.00 0.00 0.00 1 143.93820 -  
 744600.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12590.000  
 9.061545810D+06-1.658675979D+05 1.230236799D+03-4.691503730D+00  
 9.965828580D-03  
 -1.109194136D-05 5.065628490D-09 6.590937470D+05-  
 6.461598540D+03  
 500.000 1075.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12590.000  
 -9.462974968D+04 0.000000000D+00 8.841771794D+00 4.197842086D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -9.269445280D+04-  
 4.282025959D+01  
 MoO3(L) Liquid. Gurvich,1982 pt1 p30 pt2 p34.  
 1 tpis82 MO 1.000 3.00 0.00 0.00 0.00 3 143.93820 -  
 744600.000  
 1075.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12590.000

0.000000000D+00 0.000000000D+00 1.527450205D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -9.123881420D+04-  
 7.771899557D+01  
 NH4CL(II) Chase,1998 p765.  
 1 j 9/65 N 1.00H 4.00CL 1.00 0.00 0.00 1 53.49120 -  
 314553.000  
 298.150 457.7007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22698.000  
 1.593389657D+05 0.000000000D+00-5.965854940D+00 6.494193170D-02-  
 5.391456890D-05  
 0.000000000D+00 0.000000000D+00 -3.792881500D+04  
 2.933013040D+01  
 NH4CL(III) Chase,1998 p765.  
 2 j 9/65 N 1.00H 4.00CL 1.00 0.00 0.00 2 53.49120 -  
 314553.000  
 457.700 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22698.000  
 -1.641820157D+07 1.639262758D+05-6.654529630D+02 1.447086973D+00-  
 1.698254160D-03  
 1.056255415D-06-2.697574651D-10 -8.787975900D+05  
 3.897936900D+03  
 1000.000 1500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22698.000  
 8.409592660D+08-3.426760780D+06 5.548091470D+03-4.435674300D+00  
 1.772486202D-03  
 -2.817160120D-07 0.000000000D+00 2.063363145D+07-  
 3.765976360D+04  
 NH4F(cr) Hexagonal. Gurvich,1989 pt1 p388 pt2 p324.  
 2 tpi89 N 1.00H 4.00F 1.00 0.00 0.00 1 37.03690 -  
 467560.000  
 200.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11108.000  
 -2.975636383D+06 7.208754230D+04-7.346289470D+02 4.075299810D+00-  
 1.264044498D-02  
 2.111837237D-05-1.479873524D-08 -3.621184440D+05  
 3.608760970D+03  
 298.150 511.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11108.000  
 0.000000000D+00 0.000000000D+00 1.563531705D+00 2.108482641D-02  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.763754000D+04-  
 6.538862038D+00  
 NH4F(L) Liquid. Gurvich,1989 pt1 p388 pt2 p324.  
 1 tpi89 N 1.00H 4.00F 1.00 0.00 0.00 2 37.03690 -  
 467560.000  
 511.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11108.000  
 0.000000000D+00 0.000000000D+00 1.359069867D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.951515380D+04-  
 6.780477125D+01  
 Na(cr) Cubic. Ref-Elm. Cox,1989 p254.  
 1 coda89 NA 1.00 0.00 0.00 0.00 0.00 1 22.98977  
 0.000  
 200.000 371.0107 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6460.000  
 -3.584458010D+04 0.000000000D+00 6.479414690D+00-1.898697341D-02  
 3.352387090D-05  
 0.000000000D+00 0.000000000D+00 -1.504319740D+03-  
 2.677783039D+01

Na(L) Liquid. Ref-Elm. Cox,1989 p254.

1 coda89 NA 1.00 0.00 0.00 0.00 0.00 2 22.98977  
0.000  
371.010 2300.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6460.000  
2.694818670D+04-2.319000780D+02 5.162435690D+00-3.058571990D-03  
1.696407999D-06  
-1.519633426D-10 1.962859159D-14 2.842114288D+02-  
2.225763980D+01

NaALO2 (a) Alpha.Chase,1998 p131.

1 j 3/63 NA 1.00AL 1.000 2.00 0.00 0.00 1 81.97011 -  
1133190.000  
200.000 740.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
23794.000  
4.527204140D+05-7.722924360D+03 5.000166380D+01-1.091293529D-01  
1.762084005D-04  
-1.452865027D-07 4.918123650D-11 -1.021205450D+05-  
2.738871707D+02

NaALO2 (b) Beta. Chase,1998 p131.

1 j 3/63 NA 1.00AL 1.000 2.00 0.00 0.00 2 81.97011 -  
1133190.000  
740.000 3000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
23794.000  
3.197980170D+06-1.525937524D+04 3.932924030D+01-2.623291355D-02  
1.465112353D-05  
-3.740532770D-09 3.560249390D-13 -4.988553210D+04-  
2.434131708D+02

NaBO2 (cr) Hexagonal. Gurvich,1982 pt1 p357 pt2 p391.

2 tpis82 NA 1.00B 1.000 2.00 0.00 0.00 1 65.79957 -  
976500.000  
200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
11632.000  
-1.074702306D+05 2.343688910D+03-1.964636192D+01 1.319434021D-01-  
2.997058540D-04  
3.640103610D-07-1.796104124D-10 -1.291527393D+05  
9.915788280D+01  
500.000 1239.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
11632.000  
-5.597627870D+04 0.000000000D+00 5.491743560D+00 1.171509302D-02-  
4.773472260D-06  
0.000000000D+00 0.000000000D+00 -1.197489098D+05-  
2.604168849D+01

NaBO2 (L) Liquid. Gurvich,1982 pt1 p357 pt2 p391.

1 tpis82 NA 1.00B 1.000 2.00 0.00 0.00 2 65.79957 -  
976500.000  
1239.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
11632.000  
0.000000000D+00 0.000000000D+00 1.743939210D+01 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -1.245121293D+05-  
9.701235601D+01

NaBr (cr) Cubic. Gurvich,1982 pt1 p340 pt2 p378.

2 tpis82 NA 1.00BR 1.00 0.00 0.00 0.00 1 102.89377 -  
361160.000  
200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
11590.000  
3.210289070D+06-5.986721400D+04 4.572531830D+02-1.768432397D+00  
3.814169490D-03  
-4.295102010D-06 1.980139146D-09 2.245558598D+05-  
2.385763453D+03



500.000 1020.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11590.000  
 1.593247644D+04 0.000000000D+00 5.272913580D+00 2.440774360D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.506450850D+04-  
 2.022580453D+01  
 NaBr(L) Liquid. Gurvich,1982 pt1 p340 pt2 p378.  
 1 tpi82 NA 1.00BR 1.00 0.00 0.00 0.00 2 102.89377 -  
 361160.000  
 1020.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11590.000  
 0.000000000D+00 0.000000000D+00 8.178473536D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.361938300D+04-  
 3.477943790D+01  
 NaCN(II) Lambda trans@288.5K. Chase,1998(3/66) pp631-3.  
 Messer,1941.  
 6 g 8/01 NA 1.00C 1.00N 1.00 0.00 0.00 1 49.00721 -  
 90709.000  
 197.700 245.9007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19422.128  
 4.995073610D+08-1.007656780D+07 7.458386410D+04-2.134406974D+02-  
 6.965856220D-02  
 1.540182072D-03-2.204709373D-06 4.493712560D+07-  
 3.984423000D+05  
 245.900 273.1007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19422.128  
 -4.546907220D+08 4.339535660D+06 5.476070770D+02-1.324240852D+02  
 5.045446840D-01  
 -5.791737950D-04 0.000000000D+00 -2.385188911D+07  
 3.106410058D+04  
 273.100 284.2007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19422.128  
 -4.415096320D+08 0.000000000D+00 3.452631670D+04-1.661761169D+02  
 2.250608921D-01  
 0.000000000D+00 0.000000000D+00 -6.388306670D+06-  
 1.596447272D+05  
 284.200 286.3007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19422.128  
 1.647379186D+09 0.000000000D+00-6.100370390D+04 1.429224260D+02  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 1.735057318D+07  
 3.142435378D+05  
 286.300 287.7007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19422.128  
 1.607424258D+11 0.000000000D+00-8.629992400D+06 3.290155880D+04-  
 3.355904228D+01  
 0.000000000D+00 0.000000000D+00 1.946284579D+09  
 4.175641230D+07  
 287.700 288.5007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19422.128  
 -1.494237648D+11 0.000000000D+00 8.652205900D+06-3.521604880D+04  
 3.968501633D+01  
 0.000000000D+00 0.000000000D+00 -1.866195945D+09-  
 4.140143280D+07  
 NaCN(III) Lambda trans@288.5K. Chase,1998(3/66) pp631-3.  
 Messer,1941.  
 3 g 8/01 NA 1.00C 1.00N 1.00 0.00 0.00 2 49.00721 -  
 90709.000  
 288.500 290.4007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19422.128

0.000000000D+00 0.000000000D+00 5.590153690D+06-4.787600130D+04  
 1.309325625D+02  
 -1.114230434D-01 0.000000000D+00 -4.753893060D+08-  
 2.241133349D+07  
 290.400 293.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19422.128  
 0.000000000D+00 0.000000000D+00 1.752406137D+07-1.788423367D+05  
 6.083847560D+02  
 -6.898560518D-01 0.000000000D+00 -1.287828620D+09-  
 6.746932890D+07  
 293.150 835.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19422.128  
 0.000000000D+00 0.000000000D+00 8.303074986D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.338528469D+04-  
 3.306050253D+01  
 NaCN(L) Chase,1998(3/66) pp631-3. Messer,1941.  
 1 g 8/01 NA 1.00C 1.00N 1.00 0.00 0.00 3 49.00721 -  
 90709.000  
 835.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19422.128  
 0.000000000D+00 0.000000000D+00 9.561116650D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.337899448D+04-  
 4.025831708D+01  
 NaCl(cr) Cubic. Gurvich,1982 pt1 p335 pt2 p374.  
 2 tpis82 NA 1.00CL 1.00 0.00 0.00 0.00 1 58.44247 -  
 411260.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10600.000  
 2.725695501D+06-5.160958750D+04 3.984582310D+02-1.547496756D+00  
 3.352172310D-03  
 -3.787781590D-06 1.751729541D-09 1.807530763D+05-  
 2.076949046D+03  
 500.000 1074.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10600.000  
 2.657827371D+03 0.000000000D+00 5.665718690D+00 8.708901490D-04  
 1.340560030D-06  
 0.000000000D+00 0.000000000D+00 -5.119384720D+04-  
 2.390773149D+01  
 NaCl(L) Liquid. Gurvich,1982 pt1 p335 pt2 p374.  
 1 tpis82 NA 1.00CL 1.00 0.00 0.00 0.00 2 58.44247 -  
 411260.000  
 1074.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10600.000  
 0.000000000D+00 0.000000000D+00 8.166446369D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.943459010D+04-  
 3.649536621D+01  
 NaF(cr) Cubic. Gurvich,1982 pt1 p330 pt2 p370.  
 2 tpis82 NA 1.00F 1.00 0.00 0.00 0.00 1 41.98817 -  
 576600.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8482.000  
 -6.479380410D+06 1.203694117D+05-9.069923560D+02 3.596486550D+00-  
 7.775987760D-03  
 8.784072120D-06-4.059177020D-09 -6.130723750D+05  
 4.744846560D+03  
 500.000 1269.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8482.000

-1.103659993D+05 0.000000000D+00 7.264294880D+00-1.973449856D-03  
2.198504269D-06  
0.000000000D+00 0.000000000D+00 -7.181627510D+04-  
3.536594020D+01  
NaF(L) Liquid. Gurvich,1982 pt1 p330 pt2 p370.  
1 tpris82 NA 1.00F 1.00 0.00 0.00 0.00 2 41.98817 -  
576600.000  
1269.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
8482.000  
0.000000000D+00 0.000000000D+00 8.431044042D+00 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -6.918200450D+04-  
4.115725624D+01  
NaH(cr) Cubic. Gurvich,1982 pt1 p324 pt2 p365.  
2 tpris82 NA 1.00H 1.00 0.00 0.00 0.00 1 23.99771 -  
56380.000  
200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6259.000  
-7.991749220D+05 1.540118135D+04-1.207582590D+02 5.162361030D-01-  
1.142424910D-03  
1.321529809D-06-6.221705120D-10 -7.637675350D+04  
6.264186650D+02  
500.000 911.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6259.000  
-5.921209820D+04 0.000000000D+00 3.776579530D+00 4.250132020D-03  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -8.294394750D+03-  
1.830678857D+01  
NaH(L) Liquid. Gurvich,1982 pt1 p324 pt2 p365.  
1 tpris82 NA 1.00H 1.00 0.00 0.00 0.00 2 23.99771 -  
56380.000  
911.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6259.000  
0.000000000D+00 0.000000000D+00 6.735213500D+00 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -6.034013160D+03-  
3.112842170D+01  
NaI(cr) Cubic. Gurvich,1982 pt1 p343 pt2 p381.  
2 tpris82 NA 1.00I 1.00 0.00 0.00 0.00 1 149.89424 -  
289630.000  
200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
12260.000  
3.500848300D+06-6.540492260D+04 5.005676630D+02-1.943541204D+00  
4.201134090D-03  
-4.738515580D-06 2.187428593D-09 2.579135069D+05-  
2.609575154D+03  
500.000 934.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
12260.000  
2.799960757D+04 0.000000000D+00 5.047026160D+00 3.029892968D-03  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -3.637984440D+04-  
1.764780816D+01  
NaI(L) Liquid. Gurvich,1982 pt1 p343 pt2 p381.  
1 tpris82 NA 1.00I 1.00 0.00 0.00 0.00 2 149.89424 -  
289630.000  
934.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
12260.000  
0.000000000D+00 0.000000000D+00 8.058201866D+00 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -3.505265490D+04-  
3.237951568D+01

NaNO<sub>2</sub>(I) Rhombic. Gurvich,1982 pt1 p350 pt2 p386. -  
 2 tps82 NA 1.00N 1.000 2.00 0.00 0.00 1 68.99531  
 354600.000  
 298.150 400.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16500.000  
 1.090298767D+06 0.000000000D+00-3.023894373D+01 8.811824148D-02  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.389227900D+04  
 1.648982675D+02  
 400.000 436.7007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16500.000  
 0.000000000D+00 0.000000000D+00 5.419446245D+02-1.998525469D+00  
 0.000000000D+00  
 4.207630035D-06 0.000000000D+00 -1.254887886D+05-  
 2.521831769D+03

NaNO<sub>2</sub>(I') Rhombic. Gurvich,1982 pt1 p350 pt2 p386. -  
 1 tps82 NA 1.00N 1.000 2.00 0.00 0.00 2 68.99531  
 354600.000  
 436.700 557.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16500.000  
 0.000000000D+00 0.000000000D+00 1.599613206D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.773155280D+04-  
 7.952982535D+01

NaNO<sub>2</sub>(L) Liquid. Gurvich,1982 pt1 p350 pt2 p386. -  
 1 tps82 NA 1.00N 1.000 2.00 0.00 0.00 3 68.99531  
 354600.000  
 557.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16500.000  
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.372398050D+04-  
 5.120982634D+01

NaNO<sub>3</sub>(a) Hexagonal. Gurvich,1982 pt1 p353 pt2 p388. -  
 2 tps82 NA 1.00N 1.000 3.00 0.00 0.00 1 84.99471  
 467700.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17230.000  
 -4.851300240D+07 9.186316330D+05-7.046384650D+03 2.807834358D+01-  
 6.098595830D-02  
 6.858389720D-05-3.110743577D-08 -4.182115940D+06  
 3.676430560D+04  
 500.000 549.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17230.000  
 0.000000000D+00 0.000000000D+00 2.680735245D+01-1.753272291D-01  
 3.165502236D-04  
 0.000000000D+00 0.000000000D+00 -5.811076460D+04-  
 9.741742276D+01

NaNO<sub>3</sub>(b) Hexagonal. Gurvich,1982 pt1 p353 pt2 p388. -  
 1 tps82 NA 1.00N 1.000 3.00 0.00 0.00 2 84.99471  
 467700.000  
 549.000 579.6007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17230.000  
 0.000000000D+00 0.000000000D+00 1.683803375D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.159974430D+04-  
 8.308035085D+01

NaNO<sub>3</sub>(L) Liquid. Gurvich,1982 pt1 p353 pt2 p388. -  
 1 tps82 NA 1.00N 1.000 3.00 0.00 0.00 3 84.99471  
 467700.000

579.600 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17230.000  
 0.000000000D+00 0.000000000D+00 1.695830542D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.985936520D+04-  
 8.072256364D+01  
 NaOH(a) Alpha. Gurvich,1996b.  
 2 g 5/99 NA 1.000 1.00H 1.00 0.00 0.00 1 39.99711 -  
 425800.000  
 100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10490.000  
 2.008329119D+04-7.714677160D+02 8.694171090D+00 3.850883340D-03-  
 3.610498540D-06  
 0.000000000D+00 0.000000000D+00 -4.948023450D+04-  
 4.524899570D+01  
 298.150 514.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10490.000  
 1.048215710D+06 0.000000000D+00-9.592892425D+01 6.189564989D-01-  
 1.367212259D-03  
 1.067453163D-06 0.000000000D+00 -3.663541040D+04  
 4.270051072D+02  
 NaOH(b) Beta. Gurvich,1996b.  
 1 g 5/99 NA 1.000 1.00H 1.00 0.00 0.00 2 39.99711 -  
 425800.000  
 514.000 568.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10490.000  
 0.000000000D+00 0.000000000D+00 9.621733572D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.442558950D+04-  
 4.799292559D+01  
 NaOH(c) Gamma. Gurvich,1996b.  
 1 g 5/99 NA 1.000 1.00H 1.00 0.00 0.00 3 39.99711 -  
 425800.000  
 568.000 594.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10490.000  
 0.000000000D+00 0.000000000D+00 1.034336359D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.407054750D+04-  
 5.122288687D+01  
 NaOH(L) Liquid. Gurvich,1996b.  
 2 g 5/99 NA 1.000 1.00H 1.00 0.00 0.00 4 39.99711 -  
 425800.000  
 594.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10490.000  
 0.000000000D+00 0.000000000D+00 1.077790513D+01-7.111663826D-04  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.343827480D+04-  
 5.228806116D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10490.000  
 0.000000000D+00 0.000000000D+00 1.006673875D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.308269160D+04-  
 4.808666421D+01  
 NaO2(cr) Cubic. Gurvich,1982 pt1 p319 pt2 p359.Chase,1998 p1646  
 6/63.  
 1 g10/99 NA 1.000 2.00 0.00 0.00 0.00 1 54.98857 -  
 261000.000  
 223.300 825.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18300.000

0.000000000D+00 0.000000000D+00 7.541274230D+00 3.803351009D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.380838310D+04-  
 3.016162188D+01  
 Na2O (L) Liq. Gurvich,1982 pt1 p319 pt2 p359.Chase,1998 p1646  
 6/63.  
 1 g10/99 NA 1.000 2.00 0.00 0.00 0.00 2 54.98857 -  
 261000.000  
 825.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18300.000  
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.374934750D+04-  
 5.415977808D+01  
 Na2CO3 (a) Alpha,monoclinic. Gurvich,1982 pt1 p356 pt2 p390.  
 1 tpis82 NA 2.00C 1.000 3.00 0.00 0.00 1 105.98844 -  
 1129190.000  
 200.000 623.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 20750.000  
 -2.240230091D+06 3.426046630D+04-2.061520520D+02 7.168720430D-01-  
 1.253560327D-03  
 1.178136083D-06-4.526962410D-10 -2.999635262D+05  
 1.125584713D+03  
 Na2CO3 (b) Beta,monoclinic. Gurvich,1982 pt1 p356 pt2 p390.  
 1 tpis82 NA 2.00C 1.000 3.00 0.00 0.00 2 105.98844 -  
 1129190.000  
 623.000 752.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 20750.000  
 0.000000000D+00 0.000000000D+00 7.711578914D+00 1.943638290D-02  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.388766027D+05-  
 3.334178005D+01  
 Na2CO3 (c) Gamma,hexagonal. Gurvich,1982 pt1 p356 pt2 p390.  
 1 tpis82 NA 2.00C 1.000 3.00 0.00 0.00 3 105.98844 -  
 1129190.000  
 752.000 1131.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 20750.000  
 0.000000000D+00 0.000000000D+00 4.430327223D+00 1.645316441D-02  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.353130199D+05-  
 9.031669943D+00  
 Na2CO3 (L) Liquid. Gurvich,1982 pt1 p356 pt2 p390.  
 1 tpis82 NA 2.00C 1.000 3.00 0.00 0.00 4 105.98844 -  
 1129190.000  
 1131.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 20750.000  
 0.000000000D+00 0.000000000D+00 2.345297558D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.429369053D+05-  
 1.211911225D+02  
 Na2O (c) Gamma. Gurvich,1982 pt1 p320 pt2 p360.  
 2 tpis82 NA 2.000 1.00 0.00 0.00 0.00 1 61.97894 -  
 414570.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12400.000  
 1.662637910D+06-3.189091340D+04 2.474349303D+02-9.313593580D-01  
 2.006501256D-03  
 -2.253952071D-06 1.037067374D-09 9.127774380D+04-  
 1.292003778D+03  
 500.000 1023.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12400.000

2.551096288D+05-2.539111311D+03 1.659817003D+01-1.233767744D-02  
 1.540713549D-05  
 -8.084697830D-09 1.747972425D-12 -3.906526610D+04-  
 8.958024740D+01

Na2O (b) Beta. Gurvich,1982 pt1 p320 pt2 p360.  
 1 tpris82 NA 2.000 1.00 0.00 0.00 0.00 2 61.97894 -  
 414570.000  
 1023.000 1243.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12400.000  
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.485897470D+04-  
 6.235394464D+01

Na2O (a) Alpha. Gurvich,1982 pt1 p320 pt2 p360.  
 1 tpris82 NA 2.000 1.00 0.00 0.00 0.00 3 61.97894 -  
 414570.000  
 1243.000 1405.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12400.000  
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.377652960D+04-  
 6.148311196D+01

Na2O (L) Liquid. Gurvich,1982 pt1 p320 pt2 p360.  
 1 tpris82 NA 2.000 1.00 0.00 0.00 0.00 4 61.97894 -  
 414570.000  
 1405.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12400.000  
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.944674950D+04-  
 5.840141793D+01

Na2O2 (b) Beta. Gurvich,1982 pt1 p323 pt2 p363.  
 2 tpris82 NA 2.000 2.00 0.00 0.00 0.00 1 77.97834 -  
 512000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15694.000  
 -8.122024280D+05 1.451270156D+04-1.058114918D+02 4.802903390D-01-  
 1.057140356D-03  
 1.219343411D-06-5.728124010D-10 -1.295899700D+05  
 5.525239130D+02  
 500.000 785.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15694.000  
 -1.051839392D+05 0.000000000D+00 1.054275850D+01 4.638430480D-03  
 4.381769570D-09  
 0.000000000D+00 0.000000000D+00 -6.528135100D+04-  
 5.064487560D+01

Na2O2 (a) Alpha. Gurvich,1982 pt1 p323 pt2 p363.  
 1 tpris82 NA 2.000 2.00 0.00 0.00 0.00 2 77.97834 -  
 512000.000  
 785.000 948.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15694.000  
 0.000000000D+00 0.000000000D+00 1.359069867D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.546547070D+04-  
 6.641239933D+01

Na2O2 (L) Liquid. Gurvich,1982 pt1 p323 pt2 p363.  
 1 tpris82 NA 2.000 2.00 0.00 0.00 0.00 3 77.97834 -  
 512000.000  
 948.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15694.000

0.000000000D+00 0.000000000D+00 1.611640373D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.581522070D+04-  
 8.156770675D+01  
 Na2S(cr) Below lambda trans. Chase,1998 pp1667-9.  
 2 j 3/78 NA 2.00S 1.00 0.00 0.00 0.00 1 78.04554 -  
 366100.000  
 298.150 700.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 -4.541358110D+05 4.959201300D+03-1.171687783D+01 4.586680300D-02-  
 4.501505030D-05  
 1.801159260D-08 0.000000000D+00 -7.199330320D+04  
 8.057734670D+01  
 700.000 1276.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 -3.527498880D+09 2.408466098D+07-6.783369110D+04 1.008062531D+02-  
 8.320894540D-02  
 3.611294520D-05-6.422558180D-09 -1.325119033D+08  
 4.212898800D+05  
 Na2S(cr) Above lambda trans. Chase,1998 pp1667-9.  
 1 j 3/78 NA 2.00S 1.00 0.00 0.00 0.00 2 78.04554 -  
 366100.000  
 1276.000 1445.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 8.868348820D+08 0.000000000D+00-2.045962174D+03 1.675387705D+00-  
 3.752802310D-04  
 0.000000000D+00 0.000000000D+00 2.169500522D+06  
 1.309983113D+04  
 Na2S(L) Chase,1998 pp1667-9.  
 1 j 3/78 NA 2.00S 1.00 0.00 0.00 0.00 3 78.04554 -  
 366100.000  
 1445.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 0.000000000D+00 0.000000000D+00 1.107076665D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.262953690D+04-  
 4.848427350D+01  
 Na2SO3(cr) Crystal. Barin,1989 pt2 p1002.  
 1 bar 89 NA 2.00S 1.000 3.00 0.00 0.00 1 126.04374 -  
 1100802.000  
 298.150 1184.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 0.000000000D+00 0.000000000D+00 1.290193602D+01 5.233511440D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.364746191D+05-  
 5.751819280D+01  
 Na2SO3(L) Liquid. Barin,1989 pt2 p1002.  
 1 bar 89 NA 2.00S 1.000 3.00 0.00 0.00 2 126.04374 -  
 1100802.000  
 1184.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 0.000000000D+00 0.000000000D+00 2.188992496D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.403382187D+05-  
 1.123000267D+02  
 Na2SO4(V) Rhombic. Gurvich,1982 pt1 p346 pt2 p384.  
 1 tps182 NA 2.00S 1.000 4.00 0.00 0.00 1 142.04314 -  
 1387900.000  
 200.000 458.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 23204.000



-8.689043820D+05 1.449012038D+04-9.087576950D+01 3.621919930D-01-  
 5.592870850D-04  
 3.463421130D-07 0.000000000D+00 -2.371450313D+05  
 4.932876470D+02  
 Na2SO4(IV) Rhombic. Gurvich,1982 pt1 p346 pt2 p384.  
 1 tpris82 NA 2.00S 1.00O 4.00 0.00 0.00 2 142.04314 -  
 1387900.000  
 458.000 514.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 23204.000  
 -1.455046659D+05 0.000000000D+00 1.308904554D+01 1.323950539D-02  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.718682018D+05-  
 6.127355231D+01  
 Na2SO4(I) Hexagonal. Gurvich,1982 pt1 p346 pt2 p384.  
 1 tpris82 NA 2.00S 1.00O 4.00 0.00 0.00 3 142.04314 -  
 1387900.000  
 514.000 1157.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 23204.000  
 0.000000000D+00 0.000000000D+00 2.503069934D+01-1.581223668D-02  
 1.591831629D-05  
 0.000000000D+00 0.000000000D+00 -1.732950425D+05-  
 1.201603231D+02  
 Na2SO4(L) Liquid. Gurvich,1982 pt1 p346 pt2 p384.  
 1 tpris82 NA 2.00S 1.00O 4.00 0.00 0.00 4 142.04314 -  
 1387900.000  
 1157.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 23204.000  
 0.000000000D+00 0.000000000D+00 2.453542061D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.722609524D+05-  
 1.218642150D+02  
 Na3ALF6(a) Monoclinic. Gurvich,1982 pt1 p361 pt2 p394.  
 2 tpris82 NA 3.00AL 1.00F 6.00 0.00 0.00 1 209.94127 -  
 3322400.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 38070.000  
 1.564580425D+07-2.923454204D+05 2.211217567D+03-8.502636700D+00  
 1.825363780D-02  
 -2.047448239D-05 9.409455420D-09 9.119433290D+05-  
 1.157646461D+04  
 500.000 838.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 38070.000  
 -1.416702978D+05 0.000000000D+00 2.315158739D+01 1.479360403D-02  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.076260850D+05-  
 1.084672805D+02  
 Na3ALF6(b) Cubic. Gurvich,1982 pt1 p361 pt2 p394.  
 1 tpris82 NA 3.00AL 1.00F 6.00 0.00 0.00 2 209.94127 -  
 3322400.000  
 838.000 1286.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 38070.000  
 0.000000000D+00 0.000000000D+00 2.624279723D+01 7.980987454D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.065549160D+05-  
 1.221511986D+02  
 Na3ALF6(L) Liquid. Gurvich,1982 pt1 p361 pt2 p394.  
 1 tpris82 NA 3.00AL 1.00F 6.00 0.00 0.00 3 209.94127 -  
 3322400.000  
 1286.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 38070.000

0.000000000D+00 0.000000000D+00 4.702622283D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.129238590D+05-  
 2.499831311D+02  
 Na5AL3F14(cr) Tetragonal. Gurvich,1982 pt1 p362 pt2 p395.  
 2 tps82 NA 5.00AL 3.00F 14.00 0.00 0.00 1 461.87111 -  
 7555000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 80830.000  
 -2.302157125D+07 4.240174110D+05-3.188373880D+03 1.288416515D+01-  
 2.796179544D-02  
 3.169729270D-05-1.469118702D-08 -2.832459181D+06  
 1.667109223D+04  
 500.000 1010.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 80830.000  
 -8.720901540D+05 0.000000000D+00 6.109021050D+01 1.113784152D-02  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -9.302863450D+05-  
 2.943295261D+02  
 Na5AL3F14(L) Liquid. Gurvich,1982 pt1 p362 pt2 p395.  
 1 tps82 NA 5.00AL 3.00F 14.00 0.00 0.00 2 461.87111 -  
 7555000.000  
 1010.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 80830.000  
 0.000000000D+00 0.000000000D+00 1.171446062D+02 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -9.528147600D+05-  
 6.431511436D+02  
 Nb(cr) Crystal. Ref-Elm. Chase,1998 pp1675-8.  
 3 j12/73 NB 1.00 0.00 0.00 0.00 0.00 1 92.90638  
 0.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 5241.000  
 -4.254811710D+04 3.875297090D+02 1.184449739D+00 4.507436620D-03-  
 5.232091980D-06  
 3.513452460D-09-9.507605800D-13 -2.864449323D+03-  
 2.442975114D+00  
 1000.000 2000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 5241.000  
 2.527695630D+07-1.085720528D+05 1.929168202D+02-1.727427651D-01  
 8.671274570D-05  
 -2.266162374D-08 2.437387316D-12 6.472317770D+05-  
 1.284027328D+03  
 2000.000 2750.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 5241.000  
 9.016788690D+08-1.888649522D+06 1.578845370D+03-6.588882220D-01  
 1.416307803D-04  
 -1.396561356D-08 4.411624050D-13 1.264760547D+07-  
 1.175157316D+04  
 Nb(L) Liquid. Ref-Elm. Chase,1998 pp1675-8.  
 1 j12/73 NB 1.00 0.00 0.00 0.00 0.00 2 92.90638  
 0.000  
 2750.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 5241.000  
 0.000000000D+00 0.000000000D+00 4.025733326D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 1.427029683D+03-  
 1.857965621D+01  
 NbO(cr) Cubic. Gurvich,1982 pt1 p75 pt2 p77.  
 1 tps82 NB 1.000 1.00 0.00 0.00 0.00 1 108.90578 -  
 406000.000

298.150 2217.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7200.000  
 -4.430808310D+04 0.000000000D+00 5.073540112D+00 1.194297680D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.054466650D+04-  
 2.397978879D+01  
 NbO(L) Liquid. Gurvich,1982 pt1 p75 pt2 p77.  
 1 tpis82 NB 1.000 1.00 0.00 0.00 0.00 2 108.90578 -  
 406000.000  
 2217.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7200.000  
 0.000000000D+00 0.000000000D+00 7.817658527D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.765976820D+04-  
 3.975547844D+01  
 NbOCL3(cr) Barin,1989 pt2 p1030. Wagman,1982 p207.  
 1 bar 89 NB 1.000 1.00CL 3.00 0.00 0.00 1 215.26388 -  
 879500.000  
 298.150 702.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 -1.822304138D+05 4.828593360D+02 1.341861113D+01 7.546458250D-03-  
 1.198129404D-05  
 9.997155720D-09-3.425554610D-12 -1.133897355D+05-  
 6.057973360D+01  
 NbO2(II) Tetragonal. Gurvich,1982 pt1 p78 pt2 p80.  
 2 tpis82 NB 1.000 2.00 0.00 0.00 0.00 1 124.90518 -  
 795000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9267.000  
 -3.914505940D+06 7.500739880D+04-5.854724840D+02 2.416380822D+00-  
 5.358130280D-03  
 6.172498470D-06-2.893870224D-09 -4.324424750D+05  
 3.040766836D+03  
 500.000 1082.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9267.000  
 -2.074227934D+05 0.000000000D+00 1.075172627D+01-7.363421090D-03  
 7.988904160D-06  
 0.000000000D+00 0.000000000D+00 -9.926049480D+04-  
 5.405566340D+01  
 NbO2(I) Tetragonal. Gurvich,1982 pt1 p78 pt2 p80.  
 1 tpis82 NB 1.000 2.00 0.00 0.00 0.00 2 124.90518 -  
 795000.000  
 1082.000 2360.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9267.000  
 -2.470500366D+05 0.000000000D+00 1.027937906D+01 1.610437657D-04  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -9.951665200D+04-  
 5.395968051D+01  
 NbO2(L) Liquid. Gurvich,1982 pt1 p78 pt2 p80.  
 1 tpis82 NB 1.000 2.00 0.00 0.00 0.00 3 124.90518 -  
 795000.000  
 2360.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9267.000  
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -9.406789930D+04-  
 6.330929540D+01  
 Nb2O5(cr) Monoclinic. Gurvich,1982 pt1 p81 pt2 p82.  
 2 tpis82 NB 2.000 5.00 0.00 0.00 0.00 1 265.80976 -  
 1897000.000

200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22240.000  
 2.640209200D+07-4.944721050D+05 3.755171780D+03-1.472158158D+01  
 3.190561080D-02  
 -3.609939830D-05 1.669960716D-08 1.993996743D+06-  
 1.963185769D+04  
 500.000 1783.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22240.000  
 2.666894830D+05 0.000000000D+00-3.157808421D+00 7.820838380D-02-  
 9.622327490D-05  
 5.100828450D-08-9.357603760D-12 -2.290426814D+05  
 1.650612260D+01  
 Nb2O5(L) Liquid. Gurvich,1982 pt1 p81 pt2 p82.  
 1 tpis82 NB 2.000 5.00 0.00 0.00 0.00 2 265.80976 -  
 1897000.000  
 1783.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22240.000  
 0.000000000D+00 0.000000000D+00 2.405433393D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.279011100D+05-  
 1.212064449D+02  
 Ni(cr) Crystal Ref-Elm. <lambda trans 631K. Chase,1998 pp1697-  
 700.  
 2 j12/76 NI 1.00 0.00 0.00 0.00 0.00 1 58.69340  
 0.000  
 200.000 400.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 4786.000  
 -7.689131090D+05 1.433956218D+04-1.042751331D+02 3.926261320D-01-  
 6.986906890D-04  
 4.906078910D-07 0.000000000D+00 -6.543789970D+04  
 5.511391170D+02  
 400.000 631.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 4786.000  
 -3.345887340D+08 3.424527970D+06-1.394425564D+04 2.825654843D+01-  
 2.847789131D-02  
 1.142789828D-05 0.000000000D+00 -1.750250768D+07  
 8.179861400D+04  
 Ni(cr) Crystal Ref-Elm. >lambda trans 631K. Chase,1998 pp1697-  
 700.  
 2 j12/76 NI 1.00 0.00 0.00 0.00 0.00 2 58.69340  
 0.000  
 631.000 1200.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 4786.000  
 1.036354737D+09-6.813278550D+06 1.854367615D+04-2.673006535D+01  
 2.153531609D-02  
 -9.192464140D-06 1.624332987D-09 3.771960950D+07-  
 1.157617522D+05  
 1200.000 1728.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 4786.000  
 2.518440662D+09-9.895465230D+06 1.609737530D+04-1.386478566D+01  
 6.671320910D-03  
 -1.698988160D-06 1.788537986D-10 5.987658740D+07-  
 1.087743318D+05  
 Ni(L) Liquid. Ref-Elm. Chase,1998 pp1697-700.  
 1 j12/76 NI 1.00 0.00 0.00 0.00 0.00 3 58.69340  
 0.000  
 1728.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 4786.000  
 0.000000000D+00 0.000000000D+00 4.679890938D+00 0.000000000D+00  
 0.000000000D+00

0.000000000D+00 0.000000000D+00 -3.216258550D+02-  
2.335474714D+01  
NiS (b) Beta. Chase, 1998 pp1704-6.  
1 j12/76 NI 1.00S 1.00 0.00 0.00 0.00 1 90.75940 -  
87864.000  
200.000 652.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
8465.000  
9.281477840D+04-2.341897035D+03 2.156233266D+01-5.304222560D-02  
9.993984760D-05  
-9.111093130D-08 3.288570290D-11 -1.702746009D+03-  
1.117002463D+02  
NiS (a) ALpha. Chase, 1998 pp1704-6.  
1 j12/76 NI 1.00S 1.00 0.00 0.00 0.00 2 90.75940 -  
87864.000  
652.000 1249.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
8465.000  
2.424566967D+05-1.320914239D+03 7.077218200D+00 9.029383650D-05  
2.068184040D-06  
-6.559770780D-10 8.194048850D-14 -3.434758890D+03-  
3.562024750D+01  
NiS (L) Liquid. Chase, 1998 pp1704-6.  
1 j12/76 NI 1.00S 1.00 0.00 0.00 0.00 3 90.75940 -  
87864.000  
1249.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
8465.000  
0.000000000D+00 0.000000000D+00 9.233977709D+00 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -1.105334670D+04-  
4.576765033D+01  
NiS2 (cr) Crystal. Chase, 1998 pp1708-10.  
1 j 3/77 NI 1.00S 2.00 0.00 0.00 0.00 1 122.82540 -  
131377.600  
298.150 1280.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
0.000  
-1.676910840D+03 1.842877438D+01 7.671341480D+00 2.663682250D-03-  
1.892467189D-07  
1.078337009D-10-2.438956464D-14 -1.831575942D+04-  
3.578715100D+01  
NiS2 (L) Liquid. Chase, 1998 pp1708-10.  
1 j 3/77 NI 1.00S 2.00 0.00 0.00 0.00 2 122.82540 -  
131377.600  
1280.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
0.000  
0.000000000D+00 0.000000000D+00 1.094496248D+01 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -1.234477669D+04-  
4.971946503D+01  
Ni3S2 (a) Alpha. Pankratz, 1987 p225-6. Chase, 1998 pp1711-3 12/83.  
1 g12/00 NI 3.00S 2.00 0.00 0.00 0.00 1 240.21220 -  
217986.400  
200.000 834.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
21155.978  
-6.710970630D+05 9.870810610D+03-5.338151110D+01 2.311567743D-01-  
3.933292800D-04  
3.340311640D-07-1.054748249D-10 -7.620212300D+04  
2.954015489D+02  
Ni3S2 (b) Beta. Pankratz, 1987 p225-6.  
1 g12/00 NI 3.00S 2.00 0.00 0.00 0.00 2 240.21220 -  
217986.400  
834.000 1064.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
21155.978

-5.072819670D+04 0.000000000D+00 2.665250520D+01-4.426613790D-03  
 3.885431570D-07  
 0.000000000D+00 0.000000000D+00 -3.142142347D+04-  
 1.348956828D+02  
 Ni3S2(L) Liquid. Pankratz,1987 p225-6.  
 1 g12/00 NI 3.00S 2.00 0.00 0.00 0.00 3 240.21220 -  
 217986.400  
 1064.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 21155.978  
 0.000000000D+00 0.000000000D+00 2.274539329D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.720113051D+04-  
 1.099086536D+02  
 Ni3S4(cr) Crystal. Chase,1998 p1714.  
 1 j 3/77 NI 3.00S 4.00 0.00 0.00 0.00 1 304.34420 -  
 301115.000  
 298.150 1100.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 7.214883180D+03-7.806476430D+01 1.500658024D+01 1.653827825D-02  
 8.768311110D-07  
 -5.301784170D-10 1.279272852D-13 -4.096266670D+04-  
 6.825975310D+01  
 P(cr) White. Ref-Elm. Gurvich,1989 pt1 p395 pt2 p326.  
 Chase,1998a.  
 1 tpis89 P 1.00 0.00 0.00 0.00 0.00 1 30.97376  
 0.000  
 195.400 317.3007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 5360.000  
 -4.761561170D+06 1.135422659D+05-1.120481079D+03 5.889005080D+00-  
 1.727002916D-02  
 2.689248597D-05-1.737186959D-08 -4.829321490D+05  
 5.551556600D+03  
 P(L) Liquid. Ref-Elm. Gurvich,1989 pt1 p395 pt2 p326.  
 1 tpis89 P 1.00 0.00 0.00 0.00 0.00 2 30.97376  
 0.000  
 317.300 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 5360.000  
 0.000000000D+00 0.000000000D+00 3.141496011D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -8.621436240D+02-  
 1.272272999D+01  
 P4O10(cr) Crystal. Gurvich,1989 pt1 p417 pt2 p270.  
 2 tpis89 P 4.000 10.00 0.00 0.00 0.00 1 283.88904 -  
 3010100.000  
 100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 34220.000  
 -2.910475984D+04 0.000000000D+00 5.209612140D+00 7.058407940D-02  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.668178470D+05-  
 2.310786251D+01  
 298.150 699.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 34220.000  
 0.000000000D+00 0.000000000D+00 5.461897334D+00 8.078166964D-02-  
 4.072398734D-05  
 0.000000000D+00 0.000000000D+00 -3.668889200D+05-  
 2.561194012D+01  
 P4O10(L) Liquid. Gurvich,1989 pt1 p417 pt2 p270.  
 1 tpis89 P 4.000 10.00 0.00 0.00 0.00 3 283.88904 -  
 3010100.000  
 699.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 34220.000

0.000000000D+00 0.000000000D+00 4.450051777D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.765523910D+05-  
 2.311704609D+02  
 Pb(cr) Cubic. Ref-Elm. Gurvich,1991 pt1 p400 pt2 p337.  
 1 tpris91 PB 1.00 0.00 0.00 0.00 0.00 1 207.20000  
 0.000  
 200.000 600.6507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6870.000  
 -6.149670140D+05 1.065718060D+04-7.129898940D+01 2.668406702D-01-  
 5.182017320D-04  
 5.238665090D-07-2.151645616D-10 -4.974077560D+04  
 3.855826030D+02  
 Pb(L) Liquid. Ref-Elm. Gurvich,1991 pt1 p400 pt2 p337.  
 1 tpris91 PB 1.00 0.00 0.00 0.00 0.00 2 207.20000  
 0.000  
 600.650 3600.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6870.000  
 -3.798179327D+04 0.000000000D+00 4.364298076D+00-1.236392764D-03  
 4.946773773D-07  
 -5.231817630D-11 0.000000000D+00 -8.887330420D+02-  
 1.619559677D+01  
 PbBr2(cr) Rhombic Crystal. Gurvich,1991 pt1 p435 pt2 p361. -  
 2 tpris91 PB 1.00BR 2.00 0.00 0.00 0.00 1 367.00800  
 276700.000  
 100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19230.000  
 0.000000000D+00 0.000000000D+00 6.565717260D+00 1.959605208D-02-  
 3.191530530D-05  
 0.000000000D+00 0.000000000D+00 -3.582576310D+04-  
 2.245707569D+01  
 298.150 644.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19230.000  
 8.046174699D+04 0.000000000D+00 6.899264058D+00 5.925905435D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.532970360D+04-  
 2.124769272D+01  
 PbBr2(L) Liquid. Gurvich,1991 pt1 p435 pt2 p361. -  
 1 tpris91 PB 1.00BR 2.00 0.00 0.00 0.00 2 367.00800  
 276700.000  
 644.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19230.000  
 0.000000000D+00 0.000000000D+00 1.347042700D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.648036370D+04-  
 5.695842618D+01  
 PbCl2(cr) Rhombic Crystal. Gurvich,1991 pt1 p428 pt2 p356. -  
 1 tpris91 PB 1.00CL 2.00 0.00 0.00 0.00 1 278.10540  
 359400.000  
 200.000 774.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17150.000  
 2.697281121D+06-4.212942350D+04 2.651641932D+02-7.891350070D-01  
 1.316948609D-03  
 -1.123561948D-06 3.854416550D-10 1.522766773D+05-  
 1.434661776D+03  
 PbCl2(L) Liquid. Gurvich,1991 pt1 p428 pt2 p356. -  
 1 tpris91 PB 1.00CL 2.00 0.00 0.00 0.00 2 278.10540  
 359400.000  
 774.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17150.000

0.000000000D+00 0.000000000D+00 1.335015533D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.613690180D+04-  
 5.953419614D+01  
 PbF2 (II) Rhombic Crystal (II). Gurvich, 1991 pt1 p421 pt2 p351.  
 1 tpris91 PB 1.00F 2.00 0.00 0.00 0.00 1 245.19681 -  
 676000.000  
 298.150 583.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15000.000  
 1.363880734D+04 0.000000000D+00 7.104086711D+00 4.806777549D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -8.358963280D+04-  
 2.908385048D+01  
 PbF2 (I) Cubic Crystal (I). Gurvich, 1991 pt1 p421 pt2 p351.  
 2 tpris91 PB 1.00F 2.00 0.00 0.00 0.00 2 245.19681 -  
 676000.000  
 583.000 716.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15000.000  
 -7.862766417D+07 0.000000000D+00 1.154013526D+03 -2.413080386D+00  
 1.453441514D-03  
 0.000000000D+00 0.000000000D+00 -5.720487300D+05-  
 6.285579567D+03  
 716.000 1103.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15000.000  
 3.516663038D+07 0.000000000D+00 -1.580925394D+02 1.905776769D-01-  
 5.650555475D-05  
 0.000000000D+00 0.000000000D+00 4.370723820D+04  
 9.735936305D+02  
 PbF2 (L) Liquid. Gurvich, 1991 pt1 p421 pt2 p351.  
 1 tpris91 PB 1.00F 2.00 0.00 0.00 0.00 3 245.19681 -  
 676000.000  
 1103.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15000.000  
 0.000000000D+00 0.000000000D+00 1.310961199D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -8.458950020D+04-  
 6.282775717D+01  
 PbI2 (cr) Hexagonal Crystal. Gurvich, 1991 pt1 p441 pt2 p366.  
 2 tpris91 PB 1.00I 2.00 0.00 0.00 0.00 1 461.00894 -  
 176000.000  
 100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19500.000  
 -6.615857400D+03 0.000000000D+00 8.879658690D+00 1.758307313D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.391562477D+04-  
 3.012466437D+01  
 298.150 683.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19500.000  
 4.428402876D+04 0.000000000D+00 7.731062925D+00 3.690055096D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.348831172D+04-  
 2.387008226D+01  
 PbI2 (L) Liquid. Gurvich, 1991 pt1 p441 pt2 p366.  
 1 tpris91 PB 1.00I 2.00 0.00 0.00 0.00 2 461.00894 -  
 176000.000  
 683.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19500.000  
 0.000000000D+00 0.000000000D+00 1.310961199D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.355165613D+04-  
 5.237973135D+01



PbO(II-r) Tetragonal (II-red).Gurvich,1991 pt1 p409 pt2 p343.  
 2 tps91 PB 1.000 1.00 0.00 0.00 0.00 1 223.19940 -  
 218600.000  
 100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9225.000  
 0.000000000D+00 0.000000000D+00 8.050624580D-01 2.884978163D-02-  
 4.302158100D-05  
 0.000000000D+00 0.000000000D+00 -2.743361905D+04-  
 3.117085753D+00  
 298.150 762.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9225.000  
 -6.651023332D+03 0.000000000D+00 4.939557472D+00 2.406636110D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.789339075D+04-  
 2.073932502D+01

PbO(I-y) Rhombic (I-yellow).Gurvich,1991 pt1 p409 pt2 p343.  
 1 tps91 PB 1.000 1.00 0.00 0.00 0.00 2 223.19940 -  
 218600.000  
 762.000 1160.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9225.000  
 -3.360390450D+04 0.000000000D+00 5.407414267D+00 1.595644241D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.802576574D+04-  
 2.321766400D+01

PbO(L) Liquid.Gurvich,1991 pt1 p409 pt2 p343.  
 1 tps91 PB 1.000 1.00 0.00 0.00 0.00 3 223.19940 -  
 218600.000  
 1160.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9225.000  
 0.000000000D+00 0.000000000D+00 7.817658527D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.664258145D+04-  
 3.570913839D+01

PbO2(cr) Tetragonal. Gurvich,1991 pt1 p415 p52 p346.  
 2 tps91 PB 1.000 2.00 0.00 0.00 0.00 1 239.19880 -  
 276000.000  
 100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10962.000  
 0.000000000D+00 0.000000000D+00 1.007530476D-01 4.035527600D-02-  
 5.395750800D-05  
 0.000000000D+00 0.000000000D+00 -3.454199070D+04-  
 1.557803514D+00  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10962.000  
 -2.593057198D+05 0.000000000D+00 1.010402297D+01 5.003301457D-04  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.709944890D+04-  
 5.052640331D+01

PbS(cr) Cubic. Gurvich,1991 pt1 p445 p52 p370.  
 2 tps91 PB 1.00S 1.00 0.00 0.00 0.00 1 239.26600 -  
 99474.800  
 100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11510.000  
 -1.110196130D+04 0.000000000D+00 5.788552660D+00 9.715425300D-04  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.377027529D+04-  
 2.236417313D+01  
 298.150 1386.5007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11510.000  
 -7.529006520D+04 0.000000000D+00 7.331760982D+00-2.262310106D-03  
 1.609234940D-06

0.000000000D+00 0.000000000D+00 -1.431615352D+04-  
 3.062514348D+01  
 PbS(L) Liquid. Gurvich,1991 pt1 p445 p52 p370.  
 1 tps91 PB 1.00S 1.00 0.00 0.00 0.00 2 239.26600 -  
 99474.800  
 1386.500 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11510.000  
 0.000000000D+00 0.000000000D+00 8.058201866D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.007241100D+04-  
 3.316574241D+01  
 Pb2O3(cr) Monoclinic. Gurvich,1991 pt1 p417 pt2 p348.  
 2 tps91 PB 2.00O 3.00 0.00 0.00 0.00 1 462.39820 -  
 491700.000  
 100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 20880.000  
 0.000000000D+00 0.000000000D+00 1.574967406D+00 6.633690300D-02-  
 9.449445980D-05  
 0.000000000D+00 0.000000000D+00 -6.172080000D+04-  
 6.282642160D+00  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 20880.000  
 -3.314687215D+05 0.000000000D+00 1.505921576D+01 5.443495768D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.498118220D+04-  
 7.101946635D+01  
 Pb3O4(cr) Tetragonal. Gurvich,1991 pt1 p418 pt2 p349.  
 1 tps91 PB 3.00O 4.00 0.00 0.00 0.00 1 685.59760 -  
 720000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 29830.000  
 7.031601470D+06-8.770415980D+04 4.195886490D+02-9.058738460D-01  
 1.138287119D-03  
 -7.358926050D-07 1.922732625D-10 3.431611340D+05-  
 2.394229365D+03  
 Rb(cr) Cubic. Ref-Elm. Cox,1989 p260. Chase,1998a p1849 12/83.  
 1 coda89 RB 1.00 0.00 0.00 0.00 0.00 1 85.46780 -  
 0.000  
 100.000 312.4707 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7489.000  
 -1.693678854D+05 5.116764690D+03-5.686760910D+01 3.403543550D-01-  
 9.347996350D-04  
 1.017512352D-06 0.000000000D+00 -2.164547399D+04  
 2.805351095D+02  
 Rb(L) Liquid. Ref-Elm. Cox,1989 p260.  
 2 coda89 RB 1.00 0.00 0.00 0.00 0.00 2 85.46780  
 0.000  
 312.470 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7489.000  
 2.365752770D+04 2.865695009D+02 1.546589030D+00 5.164698120D-03-  
 6.065846790D-06  
 3.347806150D-09-5.178101420D-13 -1.933656171D+03  
 1.060307276D+00  
 1000.000 2100.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 7489.000  
 -3.672685780D+05 1.779065421D+03-3.414096790D-01 5.322070690D-03-  
 4.262302730D-06  
 1.699676170D-09-4.416789770D-14 -1.110894373D+04  
 1.477099469D+01  
 RbBO2(b) Gurvich,1982 pt1 p458 pt2 p482.

2 tps82 RB 1.00B 1.000 2.00 0.00 0.00 1 128.27760 -  
 975000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13310.000  
 1.320700184D+06-2.114255330D+04 1.338015047D+02-3.804509820D-01  
 6.570568430D-04  
 -5.884791840D-07 2.152384344D-10 -2.010026759D+04-  
 7.254857290D+02  
 500.000 968.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13310.000  
 -1.553422560D+05 0.000000000D+00 9.425074910D+00 3.853433670D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.207672511D+05-  
 4.437890740D+01  
 RbBO2 (a) Gurvich,1982 pt1 p458 pt2 p482.  
 1 tps82 RB 1.00B 1.000 2.00 0.00 0.00 2 128.27760 -  
 975000.000  
 968.000 1133.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13310.000  
 0.000000000D+00 0.000000000D+00 1.298934032D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.222516025D+05-  
 6.507104425D+01  
 RbBO2 (L) Gurvich,1982 pt1 p458 pt2 p482.  
 1 tps82 RB 1.00B 1.000 2.00 0.00 0.00 3 128.27760 -  
 975000.000  
 1133.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13310.000  
 0.000000000D+00 0.000000000D+00 1.743939210D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.235650894D+05-  
 9.307583456D+01  
 RbBr (cr) Cubic. Gurvich,1982 pt1 p445 pt2 p469.  
 1 tps82 RB 1.00BR 1.00 0.00 0.00 0.00 1 165.37180 -  
 394770.000  
 200.000 965.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13060.000  
 -5.724525880D+04 9.082670760D+02 4.275929780D-01 1.751269798D-02-  
 2.421969308D-05  
 1.854230436D-08-5.603980870D-12 -5.357247720D+04  
 9.232346100D+00  
 RbBr (L) Liquid. Gurvich,1982 pt1 p445 pt2 p469.  
 1 tps82 RB 1.00BR 1.00 0.00 0.00 0.00 2 165.37180 -  
 394770.000  
 965.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13060.000  
 0.000000000D+00 0.000000000D+00 8.755777550D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.852456540D+04-  
 3.604442573D+01  
 RbCL (cr) Cubic. Gurvich,1982 pt1 p441 pt2 p466.  
 1 tps82 RB 1.00CL 1.00 0.00 0.00 0.00 1 120.92050 -  
 435220.000  
 200.000 997.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12160.000  
 -5.731907690D+04 4.298433250D+02 4.955874940D+00 9.930643910D-04  
 3.857679940D-06  
 -4.516778380D-09 1.683809372D-12 -5.653364290D+04-  
 1.609477359D+01  
 RbCL (L) Liquid. Gurvich,1982 pt1 p441 pt2 p466.

1 tps82 RB 1.00CL 1.00 0.00 0.00 0.00 2 120.92050 -  
 435220.000  
 997.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12160.000  
 0.000000000D+00 0.000000000D+00 8.827940552D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.345006300D+04-  
 3.845805693D+01  
 RbF(cr) Cubic. Gurvich,1982 pt1 p438 pt2 p463.  
 1 tps82 RB 1.00F 1.00 0.00 0.00 0.00 1 104.46620 -  
 559700.000  
 298.150 1068.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10900.000  
 5.640741306D+03 0.000000000D+00 5.092663308D+00 3.129949931D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.895462790D+04-  
 2.057230003D+01  
 RbF(L) Liquid. Gurvich,1982 pt1 p438 pt2 p463.  
 1 tps82 RB 1.00F 1.00 0.00 0.00 0.00 2 104.46620 -  
 559700.000  
 1068.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10900.000  
 0.000000000D+00 0.000000000D+00 8.539288545D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.775044270D+04-  
 3.835948403D+01  
 RbH(cr) Cubic. Gurvich,1982 pt1 p434 pt2 p458.  
 1 tps82 RB 1.00H 1.00 0.00 0.00 0.00 1 86.47574 -  
 52300.000  
 298.150 858.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9100.000  
 -6.384020225D+04 0.000000000D+00 4.263149602D+00 3.963552873D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -7.951554350D+03-  
 1.816921793D+01  
 RbH(L) Liquid. Gurvich,1982 pt1 p434 pt2 p458.  
 1 tps82 RB 1.00H 1.00 0.00 0.00 0.00 2 86.47574 -  
 52300.000  
 858.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9100.000  
 0.000000000D+00 0.000000000D+00 6.735213500D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.893290150D+03-  
 2.833905350D+01  
 RbI(cr) Cubic. Gurvich,1982 pt1 p448 pt2 p472.  
 1 tps82 RB 1.00I 1.00 0.00 0.00 0.00 1 212.37227 -  
 333600.000  
 200.000 929.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13340.000  
 -1.871461077D+05 2.207646572D+03-3.199388250D+00 1.739850250D-02-  
 1.184152545D-05  
 3.313152520D-09 3.472456000D-13 -5.305010310D+04  
 3.417793530D+01  
 RbI(L) Liquid. Gurvich,1982 pt1 p448 pt2 p472.  
 1 tps82 RB 1.00I 1.00 0.00 0.00 0.00 2 212.37227 -  
 333600.000  
 929.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13340.000  
 0.000000000D+00 0.000000000D+00 8.671587382D+00 0.000000000D+00  
 0.000000000D+00

0.000000000D+00 0.000000000D+00 -4.112940250D+04-  
3.435941214D+01  
RbNO2 (I) Cubic. Gurvich,1982 pt1 p453 pt2 p477.  
1 tps82 RB 1.00N 1.000 2.00 0.00 0.00 1 131.47334 -  
367000.000  
298.150 695.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
23400.000  
0.000000000D+00 0.000000000D+00 9.108895172D+00 3.333690139D-03  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -4.700369140D+04-  
3.340874045D+01  
RbNO2 (L) Liquid. Gurvich,1982 pt1 p453 pt2 p477.  
1 tps82 RB 1.00N 1.000 2.00 0.00 0.00 2 131.47334 -  
367000.000  
695.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
23400.000  
0.000000000D+00 0.000000000D+00 1.250825364D+01 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -4.710583050D+04-  
5.124298955D+01  
RbNO3 (IV) Hexagonal. Gurvich,1982 pt1 p455 pt2 p479.  
1 tps82 RB 1.00N 1.000 3.00 0.00 0.00 1 147.47274 -  
494700.000  
200.000 437.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
19640.000  
1.211253372D+07-2.028159094D+05 1.325899840D+03-4.151421820D+00  
6.401606600D-03  
-3.822822630D-06 0.000000000D+00 8.768873850D+05-  
7.162144700D+03  
RbNO3 (III) Cubic. Gurvich,1982 pt1 p455 pt2 p479.  
1 tps82 RB 1.00N 1.000 3.00 0.00 0.00 2 147.47274 -  
494700.000  
437.000 493.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
19640.000  
0.000000000D+00 0.000000000D+00 9.120561524D+00 1.643716828D-02  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -6.277664760D+04-  
3.918776498D+01  
RbNO3 (II) Hexagonal. Gurvich,1982 pt1 p455 pt2 p479.  
1 tps82 RB 1.00N 1.000 3.00 0.00 0.00 3 147.47274 -  
494700.000  
493.000 556.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
19640.000  
0.000000000D+00 0.000000000D+00 1.078616780D+02-2.821762196D-01  
0.000000000D+00  
3.922207081D-07 0.000000000D+00 -8.057470150D+04-  
5.191016028D+02  
RbNO3 (I) Cubic. Gurvich,1982 pt1 p455 pt2 p479.  
1 tps82 RB 1.00N 1.000 3.00 0.00 0.00 4 147.47274 -  
494700.000  
556.000 583.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
19640.000  
0.000000000D+00 0.000000000D+00 1.755966377D+01 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -6.449488250D+04-  
8.253206472D+01  
RbNO3 (L) Liquid. Gurvich,1982 pt1 p455 pt2 p479.  
1 tps82 RB 1.00N 1.000 3.00 0.00 0.00 5 147.47274 -  
494700.000  
583.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
19640.000

0.000000000D+00 0.000000000D+00 1.755966377D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.394163280D+04-  
 8.158309442D+01  
 RbOH(b) Beta. Gurvich,1997.  
 1 g 8/97 RB 1.000 1.00H 1.00 0.00 0.00 1 102.47514 -  
 41880.000  
 298.150 508.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13500.000  
 0.000000000D+00 0.000000000D+00 6.589925323D+00 5.731305874D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.258929920D+04-  
 2.794998878D+01  
 RbOH(c) Gamma. Gurvich,1997.  
 1 g 8/97 RB 1.000 1.00H 1.00 0.00 0.00 2 102.47514 -  
 41880.000  
 508.000 658.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13500.000  
 0.000000000D+00 0.000000000D+00 9.140646893D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.248404970D+04-  
 3.962855491D+01  
 RbOH(L) Liquid. Gurvich,1997.  
 1 g 8/97 RB 1.000 1.00H 1.00 0.00 0.00 3 102.47514 -  
 41880.000  
 658.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13500.000  
 0.000000000D+00 0.000000000D+00 1.034336359D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.231326390D+04-  
 4.597096049D+01  
 RbO2(b) Beta,hexagonal. Gurvich,1982 pt1 p430 pt2 p453.  
 1 tpi82 RB 1.000 2.00 0.00 0.00 0.00 1 117.46660 -  
 279100.000  
 200.000 423.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16760.000  
 -5.914373690D+05 9.356154690D+03-5.173703230D+01 1.872603527D-01-  
 2.664203296D-04  
 1.581120816D-07 0.000000000D+00 -7.971547560D+04  
 2.930911089D+02  
 RbO2(a) Alpha,cubic. Gurvich,1982 pt1 p430 pt2 p453.  
 1 tpi82 RB 1.000 2.00 0.00 0.00 0.00 2 117.46660 -  
 279100.000  
 423.000 813.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16760.000  
 0.000000000D+00 0.000000000D+00 1.058390693D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.680173520D+04-  
 4.488768335D+01  
 RbO2(L) Liquid. Gurvich,1982 pt1 p430 pt2 p453.  
 1 tpi82 RB 1.000 2.00 0.00 0.00 0.00 3 117.46660 -  
 279100.000  
 813.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16760.000  
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.544940050D+04-  
 5.145193248D+01  
 Rb2CO3(a) Alpha,monoclinic. Gurvich,1982 pt1 p457 pt2 p481.  
 1 tpi82 RB 2.00C 1.000 3.00 0.00 0.00 1 230.94450 -  
 1132600.000

200.000 576.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 24480.000  
 -1.377487286D+06 2.415872404D+04-1.620555595D+02 6.425655960D-01-  
 1.249826185D-03  
 1.304525231D-06-5.552423710D-10 -2.500033904D+05  
 8.719586300D+02  
 Rb2CO3 (b) Beta, hexagonal. Gurvich, 1982 pt1 p457 pt2 p481.  
 1 tpris82 RB 2.00C 1.000 3.00 0.00 0.00 2 230.94450 -  
 1132600.000  
 576.000 1146.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 24480.000  
 0.000000000D+00 0.000000000D+00 1.355678206D+01 8.280944999D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.405896222D+05-  
 5.801044809D+01  
 Rb2CO3 (L) Liquid. Gurvich, 1982 pt1 457 pt2 p481.  
 1 tpris82 RB 2.00C 1.000 3.00 0.00 0.00 3 230.94450 -  
 1132600.000  
 1146.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 24480.000  
 0.000000000D+00 0.000000000D+00 2.465569228D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.442630744D+05-  
 1.235531008D+02  
 Rb2O (c) Gamma, cubic. Gurvich, 1982 pt1 p431 pt2 p454.  
 1 tpris82 RB 2.00O 1.00 0.00 0.00 0.00 1 186.93500 -  
 338000.000  
 298.150 543.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15600.000  
 0.000000000D+00 0.000000000D+00 6.190743652D+00 9.087246272D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.290149280D+04-  
 2.294776447D+01  
 Rb2O (b) Beta, cubic. Gurvich, 1982 pt1 p431 pt2 p454.  
 1 tpris82 RB 2.00O 1.00 0.00 0.00 0.00 2 186.93500 -  
 338000.000  
 543.000 613.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15600.000  
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.464679770D+04-  
 5.461093903D+01  
 Rb2O (a) Alpha, hexagonal. Gurvich, 1982 pt1 p431 pt2 p454.  
 1 tpris82 RB 2.00O 1.00 0.00 0.00 0.00 3 186.93500 -  
 338000.000  
 613.000 778.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15600.000  
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.416571100D+04-  
 5.382613205D+01  
 Rb2O (L) Liquid. Gurvich, 1982 pt1 p431 pt2 p454.  
 1 tpris82 RB 2.00O 1.00 0.00 0.00 0.00 4 186.93500 -  
 338000.000  
 778.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15600.000  
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.176027770D+04-  
 5.073431535D+01  
 Rb2O2 (b) Beta, rhombic Gurvich, 1982 pt1 p433 pt2 p456.

1 tpis82 RB 2.000 2.00 0.00 0.00 0.00 1 202.93440 -  
 410000.000  
 298.150 398.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19700.000  
 0.000000000D+00 0.000000000D+00 2.566116344D+00 2.890861879D-02  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.136136520D+04-  
 3.996333599D+00  
 Rb2O2(a) Alpha,cubic. Gurvich,1982 pt1 p433 pt2 p456.  
 1 tpis82 RB 2.000 2.00 0.00 0.00 0.00 2 202.93440 -  
 410000.000  
 398.000 843.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19700.000  
 0.000000000D+00 0.000000000D+00 1.407178535D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.365100100D+04-  
 6.136883861D+01  
 Rb2O2(L) Liquid. Gurvich,1982 pt1 p433 pt2 p456.  
 1 tpis82 RB 2.000 2.00 0.00 0.00 0.00 3 202.93440 -  
 410000.000  
 843.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19700.000  
 0.000000000D+00 0.000000000D+00 1.611640373D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.284890920D+04-  
 7.214727369D+01  
 Rb2SO4(a) Alpha,rhombic. Gurvich,1982 pt1 p451 pt2 p475. -  
 3 tpis82 RB 2.00S 1.000 4.00 0.00 0.00 1 266.99920 -  
 1435900.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 27014.000  
 -1.192448350D+07 2.294293959D+05-1.785117228D+03 7.309062720D+00-  
 1.617521748D-02  
 1.861676545D-05-8.714648070D-09 -1.202291196D+06  
 9.289553650D+03  
 500.000 800.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 27014.000  
 -4.871322610D+05 0.000000000D+00 2.853725036D+01-3.587804810D-02  
 4.220439770D-05  
 0.000000000D+00 0.000000000D+00 -1.816178572D+05-  
 1.327574146D+02  
 800.000 931.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 27014.000  
 0.000000000D+00 0.000000000D+00 3.464686434D+02-6.082068577D-01  
 0.000000000D+00  
 3.246132364D-07 0.000000000D+00 -2.782463487D+05-  
 1.841656965D+03  
 Rb2SO4(b) Beta,hexagonal. Gurvich,1982 pt1 p451 pt2 p475. -  
 1 tpis82 RB 2.00S 1.000 4.00 0.00 0.00 2 266.99920 -  
 1435900.000  
 931.000 1343.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 27014.000  
 0.000000000D+00 0.000000000D+00 1.107353290D+01 1.230667833D-02  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.739435450D+05-  
 3.919109508D+01  
 Rb2SO4(L) Liquid. Gurvich,1982 pt1 p451 pt2 p475. -  
 1 tpis82 RB 2.00S 1.000 4.00 0.00 0.00 3 266.99920 -  
 1435900.000  
 1343.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 27014.000



```

0.000000000D+00 0.000000000D+00 2.483609978D+01 0.000000000D+00
0.000000000D+00
0.000000000D+00 0.000000000D+00 -1.768420750D+05-
1.184499504D+02
S(a) Alpha. Ref-Elm. Gurvich,1989 pt1 p265 pt2 p160.
1 tpris89 S 1.00 0.00 0.00 0.00 0.00 1 32.06600
0.000
200.000 368.3007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
4412.000
-1.035710779D+04 0.000000000D+00 1.866766938D+00 4.256140250D-03-
3.265252270D-06
0.000000000D+00 0.000000000D+00 -7.516389580D+02-
7.961066980D+00
S(b) Beta. Ref-Elm. Gurvich,1989 pt1 p265 pt2 p160.
1 tpris89 S 1.00 0.00 0.00 0.00 0.00 2 32.06600
0.000
368.300 388.3607 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
4412.000
0.000000000D+00 0.000000000D+00 2.080514131D+00 2.440879557D-03
0.000000000D+00
0.000000000D+00 0.000000000D+00 -6.852714730D+02-
8.607846750D+00
S(L) Liquid. Ref-Elm. Gurvich,1989 pt1 p265 pt2 p160.
5 tpris89 S 1.00 0.00 0.00 0.00 0.00 3 32.06600
0.000
388.360 428.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
4412.000
-6.366550765D+07 0.000000000D+00 2.376860693D+03-7.888076026D+00
7.376076522D-03
0.000000000D+00 0.000000000D+00 -6.356594920D+05-
1.186929589D+04
428.150 432.2507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
4412.000
0.000000000D+00 0.000000000D+00 6.928522306D+03-3.254655981D+01
3.824448176D-02
0.000000000D+00 0.000000000D+00 -9.832222680D+05-
3.154806751D+04
432.250 453.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
4412.000
0.000000000D+00 0.000000000D+00 1.649945697D+02-6.843534977D-01
7.315907973D-04
0.000000000D+00 0.000000000D+00 -2.638846929D+04-
7.681730097D+02
453.150 717.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
4412.000
1.972984578D+06 0.000000000D+00-2.441009753D+01 6.090352889D-02-
3.744069103D-05
0.000000000D+00 0.000000000D+00 1.113013440D+04
1.363174183D+02
717.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
4412.000
0.000000000D+00 0.000000000D+00 3.848693429D+00 0.000000000D+00
0.000000000D+00
0.000000000D+00 0.000000000D+00 -8.284589830D+02-
1.736128237D+01
SCL2(L) Chase,1998 p855.
1 j 6/78 S 1.00CL 2.00 0.00 0.00 0.00 1 102.97140 -
49790.000
298.150 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
0.000

```

0.000000000D+00 0.000000000D+00 1.094496248D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -9.251567000D+03-  
 4.026872255D+01  
 S2CL2(L) Chase,1998 p858.  
 1 j 6/78 S 2.00CL 2.00 0.00 0.00 0.00 1 135.03740 -  
 58158.000  
 298.150 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 0.000000000D+00 0.000000000D+00 1.494856582D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.145167466D+04-  
 5.824880790D+01  
 Sc(a) Alpha. Ref-Elm. Gurvich,1982 pt1 p137 pt2 p138.  
 2 tpris82 SC 1.00 0.00 0.00 0.00 0.00 1 44.95591  
 0.000  
 100.000 400.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 5207.000  
 -5.723537690D+03 0.000000000D+00 1.835072325D+00 9.478861990D-03-  
 2.317188582D-05  
 2.004221829D-08 0.000000000D+00 -8.225089040D+02-  
 8.279121410D+00  
 400.000 1609.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 5207.000  
 -2.296409436D+04 0.000000000D+00 3.590296910D+00 -1.480249906D-03  
 2.132230702D-06  
 -4.653598600D-10 0.000000000D+00 -1.099543829D+03-  
 1.605255360D+01  
 Sc(b) Beta. Ref-Elm. Gurvich,1982 pt1 p137 pt2 p138.  
 1 tpris82 SC 1.00 0.00 0.00 0.00 0.00 2 44.95591  
 0.000  
 1609.000 1814.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 5207.000  
 0.000000000D+00 0.000000000D+00 5.316007798D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.113439951D+03-  
 2.875686543D+01  
 Sc(L) Liquid. Ref-Elm. Gurvich,1982 pt1 p137 pt2 p138.  
 1 tpris82 SC 1.00 0.00 0.00 0.00 0.00 3 44.95591  
 0.000  
 1814.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 5207.000  
 0.000000000D+00 0.000000000D+00 5.291953464D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.373974847D+03-  
 2.764152183D+01  
 Sc203(cr) Cubic. Gurvich,1982 pt1 p145 pt2 p150.  
 2 tpris82 SC 2.000 3.00 0.00 0.00 0.00 1 137.91002 -  
 1908600.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13930.000  
 -2.372563268D+06 4.573798990D+04 -3.655376590D+02 1.588230977D+00-  
 3.584389210D-03  
 4.185870320D-06 -1.985472581D-09 -4.353786390D+05  
 1.884709407D+03  
 500.000 2762.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13930.000  
 -2.669869135D+05 0.000000000D+00 1.386002327D+01 1.535415402D-03  
 1.928963573D-07  
 0.000000000D+00 0.000000000D+00 -2.346482672D+05-  
 7.170005710D+01

```

Sc2O3(L)          Liquid. Gurvich,1982 pt1 p145 pt2 p150.
 1 tpis82 SC  2.000  3.00  0.00  0.00  0.00  2  137.91002  -
1908600.000
 2762.000  6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0
13930.000
 0.000000000D+00 0.000000000D+00 2.405433393D+01 0.000000000D+00
0.000000000D+00
 0.000000000D+00 0.000000000D+00 -2.402224225D+05-
1.419525042D+02
Si(cr)           Cubic. Ref-Elm. Gurvich,1991 pt1 p236 pt2 p220.
 2 tpis91 SI  1.00  0.00  0.00  0.00  0.00  1  28.08550
0.000
 200.000  298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0
3217.471
-2.323538208D+04 0.000000000D+00 2.102021680D+00 1.809220552D-03
0.000000000D+00
 0.000000000D+00 0.000000000D+00 -7.850635210D+02-
1.038427318D+01
 298.150  1690.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0
3217.471
-5.232559740D+04 0.000000000D+00 2.850169415D+00 3.975166970D-04
0.000000000D+00
 0.000000000D+00 0.000000000D+00 -1.042947234D+03-
1.438964187D+01
Si(L)           Liquid. Ref-Elm. Gurvich,1991 pt1 p236 pt2 p220.
 1 tpis91 SI  1.00  0.00  0.00  0.00  0.00  2  28.08550
0.000
 1690.000  6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0
3217.471
 0.000000000D+00 0.000000000D+00 3.271389414D+00 0.000000000D+00
0.000000000D+00
 0.000000000D+00 0.000000000D+00 4.882667110D+03-
1.326611073D+01
SiC(b)          Beta,cubic. Gurvich,1991 pt1 p298 pt2 p264.
 2 tpis91 SI  1.00C  1.00  0.00  0.00  0.00  1  40.09620  -
73000.000
 100.000  298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0
3272.000
-2.285496383D+03 0.000000000D+00-5.349100620D-01 1.271547084D-02
0.000000000D+00
 0.000000000D+00 0.000000000D+00 -9.193174900D+03
1.241441354D+00
 298.150  3105.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0
3272.000
-1.269106658D+05 0.000000000D+00 3.757286960D+00 3.481744565D-03-
1.620660748D-06
 2.611097948D-10 0.000000000D+00 -1.046667760D+04-
2.109198538D+01
SiC(L)          Liquid. Gurvich,1991 pt1 p298 pt2 p264.
 1 tpis91 SI  1.00C  1.00  0.00  0.00  0.00  2  40.09620  -
73000.000
 3103.000  6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0
3272.000
 0.000000000D+00 0.000000000D+00 7.577115188D+00 0.000000000D+00
0.000000000D+00
 0.000000000D+00 0.000000000D+00 -7.787459000D+03-
4.367596159D+01
SiO2(a-qz)      Alpha-quartz,hexagonal. Gurvich,1991 pt1 p250 pt2 p228.
 1 tpis91 SI  1.00O  2.00  0.00  0.00  0.00  1  60.08430  -
910700.000

```

200.000 848.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6916.000  
 -5.776895500D+05 7.214661110D+03-3.145730294D+01 7.412177150D-02-  
 8.670077820D-06  
 -1.080461312D-07 8.316324910D-11 -1.462398375D+05  
 1.842424399D+02  
 SiO2 (b-qz) Beta-quartz, hexagonal. Gurvich, 1991 pt1 p250 pt2 p228.  
 1 tpris91 SI 1.000 2.00 0.00 0.00 0.00 2 60.08430 -  
 910700.000  
 848.000 1200.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6916.000  
 2.317635074D+04 0.000000000D+00 7.026511484D+00 1.241925261D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.117012474D+05-  
 3.580751356D+01  
 SiO2 (b-crt) Beta-cristobalite, cubic. Gurvich, 1991 pt1 p250 pt2  
 p228.  
 1 tpris91 SI 1.000 2.00 0.00 0.00 0.00 3 60.08430 -  
 910700.000  
 1200.000 1996.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6916.000  
 -5.356419079D+05 0.000000000D+00 9.331036946D+00-7.306503931D-04  
 3.339944266D-07  
 0.000000000D+00 0.000000000D+00 -1.134326721D+05-  
 4.998768383D+01  
 SiO2 (L) Liquid. Gurvich, 1991 pt1 p250 pt2 p228.  
 1 tpris91 SI 1.000 2.00 0.00 0.00 0.00 4 60.08430 -  
 910700.000  
 1996.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6916.000  
 0.000000000D+00 0.000000000D+00 1.004268442D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.140002976D+05-  
 5.554279592D+01  
 SiS (cr) Crystal. Gurvich, 1991 pt1 p289 pt2 p257.  
 1 tpris91 SI 1.00S 1.00 0.00 0.00 0.00 1 60.15150 -  
 168737.210  
 298.150 1363.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9000.490  
 0.000000000D+00 0.000000000D+00 4.873408054D+00 1.807202108D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.182763678D+04-  
 2.072841584D+01  
 SiS (L) Liquid. Gurvich, 1991 pt1 p289 pt2 p257.  
 1 tpris91 SI 1.00S 1.00 0.00 0.00 0.00 2 60.15150 -  
 168737.210  
 1363.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9000.490  
 0.000000000D+00 0.000000000D+00 8.058201866D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.076140696D+04-  
 3.851581605D+01  
 SiS2 (cr) Tetragonal. Gurvich, 1991 pt1 p293 pt2 p259.  
 2 tpris91 SI 1.00S 2.00 0.00 0.00 0.00 1 92.21750 -  
 287000.000  
 100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11180.490  
 -1.489679569D+04 0.000000000D+00 3.921710460D+00 1.226970632D-02  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.628253940D+04-  
 1.684224727D+01

298.150 1363.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11180.490  
 0.000000000D+00 0.000000000D+00 6.423349061D+00 3.317212921D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.658052990D+04-  
 2.834259902D+01  
 SiS2(L) Liquid. Gurvich,1991 pt1 p293 pt2 p259.  
 1 tpiS91 SI 1.00S 2.00 0.00 0.00 0.00 2 92.21750 -  
 287000.000  
 1363.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11180.490  
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.909260770D+04-  
 6.276638967D+01  
 Si2N2O(cr) Fegley,1981.  
 2 g 7/95 SI 2.00N 2.000 1.00 0.00 0.00 1 100.18388 -  
 947700.000  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 -7.783293180D+06 7.787697680D+04-3.226727260D+02 7.513788890D-01-  
 9.139450720D-04  
 5.774402010D-07-1.479973902D-10 -5.139865410D+05  
 1.873124449D+03  
 1000.000 2500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 -7.414096340D+06 2.559424417D+04-2.535540920D+01 3.208894230D-02-  
 1.340182230D-05  
 3.075006784D-09-2.892800339D-13 -2.762647725D+05  
 1.907774092D+02  
 Si3N4(cr) Hexagonal. Gurvich,1991 pt1 p297 pt2 p262.  
 2 tpiS91 SI 3.00N 4.00 0.00 0.00 0.00 1 140.28346 -  
 787800.000  
 100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12113.490  
 -1.136434515D+04 0.000000000D+00-4.993435710D-01 3.962318940D-02  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -9.640037870D+04-  
 1.086768954D+00  
 298.150 4000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 12113.490  
 -2.910454134D+05 0.000000000D+00 1.189210188D+01 9.349799327D-03-  
 2.551082385D-06  
 2.857654871D-10 0.000000000D+00 -9.966541740D+04-  
 6.412447976D+01  
 Sn(cr) CrI,tetragonal. Ref-Elm. Gurvich,1991 pt1 p350 pt2  
 p300.  
 1 tpiS91 SN 1.00 0.00 0.00 0.00 0.00 1 118.71000  
 0.000  
 200.000 505.1187 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6323.000  
 -9.970568110D+05 1.865056292D+04-1.393005103D+02 5.652800870D-01-  
 1.229162587D-03  
 1.398259924D-06-6.465843270D-10 -8.479846440D+04  
 7.317981190D+02  
 Sn(L) Liquid. Ref-Elm. Gurvich,1991 pt1 p350 pt2 p300.  
 1 tpiS91 SN 1.00 0.00 0.00 0.00 0.00 2 118.71000  
 0.000  
 505.118 4700.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6323.000

9.847844311D+04 0.000000000D+00 3.028921728D+00 2.531718646D-04-  
 1.960428215D-08  
 0.000000000D+00 0.000000000D+00 2.209652103D+02-  
 9.089783541D+00  
 SnBr2(cr) Rhombic. Gurvich,1991 pt1 p379 pt2 p322.  
 2 tps91 SN 1.00BR 2.00 0.00 0.00 0.00 1 278.51800 -  
 253600.000  
 100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18670.000  
 -1.072142073D+04 0.000000000D+00 8.650388720D+00 3.246938990D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.326028440D+04-  
 3.191324070D+01  
 298.150 503.4007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18670.000  
 1.596365871D+05 0.000000000D+00 4.310656912D+00 1.137469316D-02  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.175626170D+04-  
 8.652273965D+00  
 SnBr2(L) Liquid. Gurvich,1991 pt1 p379 pt2 p322.  
 2 tps91 SN 1.00BR 2.00 0.00 0.00 0.00 2 278.51800 -  
 253600.000  
 503.400 860.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18670.000  
 2.804494793D+05 0.000000000D+00 1.427732963D+01-2.218170403D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.305162210D+04-  
 6.008238208D+01  
 860.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18670.000  
 0.000000000D+00 0.000000000D+00 1.274879698D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.288346740D+04-  
 5.185141223D+01  
 SnBr4(cr) Monoclinic. Gurvich,1991 pt1 p382 pt2 p325.  
 1 tps91 SN 1.00BR 4.00 0.00 0.00 0.00 1 438.32600 -  
 388000.000  
 200.000 302.2507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 31260.000  
 -3.870038960D+06 0.000000000D+00 3.663330300D+02-1.775658617D+00  
 2.504656832D-03  
 0.000000000D+00 0.000000000D+00 -1.120730416D+05-  
 1.659626236D+03  
 SnBr4(L) Liquid. Gurvich,1991 pt1 p382 pt2 p325.  
 2 tps91 SN 1.00BR 4.00 0.00 0.00 0.00 2 438.32600 -  
 388000.000  
 302.250 470.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 31260.000  
 1.124780655D+05 0.000000000D+00 1.859869072D+01-4.792826035D-04  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.036569340D+04-  
 6.913668591D+01  
 470.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 31260.000  
 0.000000000D+00 0.000000000D+00 1.888265213D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.079140710D+04-  
 7.136367786D+01  
 SnCL2(cr) Rhombic. Gurvich,1991 pt1 p372 pt2 p316.  
 1 tps91 SN 1.00CL 2.00 0.00 0.00 0.00 1 189.61540 -  
 333000.000

200.000 520.2007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17330.000  
 -3.455659100D+05 5.121048940D+03-2.179939832D+01 8.738265750D-02-  
 1.087380837D-04  
 5.701191040D-08 0.000000000D+00 -6.692353080D+04  
 1.338412221D+02  
 SnCL2(L) Liquid. Gurvich,1991 pt1 p372 pt2 p316.  
 1 tpis91 SN 1.00CL 2.00 0.00 0.00 0.00 2 189.61540 -  
 333000.000  
 520.200 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17330.000  
 0.000000000D+00 0.000000000D+00 1.322988366D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.294240400D+04-  
 5.766924967D+01  
 SnCL4(L) Liquid. Gurvich,1991 pt1 p375 pt2 p319.  
 2 tpis91 SN 1.00CL 4.00 0.00 0.00 0.00 1 260.52080 -  
 517000.000  
 239.050 350.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 38740.000  
 0.000000000D+00 0.000000000D+00 2.059050984D+01-5.567014773D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.807207820D+04-  
 8.378462335D+01  
 350.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 38740.000  
 0.000000000D+00 0.000000000D+00 1.864210880D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.773111750D+04-  
 7.431947542D+01  
 SnF2(cr) Monoclinic. Gurvich,1991 pt1 p367 pt2 p311.  
 1 tpis91 SN 1.00F 2.00 0.00 0.00 0.00 1 156.70681 -  
 677000.000  
 298.150 488.2007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14200.000  
 0.000000000D+00 0.000000000D+00 6.575252180D+00 7.150150760D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -8.370213250D+04-  
 2.802481800D+01  
 SnF2(L) Liquid. Gurvich,1991 pt1 p367 pt2 p311.  
 1 tpis91 SN 1.00F 2.00 0.00 0.00 0.00 2 156.70681 -  
 677000.000  
 488.200 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14200.000  
 0.000000000D+00 0.000000000D+00 1.202716700D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -8.424882400D+04-  
 5.569866810D+01  
 SnI2(cr) Monoclinic. Gurvich,1991 pt1 p386 pt2 p328.  
 1 tpis91 SN 1.00I 2.00 0.00 0.00 0.00 1 372.51894 -  
 153000.000  
 200.000 595.7007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18950.000  
 8.194427570D+05-1.285027272D+04 8.314392190D+01-1.959449848D-01  
 2.384765022D-04  
 -9.891789320D-08 0.000000000D+00 3.957086730D+04-  
 4.432502620D+02  
 SnI2(L) Liquid. Gurvich,1991 pt1 p386 pt2 p328.  
 2 tpis91 SN 1.00I 2.00 0.00 0.00 0.00 2 372.51894 -  
 153000.000

595.700 960.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18950.000  
 3.807680789D+05 0.000000000D+00 1.313799611D+01-7.105650243D-04  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.013964325D+04-  
 5.193401798D+01  
 960.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18950.000  
 0.000000000D+00 0.000000000D+00 1.286906865D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.060553468D+04-  
 5.097603343D+01  
 SnI4(cr) Cubic. Gurvich,1991 pt1 p389 pt2 p331  
 1 tpris91 SN 1.00I 4.00 0.00 0.00 0.00 1 626.32788 -  
 207500.000  
 200.000 418.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 31600.000  
 1.365815960D+06-2.186441599D+04 1.411768692D+02-3.151970333D-01  
 2.991203201D-04  
 0.000000000D+00 0.000000000D+00 7.347422460D+04-  
 7.553382720D+02  
 SnI4(L) Liquid. Gurvich,1991 pt1 p389 pt2 p331  
 2 tpris91 SN 1.00I 4.00 0.00 0.00 0.00 2 626.32788 -  
 207500.000  
 418.000 580.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 31600.000  
 3.125499879D+05 0.000000000D+00 2.114568387D+01-5.918328320D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.828678876D+04-  
 7.927900653D+01  
 580.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 31600.000  
 0.000000000D+00 0.000000000D+00 1.864210880D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.836905732D+04-  
 6.724586950D+01  
 SnO(cr) Tetragonal. Gurvich,1991 pt1 p356 pt2 p306.  
 2 tpris91 SN 1.00O 1.00 0.00 0.00 0.00 1 134.70940 -  
 280710.000  
 100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8736.000  
 0.000000000D+00 0.000000000D+00 7.279467580D-02 3.307685420D-02-  
 4.710942000D-05  
 0.000000000D+00 0.000000000D+00 -3.483713220D+04-  
 1.306828645D+00  
 298.150 1250.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8736.000  
 0.000000000D+00 0.000000000D+00 5.260682830D+00 1.630883840D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.540242040D+04-  
 2.358356588D+01  
 SnO(L) Liquid. Gurvich,1991 pt1 p356 pt2 p306.  
 1 tpris91 SN 1.00O 1.00 0.00 0.00 0.00 2 134.70940 -  
 280710.000  
 1250.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8736.000  
 0.000000000D+00 0.000000000D+00 7.577115188D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.369230760D+04-  
 3.539798567D+01  
 SnO2(cr) Tetragonal. Gurvich,1991 pt1 p361 pt2 p308.



2 tpis91 SN 1.000 2.00 0.00 0.00 0.00 1 150.70880 -  
 577630.000  
 100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8384.000  
 0.000000000D+00 0.000000000D+00 -1.177647966D+00 3.970167880D-02-  
 4.790758920D-05  
 0.000000000D+00 0.000000000D+00 -7.046277710D+04  
 2.896556966D+00  
 298.150 1903.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8384.000  
 -2.674601390D+05 0.000000000D+00 9.145457760D+00 8.856805753D-04  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -7.313567410D+04-  
 4.798106778D+01  
 SnO2(L) Liquid. Gurvich,1991 pt1 p361 pt2 p308.  
 1 tpis91 SN 1.000 2.00 0.00 0.00 0.00 2 150.70880 -  
 577630.000  
 1903.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8384.000  
 0.000000000D+00 0.000000000D+00 1.106499361D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -7.222994130D+04-  
 5.927455845D+01  
 SnS(cr) Rhombic. Gurvich,1991 pt1 p392 pt2 p333.  
 2 tpis91 SN 1.00S 1.00 0.00 0.00 0.00 1 150.77600 -  
 109662.000  
 100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10530.000  
 -1.473490121D+04 0.000000000D+00 5.317316410D+00 2.586688381D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.493898062D+04-  
 2.188910671D+01  
 298.150 875.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10530.000  
 3.056103126D+04 0.000000000D+00 4.511751143D+00 3.579405160D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.459100103D+04-  
 1.734052255D+01  
 SnS(cr) Cubic. Gurvich,1991 pt1 p392 pt2 p333.  
 1 tpis91 SN 1.00S 1.00 0.00 0.00 0.00 2 150.77600 -  
 109662.000  
 875.000 1154.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10530.000  
 0.000000000D+00 0.000000000D+00 4.921516722D+00 1.882251630D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.425419920D+04-  
 1.855922147D+01  
 SnS(L) Liquid. Gurvich,1991 pt1 p392 pt2 p333.  
 1 tpis91 SN 1.00S 1.00 0.00 0.00 0.00 3 150.77600 -  
 109662.000  
 1154.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 10530.000  
 0.000000000D+00 0.000000000D+00 9.008348057D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.391650549D+04-  
 4.190990669D+01  
 SnS2(cr) Hexagonal. Gurvich,1991 pt1 p396 pt2 p335.  
 2 tpis91 SN 1.00S 2.00 0.00 0.00 0.00 1 182.84200 -  
 141837.000  
 100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13310.000

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-2.817980768D+04 0.000000000D+00 6.586339710D+00 7.259692260D-03
0.000000000D+00
0.000000000D+00 0.000000000D+00 -1.943987500D+04-
2.933754416D+01
298.150 1143.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
13310.000
1.193094963D+04 0.000000000D+00 7.560277154D+00 2.479641013D-03
0.000000000D+00
0.000000000D+00 0.000000000D+00 -1.938326475D+04-
3.323586315D+01
Sr(a) Alpha. Ref-Elm. Alcock,1993.
2 srd 93 SR 1.00 0.00 0.00 0.00 0.00 1 87.62000
0.000
100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
6558.289
-4.150245670D+03 1.559823384D+02-2.623173257D-01 2.945369354D-02-
1.212940361D-04
2.401045642D-07-1.708772572D-10 -1.455791066D+03
3.435106060D+00
298.150 820.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
6558.289
1.294412876D+05-1.646179180D+03 1.111114164D+01-1.973737192D-02
2.910871519D-05
-2.163423606D-08 6.508160860D-12 7.160398040D+03-
5.671602200D+01
Sr(b) Beta. Ref-Elm. Alcock,1993.
1 srd 93 SR 1.00 0.00 0.00 0.00 0.00 2 87.62000
0.000
820.000 1041.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
6558.289
0.000000000D+00 0.000000000D+00 3.190326309D+00 4.837326553D-04
0.000000000D+00
0.000000000D+00 0.000000000D+00 -8.560991280D+02-
1.157238431D+01
Sr(L) Liquid. Ref-Elm. Alcock,1993.
1 srd 93 SR 1.00 0.00 0.00 0.00 0.00 3 87.62000
0.000
1041.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
6558.289
0.000000000D+00 0.000000000D+00 4.450051777D+00 0.000000000D+00
0.000000000D+00
0.000000000D+00 0.000000000D+00 -9.431940390D+02-
1.889703393D+01
SrBr2(a) Alpha,tetragonal. Gurvich,1996a pt1 p523 pt2 p403.
1 tpris96 SR 1.00BR 2.00 0.00 0.00 0.00 1 247.42800 -
722000.000
200.000 918.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
18060.499
-1.563862878D+05 2.048387286D+03-2.389924996D+00 3.200996340D-02-
4.324517230D-05
3.247344210D-08-9.786717550D-12 -9.941922340D+04
2.897007516D+01
SrBr2(b) Beta. Gurvich,1996a pt1 p523 pt2 p403.
1 tpris96 SR 1.00BR 2.00 0.00 0.00 0.00 2 247.42800 -
722000.000
918.000 930.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
18060.499
0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00
0.000000000D+00
0.000000000D+00 0.000000000D+00 -9.021650510D+04-
5.212663905D+01

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SrBr2(L) Liquid. Gurvich,1996a pt1 p523 pt2 p403. -  
 1 tpi96 SR 1.00BR 2.00 0.00 0.00 0.00 3 247.42800  
 722000.000  
 930.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18060.499  
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -8.900176120D+04-  
 5.082046285D+01

SrCO3(a) Alpha,rhombic. Gurvich,1996a pt1 p532 pt2 p411. -  
 2 tpi96 SR 1.00C 1.000 3.00 0.00 0.00 1 147.62890  
 1226000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15120.499  
 -3.185109310D+07 5.983944250D+05-4.555778730D+03 1.807422903D+01-  
 3.922550990D-02  
 4.443338240D-05-2.057838162D-08 -2.840270234D+06  
 2.379927032D+04  
 500.000 1198.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15120.499  
 -4.737741611D+05 0.000000000D+00 1.829247905D+01-1.342833192D-02  
 1.073412624D-05  
 0.000000000D+00 0.000000000D+00 -1.539939771D+05-  
 9.167197246D+01

SrCO3(b) Beta,rhombic. Gurvich,1996a pt1 p532 pt2 p411. -  
 1 tpi96 SR 1.00C 1.000 3.00 0.00 0.00 2 147.62890  
 1226000.000  
 1198.000 1689.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15120.499  
 0.000000000D+00 0.000000000D+00 1.755966377D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.541962605D+05-  
 9.302015968D+01

SrCO3(c) Gamma,cubic. Gurvich,1996a pt1 p532 pt2 p411. -  
 1 tpi96 SR 1.00C 1.000 3.00 0.00 0.00 3 147.62890  
 1226000.000  
 1689.000 1767.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15120.499  
 0.000000000D+00 0.000000000D+00 1.755966377D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.541962605D+05-  
 9.302015968D+01

SrCO3(L) Liquid. Gurvich,1996a pt1 p532 pt2 p411. -  
 1 tpi96 SR 1.00C 1.000 3.00 0.00 0.00 4 147.62890  
 1226000.000  
 1767.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 15120.499  
 0.000000000D+00 0.000000000D+00 1.984482549D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.534232745D+05-  
 1.073837834D+02

SrCL2(a) Alpha,cubic. Gurvich,1996a pt1 p518 pt2 p400. -  
 2 tpi96 SR 1.00CL 2.00 0.00 0.00 0.00 1 158.52540  
 833000.000  
 200.000 700.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16230.000  
 -8.219302560D+05 1.414627236D+04-9.066868860D+01 3.537351300D-01-  
 6.601840230D-04  
 6.294183590D-07-2.405335168D-10 -1.675299882D+05  
 4.920219760D+02

700.000 990.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16230.000  
 1.112527665D+09 0.000000000D+00-1.718772952D+04 4.254819093D+01-  
 3.935556431D-02  
 1.290928281D-05 0.000000000D+00 6.824931370D+06  
 9.213791630D+04  
 SrCL2 (b) Beta, cubic. Gurvich, 1996a pt1 p518 pt2 p400.  
 1 tpi96 SR 1.00CL 2.00 0.00 0.00 0.00 2 158.52540 -  
 833000.000  
 900.000 1147.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16230.000  
 2.652616089D+08 0.000000000D+00-6.137593196D+02 3.705888862D-01  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 6.013938810D+05  
 4.028366895D+03  
 SrCL2 (L) Liquid. Gurvich, 1996a pt1 p518 pt2 p400.  
 1 tpi96 SR 1.00CL 2.00 0.00 0.00 0.00 3 158.52540 -  
 833000.000  
 1147.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16230.000  
 -1.621863465D+06 0.000000000D+00 1.278463794D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.040518221D+05-  
 6.010500872D+01  
 SrF2 (a) Alpha, cubic. Gurvich, 1996a pt1 p513 pt2 p396.  
 2 tpi96 SR 1.00F 2.00 0.00 0.00 0.00 1 125.61681 -  
 1229000.000  
 200.000 800.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13075.000  
 -1.436181472D+04-3.902704550D+02 9.084528850D+00 4.747017010D-03-  
 9.922331280D-06  
 1.169135473D-08-4.825603120D-12 -1.484911532D+05-  
 4.433988680D+01  
 800.000 1484.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13075.000  
 -1.706744719D+07 2.576630531D+04 3.257893350D+01-3.032276697D-02-  
 2.832102640D-05  
 2.982419101D-08-2.378577761D-12 -3.511043830D+05-  
 1.514196992D+02  
 SrF2 (b) Beta, cubic. Gurvich, 1996a pt1 p513 pt2 p396.  
 1 tpi96 SR 1.00F 2.00 0.00 0.00 0.00 2 125.61681 -  
 1229000.000  
 1484.000 1750.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13075.000  
 5.274154560D+09-9.287005960D+04-1.188369557D+04 9.829240680D+00-  
 2.277347958D-03  
 0.000000000D+00 0.000000000D+00 1.339064905D+07  
 7.586298750D+04  
 SrF2 (L) Liquid. Gurvich, 1996a pt1 p515 pt2 p396.  
 1 tpi96 SR 1.00F 2.00 0.00 0.00 0.00 3 125.61681 -  
 1229000.000  
 1750.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13075.000  
 0.000000000D+00 0.000000000D+00 1.190689530D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.478877648D+05-  
 5.796718683D+01  
 SrH2 (a) Alpha, rhombic. Gurvich, 1996a pt1 p501 pt2 p389.  
 1 tpi96 SR 1.00H 2.00 0.00 0.00 0.00 1 89.63588 -  
 180000.000

298.000 1128.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8000.499  
 0.000000000D+00 0.000000000D+00 4.125438541D+00 3.912437414D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.305279501D+04-  
 1.841745147D+01  
 SrH2 (b) Beta. Gurvich,1996a pt1 p501 pt2 p389.  
 1 tpi96 SR 1.00H 2.00 0.00 0.00 0.00 2 89.63588 -  
 180000.000  
 1128.000 1323.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8000.499  
 0.000000000D+00 0.000000000D+00 8.539288545D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.467660041D+04-  
 4.425795748D+01  
 SrH2 (L) Liquid. Gurvich,1996a pt1 p501 pt2 p389.  
 1 tpi96 SR 1.00H 2.00 0.00 0.00 0.00 3 89.63588 -  
 180000.000  
 1323.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8000.499  
 0.000000000D+00 0.000000000D+00 9.020375224D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.254682969D+04-  
 4.562495289D+01  
 SrI2 (cr) Rhombic. Gurvich,1996a pt1 p527 pt2 p406.  
 1 tpi96 SR 1.00I 2.00 0.00 0.00 0.00 1 341.42894 -  
 568000.000  
 200.000 811.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18920.499  
 -8.531836590D+05 1.396294943D+04-8.134381170D+01 2.923620048D-01-  
 4.941293260D-04  
 4.280629170D-07-1.479234641D-10 -1.358835709D+05  
 4.559376890D+02  
 SrI2 (L) Liquid. Gurvich,1996a pt1 p527 pt2 p406.  
 1 tpi96 SR 1.00I 2.00 0.00 0.00 0.00 2 341.42894 -  
 568000.000  
 811.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18920.499  
 0.000000000D+00 0.000000000D+00 1.322988366D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -7.143040870D+04-  
 5.646969655D+01  
 SrO (cr) Cubic. Gurvich,1996a pt1 p494 pt2 p383.  
 3 tpi96 SR 1.00O 1.00 0.00 0.00 0.00 1 103.61940 -  
 591000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8680.499  
 -1.625438799D+06 2.932375088D+04-2.136643281D+02 8.526581540D-01-  
 1.819594223D-03  
 2.035599655D-06-9.340883290D-10 -2.053069998D+05  
 1.123784285D+03  
 500.000 1800.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8680.499  
 -3.410904551D+04 0.000000000D+00 5.049245235D+00 3.431471007D-03-  
 3.042151612D-06  
 9.069686608D-10 0.000000000D+00 -7.282782040D+04-  
 2.317163697D+01  
 1800.000 2805.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8680.499  
 -3.971117961D+07 0.000000000D+00 7.850733236D+01-5.336790743D-02  
 1.125297823D-05

0.000000000D+00 0.000000000D+00 -1.604896850D+05-  
4.990588969D+02  
SrO(L) Liquid. Gurvich,1996a pt1 p494 pt2 p383.  
1 tpi96 SR 1.000 1.00 0.00 0.00 0.00 2 103.61940 -  
591000.000  
2805.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
8680.499  
0.000000000D+00 0.000000000D+00 1.010282025D+01 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -7.188203330D+04-  
5.541556063D+01  
Sr(OH)2(b) Beta,tetragonal. Gurvich,1996a pt1 p505 pt2 p392.  
1 tpi96 SR 1.000 2.00H 2.00 0.00 0.00 1 121.63468 -  
964300.000  
200.000 753.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
15272.499  
5.749774650D+05-9.564782420D+03 6.310466570D+01-1.470270543D-01  
2.468488663D-04  
-2.041763520D-07 6.865596260D-11 -7.364279180D+04-  
3.424340180D+02  
Sr(OH)2(a) Alpha. Gurvich,1996a pt1 p505 pt2 p392.  
1 tpi96 SR 1.000 2.00H 2.00 0.00 0.00 2 121.63468 -  
964300.000  
753.000 808.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
15272.499  
0.000000000D+00 0.000000000D+00 1.563531705D+01 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -1.216576455D+05-  
8.006737394D+01  
Sr(OH)2(L) Liquid. Gurvich,1996a pt1 p505 pt2 p392.  
1 tpi96 SR 1.000 2.00H 2.00 0.00 0.00 3 121.63468 -  
964300.000  
808.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
15272.499  
0.000000000D+00 0.000000000D+00 1.840156546D+01 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -1.211265258D+05-  
9.516262078D+01  
SrS(cr) Cubic. Gurvich,1996a pt1 p528 pt2 p408.  
2 tpi96 SR 1.00S 1.00 0.00 0.00 0.00 1 119.68600 -  
480000.000  
200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
10040.499  
2.688173776D+06-5.010846740D+04 3.813026790D+02-1.462623236D+00  
3.138875273D-03  
-3.522660370D-06 1.619531388D-09 1.665724752D+05-  
1.992760719D+03  
500.000 2500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
10040.499  
-1.221960164D+04 0.000000000D+00 5.716873273D+00 9.316243531D-04  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -5.951728090D+04-  
2.471633956D+01  
SrS(L) Liquid. Gurvich,1996a pt1 p528 pt2 p408.  
1 tpi96 SR 1.00S 1.00 0.00 0.00 0.00 2 119.68600 -  
480000.000  
2500.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
10040.499  
0.000000000D+00 0.000000000D+00 8.058201866D+00 0.000000000D+00  
0.000000000D+00

0.000000000D+00 0.000000000D+00 -5.487727330D+04-  
3.767411768D+01  
SrS04(a) Alpha,Rhombic. Gurvich,1996a pt1 p531 pt2 p410.  
1 tpi96 SR 1.00S 1.000 4.00 0.00 0.00 1 183.68360 -  
1457000.000  
298.150 1430.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
18400.499  
-2.524863161D+05 0.000000000D+00 1.319271972D+01 6.424070691D-03  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -1.803016041D+05-  
6.394942426D+01  
SrS04(b) Beta,hexagonal. Gurvich,1996a pt1 p531 pt2 p410.  
1 tpi96 SR 1.00S 1.000 4.00 0.00 0.00 2 183.68360 -  
1457000.000  
1430.000 1880.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
18400.499  
0.000000000D+00 0.000000000D+00 2.044618384D+01 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -1.827264862D+05-  
1.065597408D+02  
SrS04(L) Liquid. Gurvich,1996a pt1 p531 pt2 p410.  
1 tpi96 SR 1.00S 1.000 4.00 0.00 0.00 3 183.68360 -  
1457000.000  
1880.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
18400.499  
0.000000000D+00 0.000000000D+00 2.044618384D+01 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -1.783967061D+05-  
1.042566663D+02  
Ta(cr) Crystal. Ref-Elm. Chase,1998 pp1899-1901.  
3 j12/72 TA 1.00 0.00 0.00 0.00 0.00 1 180.94790  
0.000  
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
5681.000  
1.519941999D+04-4.927143830D+02 6.855605760D+00-1.366625579D-02  
2.561466303D-05  
-2.235631116D-08 7.389831320D-12 1.236077891D+03-  
3.252075490D+01  
1000.000 2000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
5681.000  
-1.002219854D+08 4.696591430D+05-8.992639340D+02 9.084714280D-01-  
5.043323480D-04  
1.463919859D-07-1.734426993D-11 -2.762235634D+06  
5.939534460D+03  
2000.000 3258.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
5681.000  
3.305034810D+05 8.564351680D+01-1.797593491D+00 6.549784340D-03-  
2.878793550D-06  
4.952725110D-10-7.703452530D-15 1.556933077D+03  
1.641047132D+01  
Ta(L) Liquid. Ref-Elm. Chase,1998 pp1899-1901.  
1 j12/72 TA 1.00 0.00 0.00 0.00 0.00 2 180.94790  
0.000  
3258.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
5681.000  
0.000000000D+00 0.000000000D+00 5.032166658D+00 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -7.436042760D+02-  
2.597362534D+01  
TaC(cr) Chase,1998 pp652-4.

2 j12/73 TA 1.00C 1.00 0.00 0.00 0.00 1 192.95860 -  
 144096.960  
 200.000 800.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6514.488  
 -1.182153887D+04 2.152843262D+02-1.710781252D+00 3.226351270D-02-  
 6.059170690D-05  
 5.540177420D-08-1.961814434D-11 -1.908587628D+04  
 8.122034510D+00  
 800.000 4273.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6514.488  
 -1.540090534D+05 2.156690707D+02 5.001633620D+00 1.161840292D-03-  
 1.062186764D-07  
 2.082367078D-11-1.580991193D-15 -2.062101769D+04-  
 2.388952788D+01  
 TaC(L) Chase, 1998 pp652-4.  
 1 j12/73 TA 1.00C 1.00 0.00 0.00 0.00 2 192.95860 -  
 144096.960  
 4273.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6514.488  
 0.000000000D+00 0.000000000D+00 8.051466653D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.010399602D+04-  
 4.208381497D+01  
 Ta2O5(II) Rhombic. Gurvich, 1982 pt1 p91 pt2 p92.  
 2 tpis82 TA 2.000 5.00 0.00 0.00 0.00 1 441.89280 -  
 2049000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22950.000  
 -3.279677980D+06 6.126833460D+04-4.710233330D+02 1.998455231D+00-  
 4.425553760D-03  
 5.098341430D-06-2.392974558D-09 -5.247547580D+05  
 2.448363106D+03  
 500.000 1633.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22950.000  
 -2.735481912D+05 0.000000000D+00 1.819193368D+01 3.735655440D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.529440756D+05-  
 8.923622860D+01  
 Ta2O5(I) Monoclinic. Gurvich, 1982 pt1 p91 pt2 p92.  
 1 tpis82 TA 2.000 5.00 0.00 0.00 0.00 2 441.89280 -  
 2049000.000  
 1633.000 2150.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22950.000  
 0.000000000D+00 0.000000000D+00 2.525705063D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.590924400D+05-  
 1.352062771D+02  
 Ta2O5(L) Liquid. Gurvich, 1982 pt1 p91 pt2 p92.  
 1 tpis82 TA 2.000 5.00 0.00 0.00 0.00 3 441.89280 -  
 2049000.000  
 2150.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22950.000  
 0.000000000D+00 0.000000000D+00 2.645976732D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.472456805D+05-  
 1.377221533D+02  
 Th(a) Alpha. Ref-Elm. Cox, 1989 p239.  
 1 coda89 TH 1.00 0.00 0.00 0.00 0.00 1 232.03810  
 0.000  
 200.000 1650.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6350.000



-1.453247151D+04 1.505222433D+02 2.270694767D+00 2.058614354D-03-  
9.216614670D-07  
4.316796340D-10-7.950656800D-14 -1.667536353D+03-  
6.857176980D+00

Th(b) Beta. Ref-Elm. Cox,1989 p239.  
1 coda89 TH 1.00 0.00 0.00 0.00 0.00 2 232.03810  
0.000  
1650.000 2023.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6350.000  
8.360316570D+06-2.333327743D+04 2.783594798D+01-1.293559561D-02  
3.966098040D-06  
-4.361984440D-10 0.000000000D+00 1.501326293D+05-  
1.894583434D+02

Th(L) Liquid. Ref-Elm. Cox,1989 p239.  
1 coda89 TH 1.00 0.00 0.00 0.00 0.00 3 232.03810  
0.000  
2023.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6350.000  
0.000000000D+00 0.000000000D+00 5.532496804D+00 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -2.191824935D+03-  
2.760071917D+01

Ti(a) Alpha. Ref-Elm. Cox,1989 p230.  
2 coda89 TI 1.00 0.00 0.00 0.00 0.00 1 47.86700  
0.000  
200.000 900.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
4824.000  
3.598601350D+04-8.272305960D+02 7.689097770D+00-1.143968449D-02  
1.392105464D-05  
-4.691057160D-09-9.852130400D-13 2.936621421D+03-  
3.985138010D+01  
900.000 1156.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
4824.000  
-2.876235910D+06 0.000000000D+00 4.573153420D+01-7.692381600D-02  
3.799919490D-05  
0.000000000D+00 0.000000000D+00 -2.038023972D+04-  
2.516270281D+02

Ti(b) Beta. Ref-Elm. Cox,1989 p230.  
1 coda89 TI 1.00 0.00 0.00 0.00 0.00 2 47.86700  
0.000  
1156.000 1944.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
4824.000  
-1.698740574D+06 6.576601240D+03-8.556182950D+00 9.789585830D-03-  
3.992418760D-06  
1.123642773D-09-1.201048055D-13 -3.929918290D+04  
6.506590190D+01

Ti(L) Liquid. Ref-Elm. Cox,1989 p230.  
1 coda89 TI 1.00 0.00 0.00 0.00 0.00 3 47.86700  
0.000  
1944.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
4824.000  
0.000000000D+00 0.000000000D+00 5.628714139D+00 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -2.377354619D+03-  
3.079443471D+01

TiB(cr) Crystal. Chase,1998. p258.  
2 j 6/65 TI 1.00B 1.00 0.00 0.00 0.00 1 58.67800 -  
160247.000  
298.150 1100.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
0.000

5.892962460D+05-7.628387170D+03 3.264504220D+01-4.438679670D-02  
 4.037756110D-05  
 -1.901806786D-08 3.662438970D-12 1.808566462D+04-  
 1.924926707D+02  
 1100.000 4000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 9.736238960D+05-2.744306202D+03 9.195602010D+00-1.636706129D-03  
 5.676930840D-07  
 -9.258425040D-11 6.105669480D-15 -3.925082340D+03-  
 5.367424570D+01  
 TiB2(cr) Crystal. Chase,1998 pp276-8.  
 2 j 6/65 TI 1.00B 2.00 0.00 0.00 0.00 1 69.48900 -  
 279491.000  
 200.000 2300.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 5577.000  
 2.701885716D+05-3.989107020D+03 1.904595810D+01-1.467951261D-02  
 1.249126541D-05  
 -4.481179720D-09 5.932523160D-13 -1.510818691D+04-  
 1.130901290D+02  
 2300.000 3193.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 5577.000  
 2.449855642D+10-5.420046130D+07 4.984385950D+04-2.437314870D+01  
 6.688502930D-03  
 -9.763538800D-07 5.923249200D-11 3.589528270D+08-  
 3.651406280D+05  
 TiB2(L) Liquid. Chase,1998 pp276-8.  
 1 j 6/65 TI 1.00B 2.00 0.00 0.00 0.00 2 69.48900 -  
 279491.000  
 3193.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 5577.000  
 0.000000000D+00 0.000000000D+00 1.308363331D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.298172270D+04-  
 7.649131141D+01  
 TiC(cr) Chase,1998 p655-7  
 2 j 6/68 TI 1.00C 1.00 0.00 0.00 0.00 1 59.87770 -  
 184096.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 4606.584  
 -2.936209453D+05 4.040416860D+03-2.309999326D+01 8.695403030D-02-  
 1.254447445D-04  
 8.803423830D-08-2.403516957D-11 -4.217890880D+04  
 1.253486677D+02  
 1000.000 3290.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 4606.584  
 -3.586824960D+05 1.130360992D+03 4.571181220D+00 4.332844010D-04  
 4.730133770D-07  
 -1.025727737D-10 8.572441560D-15 -3.129994969D+04-  
 2.180975207D+01  
 TiC(L) Chase,1998 p655-7  
 1 j 6/68 TI 1.00C 1.00 0.00 0.00 0.00 2 59.87770 -  
 184096.000  
 3290.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 4606.584  
 0.000000000D+00 0.000000000D+00 7.548249987D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.766010062D+04-  
 4.062778302D+01  
 TiCL2(cr) Chase,1998 p865.  
 2 j12/68 TI 1.00CL 2.00 0.00 0.00 0.00 1 118.77240 -  
 515470.000

200.000 800.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13300.936  
 6.275502170D+05-1.149039253D+04 8.470916630D+01-2.539508065D-01  
 4.582690050D-04  
 -4.167293950D-07 1.508542615D-10 -1.168917881D+04-  
 4.484122170D+02  
 800.000 2000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13300.936  
 3.621030580D+06-1.684661798D+04 4.010076440D+01-2.963515568D-02  
 1.756075169D-05  
 -5.065847400D-09 5.988802280D-13 3.466967030D+04-  
 2.478759697D+02  
 TiCL3(cr) Chase,1998 p886.  
 1 j12/68 TI 1.00CL 3.00 0.00 0.00 0.00 1 154.22510 -  
 721740.000  
 298.150 1500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 20920.000  
 1.457928527D+05-1.355589207D+03 1.563840194D+01-4.771661650D-03  
 4.776265870D-06  
 -1.901286451D-09 3.011222662D-13 -8.308136940D+04-  
 7.479338350D+01  
 TiCL4(L) Chase,1998 p904.  
 2 j12/67 TI 1.00CL 4.00 0.00 0.00 0.00 1 189.67780 -  
 804164.800  
 249.046 700.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 26963.000  
 1.179781205D+06-1.710994382D+04 1.180652525D+02-3.089428313D-01  
 5.234695800D-04  
 -4.608788890D-07 1.654264781D-10 -2.053742284D+04-  
 6.204956050D+02  
 700.000 2000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 26963.000  
 0.000000000D+00 0.000000000D+00 1.714255083D+01 1.093131841D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.018779486D+05-  
 6.764318260D+01  
 TiN(cr) Chase,1998 p1612-4.  
 2 j 6/68 TI 1.00N 1.00 0.00 0.00 0.00 1 61.87374 -  
 337648.800  
 200.000 800.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 5487.000  
 -5.479117220D+05 9.328691110D+03-6.386263890D+01 2.429925456D-01-  
 4.304234520D-04  
 3.792645100D-07-1.317412256D-10 -8.424256140D+04  
 3.392988560D+02  
 800.000 3220.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 5487.000  
 -3.656247060D+05 1.265730431D+03 3.831711190D+00 1.632900455D-03-  
 1.062786626D-07  
 1.310931390D-11-5.770548410D-16 -5.027654400D+04-  
 1.652632899D+01  
 TiN(L) Chase,1998 p1612-4.  
 1 j 6/68 TI 1.00N 1.00 0.00 0.00 0.00 2 61.87374 -  
 337648.800  
 3220.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 5487.000  
 0.000000000D+00 0.000000000D+00 7.548249987D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.626039860D+04-  
 3.958296649D+01  
 TiO(a) Alpha,monoclinic. Gurvich,1982 pt1 p98 pt2 p99.

2 tpis82 TI 1.000 1.00 0.00 0.00 0.00 1 63.86640 -  
 542000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6175.000  
 -1.126115023D+07 2.107240660D+05-1.601946203D+03 6.360717840D+00-  
 1.380180278D-02  
 1.563169158D-05-7.238514780D-09 -1.014208223D+06  
 8.368056830D+03  
 500.000 1265.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6175.000  
 -2.066517895D+05 0.000000000D+00 8.243115270D+00-4.896702160D-03  
 3.806679150D-06  
 0.000000000D+00 0.000000000D+00 -6.815384410D+04-  
 4.265310470D+01  
 TiO(b) Beta,cubic. Gurvich,1982 pt1 p98 pt2 p99.  
 1 tpis82 TI 1.000 1.00 0.00 0.00 0.00 2 63.86640 -  
 542000.000  
 1265.000 1810.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6175.000  
 -1.400082506D+05 0.000000000D+00 6.173304260D+00 1.455287203D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.756357790D+04-  
 3.249519859D+01  
 TiO(c) Gamma,cubic. Gurvich,1982 pt1 p98 pt2 p99.  
 1 tpis82 TI 1.000 1.00 0.00 0.00 0.00 3 63.86640 -  
 542000.000  
 1810.000 2030.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6175.000  
 2.080459342D+05 0.000000000D+00 5.795530945D+00 1.404532558D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.627964090D+04-  
 2.933709305D+01  
 TiO(L) Liquid. Gurvich,1982 pt1 p98 pt2 p99.  
 1 tpis82 TI 1.000 1.00 0.00 0.00 0.00 4 63.86640 -  
 542000.000  
 2030.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6175.000  
 0.000000000D+00 0.000000000D+00 8.419016875D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.314903830D+04-  
 4.370051573D+01  
 TiO2(cr) Rutile,tetragonal. Gurvich,1982 pt1 p105 pt2 p105.  
 2 tpis82 TI 1.000 2.00 0.00 0.00 0.00 1 79.86580 -  
 944000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8680.000  
 1.712264157D+07-2.997059314D+05 2.143439285D+03-7.997230440D+00  
 1.661745261D-02  
 -1.817331921D-05 8.179403360D-09 1.253121023D+06-  
 1.132509587D+04  
 500.000 2185.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8680.000  
 -1.244201863D+05 0.000000000D+00 7.600577340D+00 1.421666301D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.162831515D+05-  
 3.834053430D+01  
 TiO2(L) Liquid. Gurvich,1982 pt1 p105 pt2 p105.  
 1 tpis82 TI 1.000 2.00 0.00 0.00 0.00 2 79.86580 -  
 944000.000  
 2185.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8680.000

0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.143261561D+05-  
 6.551584491D+01  
 Ti2O3(I) Hexagonal. Gurvich,1982 pt1 p109 pt2 p108.  
 2 tps82 TI 2.000 3.00 0.00 0.00 0.00 1 143.73220 -  
 152000.000  
 200.000 400.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14090.000  
 -1.771212920D+06 2.344459434D+04-1.110358342D+02 2.714352074D-01-  
 1.921153675D-04  
 0.000000000D+00 0.000000000D+00 -2.995932792D+05  
 6.382146810D+02  
 400.000 464.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14090.000  
 0.000000000D+00 0.000000000D+00 5.692590423D+01-2.558542837D-01  
 3.734811793D-04  
 0.000000000D+00 0.000000000D+00 -1.917653868D+05-  
 2.555304929D+02  
 Ti2O3(I') Hexagonal. Gurvich,1982 pt1 p109 pt2 p108.  
 2 tps82 TI 2.000 3.00 0.00 0.00 0.00 2 143.73220 -  
 152000.000  
 464.000 580.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14090.000  
 0.000000000D+00 0.000000000D+00 9.288208205D+01-2.728212486D-01  
 2.430399386D-04  
 0.000000000D+00 0.000000000D+00 -2.022790157D+05-  
 4.543828632D+02  
 580.000 2110.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14090.000  
 4.228751905D+05 0.000000000D+00 1.281963700D+01 4.013104801D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.858705711D+05-  
 6.399935229D+01  
 Ti2O3(L) Liquid. Gurvich,1982 pt1 p109 pt2 p108.  
 1 tps82 TI 2.000 3.00 0.00 0.00 0.00 3 143.73220 -  
 152000.000  
 2110.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14090.000  
 0.000000000D+00 0.000000000D+00 2.044618384D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.821646342D+05-  
 1.087120898D+02  
 Ti3O5(a) Alpha,monoclinic. Gurvich,1982 pt1 p111 pt2 p110.  
 2 tps82 TI 3.000 5.00 0.00 0.00 0.00 1 223.59800 -  
 2457000.000  
 200.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22630.000  
 0.000000000D+00 0.000000000D+00 4.315304530D+00 4.637018750D-02  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.988551027D+05-  
 2.323385163D+01  
 298.150 448.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22630.000  
 -2.175887695D+07 0.000000000D+00 1.012212506D+03-3.624156324D+00  
 3.726318087D-03  
 0.000000000D+00 0.000000000D+00 -5.421167010D+05-  
 4.959468179D+03  
 Ti3O5(b) Beta,rhombic. Gurvich,1982 pt1 p111 pt2 p110.  
 1 tps82 TI 3.000 5.00 0.00 0.00 0.00 2 223.59800 -  
 2457000.000

448.000 2050.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22630.000  
 0.000000000D+00 0.000000000D+00 2.020131072D+01 5.124775844D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.004933224D+05-  
 9.863577455D+01  
 Ti3O5(L) Liquid. Gurvich,1982 pt1 p111 pt2 p110.  
 1 tpis82 TI 3.000 5.00 0.00 0.00 0.00 3 223.59800 -  
 2457000.000  
 2050.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22630.000  
 0.000000000D+00 0.000000000D+00 3.127063411D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.923316313D+05-  
 1.627424211D+02  
 Ti4O7(cr) Triclinic. Gurvich,1982 pt1 p112 pt2 p111.  
 2 tpis82 TI 4.000 7.00 0.00 0.00 0.00 1 303.46380 -  
 3403000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 35630.000  
 4.558528430D+06-8.146955640D+04 5.758643730D+02-1.933194123D+00  
 3.842536530D-03  
 -4.030781120D-06 1.748510017D-09 -4.239230760D+04-  
 3.066670887D+03  
 500.000 1960.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 35630.000  
 -4.675287930D+05 0.000000000D+00 2.961388604D+01 5.773820220D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.199386150D+05-  
 1.488468383D+02  
 Ti4O7(L) Liquid. Gurvich,1982 pt1 p112 pt2 p111.  
 1 tpis82 TI 4.000 7.00 0.00 0.00 0.00 2 303.46380 -  
 3403000.000  
 1960.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 35630.000  
 0.000000000D+00 0.000000000D+00 4.353834441D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.142527640D+05-  
 2.319810806D+02  
 U(a) Alpha. Ref-Elm. Cox,1989 p234.  
 1 coda89 U 1.00 0.00 0.00 0.00 0.00 1 238.02890  
 0.000  
 200.000 942.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6364.000  
 -1.540899462D+04 2.318801962D+02 1.227944510D+00 7.136117480D-03-  
 1.018038579D-05  
 1.136884370D-08-3.669367430D-12 -1.986921870D+03-  
 2.035974193D+00  
 U(b) Beta. Ref-Elm. Cox,1989 p234.  
 1 coda89 U 1.00 0.00 0.00 0.00 0.00 2 238.02890  
 0.000  
 942.000 1049.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6364.000  
 0.000000000D+00 0.000000000D+00 5.099518793D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.672080149D+03-  
 2.378030116D+01  
 U(c) Gamma. Ref-Elm. Cox,1989 p234.  
 1 coda89 U 1.00 0.00 0.00 0.00 0.00 3 238.02890  
 0.000

1049.000 1408.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6364.000  
 0.000000000D+00 0.000000000D+00 4.606404947D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.859187270D+02-  
 1.980809042D+01  
 U(L) Liquid. Ref-Elm. Cox,1989 p234.  
 1 coda89 U 1.00 0.00 0.00 0.00 0.00 4 238.02890  
 0.000  
 1408.000 4000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6364.000  
 -9.466562120D+04 8.526619680D+02 4.209128020D+00 8.407200810D-04-  
 1.309545676D-07  
 1.985020032D-11-1.231574075D-15 -5.956398090D+03-  
 1.667247672D+01  
 UF3(cr) Hexagonal. Gurvich,1982 pt1 p209 pt2 p236.  
 1 tpis82 U 1.00F 3.00 0.00 0.00 0.00 1 295.02411 -  
 1508700.000  
 298.150 1768.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18380.000  
 -1.245413139D+05 0.000000000D+00 1.281362341D+01 8.479152710D-05  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.856957321D+05-  
 5.889112439D+01  
 UF3(L) Liquid. Gurvich,1982 pt1 p209 pt2 p236.  
 1 tpis82 U 1.00F 3.00 0.00 0.00 0.00 2 295.02411 -  
 1508700.000  
 1768.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 18380.000  
 0.000000000D+00 0.000000000D+00 1.611640373D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.869060867D+05-  
 8.091478353D+01  
 UF4(cr) Monoclinic. Gurvich,1982 pt1 p212 pt2 p243.  
 2 tpis82 U 1.00F 4.00 0.00 0.00 0.00 1 314.02251 -  
 1920500.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22550.000  
 -1.900846659D+06 3.555369140D+04-2.684351890D+02 1.162227739D+00-  
 2.589319495D-03  
 2.991673531D-06-1.405949560D-09 -3.939232500D+05  
 1.401148993D+03  
 500.000 1309.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22550.000  
 -1.687548936D+05 0.000000000D+00 1.670280525D+01-3.858715240D-03  
 3.366874970D-06  
 0.000000000D+00 0.000000000D+00 -2.363858828D+05-  
 7.687256170D+01  
 UF4(L) Liquid. Gurvich,1982 pt1 p212 pt2 p243.  
 1 tpis82 U 1.00F 4.00 0.00 0.00 0.00 2 314.02251 -  
 1920500.000  
 1309.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22550.000  
 0.000000000D+00 0.000000000D+00 2.008536883D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.358206485D+05-  
 9.894817389D+01  
 UF5(b) Beta,tetragonal. Gurvich,1982 pt1 p217 pt2 p250.  
 1 tpis82 U 1.00F 5.00 0.00 0.00 0.00 1 333.02092 -  
 2083000.000

298.150 398.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 26150.000  
 -2.315229641D+04 0.000000000D+00 1.505308190D+01 3.633166597D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.552530997D+05-  
 6.539107895D+01  
 UF5(a) Alpha, tetragonal. Gurvich, 1982 pt1 p217 pt2 p250.  
 1 tpis82 U 1.00F 5.00 0.00 0.00 0.00 2 333.02092 -  
 2083000.000  
 398.000 621.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 26150.000  
 -2.315229641D+04 0.000000000D+00 1.505308190D+01 3.633166597D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.542909264D+05-  
 6.297355795D+01  
 UF5(L) Liquid. Gurvich, 1982 pt1 p217 pt2 p250.  
 1 tpis82 U 1.00F 5.00 0.00 0.00 0.00 3 333.02092 -  
 2083000.000  
 621.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 26150.000  
 0.000000000D+00 0.000000000D+00 2.008536883D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.524686368D+05-  
 8.627305038D+01  
 UF6(cr) Rhombic. Gurvich, 1982 pt1 p222 pt2 p532.  
 1 tpis82 U 1.00F 6.00 0.00 0.00 0.00 1 352.01932 -  
 2197700.000  
 100.000 337.2107 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 31565.000  
 1.490516238D+05-4.412150490D+03 5.041684430D+01-1.195638409D-01  
 2.070807828D-04  
 0.000000000D+00 0.000000000D+00 -2.502294955D+05-  
 2.473731136D+02  
 UF6(L) Liquid. Gurvich, 1982 pt1 p222 pt2 p532.  
 1 tpis82 U 1.00F 6.00 0.00 0.00 0.00 2 352.01932 -  
 2197700.000  
 337.210 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 31565.000  
 0.000000000D+00 0.000000000D+00 1.750554152D+01 1.611640373D-02  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.680142931D+05-  
 7.051080543D+01  
 UO2(cr) Cubic. Gurvich, 1982 pt1 p190 pt2 p209.  
 2 tpis82 U 1.00O 2.00 0.00 0.00 0.00 1 270.02770 -  
 1085000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11280.000  
 -1.712140039D+07 3.206174610D+05-2.435851508D+03 9.665099460D+00-  
 2.095506138D-02  
 2.371859464D-05-1.097936236D-08 -1.574556829D+06  
 1.272869884D+04  
 500.000 3123.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11280.000  
 -2.775509993D+05 0.000000000D+00 1.161094006D+01-3.430918270D-03  
 2.044412020D-06  
 0.000000000D+00 0.000000000D+00 -1.347529024D+05-  
 5.751912860D+01  
 UO2(L) Liquid. Gurvich, 1982 pt1 p190 pt2 p209.  
 1 tpis82 U 1.00O 2.00 0.00 0.00 0.00 2 270.02770 -  
 1085000.000



3123.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 11280.000  
 0.000000000D+00 0.000000000D+00 1.575558872D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.342007409D+05-  
 8.859616713D+01  
 U02F2(cr) Hexagonal. Gurchich,1982 pt1 p227 pt2 p262.  
 2 tpris82 U 1.000 2.00F 2.00 0.00 0.00 1 308.02451 -  
 1653600.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19700.000  
 2.774535231D+06-5.047416500D+04 3.733097480D+02-1.349660046D+00  
 2.816624451D-03  
 -3.086048235D-06 1.391361959D-09 2.724906305D+04-  
 1.962630228D+03  
 500.000 2100.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 19700.000  
 -1.227714401D+05 0.000000000D+00 1.277741930D+01 3.406816370D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.032540376D+05-  
 5.821006900D+01  
 U03(c) Gamma,monoclinic. Gurchich,1982 pt1 p195 pt2 p217.  
 2 tpris82 U 1.000 3.00 0.00 0.00 0.00 1 286.02710 -  
 1223800.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14585.000  
 -1.956676511D+06 3.951756640D+04-3.223198540D+02 1.417862899D+00-  
 3.236211090D-03  
 3.806716410D-06-1.814492554D-09 -3.239008630D+05  
 1.660601808D+03  
 500.000 3000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 14585.000  
 -2.090516805D+05 0.000000000D+00 1.271766576D+01-2.508681376D-03  
 2.295592116D-06  
 0.000000000D+00 0.000000000D+00 -1.515901509D+05-  
 6.143076620D+01  
 U308(II) Rhombic. Gurchich,1982 pt1 p199 pt2 p222.  
 2 tpris82 U 3.000 8.00 0.00 0.00 0.00 1 842.08190 -  
 3574800.000  
 200.000 300.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 42740.000  
 -1.312654971D+05 0.000000000D+00 1.981648464D+01 3.463180280D-02  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.378350230D+05-  
 8.998750380D+01  
 300.000 483.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 42740.000  
 -2.819324251D+06 0.000000000D+00 1.227600892D+02-2.415563843D-01  
 0.000000000D+00  
 3.622285580D-07 0.000000000D+00 -4.659833440D+05-  
 6.124926920D+02  
 U308(I) Hexagonal. Gurchich,1982 pt1 p199 pt2 p222.  
 1 tpris82 U 3.000 8.00 0.00 0.00 0.00 2 842.08190 -  
 3574800.000  
 483.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 42740.000  
 -5.848811295D+04 0.000000000D+00 2.988522475D+01 6.597141623D-03-  
 4.626851131D-07  
 0.000000000D+00 0.000000000D+00 -4.394086740D+05-  
 1.388063306D+02  
 U409(III) Cubic. Gurchich,1982 pt1 p201 pt2 p223.

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1 tpis82 U 4.000 9.00 0.00 0.00 0.00 1 1096.11020 -
4512000.000
298.150 348.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
50750.000
-1.274607283D+08 0.000000000D+00 6.797154853D+03-2.205931654D+01
0.000000000D+00
4.712462238D-05 0.000000000D+00 -2.109373967D+06-
3.324352924D+04
U409(II) Cubic. Gurvich,1982 pt1 p201 pt2 p223.
2 tpis82 U 4.000 9.00 0.00 0.00 0.00 2 1096.11020 -
4512000.000
348.000 380.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
50750.000
6.572378889D+07 0.000000000D+00-1.352246013D+03 2.459469770D+00
0.000000000D+00
0.000000000D+00 0.000000000D+00 -3.013155679D+04
7.375484389D+03
380.000 1398.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
50750.000
-7.968840016D+05 0.000000000D+00 4.574063896D+01-1.083792070D-02
9.691491140D-06
0.000000000D+00 0.000000000D+00 -5.582419360D+05-
2.211132773D+02
U409(I) Gurvich,1982 pt1 p201 pt2 p223.
1 tpis82 U 4.000 9.00 0.00 0.00 0.00 3 1096.11020 -
4512000.000
1398.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
50750.000
-3.094590060D+05 0.000000000D+00 3.592971805D+01 1.009247689D-02
0.000000000D+00
0.000000000D+00 0.000000000D+00 -5.555228520D+05-
1.695188988D+02
V(cr) Crystal. Ref-Elm. Chase,1998 p1917.
3 j 6/73 V 1.00 0.00 0.00 0.00 0.00 1 50.94150
0.000
200.000 600.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
4640.000
2.845125913D+05-5.094932860D+03 3.715018720D+01-1.176030941D-01
2.255823526D-04
-2.260642686D-07 9.289596800D-11 2.254378204D+04-
1.968241679D+02
600.000 1400.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
4640.000
1.372056465D+06-7.847553620D+03 2.095142247D+01-2.055640932D-02
1.323266530D-05
-4.042182900D-09 5.087521100D-13 4.374800000D+04-
1.292763446D+02
1400.000 2190.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
4640.000
5.281067680D+08-1.907420191D+06 2.862656637D+03-2.277492896D+00
1.017078880D-03
-2.412149691D-07 2.377114537D-11 1.169890783D+07-
1.956716732D+04
V(L) Liquid. Ref-Elm. Chase,1998 p1917.
1 j 6/73 V 1.00 0.00 0.00 0.00 0.00 2 50.94150
0.000
2190.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
4640.000
0.000000000D+00 0.000000000D+00 5.557032224D+00 0.000000000D+00
0.000000000D+00

```

0.000000000D+00 0.000000000D+00 -1.899700630D+03-  
 3.070532450D+01  
 VCL2(cr) Pankratz,1984.  
 1 g10/00 V 1.00CL 2.00 0.00 0.00 0.00 1 121.84690 -  
 451872.000  
 298.000 1300.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 -3.844575327D+04 0.000000000D+00 8.648281619D+00 1.435173931D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.711862150D+04-  
 3.824393774D+01  
 VCL3(cr) Pankratz,1984.  
 1 g 8/00 V 1.00CL 3.00 0.00 0.00 0.00 1 157.29960 -  
 581115.760  
 298.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 -1.163436931D+05 0.000000000D+00 1.218941730D+01 1.091980165D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -7.396479110D+04-  
 5.467967609D+01  
 VN(cr) Chase,1998 p1635.  
 2 j12/73 V 1.00N 1.00 0.00 0.00 0.00 1 64.94824 -  
 217150.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6225.792  
 2.091900078D+05-3.051142421D+03 1.689002455D+01-2.016563261D-02  
 2.024805796D-05  
 -9.052281300D-09 1.375923345D-12 -1.233229950D+04-  
 9.561817060D+01  
 1000.000 3500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 6225.792  
 8.212748990D+05-2.203406736D+03 6.907596040D+00 1.164274622D-03-  
 3.307430080D-07  
 1.061954757D-10-1.105176783D-14 -1.341131421D+04-  
 3.925480780D+01  
 VO(cr) Cubic Gurvich,1982 pt1 p60 pt2 p63.  
 2 tpris82 V 1.000 1.00 0.00 0.00 0.00 1 66.94090 -  
 430800.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 5980.000  
 -2.040260824D+07 3.783102280D+05-2.848005957D+03 1.118080448D+01-  
 2.407270159D-02  
 2.710471323D-05-1.249526447D-08 -1.758506851D+06  
 1.490654242D+04  
 500.000 2063.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 5980.000  
 -1.970015037D+05 0.000000000D+00 6.365723760D+00 1.576630310D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.444168120D+04-  
 3.381741570D+01  
 VO(L) Liquid Gurvich,1982 pt1 p60 pt2 p63.  
 1 tpris82 V 1.000 1.00 0.00 0.00 0.00 2 66.94090 -  
 430800.000  
 2063.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 5980.000  
 0.000000000D+00 0.000000000D+00 8.419016875D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.921350390D+04-  
 4.329727468D+01  
 V2O3(cr) Hexagonal. Gurvich,1982 pt1 p65 pt2 p67.

2 t<sub>pis</sub>82 V 2.000 3.00 0.00 0.00 0.00 1 149.88120 -  
 1216800.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17130.000  
 -2.445935804D+07 4.555627240D+05-3.448966200D+03 1.365879117D+01-  
 2.955666350D-02  
 3.340613030D-05-1.544661718D-08 -2.200372063D+06  
 1.802928653D+04  
 500.000 2230.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17130.000  
 -4.148342860D+05 0.000000000D+00 1.735995875D+01-2.248234102D-03  
 1.310940149D-06  
 0.000000000D+00 0.000000000D+00 -1.528252156D+05-  
 8.926688900D+01  
 V203(L) Liquid. Gurvich,1982 pt1 p65 pt2 p67.  
 1 t<sub>pis</sub>82 V 2.000 3.00 0.00 0.00 0.00 2 149.88120 -  
 1216800.000  
 2230.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17130.000  
 0.000000000D+00 0.000000000D+00 1.924346714D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.407455834D+05-  
 9.794985841D+01  
 V204(II) Monoclinic. Gurvich,1982 pt1 p67 pt2 p68.  
 1 t<sub>pis</sub>82 V 2.000 4.00 0.00 0.00 0.00 1 165.88060 -  
 1432600.000  
 200.000 338.7007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16720.000  
 -4.872822280D+05 0.000000000D+00 4.755837160D+01-1.909710602D-01  
 3.188918050D-04  
 0.000000000D+00 0.000000000D+00 -1.824442970D+05-  
 2.197380006D+02  
 V204(I) Tetragonal. Gurvich,1982 pt1 p67 pt2 p68.  
 1 t<sub>pis</sub>82 V 2.000 4.00 0.00 0.00 0.00 2 165.88060 -  
 1432600.000  
 338.700 1818.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16720.000  
 -3.456246971D+05 0.000000000D+00 1.740258897D+01 2.292498295D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.776670154D+05-  
 8.737764367D+01  
 V204(L) Liquid. Gurvich,1982 pt1 p67 pt2 p68.  
 1 t<sub>pis</sub>82 V 2.000 4.00 0.00 0.00 0.00 3 165.88060 -  
 1432600.000  
 1818.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 16720.000  
 0.000000000D+00 0.000000000D+00 2.164890054D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.679377747D+05-  
 1.076187785D+02  
 V205(cr) Rhombic. Gurvich,1982 pt1 p68 pt2 p69.  
 2 t<sub>pis</sub>82 V 2.000 5.00 0.00 0.00 0.00 1 181.88000 -  
 1551000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 21210.000  
 -1.149585895D+07 2.200852292D+05-1.711429444D+03 6.997610220D+00-  
 1.543892990D-02  
 1.771425949D-05-8.283987620D-09 -1.174509299D+06  
 8.899979010D+03  
 500.000 954.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 21210.000

-4.708328420D+05 0.000000000D+00 2.297387367D+01-1.118831481D-02  
 1.146815480D-05  
 0.000000000D+00 0.000000000D+00 -1.945738450D+05-  
 1.150219507D+02  
 V205(L) Liquid. Gurvich,1982 pt1 p68 pt2 p69.  
 1 tpi82 V 2.000 5.00 0.00 0.00 0.00 2 181.88000 -  
 1551000.000  
 954.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 21210.000  
 0.000000000D+00 0.000000000D+00 2.285161723D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.880385445D+05-  
 1.113109611D+02  
 W(cr) Crystal. Ref-Elm. Chase,1998 pp1925-8.  
 4 j 6/66 W 1.00 0.00 0.00 0.00 0.00 1 183.84000  
 0.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 4973.000  
 -6.824541400D+03-2.254249090D+02 4.976604610D+00-6.926436340D-03  
 1.202272986D-05  
 -9.344133510D-09 2.818887123D-12 -3.510679270D+00-  
 2.361334984D+01  
 1000.000 2600.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 4973.000  
 5.530134840D+05-2.041485344D+03 5.870839470D+00-1.920714198D-03  
 1.067652983D-06  
 -2.355109022D-10 2.160679310D-14 1.163812518D+04-  
 3.319171800D+01  
 2600.000 3200.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 4973.000  
 2.474736879D+09 4.488921620D+06-1.235978300D+04 9.678565660D+00-  
 3.556364610D-03  
 6.380420610D-07-4.521123450D-11 -2.029500909D+07  
 8.274369690D+04  
 3200.000 3680.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 4973.000  
 -1.755550399D+10 1.179059156D+07 1.177715365D+03-2.675166841D+00  
 7.252172480D-04  
 -6.128007580D-08 0.000000000D+00 -9.702249190D+07-  
 1.148926234D+03  
 W(L) Liquid. Ref-Elm. Chase,1998 pp1925-8.  
 1 j 6/66 W 1.00 0.00 0.00 0.00 0.00 2 183.84000  
 0.000  
 3680.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 4973.000  
 0.000000000D+00 0.000000000D+00 4.277341659D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 2.755443078D+03-  
 2.086449853D+01  
 WC(cr) Hf:Wagman,1982 p203. Barin,1989 pt2 p1642.  
 1 bar 89 W 1.00C 1.00 0.00 0.00 0.00 1 195.85070 -  
 40540.000  
 298.150 2500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 -1.119754391D+05-5.553268210D-01 5.217965240D+00 1.037888263D-03-  
 1.229060652D-07  
 2.880427321D-13-7.236307119D-17 -6.848998700D+03-  
 2.677066218D+01  
 WCL6(I) Alpha1. Chase,1998 pp931-4.  
 1 j12/66 W 1.00CL 6.00 0.00 0.00 0.00 1 396.55620 -  
 593710.000

298.150 450.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 1.661826519D+02 0.000000000D+00 1.508873100D+01 2.015651227D-02-  
 2.754798370D-08  
 0.000000000D+00 0.000000000D+00 -7.680028810D+04-  
 6.329365920D+01  
 WCL6(II) Alpha2. Chase,1998 pp931-4.  
 1 j12/66 W 1.00CL 6.00 0.00 0.00 0.00 2 396.55620 -  
 593710.000  
 450.000 503.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 -9.897046360D+03 0.000000000D+00 1.522857952D+01 1.994376611D-02  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -7.636166220D+04-  
 6.296167010D+01  
 WCL6(III) Beta. Chase,1998 pp931-4.  
 1 j12/66 W 1.00CL 6.00 0.00 0.00 0.00 3 396.55620 -  
 593710.000  
 503.000 555.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 0.000000000D+00 0.000000000D+00 2.264474996D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -7.565217840D+04-  
 9.527165358D+01  
 WCL6(L) Liquid. Chase,1998 pp931-4.  
 1 j12/66 W 1.00CL 6.00 0.00 0.00 0.00 4 396.55620 -  
 593710.000  
 555.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 0.000000000D+00 0.000000000D+00 2.415439996D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -7.568493560D+04-  
 1.033604557D+02  
 WOCL4(cr) Crystal. Chase,1998 pp897-9.  
 1 j 3/67 W 1.00O 1.00CL 4.00 0.00 0.00 1 341.65020 -  
 671114.000  
 298.150 484.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 1.295153216D+03 0.000000000D+00 1.378522135D+01 1.276179773D-02-  
 1.713279395D-07  
 0.000000000D+00 0.000000000D+00 -8.538742740D+04-  
 6.154983780D+01  
 WOCL4(L) Liquid. Chase,1998 pp897-9.  
 1 j 3/67 W 1.00O 1.00CL 4.00 0.00 0.00 2 341.65020 -  
 671114.000  
 484.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 0.000000000D+00 0.000000000D+00 2.188992496D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -8.236656270D+04-  
 9.422321377D+01  
 WO2(cr) Gurvich,1982 pt1 p46 pt2 p49.  
 2 tpris82 W 1.00O 2.00 0.00 0.00 0.00 1 215.83880 -  
 588100.000  
 100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8711.000  
 -1.733842408D+04 0.000000000D+00 2.558979845D+00 1.457260175D-02  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -7.220058630D+04-  
 1.293182268D+01

298.150 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 8711.000  
 -1.555714047D+05 0.000000000D+00 7.983272616D+00 1.595163155D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -7.370467050D+04-  
 4.074555290D+01  
 WO2CL2(cr) Chase,1998 p848.  
 1 j 3/67 W 1.000 2.00CL 2.00 0.00 0.00 1 286.74420 -  
 780316.000  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 -3.819410020D+05 2.367029691D+03 9.834455770D+00-2.508443012D-02  
 1.017169638D-04  
 -1.040117941D-07 3.468311980D-11 -1.111440350D+05-  
 2.227929881D+01  
 WO3(III) Gurvich,1982 pt1 p49 pt2 p51.  
 1 tpis82 W 1.000 3.00 0.00 0.00 0.00 1 231.83820 -  
 841300.000  
 100.000 325.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13280.000  
 -2.841140443D+05 7.257714840D+03-6.708405120D+01 3.092936300D-01-  
 4.127635650D-04  
 0.000000000D+00 0.000000000D+00 -1.335884160D+05  
 3.409113710D+02  
 WO3(III,II) Gurvich,1982 pt1 p49 pt2 p51.  
 1 tpis82 W 1.000 3.00 0.00 0.00 0.00 2 231.83820 -  
 841300.000  
 325.000 1013.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13280.000  
 -5.186114395D+04 0.000000000D+00 8.548308920D+00 4.317151582D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.040935177D+05-  
 4.044670662D+01  
 WO3(I) Gurvich,1982 pt1 p49 pt2 p51.  
 1 tpis82 W 1.000 3.00 0.00 0.00 0.00 3 231.83820 -  
 841300.000  
 1013.000 1747.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13280.000  
 0.000000000D+00 0.000000000D+00 9.737555190D+00 1.958624140D-03  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.039166330D+05-  
 4.614390358D+01  
 WO3(L) Liquid. Gurvich,1982 pt1 p49 pt2 p51.  
 1 tpis82 W 1.000 3.00 0.00 0.00 0.00 4 231.83820 -  
 841300.000  
 1747.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 13280.000  
 0.000000000D+00 0.000000000D+00 1.551504538D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.022412072D+05-  
 8.082927535D+01  
 Zn(cr) Crystal. Ref-Elm. Cox,1989 p221.  
 1 coda89 ZN 1.00 0.00 0.00 0.00 0.00 1 65.39000  
 0.000  
 200.000 692.7307 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 5657.000  
 3.702080380D+05-5.915475500D+03 3.959500360D+01-1.143735885D-01  
 1.934363797D-04  
 -1.675385126D-07 6.078189940D-11 2.681737238D+04-  
 2.114848186D+02  
 Zn(L) Liquid. Ref-Elm. Cox,1989 p221.

1 coda89 ZN 1.00 0.00 0.00 0.00 0.00 2 65.39000  
 0.000  
 692.730 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 5657.000  
 0.000000000D+00 0.000000000D+00 3.776530427D+00 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.317345880D+02-  
 1.567077937D+01  
 ZnSO4(a) Alpha. Chase,1998 p1788.  
 1 j 3/79 ZN 1.00S 1.000 4.00 0.00 0.00 1 161.45360 -  
 980143.840  
 200.000 540.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17238.080  
 4.103530390D+05-7.357987120D+03 5.215317850D+01-1.152180317D-01  
 1.922132213D-04  
 -1.099361720D-07 0.000000000D+00 -8.649370210D+04-  
 2.794432413D+02  
 ZnSO4(a') Alpha'.Chase,1998 p1788.  
 1 j 3/79 ZN 1.00S 1.000 4.00 0.00 0.00 2 161.45360 -  
 980143.840  
 540.000 1013.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17238.080  
 -3.253792010D+06 3.252313710D+04-1.146490609D+02 2.718567520D-01-  
 3.079986965D-04  
 1.830520033D-07-4.445112450D-11 -2.895173465D+05  
 6.881710230D+02  
 ZnSO4(b) Beta. Chase,1998 p1788.  
 1 j 3/79 ZN 1.00S 1.000 4.00 0.00 0.00 3 161.45360 -  
 980143.840  
 1013.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 17238.080  
 0.000000000D+00 0.000000000D+00 1.746161830D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.211366813D+05-  
 8.514209609D+01  
 Zr(a) Alpha. Ref-Elm. Chase,1998 pp1943-7.  
 1 j 6/79 ZR 1.00 0.00 0.00 0.00 0.00 1 91.22400  
 0.000  
 200.000 1135.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 5497.000  
 -1.153699220D+04 2.626203401D+01 2.932054698D+00 5.743358570D-04-  
 7.651710410D-07  
 1.597202829D-09-6.097129620D-13 -1.084153260D+03-  
 1.215776960D+01  
 Zr(b) Beta. Ref-Elm. Chase,1998 pp1943-7.  
 1 j 6/79 ZR 1.00 0.00 0.00 0.00 0.00 2 91.22400  
 0.000  
 1135.000 2125.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 5497.000  
 -1.065463955D+06 4.273000010D+03-3.173856480D+00 5.018842560D-03-  
 2.363431747D-06  
 7.707582390D-10-8.156156570D-14 -2.641247444D+04  
 3.072041827D+01  
 Zr(L) Liquid. Ref-Elm. Chase,1998 pp1943-7.  
 1 j 6/79 ZR 1.00 0.00 0.00 0.00 0.00 3 91.22400  
 0.000  
 2125.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 5497.000  
 0.000000000D+00 0.000000000D+00 5.032166658D+00 0.000000000D+00  
 0.000000000D+00



0.000000000D+00 0.000000000D+00 -1.100795852D+03-  
2.548066000D+01  
ZrC(cr) Crystal. Chase,1998 pp658-60.  
2 j12/64 ZR 1.00C 1.00 0.00 0.00 0.00 1 103.23470 -  
196648.000  
200.000 800.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
5862.000  
-1.329596558D+05 1.766908163D+03-9.907099000D+00 5.427909170D-02-  
8.887722520D-05  
7.332246190D-08-2.420411623D-11 -3.297124410D+04  
5.279964170D+01  
800.000 3805.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
5862.000  
8.297591180D+05-4.224196050D+03 1.308509211D+01-5.018095870D-03  
2.155019459D-06  
-4.233046770D-10 3.266859200D-14 -7.112782350D+02-  
7.921945570D+01  
ZrC(L) Liquid. Chase,1998 pp658-60.  
1 j12/64 ZR 1.00C 1.00 0.00 0.00 0.00 2 103.23470 -  
196648.000  
3805.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
5862.000  
0.000000000D+00 0.000000000D+00 7.548249987D+00 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -1.885005134D+04-  
3.953387107D+01  
ZrN(cr) Chase,1998 pp1617-9 6/61.  
2 g11/00 ZR 1.00N 1.00 0.00 0.00 0.00 1 105.23074 -  
371238.000  
200.000 800.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6590.000  
2.548624207D+05-4.476456170D+03 2.958601499D+01-6.635810940D-02  
1.033814686D-04  
-8.272994600D-08 2.689947231D-11 -2.492379728D+04-  
1.616084405D+02  
800.000 3225.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6590.000  
2.174089790D+05-1.074470994D+03 7.053124150D+00-1.447713245D-04  
3.458043010D-07  
-5.893486000D-11 3.787112980D-15 -3.999164210D+04-  
3.811591880D+01  
ZrN(L) Chase,1998 pp1617-9 6/61.  
1 g11/00 ZR 1.00N 1.00 0.00 0.00 0.00 2 105.23074 -  
371238.000  
3225.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
6590.000  
0.000000000D+00 0.000000000D+00 7.045033321D+00 0.000000000D+00  
0.000000000D+00  
0.000000000D+00 0.000000000D+00 -3.882762780D+04-  
3.444078302D+01  
ZrO2(III) Monoclinic. Gurvich,1982 pt1 p123 pt2 p122.  
2 tpris82 ZR 1.00O 2.00 0.00 0.00 0.00 1 123.22280 -  
1100300.000  
200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
8751.000  
-4.214621830D+06 7.918732350D+04-6.071267910D+02 2.463358622D+00-  
5.388665930D-03  
6.144154000D-06-2.860860736D-09 -4.893051030D+05  
3.163542730D+03  
500.000 1445.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
8751.000

```

-1.616911113D+05 0.000000000D+00 8.218464380D+00 1.091902502D-03
0.000000000D+00
0.000000000D+00 0.000000000D+00 -1.353760676D+05-
4.200007680D+01
ZrO2(II) Tetragonal. Gurvich,1982 pt1 p123 pt2 p122.
1 tps82 ZR 1.000 2.00 0.00 0.00 0.00 2 123.22280 -
1100300.000
1445.000 2620.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
8751.000
0.000000000D+00 0.000000000D+00 9.393217399D+00 0.000000000D+00
0.000000000D+00
0.000000000D+00 0.000000000D+00 -1.348114469D+05-
4.823174581D+01
ZrO2(I) Cubic. Gurvich,1982 pt1 p123 pt2 p122.
1 tps82 ZR 1.000 2.00 0.00 0.00 0.00 3 123.22280 -
1100300.000
2620.000 2983.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
8751.000
0.000000000D+00 0.000000000D+00 9.621733572D+00 0.000000000D+00
0.000000000D+00
0.000000000D+00 0.000000000D+00 -1.338466275D+05-
4.943361269D+01
ZrO2(L) Liquid. Gurvich,1982 pt1 p123 pt2 p122.
1 tps82 ZR 1.000 2.00 0.00 0.00 0.00 4 123.22280 -
1100300.000
2983.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
8751.000
0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00
0.000000000D+00
0.000000000D+00 0.000000000D+00 -1.301975851D+05-
6.505001424D+01
END PRODUCTS
Air Mole%:N2 78.084,O2 20.9476,Ar .9365,CO2
.0319.Gordon,1982.Reac
2 g 9/95 N 1.56170 .41959AR.00937C .00032 .00000 0 28.9651784 -
125.530
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
8649.264
1.009950160D+04-1.968275610D+02 5.009155110D+00-5.761013730D-03
1.066859930D-05
-7.940297970D-09 2.185231910D-12 -1.767967310D+02-
3.921500990D+00
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
8649.264
2.415214430D+05-1.257874600D+03 5.144558670D+00-2.138541790D-04
7.065227840D-08
-1.071483490D-11 6.577800150D-16 6.462263190D+03-
8.147408670D+00
B2H6(L) Diborane. McBride,1996 pp84,92.
0 g 6/96 B 2.00H 6.00 0.00 0.00 0.00 1 27.66964
16445.000
180.590 0.0000 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
0.000
B5H9(L) Pentaborane. Chase,1998 p302.
0 j 3/65 B 5.00H 9.00 0.00 0.00 0.00 1 63.12646
42840.000
298.150 0.0000 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
0.000
(CH2)x(cr) Ethylene polymer. McBride,1996 pp84,92.
0 g 6/96 C 1.00H 2.00 0.00 0.00 0.00 1 14.02658 -
25600.000

```

298.150	0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
0.000											
CH3NO2(L)		Nitromethane. McBride,1996 pp85,93.									
0 g 6/96 C	1.00H	3.00N	1.00O	2.00	0.00	1		61.04006			-
113100.000											
298.150	0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
0.000											
CH4(L)		Methane. McBride,1996 pp85,93.									
0 g 6/96 C	1.00H	4.00	0.00	0.00	0.00	1		16.04246			-
89233.000											
111.643	0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
0.000											
CH3OH(L)		MeOH. TRC(12/87) p5000 (12/84)tc,uc,vc5031,5033.									
React.											
1 n12/84 C	1.00H	4.00O	1.00	0.00	0.00	1		32.04186			-
238910.000											
175.610	390.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		
18995.000											
-1.302004763D+06	3.166984180D+04	-3.031242152D+02	1.602231130D+00	-4.594507340D-03							
6.990178310D-06	-4.207388950D-09										
1.514346642D+03											
CH6N2(L)		Monomethyl Hydrazine. TRC(12/93) p9220.									
0 n12/93 C	1.00H	6.00N	2.00	0.00	0.00	1		46.07182			
54200.000											
298.150	0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
0.000											
C2H2(L),acetylene		Acetylene. McBride,1996 pp84,92.									
0 g 6/96 C	2.00H	2.00	0.00	0.00	0.00	1		26.03728			
207599.000											
192.350	0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
0.000											
CH3CN(L)		Ethanenitrile (Acetonitrile). McBride,1996 pp84,92.									
0 g 6/96 C	2.00H	3.00N	1.00	0.00	0.00	1		41.05196			
31380.000											
298.150	0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
0.000											
C2H4(L)		Ethylene. McBride,1996 pp84,92.									
0 g 6/96 C	2.00H	4.00	0.00	0.00	0.00	1		28.05316			
33945.000											
169.420	0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
0.000											
C2H4O(L),ethylene		Ethylene oxide (Oxirane). McBride,1996 pp84,92.									
0 g 6/96 C	2.00H	4.00O	1.00	0.00	0.00	1		44.05256			-
78841.000											
283.650	0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
0.000											
C2H6(L)		Ethane. McBride,1996 pp84,92.									
0 g 6/96 C	2.00H	6.00	0.00	0.00	0.00	1		30.06904			-
103819.000											
184.559	0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
0.000											
C2H5OH(L)		Ethanol. TRC(12/87) p5000 (12/84)tc,uc,vc5031-3.									
React.											
1 n12/84 C	2.00H	6.00O	1.00	0.00	0.00	1		46.06844			-
277510.000											
159.000	390.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		
24082.000											
4.501115940D+05	-1.020828990D+04	1.014266780D+02	-3.874672610D-01	7.121392610D-04							

-1.857071450D-07-2.037622570D-10 7.448557900D+03-  
5.044255520D+02  
C2H8N2(L),UDMH Unsymmetrical Dimethyl Hydrazine. McBride,1996 pp85,93.  
0 g 6/96 C 2.00H 8.00N 2.00 0.00 0.00 1 60.09840  
48900.000  
298.150 0.0000 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0  
0.000  
C2N2(L) Cyanogen. McBride,1996 pp84,92.  
0 g 6/96 C 2.00N 2.00 0.00 0.00 0.00 1 52.03488  
283209.000  
252.050 0.0000 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0  
0.000  
C3H6(L),propyle Propylene. McBride,1996 pp85,93.  
0 g 6/96 C 3.00H 6.00 0.00 0.00 0.00 1 42.07974 -  
2704.000  
225.460 0.0000 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0  
0.000  
C3H7NO3(L) Propyl Nitrate. McBride,1996 pp85,93.  
0 g 6/96 C 3.00H 7.00N 1.00O 3.00 0.00 1 105.09262 -  
214500.000  
298.150 0.0000 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0  
0.000  
C3H8(L) Propane. McBride,1996 pp85,93.  
0 g 6/96 C 3.00H 8.00 0.00 0.00 0.00 1 44.09562 -  
128228.000  
231.076 0.0000 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0  
0.000  
C4H8(L),1-buten 1-Butene. McBride,1996 pp84,92.  
0 g 6/96 C 4.00H 8.00 0.00 0.00 0.00 1 56.10632 -  
25173.000  
266.920 0.0000 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0  
0.000  
C4H10(L),n-buta n-Butane. McBride,1996 pp84,92.  
0 g 6/96 C 4.00H 10.00 0.00 0.00 0.00 1 58.12220 -  
150664.000  
272.638 0.0000 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0  
0.000  
C4H10(L),isobut Isobutane(2-methyl propane). McBride,1996 pp84,92.  
0 g 6/96 C 4.00H 10.00 0.00 0.00 0.00 1 58.12220 -  
159664.000  
261.361 0.0000 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0  
0.000  
C5H12(L),n-pent n-Pentane. McBride,1996 pp85,93.  
0 g 6/96 C 5.00H 12.00 0.00 0.00 0.00 1 72.14878 -  
173490.000  
298.150 0.0000 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0  
0.000  
C6H6(L) TRC(10/86) tc,uc,vc3201 (4/83) p3200.  
React  
1 n10/86 C 6.00H 6.00 0.00 0.00 0.00 1 78.11184  
49080.000  
278.680 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
30110.000  
-2.291003940D+06 3.692058160D+04-1.820019971D+02 2.634137216D-01  
9.742585920D-04  
-3.307909150D-06 2.888191394D-09 -1.730169095D+05  
1.070458659D+03  
C6H5NH2(L) Aniline. TRC(12/88) tc,uc,vc9370. TRC(6/95) p9370.  
React.  
1 n12/88 C 6.00H 7.00N 1.00 0.00 0.00 1 93.12652  
31500.000

267.130 460.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 34020.000  
 6.257653490D+07-8.930118090D+05 5.055201440D+03-1.397470822D+01  
 1.889729680D-02  
 -9.205910240D-06-1.289458554D-09 4.267459270D+06-  
 2.801220752D+04  
 C6H14(L),n-hexa n-hexane. TRC(4/85) p,tc,uc,vc1440,1441.  
 React.  
 1 n 4/85 C 6.00H 14.00 0.00 0.00 0.00 1 86.17536 -  
 198660.000  
 177.860 300.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 46920.000  
 7.721016130D+06-2.249298616D+05 2.717090647D+03-1.698251992D+01  
 5.907215180D-02  
 -1.074528475D-04 8.024238270D-08 8.808691730D+05-  
 1.292771483D+04  
 C7H8(L) TRC(10/86) tc uc vc3200-1 (4/83) p-3200.  
 React.  
 1 n10/86 C 7.00H 8.00 0.00 0.00 0.00 1 92.13842  
 12180.000  
 178.150 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 33470.000  
 -3.713549510D+06 7.772529030D+04-6.312269860D+02 2.724391982D+00-  
 6.103535080D-03  
 7.022421900D-06-3.113715680D-09 -3.452115500D+05  
 3.265980710D+03  
 C7H16(L),n-hept TRC(10/84) p-1010 (10/75) tc,uc,vc1460.  
 React.  
 1 n10/75 C 7.00H 16.00 0.00 0.00 0.00 1 100.20194 -  
 224350.000  
 182.580 380.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 52640.000  
 1.759947367D+06-3.749396790D+04 3.963064900D+02-2.117827431D+00  
 6.828248670D-03  
 -1.131862116D-05 7.736860130D-09 1.269072572D+05-  
 1.921686840D+03  
 C8H18(L),n-octa TRC(10/76) tc,uc,vc1491,1492. Hf:(10/84) p1010.  
 React.  
 1 n10/84 C 8.00H 18.00 0.00 0.00 0.00 1 114.22852 -  
 250260.000  
 216.370 400.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 61490.000  
 -1.683314826D+07 3.532615080D+05-2.967857531D+03 1.316703807D+01-  
 3.186822410D-02  
 4.075748010D-05-2.153277285D-08 -1.588494258D+06  
 1.521639569D+04  
 C8H18(L),isooct TRC(10/76) tc,uc,vc1491,1492. Hf:(10/82) p1490.  
 React.  
 1 n10/82 C 8.00H 18.00 0.00 0.00 0.00 1 114.22852 -  
 259160.000  
 165.790 380.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 50190.000  
 1.419157943D+05-2.937251288D+03 4.168834760D+01-8.436942210D-02  
 2.894147919D-04  
 -2.200563712D-07 7.234225570D-11 -2.479398829D+04-  
 1.930220201D+02  
 CLF3(L) Chlorine Trifluoride. McBride,1996 pp84,92.  
 0 g 6/96 CL 1.00F 3.00 0.00 0.00 0.00 1 92.44791 -  
 193386.000  
 284.890 0.0000 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0  
 0.000

CLO3F Hf:Wagman,1982 p49. Chase,1998 p755.

React.

2 g 5/95 CL	1.000	3.00F	1.00	0.00	0.00	0	102.44930	-
23800.000								
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
13298.823								
4.461077310D+04	-5.892352210D+02	3.558850810D+00	2.809585831D-02					
3.610880350D-05								
2.273331859D-08	-5.716733040D-12							-1.388667752D+03
4.590737000D+00								
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
13298.823								
-3.910495440D+05	-1.193220687D+03	1.388657545D+01	-3.541312060D-04					
7.825464770D-08								
-8.978325430D-12	4.163869660D-16							-1.275082535D+03-
5.106453430D+01								

CLO3F(L) Perchloryl Fluoride. McBride,1996 pp85,93.

0 g 6/96 CL	1.000	3.00F	1.00	0.00	0.00	1	102.44930	-
47436.000								
226.400	0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.000								

CL2(L) Chlorine. McBride,1996 pp84,92.

0 g 6/96 CL	2.00	0.00	0.00	0.00	0.00	1	70.90540	-
22550.000								
239.120	0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.000								

F2(L) Fluorine. McBride,1996 pp84,92.

0 g 6/96 F	2.00	0.00	0.00	0.00	0.00	1	37.99681	-
13091.000								
85.020	0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.000								

F2O(L) Oxygen Difluoride. McBride,1996 pp85,93.

0 g 6/96 F	2.000	1.00	0.00	0.00	0.00	1	53.99621	
6672.000								
128.400	0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.000								

HNO3(L) Nitric Acid. McBride,1996 pp85,93.

0 g 6/96 H	1.00N	1.000	3.00	0.00	0.00	1	63.01288	-
173013.000								
298.150	0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.000								

H2(L) Hydrogen. McBride,1996 pp84,92.

0 g 6/96 H	2.00	0.00	0.00	0.00	0.00	1	2.01588	-
9012.000								
20.270	0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.000								

H2O2(L) Gurvich, 1989 v1 pt1 p126 pt2 p303.

React.

1 tpris89 H	2.000	2.00	0.00	0.00	0.00	1	34.01468	-
187780.000								
272.740	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
22949.000								
0.000000000D+00	0.000000000D+00	1.074386825D+01	0.000000000D+00					
0.000000000D+00								
0.000000000D+00	0.000000000D+00							-2.578789845D+04-
4.803221291D+01								

IRFNA Inhibited Red Fuming Nitric Acid. McBride,1996 pp84,93.

0 g 6/96 H	1.57N	1.630	4.70F	0.02	0.00	1	100.00000	-
270496.000								
298.150	0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.000								

JP-4 McBride,1996 pp85,93. Hcomb = 18640.BTU/#  
 0 g 6/96 C 1.00H 1.94 0.00 0.00 0.00 1 13.96842 -  
 22723.000  
 298.150 0.0000 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0  
 0.000

JP-5 Or ASTM A1(L). McBride,1996 pp85,93. Hcomb = 18600.BTU/#  
 0 g 6/96 C 1.00H 1.92 0.00 0.00 0.00 1 13.94443 -  
 22183.000  
 298.150 0.0000 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0  
 0.000

JP-10(g) Exo-tetrahydrodicyclopentadiene.Pri.Com.R.Jaffe 12/00.  
 React.  
 2 g 6/01 C 10.00H 16.00 0.00 0.00 0.00 0 136.23404 -  
 86855.900  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22997.434  
 -7.310769440D+05 1.521764245D+04-1.139312644D+02 4.281501620D-01-  
 5.218740440D-04  
 3.357233400D-07-8.805750980D-11 -8.067482120D+04  
 6.320148610D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 22997.434  
 1.220329594D+07-5.794846240D+04 1.092281156D+02-1.082406215D-02  
 2.034992622D-06  
 -2.052060369D-10 8.575760210D-15 3.257334050D+05-  
 7.092350760D+02

Jet-A(L) McBride,1996. Faith,1971. Gracia-Salcedo,1988.  
 React.  
 1 g 2/96 C 12.00H 23.00 0.00 0.00 0.00 1 167.31102 -  
 303403.000  
 220.000 550.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 -4.218262130D+05-5.576600450D+03 1.522120958D+02-8.610197550D-01  
 3.071662234D-03  
 -4.702789540D-06 2.743019833D-09 -3.238369150D+04-  
 6.781094910D+02

Jet-A(g) McBride,1996. Faith,1971. Gracia-Salcedo,1988.  
 React.  
 2 g 8/01 C 12.00H 23.00 0.00 0.00 0.00 0 167.31102 -  
 249657.000  
 273.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 -6.068695590D+05 8.328259590D+03-4.312321270D+01 2.572390455D-01-  
 2.629316040D-04  
 1.644988940D-07-4.645335140D-11 -7.606962760D+04  
 2.794305937D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 1.858356102D+07-7.677219890D+04 1.419826133D+02-7.437524530D-03  
 5.856202550D-07  
 1.223955647D-11-3.149201922D-15 4.221989520D+05-  
 8.986061040D+02

LiClO4(cr) Lithium Perchlorate. Chase,1998 p782.  
 0 g 6/96 LI 1.00CL 1.000 4.00 0.00 0.00 1 106.39130 -  
 380700.000  
 298.150 0.0000 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0  
 0.000

NF3(L) Nitrogen trifluoride. McBride,1996 pp85,93.  
 0 g 6/96 N 1.00F 3.00 0.00 0.00 0.00 1 71.00195 -  
 150387.000





1 tps89 N 2.00H 4.000 3.00 0.00 0.00 3 80.04344 -  
 365600.000  
 357.250 399.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 23662.000  
 0.000000000D+00 0.000000000D+00 6.023205216D+01-1.767993544D-01  
 0.000000000D+00  
 4.528829721D-07 0.000000000D+00 -5.478633510D+04-  
 2.757806209D+02  
 NH4NO3(I) Cubic(I). Gurvich,1989 pt1 p370 pt2 p322.  
 React.  
 1 tps89 N 2.00H 4.000 3.00 0.00 0.00 4 80.04344 -  
 365600.000  
 399.000 442.8507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 23662.000  
 0.000000000D+00 0.000000000D+00 1.295325882D+01 1.563531705D-02  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.783701280D+04-  
 5.848510823D+01  
 NH4NO3(L) Liquid Gurvich,1989 pt1 p370 pt2 p322.  
 React.  
 1 tps89 N 2.00H 4.000 3.00 0.00 0.00 5 80.04344 -  
 365600.000  
 442.850 900.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 23662.000  
 0.000000000D+00 0.000000000D+00 1.936373881D+01 0.000000000D+00  
 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.843793300D+04-  
 8.903005276D+01  
 N2(L) Nitrogen. McBride,1996 pp85,93.  
 0 g 6/96 N 2.00 0.00 0.00 0.00 0.00 1 28.01348 -  
 12107.000  
 77.352 0.0000 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0  
 0.000  
 N2H4(L) Hydrazine.Hf:Gurvich,1989 pt1 p360. Chase,1998(12/65).  
 React.  
 1 g11/99 N 2.00H 4.00 0.00 0.00 0.00 1 32.04524  
 50380.000  
 100.000 800.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000  
 2.080965738D+04-7.418167630D+02 1.916569184D+01-4.539330120D-02  
 1.342024252D-04  
 -1.470873931D-07 6.056288260D-11 5.735408180D+03-  
 8.820213940D+01  
 N2O4(L) Dinitrogen tetroxide. McBride,1996 pp85,93.  
 0 g 6/96 N 2.000 4.00 0.00 0.00 0.00 1 92.01108 -  
 17549.000  
 298.150 0.0000 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0  
 0.000  
 O2(L) Oxygen. McBride,1996 pp85,93.  
 0 g 6/96 O 2.00 0.00 0.00 0.00 0.00 1 31.99880 -  
 12979.000  
 90.170 0.0000 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0  
 0.000  
 O3(L) Ozone. McBride,1996 pp85,93.  
 0 g 6/96 O 3.00 0.00 0.00 0.00 0.00 1 47.99820  
 122527.000  
 161.850 0.0000 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0  
 0.000  
 RP-1 Mehta et.al. AIAA 95-2962 1995. Hcomb(high) =  
 19923.BTU/#

0 g11/00 C 1.00H 1.95 0.00 0.00 0.00 1 13.97820 -  
24717.700  
298.150 0.0000 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0  
0.000  
END REACTANTS