Thermodynamic Database Update to Model Synthetic Chelating Agents in Soil Systems

F. Yunta[a], S. Lopez-Rayo[b] and J.J. Lucena[b]

[a]*Departamento de Geología y Geoquímica, Facultad de Ciencias, Universidad de Madrid, 28049 Madrid, Spain*

[b]*Departamento de Química Agrícola, Facultad de Ciencias, Universidad de Madrid, 28049 Madrid, Spain*

SUPPORTING INFORMATION

Final Updated Component Database

```
1,"E-1",-1,0,0,0
2,"H2O",0,0,0,18.0153
20,"Ag+1",1,0,0,107.868
30,"Al+3",3,9,0,26.9815
60,"H3AsO3",0,0,0,125.9437
61,"H3AsO4",0,0,0,141.9431
90,"H3BO3",0,0,0,61.8331
100,"Ba+2",2,5,0,137.34
130,"Br-1",-1,4,0,79.904
140,"CO3-2",-2,5.4,0,60.0094
143,"CN-",-1,0,0,26.018
144,"DOM1",-2.8,0,0,0
145,"DOM2",-2.8,0,0,0
146,"DOM3",-2.8,0,0,0
150,"Ca+2",2,6,.165,40.08
160,"Cd+2",2,0,0,112.3994
180,"Cl-1",-1,3,.015,35.453
182,"Co+2",2,0,0,58.9332
183,"Co+3",3,0,0,58.9332
210,"Cr+2",2,0,0,51.996
211,"Cr(OH)2+",1,0,0,86.011
212,"CrO4-2",-2,4,0,115.994
230,"Cu+1",1,2.5,0,63.546
231,"Cu+2",2,6,0,63.546
270,"F-1",-1,3.5,0,18.9984
280,"Fe+2",2,6,0,55.847
281,"Fe+3",3,9,0,55.847
330,"H+1",1,9,0,1.008
360,"Hg2+2",2,4,0,401.18
361,"Hg(OH)2",0,0,0,234.61
362,"Hg+2",2,0,0,200.59
380,"I-1",-1,0,0,126.9044
410,"K+1",1,3,.015,39.102
440,"Li+1",1,6,0,6.939
460,"Mg+2",2,6.5,.2,24.312
470,"Mn+2",2,6,0,54.938
471,"Mn+3",3,9,0,54.938
472,"Mn+4",4,0,0,54.938
480,"MoO4-2",-2,0,0,159.938
490,"NH4+1",1,2.5,0,18.0386
491,"NO2-1",-1,0,0,46.0055
492,"NO3-1",-1,3,0,62.0049
500,"Na+1",1,4,.075,22.9898
540,"Ni+2",2,0,0,58.71
```

```
560,"OCN-",-1,0,0,42.017
580,"PO4-3",-3,5,0,94.9714
600,"Pb+2",2,0,0,207.1899
680,"Rb+1",1,0,0,85.4699
730,"HS-1",-1,3.5,0,33.072
731,"S",0,0,0,32.064
732,"SO4-2",-2,4,-.04,96.0616
740,"Sb(OH)3",0,0,0,172.7719
741,"Sb(OH)6-",-1,0,0,223.7938
760,"HSe-1",-1,0,0,79.97
761,"HSeO3-1",-1,0,0,127.97
762,"SeO4-2",-2,4,0,142.96
770,"H4SiO4",0,0,0,96.1155
800,"Sr+2",2,5,0,87.62
870,"Tl+1",1,0,0,204.37
871,"Tl(OH)3",0,0,0,255.39
891,"U+4",4,0,0,238.029
890,"U+3",3,0,0,238.029
892,"UO2+1",1,0,0,270.0278
893,"UO2+2",2,0,0,270.0278
900,"V+2",2,0,0,50.94
901,"V+3",3,0,0,50.94
902,"VO+2",2,0,0,66.939
903,"VO2+1",1,0,0,82.939
910,"CDTA-4",-4,0,0,288.213
911,"HEDTA-3",-3,0,0,275.238
912,"EGTA-4",-4,0,0,376.319
913,"BPDS-2",-2,0,0,536.5
920,"EDDHA-4",-4,0,0,356.40
921,"rac-EDDHA-4",-4,0,0,356.40
922,"meso-EDDHA-4",-4,0,0,356.40
923,"p,p-EDDHA-4",-4,0,0,356.40
924,"EDDH4MA-4",-4,0,0,384.40
925,"rac-EDDH4MA-4",-4,0,0,384.40
926,"meso-EDDH4MA-4",-4,0,0,384.40
927,"EDDH5MA-4",-4,0,0,384.40
928,"PDDHA-4",-4,0,0,370.40
929,"XDDHA-4",-4,0,0,432.50
930,"BDDHA-4",-4,0,0,384.44
931,"o,p-EDDHA-4",-4,0,0,356.40
932,"EDDMetxA-2",-2,0,0,386.50
933,"PDDHAbis-4",-4,0,0,370.40
934,"EDDHSA-6",-6,0,0,514.40
935,"HBED-4",-4,0,0,384.40
936,"IDHA-4",-4,0,0,245.10
937,"DCHA-3",-3,0,0,316.34
938,"HJB-4",-4,0,0,412.47
939,"EDDS-4",-4,0,0,292.02
950,"Zn+2",2,6,0,65.3699
953,"DTPA-5",-5,0,0,388.31
954,"EDDHA-4(Lindsay)",-4,0,0,356.33
955,"Dietham",0,0,0,73
956,"Nbutyam",0,0,0,73
958,"Metham",0,0,0,31.018
959,"Dimetham",0,0,0,45.028
960,"Trbutph",0,0,0,265.97
961,"Hexam",0,0,0,101
963,"EN",0,0,0,60.12
964,"Npropam",0,0,0,59.04
965,"Ipropam",0,0,0,59.04
```

```
966,"Tmetham",0,0,0,59.04
967,"Citrate",-3,0,0,189.06
968,"NTA-3",-3,0,0,188.177
969,"EDTA-4",-4,0,0,288.213
970,"Nicotmine-3",-3,0,0,300.29
971,"Prpanot",-1,0,0,73.032
972,"Butanot",-1,0,0,87.043
973,"Isobuty",-1,0,0,87.043
980,"2Metpyr",0,0,0,94
981,"3Metpyr",0,0,0,94
982,"4Metpyr",0,0,0,94
983,"Formate",-1,0,0,45.02
984,"Isvaler",-1,0,0,101.13
985,"Valerat",-1,0,0,101.13
990,"Fulvate",-2,0,0,650
991,"Humate",-2,0,0,2000
992,"Acetate",-1,0,0,59.05
993,"Tartrat",-2,0,0,148.09
994,"Glycine",-1,0,0,74.07
995,"Salicyl",-2,0,0,136.12
996,"Glutama",-2,0,0,145.13
997,"Phthala",-2,0,0,164.13
998,"H+1D",1,0,0,1.008
999,"OH-D",-1,0,0,17.0074
1090,"SOC%",0,0,0,1
1091,"Clay%",0,0,0,1
1092,"Dummy3",0,0,0,1
1200,"DOC (Gaussian DOM)",0,0,0,12
1301,"Lsite1",0,0,0,1
1302,"Lsite2",0,0,0,1
1311,"LFsite1",0,0,0,1
1312,"LFsite2",0,0,0,1
1321,"NICAsite1",0,0,0,1
1322,"NICAsite2",0,0,0,2
1340,"DOC (NICA-Donnan)",0,0,0,12
1341,"HFA1-(6)",-1,0,0,1
1342,"HFA2-(6)",-1,0,0,1
1343,"HFA1-(7)",-1,0,0,1
1344,"HFA2-(7)",-1,0,0,1
1351,"HFA1-(8)",-1,0,0,1
1352,"HFA2-(8)",-1,0,0,1
1353,"HFA1-(9)",-1,0,0,1
1354,"HFA2-(9)",-1,0,0,1
1361,"HFA1-(10)",-1,0,0,1
1362,"HFA2-(10)",-1,0,0,1
1363,"HFA1-(11)",-1,0,0,1
1364,"HFA2-(11)",-1,0,0,1
1401,"Ts1-Fer",0,0,0,0
1501,"R-dum",-1,0,0,1
1601,"PSIo(1)",0,0,0,0
1602,"PSIb(1)",0,0,0,0
1603,"PSId(1)",0,0,0,0
1607,"=SX-(1)",-1,0,0,1
1608,"=IX-(1)",-1,0,0,1
1611,"=SOH(1)",0,0,0,1
1612,"=SOHs2(1)",0,0,0,1
1613,"=SOHs3(1)",0,0,0,1
1614,"=SOHs4(1)",0,0,0,1
1615,"=SOHs5(1)",0,0,0,1
1616,"=SOHs6(1)",0,0,0,1
```

```
1621,"PSIo(2)",0,0,0,0
1622,"PSIb(2)",0,0,0,0
1623,"PSId(2)",0,0,0,0
1627,"=SX-(2)",-1,0,0,1
1628,"=IX-(2)",-1,0,0,1
1631,"=SOH(2)",0,0,0,1
1632,"=SOHs2(2)",0,0,0,1
1633,"=SOHs3(2)",0,0,0,1
1634,"=SOHs4(2)",0,0,0,1
1635,"=SOHs5(2)",0,0,0,1
1636,"=SOHs6(2)",0,0,0,1
1641,"PSIo(3)",0,0,0,0
1642,"PSIb(3)",0,0,0,0
1643,"PSId(3)",0,0,0,0
1647,"=SX-(3)",-1,0,0,1
1648,"=IX-(3)",-1,0,0,1
1651,"=SOH(3)",0,0,0,1
1652,"=SOHs2(3)",0,0,0,1
1653,"=SOHs3(3)",0,0,0,1
1654,"=SOHs4(3)",0,0,0,1
1655,"=SOHs5(3)",0,0,0,1
1656,"=SOHs6(3)",0,0,0,1
1661,"PSIo(4)",0,0,0,0
1662,"PSIb(4)",0,0,0,0
1663,"PSId(4)",0,0,0,0
1667,"=SX-(4)",-1,0,0,1
1668,"=IX-(4)",-1,0,0,1
1671,"=SOH(4)",0,0,0,1
1672,"=SOHs2(4)",0,0,0,1
1673,"=SOHs3(4)",0,0,0,1
1674,"=SOHs4(4)",0,0,0,1
1675,"=SOHs5(4)",0,0,0,1
1676,"=SOHs6(4)",0,0,0,1
1681,"PSIo(5)",0,0,0,0
1682,"PSIb(5)",0,0,0,0
1683,"PSId(5)",0,0,0,0
1687,"=SX-(5)",-1,0,0,1
1688,"=IX-(5)",-1,0,0,1
1691,"=SOH(5)",0,0,0,1
1692,"=SOHs2(5)",0,0,0,1
1693,"=SOHs3(5)",0,0,0,1
1694,"=SOHs4(5)",0,0,0,1
1695,"=SOHs5(5)",0,0,0,1
1696,"=SOHs6(5)",0,0,0,1
1700,"DOC (SHM)",0,0,0,12
1701,"/HFA-haf(6)",0,0,0,1
1702,"/HFA(6)",0,0,0,1
1703,"/PSIo(6)",0,0,0,0
1704,"/PSIb(6)",0,0,0,0
1705,"/PSId(6)",0,0,0,0
1799,"HFA-dum(6)",0,0,0,0
1801,"/HFA-haf(7)",0,0,0,1
1802,"/HFA(7)",0,0,0,1
1803,"/PSIo(7)",0,0,0,0
1804,"/PSIb(7)",0,0,0,0
1805,"/PSId(7)",0,0,0,0
1899,"HFA-dum(7)",0,0,0,0
1901,"/HFA-haf(8)",0,0,0,1
1902,"/HFA(8)",0,0,0,1
1903,"/PSIo(8)",0,0,0,0
```

```
1904,"/PSIb(8)",0,0,0,0
1905,"/PSId(8)",0,0,0,0
1999,"HFA-dum(8)",0,0,0,0
2001,"/HFA-haf(9)",0,0,0,1
2002,"/HFA(9)",0,0,0,1
2003,"/PSIo(9)",0,0,0,0
2004,"/PSIb(9)",0,0,0,0
2005,"/PSId(9)",0,0,0,0
2099,"HFA-dum(9)",0,0,0,0
2101,"/HFA-haf(10)",0,0,0,1
2102,"/HFA(10)",0,0,0,1
2103,"/PSIo(10)",0,0,0,0
2104,"/PSIb(10)",0,0,0,0
2105,"/PSId(10)",0,0,0,0
2199,"HFA-dum(10)",0,0,0,0
2201,"/HFA-haf(11)",0,0,0,1
2202,"/HFA(11)",0,0,0,1
2203,"/PSIo(11)",0,0,0,0
2204,"/PSIb(11)",0,0,0,0
2205,"/PSId(11)",0,0,0,0
2299,"HFA-dum(11)",0,0,0,0
0,"",0,0,0,0
```

Final Updated Thermodynamic Database

```
3300020,"OH-",55.835,-14,0,0,-1,3.5,0,0,2
1,2,-1,330
17.0074,"WLL79",""
3307700,"H3SiO4 -",37.384,-9.93,0,0,-1,4,0,0,2
1,770,-1,330
95.107,"",""
3307701,"H2SiO4 -2",124.323,-21.619,0,0,-2,5.4,0,0,2
1,770,-2,330
94.099,"",""
7702700,"SiF6 -2",-68.032,30.18,0,0,-2,5,0,0,4
1,770,6,270,4,330,-4,2
142.076,"",""
3300900,"H2BO3 -1",13.489,-9.24,0,0,-1,2.5,0,0,2
1,90,-1,330
60.825,"",""
902700,"BF(OH)3 -",7.74,-0.399,0,0,-1,2.5,0,0,2
1,90,1,270
80.831,"",""
902701,"BF2(OH)2 -",6.841,7.63,0,0,-1,2.5,0,0,4
1,90,2,270,-1,2,1,330
82.822,"",""
902702,"BF3OH -",-6.611,13.667,0,0,-1,2.5,0,0,4
1,90,3,270,-2,2,2,330
84.813,"",""
902703,"BF4 -",-7.51,20.274,0,0,-1,2.5,0,0,4
1,90,4,270,-3,2,3,330
86.804,"",""
3304900,"NH3 AQ",52.216,-9.252,0,0,0,0,0,0,2
1,490,-1,330
17.03,"",""
4907320,"NH4SO4 -",0,1.11,0,0,-1,5,0,0,2
1,490,1,732
114.1,"",""
4603300,"MgOH +",66.672,-11.79,0,0,1,6.5,0,0,3
1,460,1,2,-1,330
41.319,"",""
4602700,"MgF +",19.556,1.82,0,0,1,4.5,0,0,2
1,460,1,270
43.31,"",""
```

```
4601400,"MgCO3 AQ",8.46,3.23,0,0,0,0,0,2,2
1,460,1,140
84.321,"WLL79",""
4601401,"MgHCO3 +",-10.167,11.39,0,0,1,4,0,1,3
1,460,1,140,1,330
85.329,"WLL79",""
4607320,"MgSO4 AQ",5.853,2.23,0,0,0,0,0,0,2
1,460,1,732
120.373,"WLL79",""
4605800,"MgPO4 -",12.97,6.589,0,0,-1,5.4,0,0,2
1,460,1,580
119.283,"",""
4605801,"MgH2PO4 +",-4.686,21.066,0,0,1,5.4,0,0,3
1,460,1,580,2,330
121.299,"",""
4605802,"MgHPO4 AQ",-0.962,15.26,0,0,0,0,0,0,3
1,460,1,580,1,330
120.291,"WLL79",""
1503300,"CaOH +",60.814,-12.598,0,0,1,6,0,0,3
1,150,1,2,-1,330
57.087,"",""
1501400,"CaHCO3 +",7.489,11.33,0,0,1,6,0,1,3
1,150,1,140,1,330
101.097,"",""
1501401,"CaCO3 AQ",16.862,3.15,0,0,0,0,0,2,2
1,150,1,140
100.089,"",""
1507320,"CaSO4 AQ",6.15,2.309,0,0,0,0,0,0,2
1,150,1,732
136.141,"",""
1505800,"CaHPO4 AQ",-0.962,15.09,0,0,0,0,0,0,3
1,150,1,580,1,330
136.059,"WLL79",""
1505801,"CaPO4 -",12.97,6.46,0,0,-1,5.4,0,0,2
1,150,1,580
135.051,"WLL79",""
1505802,"CaH2PO4 +",-4.686,20.95,0,0,1,5.4,0,0,3
1,150,1,580,2,330
137.067,"WLL79",""
1502700,"CaF +",15.891,0.94,0,0,1,5,0,0,2
1,150,1,270
59.078,"",""
5001400,"NaCO3 -",37.284,1.268,0,0,-1,5.4,0,2,2
1,500,1,140
82.999,"",""
5001401,"NaHCO3 AQ",0,10.08,0,0,0,0,0,1,3
1,500,1,140,1,330
84.007,"",""
5007320,"NaSO4 -",4.686,0.7,0,0,-1,5.4,0,0,2
1,500,1,732
119.051,"",""
5005800,"NaHPO4 -",0,12.636,0,0,-1,5.4,0,0,3
1,500,1,580,1,330
118.969,"",""
5002700,"NaF AQ",0,-0.79,0,0,0,0,0,0,2
1,500,1,270
41.988,"",""
4107320,"KSO4 -",9.414,0.85,0,0,-1,5.4,0,0,2
1,410,1,732
135.163,"",""
4105800,"KHPO4 -",0,12.64,0,0,-1,5.4,0,0,3
1,410,1,580,1,330
135.081,"",""
303300,"AlOH+2",49.785,-5,0,0,2,5.4,0,0,3
1,30,1,2,-1,330
43.988,"N&M89",""
303301,"Al(OH)2 +",0,-10.1,0,0,1,5.4,0,0,3
```

```
1,30,2,2,-2,330
60.996,"N&M89",""
303302,"Al(OH)4 -",184.347,-22.7,0,0,-1,4.5,0,0,3
1,30,4,2,-4,330
95.011,"N&M89",""
303304,"Al2(OH)2+4",0,-7.69,0,0,4,0,0,0,3
2,30,2,2,-2,330
87.978,"WLL79",""
302700,"AlF +2",0,7,0,0,2,5.4,0,0,2
1,30,1,270
45.979,"N&M89",""
302701,"AlF2 +",83.68,12.7,0,0,1,5.4,0,0,2
1,30,2,270
64.978,"N&M89",""
302702,"AlF3 AQ",10.46,16.8,0,0,0,0,0,0,2
1,30,3,270
83.976,"N&M89",""
302703,"AlF4 -",0,19.4,0,0,-1,4.5,0,0,2
1,30,4,270
102.975,"N&M89",""
302704,"AlF5-2",0,20.6,0,0,-2,0,0,0,2
1,30,5,270
126.974,"WLL79",""
302705,"AlF6-3",0,20.6,0,0,-3,0,0,0,2
1,30,6,270
137.972,"WLL79",""
307320,"AlSO4 +",8.996,3.5,0,0,1,4.5,0,0,2
1,30,1,732
123.043,"N&M89",""
307321,"Al(SO4)2 -",11.883,5,0,0,-1,4.5,0,0,2
1,30,2,732
219.104,"N&M89",""
303303,"Al(OH)3 AQ",0,-16.8,0,0,0,0,0,0,3
1,30,3,2,-3,330
78.003,"N&M89",""
305800,"AlH2PO4 +2",0,22.65,0,0,2,0,0,0,3
1,30,2,330,1,580
123.969,"N&M89",""
305801,"AlHPO4+",0,19.75,0,0,1,0,0,0,3
1,30,1,330,1,580
122.961,"N&M89",""
2803300,"FeOH +",55.225,-6.74,0,0,1,5,0,0,3
1,280,1,2,-1,330
72.854,"WLL79",""
2803301,"Fe(OH)3-",126.775,-31.99,0,0,-1,5,0,0,3
1,280,3,2,-3,330
106.869,"WLL79",""
2807320,"FeSO4 AQ",13.514,2.2,0,0,0,0,0,0,2
1,280,1,732
151.908,"WLL79",""
2805800,"FeH2PO4 +",0,22.25,0,0,1,5.4,0,0,3
1,280,1,580,2,330
152.834,"WLL79",""
2803302,"Fe(OH)2 AQ",119.516,-16.04,0,0,0,0,0,0,3
1,280,2,2,-2,330
89.861,"WLL79",""
2803303,"Fe(OH)4-2",0,-46.38,0,0,-2,0,0,0,3
1,280,4,2,-4,330
123.876,"WLL79",""
2803304,"Fe3(OH)4+2",0,-45.39,0,0,2,0,0,0,3
1,280,4,2,-4,330
235.57,"WLL79",""
2805801,"FeHPO4 AQ",0,15.95,0,0,0,0,0,0,3
1,280,1,580,1,330
151.826,"WLL79",""
2807300,"Fe(HS)2 AQ",0,8.95,0,0,0,0,0,0,2
1,280,2,730
```

```
121.99,"",""
2807301,"Fe(HS)3 -",0,10.987,0,0,-1,0,0,0,2
1,280,3,730
155.062,"",""
2813300,"FeOH +2",43.509,-2.19,0,0,2,5,0,0,3
1,281,1,2,-1,330
72.854,"WLL79",""
2815800,"FeHPO4 +",-30.543,23.26,0,0,1,5.4,0,0,3
1,281,1,580,1,330
151.826,"WLL79",""
2817320,"FeSO4 +",16.359,4.15,0,0,1,5,0,0,2
1,281,1,732
151.908,"WLL79",""
2811800,"FeCl +2",23.43,1.48,0,0,2,5,0,0,2
1,281,1,180
91.3,"WLL79",""
2811801,"FeCl2 +",0,2.13,0,0,1,5,0,0,2
1,281,2,180
126.753,"WLL79",""
2811802,"FeCl3 AQ",0,0.77,0,0,0,0,0,0,2
1,281,3,180
162.206,"WLL79",""
2813301,"Fe(OH)2+",0,-5.69,0,0,1,5.4,0,0,3
1,281,2,2,-2,330
89.861,"WLL79",""
2813302,"Fe(OH)3 AQ",0,-13.09,0,0,0,0,0,0,3
1,281,3,2,-3,330
106.869,"WLL79",""
2813303,"Fe(OH)4-",0,-21.59,0,0,-1,5.4,0,0,3
1,281,4,2,-4,330
123.876,"WLL79",""
2813304,"Fe2(OH)2+4",0,-2.9,0,0,4,0,0,0,3
2,281,2,2,-2,330
145.709,"WLL79",""
2815801,"FeH2PO4 +2",0,24.98,0,0,2,5.4,0,0,3
1,281,1,580,2,330
152.834,"WLL79",""
2812700,"FeF +2",11.293,6,0,0,2,5,0,0,2
1,281,1,270
74.845,"WLL79",""
2812701,"FeF2 +",20.083,9.2,0,0,1,5,0,0,2
1,281,2,270
93.843,"WLL79",""
2812702,"FeF3 AQ",22.589,11.7,0,0,0,0,0,0,2
1,281,3,270
112.842,"WLL79",""
2814920,"FeNO3 +2",0,1,0,0,2,0,0,0,2
1,281,1,492
117.852,"WLL79",""
2817321,"Fe(SO4)2 -",19.246,5.38,0,0,-1,0,0,0,2
1,281,2,732
247.97,"WLL79",""
2819900,"Fe FULVATE",0,9.399,0,0,1,0,0,0,2
1,281,1,990
705.847,"",""
2819910,"Fe HUMATE",0,9.399,0,0,1,0,0,0,2
1,281,1,991
2055.846,"",""
2813305,"Fe3(OH)4+5",59.831,-6.3,0,0,5,0,0,0,3
3,281,4,2,-4,330
235.57,"",""
4407320,"LiSO4 -",0,0.64,0,0,-1,5,0,0,2
1,440,1,732
103,"",""
8003300,"SrOH +",60.647,-13.178,0,0,1,5,0,0,3
1,800,1,2,-1,330
104.627,"",""
```

```
1003300,"BaOH +",63.157,-13.358,0,0,1,5,0,0,3
1,100,1,2,-1,330
154.347,"",""
4701800,"MnCl +",0,0.607,0,0,1,5,0,0,2
1,470,1,180
90.391,"",""
4701801,"MnCl2 AQ",0,0.041,0,0,0,0,0,0,2
1,470,2,180
125.844,"",""
4701802,"MnCl3 -",0,-0.305,0,0,-1,5,0,0,2
1,470,3,180
161.297,"",""
4703300,"MnOH +",60.245,-10.59,0,0,1,5,0,0,3
1,470,1,2,-1,330
161.297,"",""
4703301,"Mn(OH)3 -1",0,-34.8,0,0,-1,5,0,0,3
1,470,3,2,-3,330
105.96,"",""
4700020,"MnO4 -",738.978,-127.824,0,0,-1,3,0,0,4
1,470,4,2,-8,330,-5,1
118.935,"",""
4700021,"MnO4 -2",627.684,-118.44,0,0,-2,5,0,0,4
1,470,4,2,-8,330,-4,1
118.935,"",""
4702700,"MnF +",0,0.85,0,0,1,5,0,0,2
1,470,1,270
73.936,"",""
4707320,"MnSO4 AQ",9.079,2.26,0,0,0,0,0,0,2
1,470,1,732
150.999,"",""
4704920,"Mn(NO3)2AQ",-1.657,0.6,0,0,0,0,0,0,2
1,470,2,492
178.947,"",""
4701400,"MnHCO3 +",0,11.6,0,0,1,5,0,1,3
1,470,1,140,1,330
115.955,"",""
2301802,"CuCl AQ",0,2.7,0,0,0,0,0,0,2
1,230,1,180
98.999,"WLL79",""
2301803,"Cu2Cl4-2",0,13.1,0,0,-2,0,0,0,2
2,230,4,180
268.904,"WLL79",""
2301800,"CuCl2 -",-1.757,5.51,0,0,-1,4,0,0,2
1,230,2,180
134.452,"WLL79",""
2301801,"CuCl3 -2",1.088,5.7,0,0,-2,5,0,0,2
1,230,3,180
169.905,"WLL79",""
2307300,"Cu(S4)2 -3",0,3.39,0,0,-3,23,0,0,4
1,230,2,730,6,731,-2,330
320.058,"",""
2307301,"CuS4S5 -3",0,2.66,0,0,-3,25,0,0,4
1,230,2,730,7,731,-2,330
352.122,"",""
2319921,"Cu ACETATE",0,2.24,0,0,1,0,0,0,2
1,231,1,992
122.59,"",""
2319941,"Cu GLYCINE",0,8.62,0,0,1,0,0,0,2
1,231,1,994
137.61,"",""
2319942,"Cu2GLYCINE",0,15.64,0,0,3,0,0,0,2
2,231,1,994
201.15,"",""
2319951,"Cu SALICYL",0,10.64,0,0,0,0,0,0,2
1,231,1,995
199.66,"",""
2319952,"Cu2SALICYL",0,16.94,0,0,2,0,0,0,2
```

```
2,231,1,995
263.2,"",""
2319961,"Cu GLUTAMA",0,8.33,0,0,0,0,0,0,2
1,231,1,996
208.67,"",""
2319962,"Cu2GLUTAMA",0,14.84,0,0,2,0,0,0,2
2,231,1,996
272.21,"",""
2319971,"Cu PHTHALA",0,4.04,0,0,0,0,0,0,2
1,231,1,997
227.67,"",""
2319972,"Cu2PHTHALA",0,5.3,0,0,2,0,0,0,2
2,231,1,997
291.21,"",""
2311400,"CuCO3 AQ",0,6.72,0,0,0,0,0,2,2
1,231,1,140
123.555,"WLL79",""
2311401,"Cu(CO3)2-2",0,9.82,0,0,-2,0,0,4,2
1,231,2,140
183.564,"WLL79",""
2314920,"Cu(NO3)2 AQ",0,0.5,0,0,0,0,0,0,2
1,231,2,492
125.551,"WLL79",""
2315800,"CuH2PO4 +",0,21.14,0,0,1,0,0,0,3
1,231,2,330,1,580
160.533,"WLL79",""
2315801,"CuHPO4 AQ",0,15.55,0,0,0,0,0,0,3
1,231,1,330,1,580
159.525,"WLL79",""
2311800,"CuCl +",36.192,0.4,0,0,1,4,0,0,2
1,231,1,180
98.999,"WLL79",""
2311801,"CuCl2 AQ",44.183,-0.12,0,0,0,0,0,0,2
1,231,2,180
134.452,"WLL79",""
2311802,"CuCl3 -",57.279,-1.57,0,0,-1,4,0,0,2
1,231,3,180
169.905,"WLL79",""
2311803,"CuCl4 -2 1",32.552,-4.59,0,0,-2,5,0,0,2
1,231,4,180
205.358,"",""
2312700,"CuF +",6.778,1.26,0,0,1,0,0,0,2
1,231,1,270
82.544,"",""
2313300,"CuOH +",0,-7.7,0,0,1,4,0,0,3
1,231,1,2,-1,330
80.553,"WLL79",""
2313301,"Cu(OH)2 AQ",0,-13.78,0,0,0,0,0,0,3
1,231,2,2,-2,330
97.56,"WLL79",""
2313302,"Cu(OH)3 -",0,-26.75,0,0,-1,0,0,0,3
1,231,3,2,-3,330
114.568,"WLL79",""
2313303,"Cu(OH)4 -2",0,-39.59,0,0,-2,0,0,0,3
1,231,4,2,-4,330
131.575,"WLL79",""
2313304,"Cu2(OH)2+2",73.383,-10.68,0,0,2,0,0,0,3
2,231,2,2,-2,330
161.106,"WLL79",""
2317320,"CuSO4 AQ",5.104,2.36,0,0,0,0,0,0,2
1,231,1,732
159.607,"WLL79",""
2317300,"Cu(HS)3 -",0,25.899,0,0,-1,0,0,0,2
1,231,3,730
162.761,"",""
2311402,"CuHCO3 +",0,12.42,0,0,1,0,0,1,3
1,231,1,140,1,330
```

```
124.563,"WLL79",""
2319900,"Cu FULVATE",0,0,0,0,0,0,0,0,2
1,231,1,990
713.546,"",""
2319910,"Cu HUMATE",0,0,0,0,0,0,0,0,2
1,231,1,991
2063.545,"",""
9501800,"ZnCl +",32.593,0.43,0,0,1,4,0,0,2
1,950,1,180
100.823,"WLL79",""
9501801,"ZnCl2 AQ",35.564,0,0,0,0,0,0,0,2
1,950,2,180
136.276,"WLL79",""
9501802,"ZnCl3 -",39.999,0.5,0,0,-1,4,0,0,2
1,950,3,180
171.729,"WLL79",""
9501803,"ZnCl4 -2",45.857,0.2,0,0,-2,5,0,0,2
1,950,4,180
207.182,"WLL79",""
9502700,"ZnF +",9.288,1.15,0,0,1,0,0,0,2
1,950,1,270
84.368,"",""
9503300,"ZnOH +",56.061,-7.69,0,0,1,0,0,0,3
1,950,1,2,-1,330
82.377,"WLL79",""
9503301,"Zn(OH)2 AQ",0,-16.8,0,0,0,0,0,0,3
1,950,2,2,-2,330
99.384,"WLL79",""
9503302,"Zn(OH)3 -",0,-28.68,0,0,-1,0,0,0,3
1,950,3,2,-3,330
116.392,"WLL79",""
9503303,"Zn(OH)4 -2",0,-38.29,0,0,-2,0,0,0,3
1,950,4,2,-4,330
133.399,"WLL79",""
9501804,"ZnOHCl AQ",0,-7.48,0,0,0,0,0,0,4
1,950,1,2,-1,330,1,180
117.83,"",""
9507300,"Zn(HS)2 AQ",0,14.94,0,0,0,0,0,0,2
1,950,2,730
131.513,"",""
9507301,"Zn(HS)3 -",0,16.1,0,0,-1,0,0,0,2
1,950,3,730
164.585,"",""
9507320,"ZnSO4 AQ",5.69,2.33,0,0,0,0,0,0,2
1,950,1,732
161.431,"WLL79",""
9507320,"ZnH2PO4+",0,21.15,0,0,1,0,0,0,3
1,950,2,330,1,580
162.367,"WLL79",""
9505801,"ZnHPO4 AQ",0,15.65,0,0,0,0,0,0,3
1,950,1,330,1,580
161.359,"WLL79",""
9504920,"ZnNO3 +",0,0.4,0,0,1,0,0,0,2
1,950,1,492
127.385,"WLL79",""
9504921,"Zn(NO3)2 AQ",0,-0.3,0,0,0,0,0,0,2
1,950,2,492
189.39,"WLL79",""
9507321,"Zn(SO4)2-2",0,3.28,0,0,-2,0,0,0,2
1,950,2,732
257.493,"",""
9501300,"ZnBr +",0,-0.58,0,0,1,0,0,0,2
1,950,1,130
145.274,"",""
9501301,"ZnBr2 AQ",0,-0.98,0,0,0,0,0,0,2
1,950,2,130
225.178,"",""
```

```
9503800,"ZnI +",0,-2.91,0,0,1,0,0,0,2
1,950,1,380
192.274,"",""
9503801,"ZnI2 AQ",0,-1.69,0,0,0,0,0,0,2
1,950,2,380
319.178,"",""
9501400,"ZnHCO3 +",0,12.4,0,0,1,0,0,1,3
1,950,1,140,1,330
126.357,"",""
9501401,"ZnCO3 AQ",0,5.3,0,0,0,0,0,2,2
1,950,1,140
125.379,"",""
9501402,"Zn(CO3)2-2",0,9.63,0,0,-2,0,0,4,2
1,950,2,140
185.358,"",""
1601800,"CdCl +",2.469,1.98,0,0,1,0,0,0,2
1,160,1,180
147.853,"WLL79",""
1601801,"CdCl2 AQ",5.188,2.6,0,0,0,0,0,0,2
1,160,2,180
183.306,"WLL79",""
1601802,"CdCl3 -",16.318,2.4,0,0,-1,0,0,0,2
1,160,3,180
218.759,"WLL79",""
1601803,"CdCl4 -2",0,2.5,0,0,-2,0,0,0,2
1,160,4,180
254.222,"WLL79",""
1602700,"CdF +",0,1.1,0,0,1,0,0,0,2
1,160,1,270
131.398,"",""
1602701,"CdF2 AQ",0,1.5,0,0,0,0,0,0,2
1,160,2,270
150.396,"",""
1601400,"Cd(CO3)3-4",0,6.22,0,0,-4,0,0,6,2
1,160,3,140
292.428,"",""
1603300,"CdOH +",54.81,-10.1,0,0,1,0,0,0,3
1,160,1,2,-1,330
129.407,"WLL79",""
1603301,"Cd(OH)2 AQ",0,-20.3,0,0,0,0,0,0,3
1,160,2,2,-2,330
146.414,"WLL79",""
1603302,"Cd(OH)3 -",0,-33.01,0,0,-1,0,0,0,3
1,160,3,2,-3,330
163.422,"WLL79",""
1603303,"Cd(OH)4 -2",0,-47.29,0,0,-2,0,0,0,3
1,160,4,2,-4,330
180.429,"WLL79",""
1603304,"Cd2OH +3",45.601,-6.4,0,0,3,0,0,0,3
2,160,1,2,-1,330
241.8074,"WLL79",""
1603305,"Cd(OH)5 -3",0,-61.93,0,0,-3,0,0,0,3
1,160,5,2,-5,330
197.447,"WLL79",""
1603306,"Cd(OH)6 -4",0,-76.81,0,0,-4,0,0,0,3
1,160,6,2,-6,330
214.454,"WLL79",""
1603307,"Cd4(OH)4 +4",0,-27.92,0,0,4,0,0,0,3
4,160,4,2,-4,330
517.669,"WLL79",""
1601803,"CdOHCl AQ",18.221,-7.404,0,0,0,0,0,0,4
1,160,1,2,-1,330,1,180
164.86,"",""
1604920,"CdNO3 +",-21.757,0.399,0,0,1,0,0,0,2
1,160,1,492
174.404,"",""
1607320,"CdSO4 AQ",4.519,2.45,0,0,0,0,0,0,2
```

```
1,160,1,732
208.461,"WLL79",""
1605800,"CdHPO4 AQ",0,15.55,0,0,0,0,0,0,3
1,160,1,330,1,580
208.389,"WLL79",""
1607300,"CdHS +",0,10.17,0,0,1,0,0,0,2
1,160,1,730
145.472,"",""
1607301,"Cd(HS)2 AQ",0,16.53,0,0,0,0,0,0,2
1,160,2,730
178.543,"",""
1607302,"Cd(HS)3 -",0,18.71,0,0,-1,0,0,0,2
1,160,3,730
211.615,"",""
1607303,"Cd(HS)4 -2",0,20.9,0,0,-2,0,0,0,2
1,160,4,730
244.687,"",""
1601300,"CdBr +",-3.389,2.15,0,0,1,0,0,0,2
1,160,1,130
192.304,"WLL79",""
1601301,"CdBr2 AQ",0,3,0,0,0,0,0,0,2
1,160,2,130
272.208,"WLL79",""
1601302,"CdBr3 -",0,3,0,0,-1,0,0,0,2
1,160,3,130
352.122,"WLL79",""
1601303,"CdBr4 -2",0,2.9,0,0,-2,0,0,0,2
1,160,4,130
432.026,"WLL79",""
1603800,"CdI +",-9.916,2.28,0,0,1,0,0,0,2
1,160,1,380
239.304,"WLL79",""
1603801,"CdI2 AQ",0,3.59,0,0,0,0,0,0,2
1,160,2,380
366.208,"",""
1603802,"CdI3 -",0,5,0,0,-1,0,0,0,2
1,160,3,380
493.124,"WLL79",""
1603803,"CdI4 -2",0,6,0,0,-2,0,0,0,2
1,160,4,380
620.028,"WLL79",""
1601400,"CdHCO3 +",0,12.42,0,0,1,0,0,1,3
1,160,1,140,1,330
173.417,"WLL79",""
1601401,"CdCO3 AQ",0,4.09,0,0,0,0,0,2,2
1,160,1,140
172.409,"WLL79",""
1604921,"Cd(NO3)2 AQ",0,0,0,0,0,0,0,0,2
1,160,2,492
236.42,"WLL79",""
1607321,"Cd(SO4)2-2",0,3.5,0,0,-2,0,0,0,2
1,160,2,732
208.461,"",""
1609900,"Cd FULVATE",0,0,0,0,0,0,0,0,2
1,160,1,990
762.399,"",""
1609910,"Cd HUMATE",0,0,0,0,0,0,0,0,2
1,160,1,991
2112.399,"",""
6001800,"PbCl +",18.326,1.6,0,0,1,0,0,0,2
1,600,1,180
242.643,"WLL79",""
6001801,"PbCl2 AQ",4.519,1.78,0,0,0,0,0,0,2
1,600,2,180
278.096,"WLL79",""
6001802,"PbCl3 -",9.079,1.68,0,0,-1,0,0,0,2
1,600,3,180
```

```
313.549,"WLL79",""
6001803,"PbCl4 -2",14.77,1.38,0,0,-2,0,0,0,2
1,600,4,180
349.002,"WLL79",""
6001400,"Pb(CO3)2-2",0,10.64,0,0,-2,0,0,4,2
1,600,2,140
327.208,"",""
6002700,"PbF +",0,1.49,0,0,1,0,0,0,2
1,600,1,270
226.188,"WLL79",""
6002701,"PbF2 AQ",0,2.27,0,0,0,0,0,0,2
1,600,2,270
245.186,"WLL79",""
6002702,"PbF3 -",0,3.42,0,0,-1,0,0,0,2
1,600,3,270
264.185,"WLL79",""
6002703,"PbF4 -2",0,3.1,0,0,-2,0,0,0,2
1,600,4,270
283.183,"WLL79",""
6003300,"PbOH +",0,-7.7,0,0,1,0,0,0,3
1,600,1,2,-1,330
224.197,"WLL79",""
6003301,"Pb(OH)2 AQ",0,-17.75,0,0,0,0,0,0,3
1,600,2,2,-2,330
241.204,"WLL79",""
6003302,"Pb(OH)3 -",0,-28.09,0,0,-1,0,0,0,3
1,600,3,2,-3,330
258.212,"WLL79",""
6003303,"Pb2OH +3",0,-6.4,0,0,3,0,0,0,3
2,600,1,2,-1,330
431.387,"WLL79",""
6004920,"PbNO3 +",0,1.17,0,0,1,0,0,0,2
1,600,1,492
269.194,"WLL79",""
6004921,"Pb(NO3) AQ",0,1.4,0,0,0,0,0,0,2
1,600,2,492
218.981,"WLL79",""
6007320,"PbSO4 AQ",0,2.62,0,0,0,0,0,0,2
1,600,1,732
303.251,"WLL79",""
6005800,"PbH2PO4 +",0,21.05,0,0,1,0,0,0,3
1,600,2,330,1,580
304.187,"WLL79",""
6005801,"PbHPO4 AQ",0,15.45,0,0,0,0,0,0,3
1,600,1,330,1,580
303.179,"WLL79",""
6007300,"Pb(HS)2 AQ",0,15.27,0,0,0,0,0,0,2
1,600,2,730
273.333,"",""
6007301,"Pb(HS)3 -",0,16.57,0,0,-1,0,0,0,2
1,600,3,730
306.405,"",""
6003304,"Pb3(OH)4+2",110.876,-23.89,0,0,2,0,0,0,3
3,600,4,2,-4,330
689.599,"WLL79",""
6001300,"PbBr +",12.05,1.77,0,0,1,0,0,0,2
1,600,1,130
287.094,"WLL79",""
6001301,"PbBr2 AQ",0,2.6,0,0,0,0,0,0,2
1,600,2,130
366.998,"WLL79",""
6001300,"PbBr3 -",0,3,0,0,-1,0,0,0,2
1,600,3,130
446.912,"WLL79",""
6003800,"PbI +",0,1.92,0,0,1,0,0,0,2
1,600,1,380
334.094,"WLL79",""
```

```
6003801,"PbI2 AQ",0,3.15,0,0,0,0,0,0,2
1,600,2,380
460.998,"WLL79",""
6003801,"PbI3 -",0,3.92,0,0,-1,0,0,0,2
1,600,3,380
587.914,"WLL79",""
6003802,"PbI4 -2",0,4.5,0,0,-2,0,0,0,2
1,600,4,380
714.818,"WLL79",""
6001401,"PbCO3 AQ",0,7.24,0,0,0,0,0,2,2
1,600,1,140
267.199,"",""
6003305,"Pb(OH)4 -2",0,-39.49,0,0,-2,0,0,0,3
1,600,4,2,-4,330
375.219,"WLL79",""
6007321,"Pb(SO4)2-2",0,3.47,0,0,-2,0,0,0,2
1,600,2,732
399.313,"WLL79",""
6001402,"PbHCO3 +",0,13.2,0,0,1,0,0,1,3
1,600,1,140,1,330
268.207,"",""
5401300,"NiBr +",0,0.5,0,0,1,0,0,0,2
1,540,1,130
138.614,"",""
5401800,"NiCl +",0,0.399,0,0,1,0,0,0,2
1,540,1,180
94.163,"",""
5402700,"NiF +",0,1.3,0,0,1,0,0,0,2
1,540,1,270
77.708,"",""
5403300,"NiOH +",51.965,-9.86,0,0,1,0,0,0,3
1,540,1,2,-1,330
75.717,"",""
5403301,"Ni(OH)2 AQ",0,-19,0,0,0,0,0,0,3
1,540,2,2,-2,330
92.724,"",""
5403302,"Ni(OH)3 -",0,-30,0,0,-1,0,0,0,3
1,540,3,2,-3,330
109.732,"",""
5407320,"NiSO4 AQ",6.36,2.29,0,0,0,0,0,0,2
1,540,1,732
154.771,"",""
5401801,"NiCl2 AQ",0,0.96,0,0,0,0,0,0,2
1,540,2,180
129.616,"",""
5401400,"NiHCO3 +",0,12.47,0,0,1,0,0,1,3
1,540,1,140,1,330
119.727,"",""
5401401,"NiCO3 AQ",0,6.87,0,0,0,0,0,2,2
1,540,1,140
118.719,"",""
5401402,"Ni(CO3)2-2",0,10.11,0,0,-2,0,0,4,2
1,540,2,140
178.728,"",""
5407321,"Ni(SO4)2-2",0,1.02,0,0,-2,0,0,0,2
1,540,2,732
250.833,"",""
5409921,"Ni ACETATE",0,1.12,0,0,1,0,0,0,2
1,540,1,992
117.76,"",""
5409941,"Ni GLYCINE",0,6.18,0,0,1,0,0,0,2
1,540,1,994
132.78,"",""
5409942,"Ni GLYCINE",0,11.13,0,0,3,0,0,0,2
2,540,1,994
191.49,"",""
5409951,"Ni SALICYL",0,6.95,0,0,0,0,0,0,2
```

```
1,540,1,995
194.83,"",""
5409952,"Ni SALICYL",0,11.75,0,0,2,0,0,0,2
2,540,1,995
253.54,"",""
5409961,"Ni GLUTAMA",0,5.9,0,0,0,0,0,0,2
1,540,1,996
203.84,"",""
5401572,"Ni GLUTAMA",0,10.34,0,0,2,0,0,0,2
2,540,1,996
262.55,"",""
5409971,"Ni PHTHALA",0,2.95,0,0,0,0,0,0,2
1,540,1,997
222.84,"",""
201300,"AGBr AQ",0,4.24,0,0,0,0,0,0,2
1,20,1,130
187.772,"",""
201301,"AgBr2 -",0,7.28,0,0,-1,0,0,0,2
1,20,2,130
267.676,"",""
201800,"AgCL AQ",-11.213,3.27,0,0,0,0,0,0,2
1,20,1,180
143.321,"",""
201801,"AgCL2 -",-16.443,5.27,0,0,-1,0,0,0,2
1,20,2,180
178.774,"",""
201802,"AgCL3 -2",0,5.29,0,0,-2,0,0,0,2
1,20,3,180
214.227,"",""
201803,"AgCL4 -3",0,5.51,0,0,-3,0,0,0,2
1,20,4,180
249.679,"",""
202700,"AgF AQ",-11.841,0.36,0,0,0,0,0,0,2
1,20,1,270
126.866,"",""
207300,"AgHS AQ",0,14.05,0,0,0,0,0,0,2
1,20,1,730
140.939,"",""
207301,"Ag(HS)2 -",0,18.45,0,0,-1,0,0,0,2
1,20,2,730
174.011,"",""
203800,"AgI AQ",0,6.6,0,0,0,0,0,0,2
1,20,1,380
234.772,"",""
203801,"AgI2 -",0,10.68,0,0,-1,0,0,0,2
1,20,2,380
361.676,"",""
203300,"AgOH AQ",0,-12,0,0,0,0,0,0,3
1,20,1,2,-1,330
124.875,"",""
203301,"Ag(OH)2 -",0,-24,0,0,-1,0,0,0,3
1,20,2,2,-2,330
141.882,"",""
207320,"AgSO4 -",6.234,1.29,0,0,-1,0,0,0,2
1,20,1,732
203.929,"",""
204920,"AgNO3 AQ",0,-0.29,0,0,0,0,0,0,2
1,20,1,492
169.872,"",""
204910,"Ag(NO2)2 -",0,2.22,0,0,-1,0,0,0,2
1,20,2,491
199.879,"",""
201302,"AgBr3 -2",0,8.71,0,0,-2,0,0,0,2
1,20,3,130
347.58,"",""
203802,"AgI3 -2",-113.094,13.37,0,0,-2,0,0,0,2
1,20,3,380
```

```
488.581,"",""
203803,"AgI4 -3",0,14.08,0,0,-3,0,0,0,2
1,20,4,380
615.485,"",""
207302,"Ag(S4)2 -3",0,0.991,0,0,-3,22,0,0,4
1,20,2,730,-2,330,6,731
364.38,"",""
207303,"AgS4S5 -3",0,0.68,0,0,-3,24,0,0,4
1,20,2,730,-2,330,7,731
396.444,"",""
207304,"Ag(HS)S4-2",0,10.431,0,0,-2,15,0,0,4
1,20,2,730,-1,330,3,731
269.196,"",""
209900,"Ag FULVATE",0,0,0,0,-1,0,0,0,2
1,20,1,990
757.868,"",""
209910,"Ag HUMATE",0,0,0,0,-1,0,0,0,2
1,20,1,991
2107.867,"",""
3304801,"HMoO4-",0,4.23,0,0,-1,0,0,0,2
1,330,1,480
160.9455,"RED90",""
3304802,"H2MoO4aq",0,8.23,0,0,0,0,0,0,2
2,330,1,480
162.9455,"RED90",""
3304803,"MoO2(OH)+",0,8.17,0,0,1,0,0,0,3
3,330,1,480,-1,2
144.9461,"RED90",""
3304804,"MoO2+2",0,8.64,0,0,2,0,0,0,3
4,330,1,480,-2,2
127.9388,"RED90",""
1504801,"CaMoO4aq",0,-3.09,0,0,0,0,0,0,2
1,150,1,480
200.0156,"RED90",""
5004801,"NaMoO4-",0,-1.66,0,0,-1,0,0,0,2
1,500,1,480
182.9274,"RED90",""
5004802,"Na2MoO4aq",0,0.02,0,0,0,0,0,0,2
2,500,1,480
205.9172,"RED90",""
4104801,"KMoO4-",0,-1.29,0,0,-1,0,0,0,2
1,410,1,480
199.0359,"RED90",""
4104802,"K2MoO4aq",0,0.27,0,0,0,0,0,0,2
2,410,1,480
238.1342,"RED90",""
4604801,"MgMoO4aq",0,-3.7,0,0,0,0,0,0,2
1,460,1,480
184.2426,"",""
3300600,"H2AsO3 -",27.447,-9.228,0,0,-1,0,0,0,2
1,60,-1,330
124.935,"",""
3300601,"HAsO3 -2",59.409,-21.33,0,0,-2,0,0,0,2
1,60,-2,330
123.927,"",""
3300602,"AsO3 -3",84.726,-34.744,0,0,-3,0,0,0,2
1,60,-3,330
122.919,"",""
3300610,"H4AsO3 +",0,-0.305,0,0,1,0,0,0,2
1,60,1,330
126.951,"",""
3300611,"H2AsO4 -",-7.071,-2.243,0,0,-1,0,0,0,2
1,61,-1,330
140.935,"",""
3300612,"HAsO4 -2",-3.849,-9.001,0,0,-2,0,0,0,2
1,61,-2,330
139.927,"",""
```

```
3300613,"AsO4 -3",14.351,-20.597,0,0,-3,0,0,0,2
1,61,-3,330
138.919,"",""
7400021,"HSbO2",-0.063,-0.0073,0,0,0,0,0,0,2
1,740,-1,2
154.7567,"",""
7402700,"SbOF (aq)",0,6.1864,0,0,0,0,0,0,4
1,740,1,270,1,330,-2,2
156.7478,"",""
7402702,"Sb(OH)2F aq",0,6.1937,0,0,0,0,0,0,4
1,740,1,270,1,330,-1,2
174.7631,"",""
7403300,"SbO+",8.242,0.9228,0,0,1,0,0,0,3
1,740,1,330,-2,2
137.7494,"",""
7403301,"SbO2-",70.187,-11.8011,0,0,-1,0,0,0,3
1,740,-1,2,-1,330
153.7488,"",""
7403302,"Sb(OH)2+",0,1.3853,0,0,1,0,0,0,3
1,740,1,330,-1,2
155.7647,"",""
7407300,"Sb2S4-2",-316.645,49.3005,0,0,-2,0,0,0,4
2,740,4,730,2,330,-6,2
371.764,"",""
7410021,"SbO3-",0,2.9319,0,0,-1,0,0,0,2
1,741,-3,2
169.7482,"",""
7413300,"SbO2+",0,2.3895,0,0,1,0,0,0,3
1,741,2,330,-4,2
153.7488,"",""
7400020,"Sb(OH)4-1",69.852,-12.0429,0,0,-1,0,0,0,3
1,740,1,2,-1,330
189.7794,"",""
3301400,"HCO3 -",-15.134,10.33,0,0,-1,5.4,0,1,2
1,140,1,330
61.017,"WLL79",""
3301401,"H2CO3 AQ",-9.401,16.681,0,0,0,0,0,0,2
1,140,2,330
62.025,"",""
3307320,"HSO4 -",20.543,1.987,0,0,-1,4.5,0,0,2
1,732,1,330
97.069,"",""
3302700,"HF AQ",14.477,3.169,0,0,0,0,0,0,2
1,270,1,330
20.006,"",""
3302701,"HF2 -",19.037,3.749,0,0,-1,3.5,0,0,2
2,270,1,330
39.004,"",""
3302702,"H2F2 AQ",0,6.768,0,0,0,0,0,0,2
2,270,2,330
40.012,"",""
3305800,"HPO4 -2",-14.77,12.35,0,0,-2,5,0,0,2
1,580,1,330
95.979,"WLL79",""
3305801,"H2PO4 -",-18.912,19.55,0,0,-1,5.4,0,0,2
1,580,2,330
96.987,"WLL79",""
3305802,"H3PO4 AQ",0,21.7,0,0,0,0,0,0,2
1,580,3,330
97.995,"WLL79",""
3307300,"H2S AQ",-22.175,6.994,0,0,0,0,0,0,2
1,730,1,330
34.079,"",""
3307301,"S -2",50.626,-12.918,0,0,-2,5,0,0,2
1,730,-1,330
32.064,"",""
3309900,"H FULVATE",0,0,0,0,-1,0,0,0,2
```

```
1,990,1,330
651.008,"",""
3309910,"H HUMATE",0,0,0,0,-1,0,0,0,2
1,991,1,330
2001.007,"",""
8913300,"UOH +3",49.016,-0.656,0,0,3,0,0,0,3
1,891,1,2,-1,330
255.0364,"",""
8913301,"U(OH)2 +2",74.182,-2.27,0,0,2,0,0,0,3
-2,330,1,891,2,2
272.0437,"",""
8913302,"U(OH)3 +1",94.747,-4.935,0,0,1,0,0,0,3
1,891,3,2,-3,330
289.0511,"",""
8913303,"U(OH)4 AQ",103.596,-8.498,0,0,0,0,0,0,3
1,891,4,2,-4,330
306.0586,"",""
8913304,"U(OH)5 -1",115.374,-13.12,0,0,-1,0,0,0,3
1,891,5,2,-5,330
323.0659,"",""
8913305,"U6(OH)15+9",0,-17.229,0,0,9,0,0,0,3
6,891,15,2,-15,330
1683.2846,"",""
8912700,"UF +3",21.129,8.659,0,0,3,0,0,0,2
1,891,1,270
257.0274,"",""
8912701,"UF2 +2",30.125,14.457,0,0,2,0,0,0,2
1,891,2,270
276.0258,"",""
8912702,"UF3 +1",29.916,19.115,0,0,1,0,0,0,2
1,891,3,270
295.0242,"",""
8912703,"UF4 AQ",19.246,23.64,0,0,0,0,0,0,2
1,891,4,270
314.0226,"",""
8912704,"UF5 -1",20.292,25.238,0,0,-1,0,0,0,2
1,891,5,270
333.021,"",""
8912705,"UF6 -2",13.807,27.718,0,0,-2,0,0,0,2
1,891,6,270
352.0194,"",""
8911800,"UCl +3",41.56,1.338,0,0,3,0,0,0,2
1,891,1,180
273.482,"",""
8917320,"USO4 +2",15.481,5.461,0,0,2,0,0,0,2
1,891,1,732
334.0906,"",""
8917321,"U(SO4)2 AQ",31.798,9.749,0,0,0,0,0,0,2
1,891,2,732
430.1522,"",""
8915800,"UHPO4 +2",31.38,24.443,0,0,2,0,0,0,3
1,891,1,580,1,330
334.0084,"",""
8915801,"U(HPO4)2AQ",7.113,46.833,0,0,0,0,0,0,3
1,891,2,580,2,330
429.9877,"",""
8915802,"U(HPO4)3-2",-32.635,67.564,0,0,-2,0,0,0,3
1,891,3,580,3,330
525.9671,"",""
8915803,"U(HPO4)4-4",-110.876,88.483,0,0,-4,0,0,0,3
1,891,4,580,4,330
621.9465,"",""
8933300,"UO2OH +1",42.744,-5.09,0,0,1,0,0,0,3
1,893,1,2,-1,330
287.0352,"",""
8933301,"UO2)2OH2+2",42.802,-5.645,0,0,2,0,0,0,3
2,893,2,2,-2,330
```

```
574.0703,"",""
8933302,"UO2)3OH5+1",104.914,-15.593,0,0,1,0,0,0,3
3,893,5,2,-5,330
895.1203,"",""
8931400,"UO2CO3 AQ",3.515,10.071,0,0,0,0,0,2,2
1,893,1,140
330.0372,"",""
8931401,"UO2CO3)2-2",14.56,17.008,0,0,-2,0,0,4,2
1,893,2,140
390.0465,"",""
8931402,"UO2CO3)3-4",-36.736,21.384,0,0,-4,0,0,6,2
1,893,3,140
450.0559,"",""
8932700,"UO2F +1",-1.883,5.105,0,0,1,0,0,0,2
1,893,1,270
289.0262,"",""
8932701,"UO2F2 AQ",-3.766,8.92,0,0,0,0,0,0,2
1,893,2,270
308.0246,"",""
8932702,"UO2F3 -1",-3.556,11.364,0,0,-1,0,0,0,2
1,893,3,270
327.023,"",""
8932703,"UO2F4 -2",-4.602,12.607,0,0,-2,0,0,0,2
1,893,4,270
346.0214,"",""
8931800,"UO2Cl +1",5.159,0.22,0,0,1,0,0,0,2
1,893,1,180
305.4808,"",""
8937320,"UO2SO4 AQ",21.338,2.709,0,0,0,0,0,0,2
1,893,1,732
366.0894,"",""
8937321,"UO2SO4)2-2",25.522,4.183,0,0,-2,0,0,0,2
1,893,2,732
462.151,"",""
8935800,"UO2HPO4 AQ",-8.786,20.814,0,0,0,0,0,0,3
1,893,1,580,1,330
366.0072,"",""
8935801,"UO2HPO4)2",-47.693,42.988,0,0,-2,0,0,0,3
1,893,2,580,2,330
461.9865,"",""
8935802,"UO2H2PO4+1",-15.481,22.643,0,0,1,0,0,0,3
1,893,1,580,2,330
367.0151,"",""
8935803,"UO2H2PO4)2",-69.036,44.7,0,0,0,0,0,0,3
1,893,2,580,4,330
464.002,"",""
8935804,"UO2H2PO4)3",-119.662,66.245,0,0,-1,0,0,0,3
1,893,3,580,6,330
560.989,"",""
8937700,"UO2H3SIO4",0,-2.4,0,0,1,0,0,0,3
1,893,1,770,-1,330
365.135,"",""
7317300,"S2 -2",47.698,-14.528,0,0,-2,0,0,0,3
1,730,1,731,-1,330
64.128,"",""
7317301,"S3 -2",43.514,-13.282,0,0,-2,0,0,0,3
1,730,2,731,-1,330
96.192,"",""
7317302,"S4 -2",40.585,-9.829,0,0,-2,0,0,0,3
1,730,3,731,-1,330
128.236,"",""
7317303,"S5 -2",38.911,-9.595,0,0,-2,0,0,0,3
1,730,4,731,-1,330
160.32,"",""
7317304,"S6 -2",0,-9.881,0,0,-2,0,0,0,3
1,730,5,731,-1,330
192.384,"",""
```

```
9003300,"VOH +",0,-5.64,0,0,1,0,0,0,3
1,900,1,2,-1,330
67.947,"",""
9013300,"VOH +2",39.12,-2.3,0,0,2,0,0,0,3
1,901,1,2,-1,330
67.947,"",""
9013301,"V(OH)2 +1",0,-5.83,0,0,1,0,0,0,3
1,901,2,2,-2,330
84.955,"",""
9013302,"V(OH)3 AQ",0,-11.02,0,0,0,0,0,0,3
1,901,3,2,-3,330
101.962,"",""
9017320,"VSO4 +1",0,1.44,0,0,1,0,0,0,2
1,901,1,732
146.998,"",""
9013303,"V2(OH)3 +3",0,-7.5,0,0,3,0,0,0,3
2,901,3,2,-3,330
152.902,"",""
9013304,"V2(OH)2 +4",0,-3.75,0,0,4,0,0,0,3
2,901,2,2,-2,330
135.895,"",""
9023300,"V(OH)3 +1",0,-5.67,0,0,1,0,0,0,3
1,902,2,2,-1,330
101.962,"",""
9023301,"H2V2O4 +2",0,-6.44,0,0,2,0,0,0,3
2,902,2,2,-2,330
167.894,"",""
9022700,"VOF +",7.95,3.34,0,0,1,0,0,0,2
1,902,1,270
85.937,"",""
9022701,"VOF2 AQ",14.644,5.74,0,0,0,0,0,0,2
1,902,2,270
104.935,"",""
9022702,"VOF3 -1",20.502,7.3,0,0,-1,0,0,0,2
1,902,3,270
123.933,"",""
9022703,"VOF4 -2",26.778,8.11,0,0,-2,0,0,0,2
1,902,4,270
142.931,"",""
9027320,"VOSO4 AQ",15.564,2.45,0,0,0,0,0,0,2
1,902,1,732
162.997,"",""
9021800,"VOCl +1",0,0.02,0,0,1,0,0,0,2
1,902,1,180
102.392,"",""
9033300,"H3VO4 AQ",44.476,-3.3,0,0,0,0,0,0,3
1,903,2,2,-1,330
117.962,"",""
9033301,"H2VO4 -1",47.405,-7.09,0,0,-1,0,0,0,3
1,903,2,2,-2,330
116.954,"",""
9033302,"HVO4 -2",62.467,-15.15,0,0,-2,0,0,0,3
1,903,2,2,-3,330
115.946,"",""
9033303,"VO4 -3",81.714,-28.4,0,0,-3,0,0,0,3
1,903,2,2,-4,330
114.938,"",""
9030020,"V2O7 -4",0,-29.08,0,0,-4,0,0,0,3
2,903,3,2,-6,330
213.876,"",""
9030021,"HV2O7 -3",0,-16.32,0,0,-3,0,0,0,3
2,903,3,2,-5,330
214.884,"",""
9030022,"H3V2O7 -1",0,-3.79,0,0,-1,0,0,0,3
2,903,3,2,-3,330
216.9,"",""
9030023,"V3O9 -3",0,-15.88,0,0,-3,0,0,0,3
```

```
3,903,3,2,-6,330
296.815,"",""
9030024,"V4O12 -4",0,-20.79,0,0,-4,0,0,0,3
4,903,4,2,-8,330
395.753,"",""
9030025,"V10O28 -6",0,-17.53,0,0,-6,0,0,0,3
10,903,8,2,-16,330
957.383,"",""
9030026,"HV10O28 -5",90.04,-11.35,0,0,-5,0,0,0,3
10,903,8,2,-15,330
958.391,"",""
9030027,"H2V10O28 -4",0,-7.71,0,0,-4,0,0,0,3
10,903,8,2,-14,330
959.399,"",""
9032700,"VO2F AQ",0,3.12,0,0,0,0,0,0,2
1,903,1,270
101.937,"",""
9032701,"VO2F2 -1",0,5.67,0,0,-1,0,0,0,2
1,903,2,270
120.935,"",""
9032702,"VO2F3 -2",0,6.97,0,0,-2,0,0,0,2
1,903,3,270
139.933,"",""
9032703,"VO2F4 -3",0,7.07,0,0,-3,0,0,0,2
1,903,4,270
158.931,"",""
9037320,"VO2SO4 -1",0,1.71,0,0,-1,0,0,0,2
1,903,1,732
178.996,"",""
9034920,"VO2NO3 AQ",0,-0.43,0,0,0,0,0,0,2
1,903,1,492
144.944,"",""
8703300,"TlOH AQ",58.304,-13.1717,0,0,0,0,0,0,3
1,870,1,2,-1,330
221.3773,"",""
8702700,"TlF AQ",0,-0.4251,0,0,0,0,0,0,2
1,870,1,270
223.3684,"",""
8701800,"TlCl AQ",-4.799,0.6824,0,0,0,0,0,0,2
1,870,1,180
239.823,"",""
8701801,"TlCl2-1",0,0.2434,0,0,-1,0,0,0,2
1,870,2,180
275.276,"",""
8701300,"TlBr AQ",-10.297,0.9477,0,0,0,0,0,0,2
1,870,1,130
284.274,"",""
8701301,"TlBr2-1",12.544,0.9719,0,0,-1,0,0,0,2
1,870,2,130
364.178,"",""
8701302,"TlBrCl-1",0,0.8165,0,0,-1,0,0,0,3
1,870,1,130,1,180
319.727,"",""
8703800,"TlI AQ",0,1.4279,0,0,0,0,0,0,2
1,870,1,380
331.2745,"",""
8703801,"TlI2-1",0,1.8588,0,0,-1,0,0,0,2
1,870,2,380
458.179,"",""
8703802,"TlIBr-1",0,2.185,0,0,-1,0,0,0,3
1,870,1,380,1,130
411.1785,"",""
8707320,"TlSO4-1",-0.92,1.3853,0,0,-1,0,0,0,2
1,870,1,732
300.4276,"",""
8704920,"TlNO3 AQ",-2.72,0.3665,0,0,0,0,0,0,2
1,870,1,492
```

```
266.3749,"",""
8704910,"TlNO2 AQ",0,0.9969,0,0,0,0,0,0,2
1,870,1,491
250.3755,"",""
8707300,"TlHS AQ",0,1.8178,0,0,0,0,0,0,2
1,870,1,730
237.4379,"",""
8707301,"Tl2HS+1",0,7.6979,0,0,1,0,0,0,2
2,870,1,730
441.8079,"",""
8707302,"Tl2OH(HS)3-",0,1.0044,0,0,-2,0,0,0,4
2,870,3,730,1,2,-1,330
524.951,"",""
8707303,"Tl2(OH)2(HS",0,-11.0681,0,0,-2,0,0,0,4
2,870,2,730,2,2,-2,330
508.8904,"",""
8713300,"Tl+3",0,4.7424,0,0,3,0,0,0,3
1,871,3,330,-3,2
204.37,"",""
8713301,"TlOH+2",0,3.577,0,0,2,0,0,0,3
1,871,2,330,-2,2
221.3773,"",""
8713302,"Tl(OH)2+1",0,2.1183,0,0,1,0,0,0,3
1,871,1,330,-1,2
238.3846,"",""
8711800,"TlCl+2",0,12.2342,0,0,2,0,0,0,4
1,871,1,180,3,330,-3,2
239.823,"",""
8711801,"TlCl2+1",0,18.0402,0,0,1,0,0,0,4
1,871,2,180,3,330,-3,2
275.276,"",""
8711802,"TlCl3 AQ",0,21.4273,0,0,0,0,0,0,4
1,871,3,180,3,330,-3,2
310.729,"",""
8711803,"TlCl4-1",0,24.2281,0,0,-1,0,0,0,4
1,871,4,180,3,330,-3,2
346.182,"",""
8711300,"TlBr+2",0,14.2221,0,0,2,0,0,0,4
1,871,1,130,3,330,-3,2
284.274,"",""
8711301,"TlBr2+1",0,21.5761,0,0,1,0,0,0,4
1,871,2,130,3,330,-3,2
364.178,"",""
8711302,"TlBr3 AQ",0,27.0244,0,0,0,0,0,0,4
1,871,3,130,3,330,-3,2
444.082,"",""
8711303,"TlBr4-1",0,31.1533,0,0,-1,0,0,0,4
1,871,4,130,3,330,-3,2
523.986,"",""
8713800,"TlI4-1",0,34.7596,0,0,-1,0,0,0,4
1,871,4,380,3,330,-3,2
711.988,"",""
8714920,"TlNO3+2",0,7.0073,0,0,2,0,0,0,4
1,871,1,492,3,330,-3,2
266.3749,"",""
8713303,"Tl(OH)4-1",0,-10.2545,0,0,-1,0,0,0,3
1,871,1,2,-1,330
272.3992,"",""
8711804,"TlOHCl+1",0,10.629,0,0,1,0,0,0,4
1,871,1,180,2,330,-2,2
256.8303,"",""
3307601,"Se-2",48.116,-14.9529,0,0,-2,0,0,0,2
1,760,-1,330
78.96,"",""
3307600,"H2Se",3.347,3.8115,0,0,0,0,0,0,2
1,760,1,330
80.9758,"",""
```

```
4707600,"MnSe",0,-6.7435,0,0,0,0,0,0,3
1,760,1,470,-1,330
133.898,"",""
207600,"Ag2Se",0,34.0677,0,0,0,0,0,0,3
1,760,2,20,-1,330
294.696,"",""
207601,"AgOH(Se)2-4",0,-18.6237,0,0,-4,0,0,0,4
2,760,1,20,1,2,-3,330
282.7953,"",""
3307611,"SeO3-2",5.356,-7.3005,0,0,-2,0,0,0,2
1,761,-1,330
126.9582,"",""
3307610,"H2SeO3",7.071,2.5728,0,0,0,0,0,0,2
1,761,1,330
128.974,"",""
2817610,"FeHSeO3+2",0,1.8618,0,0,2,0,0,0,2
1,761,1,281
183.8131,"",""
207610,"AgSeO3-1",0,-5.5985,0,0,-1,0,0,0,3
1,761,1,20,-1,330
234.8262,"",""
207611,"Ag(SeO3)2-3",0,-10.9933,0,0,-3,0,0,0,3
2,761,1,20,-2,330
361.7844,"",""
1607610,"Cd(SeO3)2-2",0,-11.189,0,0,-2,0,0,0,3
2,761,1,160,-2,330
366.3264,"",""
3307620,"HSeO4-1",17.573,1.9058,0,0,-1,0,0,0,2
1,762,1,330
143.9655,"",""
4707620,"MnSeO4",14.477,2.4188,0,0,0,0,0,0,2
1,762,1,470
197.8956,"",""
2007620,"CoSeO4",12.175,2.712,0,0,0,0,0,0,2
1,762,1,200
201.8908,"",""
5407620,"NiSeO4",14.644,2.6387,0,0,0,0,0,0,2
1,762,1,540
201.6576,"",""
1607620,"CdSeO4",0,2.2415,0,0,0,0,0,0,2
1,762,1,160
255.3676,"",""
9507620,"ZnSeO4",0,2.2019,0,0,0,0,0,0,2
1,762,1,950
208.3376,"",""
9507621,"Zn(SeO4)2-2",0,-0.0704,0,0,-2,0,0,0,2
2,762,1,950
351.2952,"",""
3600000,"Hg (aq)",-69.475,6.9316,0,0,0,0,0,0,2
0.5,360,1,1
200.59,"",""
3613300,"Hg+2",-46.275,6.097,0,0,2,0,0,0,3
1,361,2,330,-2,2
200.59,"",""
3611301,"HgBr+",0,15.8347,0,0,1,0,0,0,4
1,361,1,130,2,330,-2,2
280.494,"",""
3611302,"HgBr2 (aq)",-129.001,23.6065,0,0,0,0,0,0,4
1,361,2,130,2,330,-2,2
360.398,"",""
3611303,"HgBr3-1",0,25.7857,0,0,-1,0,0,0,4
1,361,2,330,3,130,-2,2
440.302,"",""
3611304,"HgBr4-2",0,27.0633,0,0,-2,0,0,0,4
1,361,2,330,4,130,-2,2
520.206,"",""
3611305,"HgBrCl (aq)",0,22.0145,0,0,0,0,0,0,5
```

```
1,361,1,130,1,180,2,330,-2,2
315.947,"",""
3611306,"HgBrI (aq)",0,27.1212,0,0,0,0,0,0,5
1,361,1,130,1,380,2,330,-2,2
407.3985,"",""
3611307,"HgBrI3-2",0,34.2135,0,0,-2,0,0,0,5
1,361,1,130,3,380,2,330,-2,2
661.2075,"",""
3611308,"HgBr2I2-2",0,32.3994,0,0,-2,0,0,0,5
1,361,2,130,2,380,2,330,-2,2
614.207,"",""
3611309,"HgBr3I-2",0,30.1528,0,0,-2,0,0,0,5
1,361,3,130,1,380,2,330,-2,2
567.2065,"",""
3613301,"HgBrOH (aq)",0,11.598,0,0,0,0,0,0,4
1,361,1,130,1,330,-1,2
297.5013,"",""
3611800,"HgCl+1",0,12.85,0,0,1,0,0,0,4
1,361,1,180,2,330,-2,2
236.043,"",""
3611801,"HgCl2 (aq)",0,19.2203,0,0,0,0,0,0,4
1,361,2,180,2,330,-2,2
271.496,"",""
3811802,"HgCl3-1",0,20.1226,0,0,-1,0,0,0,4
1,361,3,180,2,330,-2,2
306.949,"",""
3611803,"HgCl4-2",0,20.5338,0,0,-2,0,0,0,4
1,361,4,180,2,330,-2,2
342.402,"",""
3611804,"HgClI (aq)",0,25.3532,0,0,0,0,0,0,5
1,361,1,180,1,380,2,330,-2,2
362.9475,"",""
3611805,"HgClOH (aq)",-52.225,9.317,0,0,0,0,0,0,4
1,361,1,180,1,330,-1,2
253.0503,"",""
3612701,"HgF+1",0,8.0848,0,0,1,0,0,0,4
1,361,1,270,2,330,-2,2
219.5884,"",""
3613801,"HGI+1",0,18.8949,0,0,1,0,0,0,4
1,361,1,380,2,330,-2,2
327.4945,"",""
3613802,"HgI2 (aq)",-186.28,30.1081,0,0,0,0,0,0,4
1,361,2,380,2,330,-2,2
454.399,"",""
3613803,"HgI3-1",-200.594,33.7935,0,0,-1,0,0,0,4
1,361,3,380,2,330,-2,2
581.3035,"",""
3613804,"HgI4-2",0,35.7858,0,0,-2,0,0,0,4
1,361,4,380,2,330,-2,2
708.208,"",""
3614900,"HgNH3+2",0,5.6139,0,0,2,0,0,0,4
1,361,1,490,1,330,-2,2
217.6204,"",""
3614901,"Hg(NH3)2+2",0,5.0341,0,0,2,0,0,0,3
1,361,2,490,-2,2
234.6508,"",""
3614902,"Hg(NH3)3+2",0,-3.2493,0,0,2,0,0,0,4
1,361,3,490,-1,330,-2,2
251.6812,"",""
3614903,"Hg(NH3)4+2",0,-11.7307,0,0,2,0,0,0,4
1,361,4,490,-2,330,-2,2
268.7116,"",""
3614920,"HgNO3+1",0,6.4503,0,0,1,0,0,0,4
1,361,1,492,2,330,-2,2
262.5949,"",""
3614921,"Hg(NO3)2 (a",0,4.7791,0,0,0,0,0,0,4
1,361,2,492,2,330,-2,2
```

```
324.5998,"",""
3613302,"HgOH+1",0,2.6974,0,0,1,0,0,0,3
1,361,1,330,-1,2
217.5973,"",""
3613303,"Hg(OH)3-1",0,-15.0042,0,0,-1,0,0,0,3
1,361,1,2,-1,330
251.6119,"",""
3617300,"HgS2-2",0,31.2398,0,0,-2,0,0,0,3
1,361,2,730,-2,2
264.71,"",""
3617301,"Hg(HS)2 (aq",0,43.8178,0,0,0,0,0,0,4
1,361,2,730,2,330,-2,2
266.7258,"",""
3617320,"HgSO4 (aq)",0,7.4911,0,0,0,0,0,0,4
1,361,1,732,2,330,-2,2
296.6476,"",""
2113300,"Cr+3",-84.266,9.62,0,0,3,0,0,0,3
1,211,2,330,-2,2
51.996,"",""
2113301,"Cr(OH)+2",0,5.62,0,0,2,0,0,0,3
1,211,1,330,-1,2
69.0033,"",""
2110020,"Cr(OH)3 AQ",0,-7.13,0,0,0,0,0,0,3
1,211,1,2,-1,330
103.0179,"",""
2110021,"Cr(OH)4-",0,-18.15,0,0,-1,0,0,0,3
1,211,2,2,-2,330
120.0252,"",""
2113304,"CrO2-",0,-17.7456,0,0,-1,0,0,0,2
1,211,-2,330
83.9948,"",""
2111300,"CrBr+2",-46.907,7.5519,0,0,2,0,0,0,4
1,211,1,130,2,330,-2,2
131.9,"",""
2111800,"CrCl+2",-57.936,9.3683,0,0,2,0,0,0,4
1,211,1,180,2,330,-2,2
87.449,"",""
2111801,"CrCl2 +",-39.221,8.658,0,0,1,0,0,0,4
1,211,2,180,2,330,-2,2
122.902,"",""
2111802,"CrOHCl2 AQ",0,2.9627,0,0,0,0,0,0,4
1,211,2,180,1,330,-1,2
139.9093,"",""
2112700,"CrF+2",-70.245,14.5424,0,0,2,0,0,0,4
1,211,1,270,2,330,-2,2
70.9944,"",""
2113800,"CrI+2",0,4.8289,0,0,2,0,0,0,4
1,211,1,380,2,330,-2,2
178.9005,"",""
2114900,"Cr(NH3)6+3",0,-32.5709,0,0,3,0,0,0,4
1,211,6,490,-4,330,-2,2
154.1784,"",""
2114901,"CrNH3)5OH+2",0,-30.2759,0,0,2,0,0,0,4
1,211,5,490,-4,330,-1,2
154.1553,"",""
2114902,"CCrNH3)4OH2",0,-29.8574,0,0,1,0,0,0,3
1,211,4,490,-4,330
154.1322,"",""
2114903,"TCrNH3)4OH2",0,-30.5537,0,0,1,0,0,0,3
1,211,4,490,-4,330
154.1322,"",""
2114904,"CrNH3)6CL+2",0,-31.7932,0,0,2,0,0,0,5
1,211,6,490,1,180,-2,2,-4,330
189.6314,"",""
2114905,"CrNH3)6BR+2",0,-31.887,0,0,2,0,0,0,5
1,211,6,490,1,130,-4,330,-2,2
234.0824,"",""
```

```
2114906,"CrNH3)6I +2",0,-32.008,0,0,2,0,0,0,5
1,211,6,490,1,380,-4,330,-2,2
281.0829,"",""
2114920,"CrNO3 +2",-65.438,8.2094,0,0,2,0,0,0,4
1,211,1,492,2,330,-2,2
114.0009,"",""
2115800,"CrH2PO4 +2",0,31.9068,0,0,2,0,0,0,4
1,211,4,330,1,580,-2,2
148.9832,"",""
2117320,"CrSO4 +",-52.802,10.9654,0,0,1,0,0,0,4
1,211,1,732,2,330,-2,2
148.0536,"",""
2117321,"CrOHSO4 AQ",0,8.2754,0,0,0,0,0,0,4
1,211,1,732,1,330,-1,2
165.0609,"",""
2117322,"Cr2OH2SO4)S",0,14.5278,0,0,0,0,0,0,4
2,211,2,732,2,330,-2,2
330.1218,"",""
2117323,"Cr2OH2SO4+2",0,16.155,0,0,2,0,0,0,4
2,211,1,732,2,330,-2,2
234.0642,"",""
2117324,"Cr2OH2SO42",0,17.9288,0,0,0,0,0,0,4
2,211,2,732,2,330,-2,2
330.1218,"",""
2123300,"HCrO4 -",3.766,6.5089,0,0,-1,0,0,0,2
1,212,1,330
117.0015,"",""
2123301,"H2CrO4 AQ",0,5.6513,0,0,0,0,0,0,2
1,212,2,330
118.0094,"",""
2123302,"Cr2O7 -2",-12.531,14.5571,0,0,-2,0,0,0,3
2,212,2,330,-1,2
215.9878,"",""
2121800,"CrO3Cl -",0,7.3086,0,0,-1,0,0,0,4
1,212,1,180,2,330,-1,2
135.4472,"",""
2125800,"Cr03H2PO4-",0,29.3634,0,0,-1,0,0,0,4
1,212,4,330,1,580,-1,2
196.9814,"",""
2125801,"CrO3HPO4-2",0,26.6806,0,0,-2,0,0,0,4
1,212,3,330,1,580,-1,2
195.9735,"",""
2127320,"CrO3SO4-2",0,8.9937,0,0,-2,0,0,0,4
1,212,1,732,2,330,-1,2
196.0518,"",""
5002120,"NaCrO4-",0,0.6963,0,0,-1,0,0,0,2
1,212,1,500
138.9834,"",""
4102120,"KCrO4-",0,0.799,0,0,-1,0,0,0,2
1,212,1,410
155.0919,"",""
1001431,"BaFe(CN)6-1",-291.541,55.435,0,0,-1,0,0,0,3
1,100,1,281,6,143
349.2804,"",""
1501434,"CaHFe(CN)6-2",-343.088,52.709,0,0,-2,0,0,0,5
1,150,1,330,1,280,6,143,1,1
253.0394,"",""
4101433,"KFe(CN)6-3",-351.456,48.12,0,0,-3,0,0,0,3
1,410,1,280,6,143
251.0517,"",""
4101434,"K2Fe(CN)6-2",-323.423,48.978,0,0,-2,0,0,0,3
2,410,1,280,6,143
290.15,"",""
4101435,"KHFe(CN)6-2",-326.77,51.47,0,0,-2,0,0,0,4
1,410,1,330,1,280,6,143
252.0597,"",""
4401432,"Li2Fe(CN)6-2",-349.356,48.533,0,0,-2,0,0,0,3
```

```
2,440,1,280,6,143
225.8354,"",""
4401433,"LiHFe(CN)6-2",-338.9,51.218,0,0,-2,0,0,0,4
1,440,1,330,1,280,6,143
219.9024,"",""
4901431,"NH4Fe(CN)6-3",-353.548,48.068,0,0,-3,0,0,0,3
1,490,1,280,6,143
314.0324,"",""
4901433,"NH5Fe(CN)6-",-351.038,51.403,0,0,-2,0,0,0,4
1,490,1,330,1,280,6,143
315.0403,"",""
5001431,"NAFe(CN)6-3",-355.222,47.988,0,0,-3,0,0,0,3
1,500,1,280,6,143
234.9432,"",""
5001432,"Na2Fe(CN)6-2",-355.64,48.743,0,0,-2,0,0,0,3
2,500,1,280,6,143
257.933,"",""
5001433,"NaHFe(CN)6-2",-358.15,51.433,0,0,-2,0,0,0,4
1,500,1,330,1,280,6,143
235.9512,"",""
4901432,"NH4)2FeCN6-2",-347.272,48.866,0,0,-2,0,0,0,3
2,490,1,280,6,143
332.0709,"",""
201431,"Ag(CN)OH-",0,-0.56,0,0,-1,0,0,0,4
1,143,1,20,1,2,-1,330
150.8933,"",""
201432,"Ag(CN)2-",-136.712,20.381,0,0,-1,0,0,0,2
2,143,1,20
159.9037,"",""
4101431,"K2H2Fe(CN)6",-359.238,52.305,0,0,0,0,0,0,4
6,143,2,410,2,330,1,280
292.1659,"",""
1501431,"CaFe(CN)6-",-290.788,55.473,0,0,-1,0,0,0,3
6,143,1,150,1,281
252.0314,"",""
1501432,"CaFe(CN)6-2",-347.69,49.689,0,0,-2,0,0,0,3
6,143,1,150,1,280
252.0314,"",""
1501433,"Ca2Fe(CN)6",-350.201,50.995,0,0,0,0,0,0,3
6,143,2,150,1,280
292.1094,"",""
1601431,"CdCN+",0,5.32,0,0,1,0,0,0,2
1,143,1,160
138.4287,"",""
1601432,"Cd(CN)2 (aq)",-54.392,10.37,0,0,0,0,0,0,2
2,143,1,160
164.4465,"",""
1601433,"Cd(CN)3-",-90.374,14.834,0,0,-1,0,0,0,2
3,143,1,160
190.4642,"",""
1601434,"Cd(CN)4-2",-98.575,18.293,0,0,-2,0,0,0,2
4,143,1,160
216.482,"",""
2301431,"Cu(CN)4-3",-215.058,30.345,0,0,-3,0,0,0,2
4,143,1,230
167.617,"",""
2301432,"Cu(CN)2-",-121.754,24.027,0,0,-1,0,0,0,2
2,143,1,230
115.5815,"",""
2301433,"Cu(CN)3-2",-168.197,28.652,0,0,-2,0,0,0,2
3,143,1,230
141.5992,"",""
2801431,"Fe(CN)6-4",-358.987,45.606,0,0,-4,0,0,0,2
6,143,1,280
211.9534,"",""
2801432,"HFe(CN)6-3",-352.125,49.996,0,0,-3,0,0,0,3
6,143,1,280,1,330
```

```
212.9614,"",""
2801433,"H2Fe(CN)6-2",-347.69,52.445,0,0,-2,0,0,0,3
6,143,2,330,1,280
213.9693,"",""
2811431,"Fe(CN)6-3",-293.298,52.628,0,0,-3,0,0,0,2
6,143,1,281
211.9534,"",""
3301431,"HCN",-43.514,9.235,0,0,0,0,0,0,2
1,143,1,330
27.0257,"",""
3305601,"HOCN",-8.368,3.445,0,0,0,0,0,0,2
1,560,1,330
43.0251,"",""
3611431,"HgCN+",-141.545,24.173,0,0,1,0,0,0,4
1,143,1,361,2,330,-2,2
226.6077,"",""
3611432,"Hg(CN)2",-239.492,40.651,0,0,0,0,0,0,4
2,143,1,361,2,330,-2,2
252.6255,"",""
3611433,"Hg(CN)3-",-271.249,44.404,0,0,-1,0,0,0,4
3,143,1,361,2,330,-2,2
278.6432,"",""
3611434,"Hg(CN)4-2",-292.587,47.409,0,0,-2,0,0,0,4
4,143,1,361,2,330,-2,2
304.661,"",""
3611435,"Hg(CN)2Cl-",0,40.373,0,0,-1,0,0,0,5
2,143,1,180,1,361,2,330,-2,2
288.0782,"",""
3611436,"Hg(CN)3Cl-2",0,43.833,0,0,-2,0,0,0,5
3,143,1,180,1,361,2,330,-2,2
314.0959,"",""
3611437,"Hg(CN)3Br-2",0,44.941,0,0,-2,0,0,0,5
3,143,1,130,1,361,2,330,-2,2
358.5472,"",""
3801432,"I2CN-",0,-11.848,0,0,-1,0,0,0,3
1,143,2,380,-2,1
279.8267,"",""
3801433,"I(CN)2-",0,-11.458,0,0,-1,0,0,0,3
2,143,1,380,-2,1
178.9399,"",""
4101432,"K3HFe(CN)6",-359.782,50.224,0,0,0,0,0,0,4
6,143,3,410,1,330,1,280
330.2563,"",""
4401431,"LiFe(CN)6-3",-335.343,47.685,0,0,-3,0,0,0,3
6,143,1,440,1,280
218.8944,"",""
4601431,"MgFe(CN)6-",-289.993,55.391,0,0,-1,0,0,0,3
6,143,1,460,1,281
236.2584,"",""
4601432,"MgFe(CN)6-2",0,49.425,0,0,-2,0,0,0,3
6,143,1,460,1,280
236.2584,"",""
5401431,"Ni(CN)4-2",-180.707,30.125,0,0,-2,0,0,0,2
4,143,1,540
162.761,"",""
8001431,"SrFe(CN)6-",-292.169,55.618,0,0,-1,0,0,0,3
1,800,1,281,6,143
299.5734,"",""
8701431,"Tl(CN)4-",0,-8.018,0,0,-1,0,0,0,3
4,143,1,870,-2,1
308.4543,"",""
8701432,"TlFe(CN)6-3",-355.138,48.75,0,0,-3,0,0,0,3
6,143,1,870,1,280
416.3367,"",""
9501431,"Zn(CN)4-2",-106.855,16.715,0,0,-2,0,0,0,2
4,143,1,950
169.461,"",""
```

```
9501432,"Zn(CN)3-",-84.513,16.048,0,0,-1,0,0,0,2
3,143,1,950
143.4432,"",""
9501430,"Zn(CN)2(aq)",-46.02,11.071,0,0,0,0,0,0,2
2,143,1,950
117.4255,"",""
5401436,"Ni(CN)3-",0,22.634,0,0,-1,0,0,0,2
3,143,1,540
136.7432,"",""
5401432,"NiH(CN)4-",0,36.748,0,0,-1,0,0,0,3
4,143,1,540,1,330
163.7689,"",""
5401433,"NiH2CN4(aq)",0,41.457,0,0,0,0,0,0,3
4,143,1,540,2,330
164.7768,"",""
5401434,"NiH3(CN)4+",0,43.949,0,0,1,0,0,0,3
4,143,1,540,3,330
165.7848,"",""
5401435,"Ni(CN)2(aq)",0,14.586,0,0,0,0,0,0,2
2,143,1,540
110.7255,"",""
2811432,"Fe2(CN)6(aq)",0,56.982,0,0,0,0,0,0,2
6,143,2,281
267.8004,"",""
205600,"Ag(OCN)2-",0,5.003,0,0,-1,0,0,0,2
2,560,1,20
191.9025,"",""
201433,"Ag(CN)3-2",-140.143,21.4,0,0,-2,0,0,0,2
3,143,1,20
185.9214,"",""
1001430,"BaFe(CN)6-2",0,49.403,0,0,-2,0,0,0,3
6,143,1,280,1,100
349.2804,"",""
3309921,"H ACETATE",0,4.76,0,0,0,0,0,0,2
1,992,1,330
60.06,"",""
3309931,"H TARTRAT",0,4.16,0,0,-1,0,0,0,2
1,993,1,330
149.1,"",""
3309932,"H TARTRAT",0,6.67,0,0,0,0,0,0,2
1,993,2,330
150.11,"",""
3309941,"H GLYCINE",0,9.78,0,0,0,0,0,0,2
1,994,1,330
75.08,"",""
3309942,"H GLYCINE",0,12.12,0,0,1,0,0,0,2
1,994,2,330
76.09,"",""
3309951,"H SALICYL",0,13.4,0,0,-1,0,0,0,2
1,995,1,330
137.13,"",""
3309952,"H SALICYL",0,16.4,0,0,0,0,0,0,2
1,995,2,330
138.14,"",""
3309961,"H GLUTAMA",0,9.95,0,0,-1,0,0,0,2
1,996,1,330
146.14,"",""
3309962,"H GLUTAMA",0,14.37,0,0,0,0,0,0,2
1,996,2,330
147.15,"",""
3309971,"H PHTHALA",0,5.4,0,0,-1,0,0,0,2
1,997,1,330
165.14,"",""
3309972,"H PHTHALA",0,8.35,0,0,0,0,0,0,2
1,997,2,330
166.15,"",""
1609921,"CD ACETATE",0,1.7,0,0,1,0,0,0,2
```

```
1,160,1,992
171.46,"",""
1609931,"CD TARTRAT",0,3.9,0,0,0,0,0,0,2
1,160,1,993
260.5,"",""
1609941,"CD GLYCINE",0,4.8,0,0,1,0,0,0,2
1,160,1,994
186.48,"",""
1609942,"CD GLYCINE",0,8.4,0,0,0,0,0,0,2
1,160,2,994
260.55,"",""
1609961,"CD GLUTAMA",0,4.78,0,0,0,0,0,0,2
1,160,1,996
257.54,"",""
1609962,"CD GLUTAMA",0,2.78,0,0,-2,0,0,0,2
1,160,2,996
402.67,"",""
1609971,"CD PHTHALA",0,2.5,0,0,0,0,0,0,2
1,160,1,997
276.54,"",""
6009931,"PB TARTRAT",0,3.78,0,0,0,0,0,0,2
1,600,1,993
355.3,"",""
6009941,"PB GLYCINE",0,5.47,0,0,1,0,0,0,2
1,600,1,994
281.28,"",""
6009942,"PB GLYCINE",0,8.32,0,0,0,0,0,0,2
1,600,2,994
355.35,"",""
1009921,"BA ACETATE",0,0.979,0,0,1,0,0,0,2
1,100,1,992
196.41,"",""
1009931,"BA TARTRATE",0,2.54,0,0,0,0,0,0,2
1,100,1,993
285.45,"",""
1009941,"BA GLYCINE",0,0.77,0,0,1,0,0,0,2
1,100,1,994
211.43,"",""
1009951,"BA SALICYL",0,0.21,0,0,0,0,0,0,2
1,100,1,995
273.48,"",""
1009961,"BA GLUTAMA",0,1.28,0,0,0,0,0,0,2
1,100,1,996
282.49,"",""
1009971,"BA PHTHALA",0,2.33,0,0,0,0,0,0,2
1,100,1,997
301.49,"",""
209921,"AG ACETATE",0,0.73,0,0,0,0,0,0,2
1,20,1,992
166.93,"",""
209922,"AG ACETATE2",0,0.64,0,0,-1,0,0,0,2
1,20,2,992
225.98,"",""
209941,"AG GLYCINE",0,3.51,0,0,0,0,0,0,2
1,20,1,994
181.95,"",""
209942,"AG GLYCINE",0,3.38,0,0,-1,0,0,0,2
1,20,2,994
256.02,"",""
2119921,"Cr ACETATE",0,14.25,0,0,2,0,0,0,4
1,211,1,992,2,330,-2,2
111.06,"",""
2119922,"Cr ACETATE2",0,16.68,0,0,1,0,0,0,4
1,211,2,992,2,330,-2,2
170.11,"",""
2119923,"Cr ACETATE3",0,19.2,0,0,0,0,0,0,4
1,211,3,992,2,330,-2,2
```

```
229,"","",
2119941,"CR GLYCINE",0,8.4,0,0,2,0,0,0,2
1,211,1,994
126.08,"","",
2119942,"CR GLYCINE",0,6.4,0,0,0,0,0,0,2
1,211,2,994
200.15,"","",
2119943,"CR GLYCINE",0,5.7,0,0,-1,0,0,0,2
1,211,3,994
274.22,"","",
2119971,"CR PHTHALA",0,5.52,0,0,1,0,0,0,2
1,211,1,997
216.14,"","",
2119972,"CR PHTHALA",0,10,0,0,-2,0,0,0,2
1,211,2,997
380.27,"","",
2119973,"CR PHTHALA",0,12.48,0,0,-4,0,0,0,2
1,211,3,997
544.4,"","",
8719931,"Tl TARTRAT",0,1.39,0,0,-1,0,0,0,2
1,870,1,993
352.48,"","",
3609941,"Hg GLYCINE",0,10.8,0,0,1,0,0,0,2
1,360,1,994
274.68,"","",
3609942,"Hg GLYCINE",0,20,0,0,1,0,0,0,2
1,360,2,994
348.75,"","",
1609721,"CdBUTANOATE",0,1.25,0,0,1,0,0,0,2
1,160,1,972
199.4,"","",
1609671,"CdCITRATE",0,5.3,0,0,-1,0,0,0,2
1,160,1,967
301.4,"","",
1609673,"CdH2CITRATE",0,2.05,0,0,1,0,0,0,3
1,160,1,967,2,330
303.4,"","",
1609672,"CdHCITRATE",0,3.37,0,0,0,0,0,0,3
1,160,1,967,1,330
302.4,"","",
1609674,"CdCITRATE2",0,5.34,0,0,-4,0,0,0,2
1,160,2,967
490.4,"","",
1609692,"CdHEDTA",0,21.54,0,0,-1,0,0,0,3
1,160,1,969,1,330
401.63,"SM89 8/1","",
1609693,"CdH2EDTA-0",0,23.6,0,0,0,0,0,0,3
1,160,1,969,2,330
402.639,"SM 89","",
1609694,"CdOHEDTA-3",0,4.1,0,0,-3,0,0,0,3
1,160,1,969,-1,330
417.63,"SM 89","",
1609922,"CdACETATE2",0,3.15,0,0,0,0,0,0,2
1,160,2,992
230.4,"","",
1609923,"CdACETATE3",0,2.17,0,0,-1,0,0,0,2
1,160,3,992
289.4,"","",
1609924,"CdACETATE4",0,2.04,0,0,-2,0,0,0,2
1,160,4,992
394.4,"","",
1609551,"CdDIETHAM",0,2.62,0,0,2,0,0,0,2
1,160,1,955
185.4,"","",
1609552,"CdDIETHAMIN2",0,4.86,0,0,2,0,0,0,2
1,160,2,955
258.41,"","",
```

```
1609553,"CdDIETHAMIN3",0,6.36,0,0,2,0,0,0,2
1,160,3,955
331.42,"",""
1609554,"CdDIETHAMIN4",0,7.31,0,0,2,0,0,0,2
1,160,4,955
404.43,"",""
1609711,"CdPROPANOATE",0,1.19,0,0,1,0,0,0,2
1,160,1,971
185.4,"",""
1609712,"CdPROPANOAT2",0,1.86,0,0,0,0,0,0,2
1,160,2,971
285.4,"",""
1609723,"CdPROPANOAT3",0,2.345,0,0,-1,0,0,0,2
1,160,3,971
331.4,"",""
1609714,"CdPROPANOAT4",0,1.98,0,0,-2,0,0,0,2
1,160,4,971
404.527,"",""
1609722,"CdBUTANOAT2",0,1.93,0,0,1,0,0,0,2
1,160,2,972
286.4,"",""
1609723,"CdBUTANOATE3",0,2.34,0,0,-1,0,0,0,2
1,160,3,972
373.4,"",""
1609724,"CdBUTANOAT4",0,1.98,0,0,-2,0,0,0,2
1,160,4,972
460.4,"",""
1609641,"CdPROPAM",0,2.62,0,0,2,0,0,0,2
1,160,1,964
171.41,"",""
1609642,"CdPROPAM2",0,4.64,0,0,2,0,0,0,2
1,160,2,964
230.41,"",""
1609643,"CdPROPAM3",0,6.03,0,0,2,0,0,0,2
1,160,3,964
289.42,"",""
1609651,"CdISOPROPAM",0,2.55,0,0,2,0,0,0,2
1,160,1,965
171.41,"",""
1609652,"CdISOPROPAM2",0,4.57,0,0,2,0,0,0,2
1,160,2,965
230.41,"",""
1609653,"CdISOPROPAM3",0,6.07,0,0,2,0,0,0,2
1,160,3,965
289.4,"",""
1609654,"CdISOPROPAM4",0,6.9,0,0,2,0,0,0,2
1,160,4,965
348.41,"",""
2109692,"CrHEDTA",0,6.1,0,0,0,0,0,0,3
1,210,1,969,1,330
341,"",""
2109711,"CrPROPANAT",0,4.7,0,0,2,0,0,0,2
1,210,1,971
125,"",""
2109712,"CrPROPANAT2",0,7.06,0,0,1,0,0,0,2
1,210,2,971
198,"",""
2109713,"CrPROPANAT3",0,9.72,0,0,0,0,0,0,2
1,210,3,971
270.996,"",""
2319691,"CuEDTA-2",0,20.41,0,0,-2,0,0,0,2
1,231,1,969
351.76,"",""
2319692,"CuHEDTA-1",0,23.84,0,0,-1,0,0,0,3
1,231,1,969,1,330
352.77,"",""
2319693,"CuH2EDTA-0",0,26.9,0,0,0,0,0,0,3
```

```
1,231,1,969,2,330
353.775,"SM 89",""
2319694,"CuOHEDTA-3",0,8.5,0,0,-3,0,0,0,3
1,231,1,969,-1,330
368.766,"SM 89",""
2319922,"CuACETATE2",0,3.63,0,0,0,0,0,0,2
1,231,2,992
181.582,"",""
2319923,"CuACETATE3",0,3.58,0,0,-1,0,0,0,2
1,231,3,992
240.603,"",""
2319924,"CuACETATE4",0,3.33,0,0,-2,0,0,0,2
1,231,4,992
299.624,"",""
2319711,"CuPROPANOAT",0,1.83,0,0,1,0,0,0,2
1,231,1,971
136.57,"",""
2319712,"CuPROPANAT2",0,2.65,0,0,0,0,0,0,2
1,231,2,971
209.6,"",""
2319713,"CuPROANAT3",0,2.3,0,0,-1,0,0,0,2
1,231,3,971
282.64,"",""
2319714,"CuPROPANAT4",0,2.7,0,0,-2,0,0,0,2
1,231,4,971
355.67,"",""
2319582,"CuMETHAM2",0,7.51,0,0,2,0,0,0,2
1,231,2,958
94.558,"",""
2319591,"CuDIMETHAM",0,3.21,0,0,2,0,0,0,2
1,231,1,959
108.57,"",""
2319592,"CUDIMETHAM2",0,5.66,0,0,2,0,0,0,2
1,231,2,959
153.598,"",""
2319593,"CuDIMETHAM3",0,7.26,0,0,2,0,0,0,2
1,231,3,959
198.628,"",""
2319721,"CuBUTANOAT",0,2.14,0,0,1,0,0,0,2
1,231,1,972
150.583,"",""
2319722,"CuBUTANOAT2",0,2.6,0,0,0,0,0,0,2
1,231,2,972
237.626,"",""
2319723,"CuBUTANOAT3",0,2.3,0,0,-1,0,0,0,2
1,231,3,972
342.67,"",""
2319724,"CuBUTANOAT4",0,2.95,0,0,-2,0,0,0,2
1,231,4,972
411.712,"",""
2319731,"CuISBUTRAT",0,2.027,0,0,1,0,0,0,2
1,231,1,973
150.583,"",""
2319732,"CuISOBUTYRT2",0,2.7,0,0,0,0,0,0,2
1,231,2,973
237.626,"",""
6009671,"PB CITRATE",0,4.34,0,0,-1,0,0,0,2
1,600,1,967
396.252,"",""
6009672,"PBCITRATE2",0,6.08,0,0,-4,0,0,0,2
1,600,2,967
585.315,"",""
6009673,"PBCITRATE3",0,6.97,0,0,-7,0,0,0,2
1,600,3,967
774.378,"",""
6009691,"PbEDTA-2",0,19.71,0,0,-2,0,0,0,2
1,600,1,969
```

```
495.41,"SM89 8/1",""
6009692,"PbHEDTA-1",0,22.51,0,0,-1,0,0,0,3
1,600,1,969,1,330
496.42,"SM89 8/1",""
6009921,"PBACETATE",0,2.87,0,0,1,0,0,0,2
1,600,1,992
266.24,"",""
6009922,"PBACETATE2",0,4.08,0,0,0,0,0,0,2
1,600,2,992
325.232,"",""
6009923,"PBACETATE3",0,3.59,0,0,-1,0,0,0,2
1,600,3,992
384.25,"",""
6009711,"PBPROPANAT",0,2.64,0,0,1,0,0,0,2
1,600,1,971
280.222,"",""
6009712,"PBPROPANOAT2",0,4.05,0,0,0,0,0,0,2
1,600,2,971
353.25,"",""
6009713,"PBPROPANOAT3",0,2.99,0,0,-1,0,0,0,2
1,600,3,971
426.286,"",""
6009714,"PBPROPANOAT4",0,4.18,0,0,-2,0,0,0,2
1,600,4,971
499.318,"",""
6009721,"PB BUTANOAT",0,2.125,0,0,1,0,0,0,2
1,600,1,972
294.23,"",""
6009722,"PBBUTANOATE2",0,3.735,0,0,0,0,0,0,2
1,600,2,972
381.28,"",""
6009723,"PBBUTANOAT3",0,4.125,0,0,-1,0,0,0,2
1,600,3,972
468.32,"",""
6009724,"PBBUTANOAT4",0,4.43,0,0,-2,0,0,0,2
1,600,4,972
555.36,"",""
5409671,"NICITRATE",0,6.62,0,0,-1,0,0,0,2
1,540,1,967
247.77,"",""
5409672,"NICITRATEH",0,4.09,0,0,0,0,0,0,3
1,540,1,967,1,330
248.77,"",""
5409673,"NICITRATEH2",0,2.13,0,0,1,0,0,0,3
1,540,1,967,2,330
249.77,"",""
5409691,"NiEDTA-2",0,20.23,0,0,-2,0,0,0,2
1,540,1,969
346.91,"",""
5409692,"NiHEDTA-1",0,23.86,0,0,-1,0,0,0,3
1,540,1,969,1,330
347.92,"",""
5409693,"NiH2EDTA-0",0,25.2,0,0,0,0,0,0,3
1,540,1,969,2,330
348.929,"SM 89",""
5409694,"NiOHEDTA-3",0,7.6,0,0,-3,0,0,0,3
1,540,1,969,-1,330
363.92,"SM 89",""
5409711,"NIPROPANOAT",0,0.83,0,0,1,0,0,0,2
1,540,1,971
131.73,"",""
5409712,"NIPROPANOAT2",0,1.2067,0,0,0,0,0,0,2
1,540,2,971
204.76,"",""
5409713,"NIPROPANOAT3",0,0.97,0,0,-1,0,0,0,2
1,540,3,971
277.795,"",""
```

```
5409721,"NI BUTANOAT",0,0.77,0,0,1,0,0,0,2
1,540,1,972
145.75,"",""
5409722,"NIBUTANOAT2",0,0.8,0,0,0,0,0,0,2
1,540,2,972
218.785,"",""
5409723,"NIBUTAOAT3",0,1.34,0,0,-1,0,0,0,2
1,540,3,972
291.82,"",""
5409641,"NINPROPYLAM",0,2.81,0,0,2,0,0,0,2
1,540,1,964
117.75,"",""
5409642,"NINPROPYLAM2",0,5.02,0,0,2,0,0,0,2
1,540,2,964
176.79,"",""
5409643,"NINPROPYLAM3",0,6.79,0,0,2,0,0,0,2
1,540,3,964
235.83,"",""
5409644,"NINPROPYLAM4",0,8.31,0,0,2,0,0,0,2
1,540,4,964
294.87,"",""
5409651,"NIIPROYLAM",0,2.71,0,0,2,0,0,0,2
1,540,1,965
117.75,"",""
5409652,"NIIPROPYLAM2",0,4.86,0,0,2,0,0,0,2
1,540,2,965
176.79,"",""
5409653,"NIIPROPYLAM3",0,6.57,0,0,2,0,0,0,2
1,540,3,965
235.83,"",""
5409654,"NIIPROPYLAM4",0,7.83,0,0,2,0,0,0,2
1,540,4,965
294.87,"",""
5409655,"NIIPROPYLAM5",0,8.43,0,0,2,0,0,0,2
1,540,5,965
353.91,"",""
209551,"AGDIETHAM",0,3.965,0,0,1,0,0,0,2
1,20,1,955
152.897,"",""
209552,"AGDIETHAM2",0,7.02,0,0,1,0,0,0,2
1,20,2,955
197.926,"",""
209581,"AGMETHAM",0,3.18,0,0,1,0,0,0,2
1,20,1,958
138.928,"",""
209582,"AGMETHAM2",0,7.14,0,0,1,0,0,0,2
1,20,2,958
169.99,"",""
209611,"AGHEXYLAM",0,3.66,0,0,1,0,0,0,2
1,20,1,961
208.868,"",""
209612,"AGHEXYLAM2",0,7.35,0,0,1,0,0,0,2
1,20,2,961
309.868,"",""
209651,"AGIPROPAM",0,3.19,0,0,1,0,0,0,2
1,20,1,965
166.91,"",""
209652,"AGIPROPYLAM2",0,6.85,0,0,1,0,0,0,2
1,20,2,965
225.948,"",""
209561,"AGNBUTYLAM",0,3.55,0,0,1,0,0,0,2
1,20,1,956
181.01,"",""
209562,"AGNBUTYLAM2",0,7.77,0,0,1,0,0,0,2
1,20,2,956
254.148,"",""
209961,"AGGLUTAM",0,3.79,0,0,0,0,0,0,2
```

```
1,20,1,996
252.998,"",""
209962,"AGGLUTAM2",0,6.55,0,0,-1,0,0,0,2
1,20,2,996
398.128,"",""
209681,"AGNTA",0,5.36,0,0,-2,0,0,0,2
1,20,1,968
295.928,"",""
209691,"AGEDTA",0,7.355,0,0,-3,0,0,0,2
1,20,1,969
383.868,"",""
209692,"AGEDTA2",0,11.355,0,0,-7,0,0,0,2
1,20,2,969
659.868,"",""
209693,"AGHEDTA",0,3.36,0,0,-2,0,0,0,3
1,20,1,969,1,330
384.868,"",""
209801,"AG2METPYR",0,2.32,0,0,1,0,0,0,2
1,20,1,980
201.868,"",""
209802,"AG2METPYR2",0,4.68,0,0,1,0,0,0,2
1,20,2,980
295.868,"",""
209811,"AG3METPYR",0,2.2,0,0,1,0,0,0,2
1,20,1,981
201.868,"",""
209812,"AG3METPYR2",0,4.46,0,0,1,0,0,0,2
1,20,2,981
295.868,"",""
209821,"AG4METPYR",0,2.21,0,0,1,0,0,0,2
1,20,1,982
201.868,"",""
209822,"AG4METPYR2",0,4.67,0,0,1,0,0,0,2
1,20,2,982
295.868,"",""
209641,"AGNPROPYLAM",0,3.47,0,0,1,0,0,0,2
1,20,1,964
166.908,"",""
209642,"AGNPROPYLAM2",0,7.51,0,0,1,0,0,0,2
1,20,2,964
225.948,"",""
9509961,"ZNGLUTAM",0,3.79,0,0,0,0,0,0,2
1,950,1,996
210.5,"",""
9509962,"ZNGLUTAM2",0,8.25,0,0,-2,0,0,0,2
1,950,2,996
355.63,"",""
9509963,"ZNGLUTAM3",0,9.8,0,0,-4,0,0,0,2
1,950,3,996
500.76,"",""
9509811,"ZN3METPYR",0,1,0,0,2,0,0,0,2
1,950,1,981
159.37,"",""
9509812,"ZN3METPYR2",0,2.1,0,0,2,0,0,0,2
1,950,2,981
224.74,"",""
9509813,"ZN3METPYR3",0,2.6,0,0,2,0,0,0,2
1,950,3,981
290.11,"",""
9509814,"ZN3METPYR4",0,3.7,0,0,2,0,0,0,2
1,950,4,981
355.48,"",""
9509941,"ZNGLYCERIN",0,5.38,0,0,1,0,0,0,2
1,950,1,994
139.44,"",""
9509942,"ZNGLYCERIN2",0,9.81,0,0,0,0,0,0,2
1,950,2,994
```

```
213.51,"",""
9509943,"ZNGLYCERN3",0,12.3,0,0,-1,0,0,0,2
1,950,3,994
287.58,"",""
9509671,"ZNCITRATE",0,6.1,0,0,-1,0,0,0,2
1,950,1,967
254.43,"",""
9509672,"ZNCITRATE2",0,6.7,0,0,-4,0,0,0,2
1,950,2,967
443.49,"",""
9509673,"ZNCITRATEH",0,3.78,0,0,0,0,0,0,3
1,950,1,967,1,330
255.43,"",""
9509674,"ZNCITRATEH2",0,1.68,0,0,1,0,0,0,3
1,950,1,967,2,330
256.43,"",""
9509971,"ZNPHTHLATE",0,2.91,0,0,0,0,0,0,2
1,950,1,997
229.5,"",""
9509972,"ZNPHTHALATE2",0,4.2,0,0,-2,0,0,0,2
1,950,2,997
393.64,"",""
6009961,"PBGLUTAM",0,4.7,0,0,0,0,0,0,2
1,600,1,996
352.32,"",""
6009962,"PBGLUTAM2",0,7.55,0,0,-2,0,0,0,2
1,600,2,996
497.45,"",""
6009971,"PBPHTHALAT",0,2.78,0,0,0,0,0,0,2
1,600,1,997
371.32,"",""
6009972,"PBPHTHALA2",0,4.01,0,0,-2,0,0,0,2
1,600,2,997
535.45,"",""
6009924,"PBACETATE4",0,3.4,0,0,-2,0,0,0,2
1,600,4,992
443.39,"",""
2319581,"CUMETHAM",0,4.11,0,0,2,0,0,0,2
1,231,1,958
94.474,"",""
2319583,"CUMETHAM3",0,10.21,0,0,2,0,0,0,2
1,231,3,958
156.51,"",""
2319584,"CUMETHAM4",0,12.08,0,0,2,0,0,0,2
1,231,4,958
187.528,"",""
2319811,"CU3METPYR",0,2.74,0,0,2,0,0,0,2
1,231,1,981
157.546,"",""
2319812,"CU3METPYR2",0,4.8,0,0,2,0,0,0,2
1,231,2,981
251.546,"",""
2319813,"CU3METPYR3",0,6.3,0,0,2,0,0,0,2
1,231,3,981
345.546,"",""
2319814,"CU3METPYR4",0,7.2,0,0,2,0,0,0,2
1,231,4,981
439.546,"",""
2319821,"CU4METPYR",0,2.88,0,0,2,0,0,0,2
1,231,1,982
157.546,"",""
2319822,"CU4METPYR2",0,5.16,0,0,2,0,0,0,2
1,231,2,982
251.546,"",""
2319823,"CU4METPYR3",0,6.77,0,0,2,0,0,0,2
1,231,3,982
345.546,"",""
```

```
2319824,"CU4METPYR4",0,8.08,0,0,2,0,0,0,2
1,231,4,982
439.546,"",""
2319825,"CU4METPYR5",0,8.3,0,0,2,0,0,0,2
1,231,5,982
533.546,"",""
2319961,"CUGLUTAM",0,8.33,0,0,0,0,0,0,2
1,231,1,996
208.676,"",""
2319671,"CUCITRATE",0,7.26,0,0,-1,0,0,0,2
1,231,1,967
252.606,"",""
2319672,"CUCITRATE2",0,8.72,0,0,-4,0,0,0,2
1,231,2,967
441.666,"",""
2319673,"CUHCITRATE",0,4.27,0,0,0,0,0,0,3
1,231,1,967,1,330
253.6,"",""
2319674,"CUH2CITRATE",0,2.2,0,0,1,0,0,0,3
1,231,1,967,2,330
254.6,"",""
2319841,"CUISVALER",0,2.08,0,0,1,0,0,0,2
1,231,1,984
164.676,"",""
2319971,"CUPHTHALAT",0,4.04,0,0,0,0,0,0,2
1,231,1,997
227.676,"",""
2319851,"CUVALERAT",0,2.12,0,0,1,0,0,0,2
1,231,1,985
164.676,"",""
2319852,"CUVALERAT2",0,3,0,0,0,0,0,0,2
1,231,2,985
265.806,"",""
1009691,"BaEDTA-2",0,10.2,0,0,-2,0,0,0,2
1,100,1,969
425.543,"SPO 80",""
1009692,"BaHEDTA-1",0,15.4,0,0,-1,0,0,0,3
1,100,1,969,1,330
426.551,"SPO 80",""
1009671,"BACITRATE",0,4.06,0,0,-1,0,0,0,2
1,100,1,967
326.4,"",""
1009672,"BACITRATEH",0,2.7,0,0,0,0,0,0,3
1,100,1,967,1,330
327.4,"",""
1009673,"BACITRATEH2",0,1.27,0,0,1,0,0,0,3
1,100,1,967,2,330
328.4,"",""
1009711,"BAPROPANOAT",0,0.34,0,0,1,0,0,0,2
1,100,1,971
210.372,"",""
1009721,"BABUTANOAT",0,0.31,0,0,1,0,0,0,2
1,100,1,972
224.413,"",""
2109691,"CR EDTA",0,13.61,0,0,-2,0,0,0,2
1,210,1,969
327.996,"",""
5409801,"NI2METPYR",0,0.4,0,0,2,0,0,0,2
1,540,1,980
152.71,"",""
5409811,"NI3METPYR",0,2.02,0,0,2,0,0,0,2
1,540,1,981
152.71,"",""
5409812,"NI3METPYR2",0,3.3,0,0,2,0,0,0,2
1,540,2,981
246.71,"",""
5409813,"NI3METPYR3",0,4.1,0,0,2,0,0,0,2
```

```
0,540,3,981
340.71,"",""
5409814,"NI3METPYR4",0,4.6,0,0,2,0,0,0,2
1,540,4,981
434.71,"",""
5409821,"NI4METPYR",0,2.11,0,0,2,0,0,0,2
1,540,1,982
152.71,"",""
5409822,"NI4METPYR2",0,3.59,0,0,2,0,0,0,2
1,540,2,982
246.71,"",""
5409823,"NI4METPYR3",0,4.34,0,0,2,0,0,0,2
1,540,3,982
340.71,"",""
5409824,"NI4METPYR4",0,4.7,0,0,2,0,0.04,0,2
1,540,4,982
34.71,"",""
5409551,"NIDIETHAM1",0,2.78,0,0,2,0,0,0,2
1,540,1,955
152.71,"",""
5409552,"NIDIETHAM2",0,4.97,0,0,2,0,0,0,2
1,540,2,955
246.71,"",""
5409553,"NIDIEHTAM3",0,6.72,0,0,2,0,0,0,2
1,540,3,955
340.71,"",""
5409554,"NIDIETHAM4",0,7.93,0,0,2,0,0,0,2
1,540,4,955
434.71,"",""
5409555,"NIDIETHAM5",0,8.87,0,0,2,0,0,0,2
1,540,5,955
529,"",""
5409943,"NIGLYCINE3",0,14.2,0,0,-1,0,0,0,2
1,540,3,994
280.92,"",""
1609811,"CD3METPYR",0,1.62,0,0,2,0,0,0,2
1,160,1,981
206.4,"",""
1609812,"CD3METPYR2",0,2.8,0,0,2,0,0,0,2
1,160,2,981
300.4,"",""
1609813,"CD3METPYR3",0,3.6,0,0,2,0,0,0,2
1,160,3,981
394.4,"",""
1609814,"CD3METPYR4",0,4,0,0,2,0,0,0,2
1,160,4,981
488.4,"",""
1609821,"CD4METPYR",0,1.51,0,0,2,0,0,0,2
1,160,1,982
206.4,"",""
1609822,"CD4METPYR2",0,2.5,0,0,2,0,0,0,2
1,160,2,982
300.4,"",""
1609823,"CD4METPYR3",0,2.9,0,0,2,0,0,0,2
1,160,3,982
394.4,"",""
1609824,"CD4METPYR4",0,4,0,0,2,0,0,0,2
1,160,4,982
488.4,"",""
1609943,"CDGLYCINE",0,10.7,0,0,1,0,0,0,2
1,160,3,994
186.47,"",""
1609972,"CDPHTHALA",0,2.88,0,0,0,0,0,0,2
1,160,2,997
276.53,"",""
1609841,"CDISVALERAT",0,1.34,0,0,1,0,0,0,2
1,160,1,984
```

```
215.53,"",""
1609842,"CDISVALERAT2",0,2.3,0,0,0,0,0,0,2
1,160,2,984
314.6,"",""
1609843,"CDISVALERAT3",0,2.5,0,0,-1,0,0,0,2
1,160,3,984
415.79,"",""
1609844,"CDISVALERAT4",0,2,0,0,-2,0,0,0,2
1,160,4,984
516.92,"",""
3609831,"HGFORMATE",0,2.94,0,0,0,0,0,0,2
0.5,360,1,983
245.61,"",""
3609832,"HGFORMATE2",0,5.45,0,0,-1,0,0,0,2
0.5,360,2,983
290.63,"",""
3609711,"HGPROPANOAT",0,3.72,0,0,0,0,0,0,2
0.5,360,1,971
273.62,"",""
3609712,"HGPROPANOT2",0,6.99,0,0,-1,0,0,0,2
0.5,360,2,971
346.654,"",""
8709671,"TL CITRATE",0,1.61,0,0,-2,0,0,0,2
1,870,1,967
393.43,"",""
8709681,"TL NTA",0,4.71,0,0,-2,0,0,0,2
1,870,1,968
392.434,"",""
8709691,"TL EDTA",0,6.41,0,0,-3,0,0,0,2
1,870,1,969
480.37,"",""
8709921,"TL ACETATE",0,-0.11,0,0,0,0,0,0,2
1,870,1,992
263.42,"",""
9509691,"ZNEDTA-2",0,18.15,0,0,-2,0,0,0,2
1,950,1,969
353.59,"",""
9509692,"ZnHEDTA-1",0,21.58,0,0,-1,0,0,0,3
1,950,1,969,1,330
354.6,"",""
9509693,"ZnH2EDTA-0",0,23.3,0,0,0,0,0,0,3
1,950,1,969,2,330
355.609,"SM 89",""
9509694,"ZnOHEDTA-3",0,6,0,0,-3,0,0,0,3
1,950,1,969,-1,330
370.6,"SM 89",""
9509921,"ZN ACETATE",0,1.21,0,0,1,0,0,0,2
1,950,1,992
124.392,"",""
9509922,"ZN ACETATE2",0,2.01,0,0,0,0,0,0,2
1,950,2,992
183.412,"",""
9509923,"ZNACETATE3",0,1.63,0,0,-1,0,0,0,2
1,950,3,992
242.433,"",""
9509924,"ZN ACETATE4",0,1.36,0,0,-2,0,0,0,2
1,950,4,992
301.454,"",""
9509551,"ZN DIETHYLAM",0,2.51,0,0,2,0,0,0,2
1,950,1,955
110.399,"",""
9509552,"ZN DIETHYLAM",83.68,4.96,0,0,2,0,0,0,2
1,950,2,955
155.428,"",""
9509553,"ZN DIETHAM3",0,7.49,0,0,2,0,0,0,2
1,950,3,955
200.457,"",""
```

```
9509554,"ZN DIETHAM4",0,9.83,0,0,2,0,0,0,2
1,950,4,955
245.486,"",""
9509711,"ZNPROPANOT",0,0.72,0,0,1,0,0,0,2
1,950,1,971
138.399,"",""
9509712,"ZNPROPANOT2",0,1.145,0,0,0,0,0,0,2
1,950,2,971
211.434,"",""
9509713,"ZNPROPANOT3",0,1.82,0,0,-1,0,0,0,2
1,950,3,971
284.47,"",""
9509714,"ZNPROPANOT4",0,1.36,0,0,-2,0,0,0,2
1,950,4,971
357.5,"",""
9509721,"ZNBUTANOAT",0,0.983,0,0,1,0,0,0,2
1,950,1,972
152.413,"",""
9509722,"ZNBUTANOT2",0,1.65,0,0,0,0,0,0,2
1,950,2,972
239.46,"",""
9509723,"ZNBUTANOT3",0,1.69,0,0,-1,0,0,0,2
1,950,3,972
326.5,"",""
9509724,"ZNBUTANOAT4",0,2.05,0,0,-2,0,0,0,2
1,950,4,972
413.54,"",""
9509641,"ZNNPRPYLAM",0,2.42,0,0,2,0,0,0,2
1,950,1,964
124.41,"",""
9509642,"ZNNPRPYLAM2",0,4.85,0,0,2,0,0,0,2
1,950,2,964
183.45,"",""
9509643,"ZNNPRPYLAM3",0,7.38,0,0,2,0,0,0,2
1,950,3,964
242.29,"",""
9509644,"ZNNPRPYLAM4",0,9.49,0,0,2,0,0,0,2
1,950,4,964
301.53,"",""
9509651,"ZNIPRPYLAM1",0,2.37,0,0,2,0,0,0,2
1,950,1,965
124.41,"",""
9509652,"ZNIPRPYLAM2",0,4.67,0,0,2,0,0,0,2
1,950,2,965
183.45,"",""
9509653,"ZNIPRPYLAM3",0,7.14,0,0,2,0,0,0,2
1,950,3,965
242.49,"",""
9509654,"ZNIPRPYLAM4",0,9.44,0,0,2,0,0,0,2
1,950,4,965
301.53,"",""
3309671,"CITRATEH",0,6.33,0,0,-2,0,0,0,2
1,330,1,967
190.062,"",""
3309672,"CITRATEH2",0,11.05,0,0,-1,0,0,0,2
2,330,1,967
191.062,"",""
3309673,"CITRATEH3",0,14.18,0,0,0,0,0,0,2
3,330,1,967
192.062,"",""
1509671,"CACITRATE",0,4.73,0,0,-1,0,0,0,2
1,150,1,967
229.143,"",""
1509672,"CACITRATEH",0,3.02,0,0,0,0,0,0,3
1,150,1,967,1,330
230.143,"",""
1509673,"CACITRATEH2",0,1.29,0,0,1,0,0,0,3
```

```
1,150,1,967,2,330
231.143,"",""
4709671,"MNCITRATE",0,5.28,0,0,-1,0,0,0,2
1,470,1,967
244.001,"",""
4709672,"MNCITRATEH",0,3.02,0,0,0,0,0,0,3
1,470,1,967,1,330
245.001,"",""
2809671,"FECITRATE",0,5.7,0,0,-1,0,0,0,2
1,280,1,967
244.91,"",""
2809672,"FECITRATEH",0,3.5,0,0,0,0,0,0,3
1,280,1,967,1,330
245.91,"",""
2819671,"FECITRATE",0,12.55,0,0,0,0,0,0,2
1,281,1,967
244.91,"",""
2819672,"FECITRATEH",0,19.8,0,0,1,0,0,0,3
1,281,1,967,1,330
245.91,"",""
3309631,"HEN",0,9.96,0,0,1,0,0,0,2
1,330,1,963
61.12,"",""
3309632,"H2EN",0,16.85,0,0,2,0,0,0,2
2,330,1,963
62.12,"",""
2319631,"CUEN",0,10.49,0,0,2,0,0,0,2
1,231,1,963
123.666,"",""
2319632,"CUEN2",0,19.62,0,0,2,0,0,0,2
1,231,2,963
183.786,"",""
1609631,"CDEN",0,5.61,0,0,2,0,0,0,2
1,160,1,963
172.591,"",""
1609632,"CDEN2",0,10.34,0,0,2,0,0,0,2
1,160,2,963
232.639,"",""
1609633,"CDEN3",0,12.26,0,0,2,0,0,0,2
1,160,3,963
292.759,"",""
209631,"AGEN",0,4.7,0,0,1,0,0,0,2
1,20,1,963
167.988,"",""
209632,"AGEN2",0,7.7,0,0,1,0,0,0,2
1,20,2,963
228.108,"",""
209633,"AGENH",0,7.31,0,0,2,0,0,0,3
1,20,1,963,1,330
168.988,"",""
209634,"AG2EN",0,1.43,0,0,2,0,0,0,2
2,20,1,963
275.856,"",""
209635,"AG2EN2",0,12.73,0,0,2,0,0,0,2
2,20,2,963
335.976,"",""
5409631,"NIEN",0,7.24,0,0,2,0,0,0,2
1,540,1,963
118.83,"",""
5409632,"NIEN2",0,13.36,0,0,2,0,0,0,2
1,540,2,963
178.95,"",""
5409633,"NIEN3",0,17.54,0,0,2,0,0,0,2
1,540,3,963
239.07,"",""
6009631,"PBEN",0,7,0,0,2,0,0,0,2
1,600,1,963
```

```
267.31,"",""
6009632,"PBEN2",0,8.45,0,0,2,0,0,0,2
1,600,2,963
326.43,"",""
9509631,"ZNEN",0,5.65,0,0,2,0,0,0,2
1,950,1,963
125.49,"",""
9509632,"ZNEN2",0,10.62,0,0,2,0,0,0,2
1,950,2,963
185.61,"",""
9509633,"ZNEN3",0,13.83,0,0,2,0,0,0,2
1,950,3,963
245.73,"",""
4709631,"MNEN",0,2.67,0,0,2,0,0,0,2
1,470,1,963
115.058,"",""
4709632,"MNEN2",0,4.2,0,0,2,0,0,0,2
1,470,2,963
175.178,"",""
2809631,"FEEN",0,4.36,0,0,2,0,0,0,2
1,280,1,963
115.967,"",""
2809632,"FEEN2",0,7.65,0,0,2,0,0,0,2
1,280,2,963
176.087,"",""
2809633,"FEEN3",0,9.68,0,0,2,0,0,0,2
1,280,3,963
236.207,"",""
3309681,"HNTA",0,10.3,0,0,-2,0,0,0,2
1,330,1,968
189.185,"DRP90",""
3309682,"H2NTA",0,13.3,0,0,-1,0,0,0,2
2,330,1,968
190.193,"DRP90",""
3309683,"H3NTA",0,15.4,0,0,0,0,0,0,2
3,330,1,968
191.201,"DRP90",""
1509681,"CaNTA-1",0,7.7,0,0,-1,0,0,0,2
1,150,1,968
228.257,"DRP90",""
1509682,"Ca(NTA)2-4",0,9.5,0,0,-4,0,0,0,2
1,150,2,968
416.434,"DRP90",""
4609681,"MgNTA-1",0,6.8,0,0,-1,0,0,0,2
1,460,1,968
212.482,"DRP90",""
8009681,"SrNTA-1",0,6.3,0,0,-1,0,0,0,2
1,800,1,968
275.797,"DRP90",""
4109681,"KNTA-2",0,1.3,0,0,-2,0,0,0,2
1,410,1,968
227.275,"DRP90",""
5009681,"NaNTA-2",0,1.9,0,0,-2,0,0,0,2
1,500,1,968
211.167,"DRP90",""
2819681,"FeNTA-0",0,17.9,0,0,0,0,0,0,2
1,281,1,968
244.024,"DRP90",""
2819682,"Fe(NTA)2-3",0,26.2,0,0,-3,0,0,0,2
1,281,2,968
432.201,"DRP90",""
2819683,"FeOHNTA-1",0,13.5,0,0,-1,0,0,0,3
1,281,1,968,-1,330
261.102,"DRP90",""
2819684,"Fe(OH)2NTA-2",0,5.3,0,0,-2,0,0,0,3
1,281,1,968,-2,330
278.18,"DRP90",""
```

```
2809681,"FeIINTA-1",0,9.6,0,0,-1,0,0,0,2
1,280,1,968
244.024,"DRP90",""
2809682,"FeII(NTA)2-4",0,13.6,0,0,-4,0,0,0,2
1,280,2,968
432.201,"DRP90",""
2809683,"FeIIHNTA-0",0,11.8,0,0,0,0,0,0,3
1,280,1,330,1,968
245.032,"DRP90",""
2809684,"FeIIOHNTA-2",0,-1.4,0,0,-2,0,0,0,3
1,280,1,968,-1,330
261.102,"DRP90",""
4709681,"MnNTA-1",0,8.8,0,0,-1,0,0,0,2
1,470,1,968
243.115,"DRP90",""
4709682,"Mn(NTA)2-4",0,11.6,0,0,-4,0,0,0,2
1,470,2,968
431.292,"DRP90",""
2319681,"CuNTA-1",0,14.4,0,0,-1,0,0,0,2
1,231,1,968
251.723,"DRP90",""
2319682,"Cu(NTA)2-4",0,18.2,0,0,-4,0,0,0,2
1,231,2,968
439.9,"DRP90",""
2319683,"CuHNTA-0",0,16.2,0,0,0,0,0,0,3
1,231,1,330,1,968
252.731,"DRP90",""
2319684,"CuOHNTA-2",0,4.8,0,0,-2,0,0,0,3
1,231,1,968,-1,330
268.801,"DRP90",""
1009681,"BaNTA-1",0,6.1,0,0,-1,0,0,0,2
1,100,1,968
325.507,"DRP90",""
1609681,"CdNTA-1",0,11.1,0,0,-1,0,0,0,2
1,160,1,968
300.587,"DRP90",""
1609682,"Cd(NTA)2-4",0,15,0,0,-4,0,0,0,2
1,160,2,968
488.764,"DRP90",""
1609683,"CdOHNTA-2",0,-0.6,0,0,-2,0,0,0,3
1,160,1,968,-1,330
317.665,"DRP90",""
9509681,"ZnNTA-1",0,12,0,0,-1,0,0,0,2
1,950,1,968
253.557,"DRP90",""
9509682,"Zn(NTA)2-4",0,14.9,0,0,-4,0,0,0,2
1,950,2,968
441.734,"DRP90",""
9509683,"ZnOHNTA-2",0,1.5,0,0,-2,0,0,0,3
1,950,1,968,-1,330
270.635,"DRP90",""
5409681,"NiNTA-1",0,12.8,0,0,-1,0,0,0,2
1,540,1,968
246.877,"DRP90",""
5409682,"Ni(NTA)2-4",0,17,0,0,-4,0,0,0,2
1,540,2,968
435.054,"DRP90",""
5409683,"NiOHNTA-2",0,1.5,0,0,-2,0,0,0,3
1,540,1,968,-1,330
263.955,"DRP90",""
3629681,"HgNTA-1",0,15.6,0,0,-1,0,0,0,2
1,362,1,968
388.767,"DRP90",""
6009681,"PbNTA-1",0,12.7,0,0,-1,0,0,0,2
1,600,1,968
395.377,"DRP90",""
1829681,"CoNTA-1",0,11.7,0,0,-1,0,0,0,2
```

```
1,182,1,968
247.11,"DRP90",""
1829682,"Co(NTA)2-4",0,15,0,0,-4,0,0,0,2
1,182,2,968
435.287,"DRP90",""
1829683,"CoOHNTA-2",0,0.4,0,0,-2,0,0,0,3
1,182,1,968,-1,330
264.188,"DRP90",""
309681,"AlNTA-0",0,13.7,0,0,0,0,0,0,2
1,30,1,968
215.159,"DRP90",""
309682,"AlHNTA+1",0,15.6,0,0,1,0,0,0,3
1,30,1,330,1,968
216.166,"DRP90",""
309683,"AlOHNTA-1",0,8.4,0,0,-1,0,0,0,3
1,30,1,968,-1,330
232.166,"DRP90",""
309684,"Al(OH)2NTA-2",0,-0.4,0,0,-2,0,0,0,3
1,30,1,968,-2,330
249.244,"DRP90",""
3309121,"HEGTA-3",0,10.3,0,0,-3,0,0,0,2
1,330,1,912
377.327,"DRP90",""
3309122,"H2EGTA-2",0,19.7,0,0,-2,0,0,0,2
2,330,1,912
378.335,"DRP90",""
3309123,"H3EGTA-1",0,22.8,0,0,-1,0,0,0,2
3,330,1,912
379.343,"DRP90",""
3309124,"H4EGTA-0",0,25,0,0,0,0,0,0,2
4,330,1,912
380.351,"DRP90",""
1509121,"CaEGTA-2",0,12.6,0,0,-2,0,0,0,2
1,150,1,912
416.399,"DRP90",""
1509122,"CaHEGTA-1",0,16.8,0,0,-1,0,0,0,3
1,150,1,330,1,912
417.407,"","",""
4609121,"MgEGTA-2",0,7,0,0,-2,0,0,0,2
1,460,1,912
400.642,"DRP90",""
4609122,"MgHEGTA-1",0,15.1,0,0,-1,0,0,0,3
1,460,1,330,1,912
401.632,"DRP90",""
8009121,"SrEGTA-2",0,10.2,0,0,-2,0,0,0,2
1,800,1,912
463.939,"DRP90",""
8009122,"SrHEGTA-1",0,15.9,0,0,-1,0,0,0,3
1,800,1,330,1,912
464.947,"DRP90",""
2819121,"FeEGTA-1",0,23.1,0,0,-1,0,0,0,2
1,281,1,912
432.166,"","",""
2809121,"FeIIEGTA-2",0,13.5,0,0,-2,0,0,0,2
1,280,1,912
432.166,"DRP90",""
2809122,"FeIIHEGTA-1",0,18.3,0,0,-1,0,0,0,3
1,280,1,330,1,912
433.174,"DRP90",""
4709121,"MnEGTA-2",0,13.9,0,0,-2,0,0,0,2
1,470,1,912
431.257,"DRP90",""
4709122,"MnHEGTA-1",0,18.4,0,0,-1,0,0,0,3
1,470,1,330,1,912
432.265,"DRP90",""
2319121,"CuEGTA-2",0,19.3,0,0,-2,0,0,0,2
1,231,1,912
```

```
439.865,"DRP90",""
2319122,"CuHEGTA-1",0,24,0,0,-1,0,0,0,3
1,231,1,330,1,912
440.873,"DRP90",""
2319123,"Cu2EGTA-0",0,24.5,0,0,0,0,0,0,2
2,231,1,912
503.411,"DRP90",""
2319124,"Cu2OHEGTA-1",0,17.4,0,0,-1,0,0,0,3
2,231,1,912,-1,330
520.489,"DRP90",""
2319125,"Cu2OH2EGTA-2",0,9,0,0,-2,0,0,0,3
2,231,1,912,-2,330
537.567,"DRP90",""
1009121,"BaEGTA-2",0,10,0,0,-2,0,0,0,2
1,100,1,912
513.649,"DRP90",""
1009122,"BaHEGTA-1",0,15.8,0,0,-1,0,0,0,3
1,100,1,330,1,912
514.657,"DRP90",""
1609121,"CdEGTA-2",0,18.2,0,0,-2,0,0,0,2
1,160,1,912
488.729,"DRP90",""
1609122,"CdHEGTA-1",0,22.1,0,0,-1,0,0,0,3
1,160,1,330,1,912
489.737,"DRP90",""
9509121,"ZnEGTA-2",0,14.3,0,0,-2,0,0,0,2
1,950,1,912
441.699,"DRP90",""
9509122,"ZnHEGTA-1",0,19.7,0,0,-1,0,0,0,3
1,950,1,330,1,912
442.707,"DRP90",""
9509123,"Zn2EGTA-0",0,18.5,0,0,0,0,0,0,2
2,950,1,912
507.079,"DRP90",""
5409121,"NiEGTA-2",0,15.2,0,0,-2,0,0,0,2
1,540,1,912
435.019,"DRP90",""
5409122,"NiHEGTA-1",0,20.8,0,0,-1,0,0,0,3
1,540,1,330,1,912
436.027,"DRP90",""
5409123,"Ni2EGTA-0",0,21,0,0,0,0,0,0,2
2,540,1,912
493.719,"DRP90",""
3629121,"HgEGTA-2",0,24.6,0,0,-2,0,0,0,2
1,362,1,912
576.909,"DRP90",""
3629122,"HgHEGTA-1",0,28.1,0,0,-1,0,0,0,3
1,362,1,330,1,912
577.917,"DRP90",""
6009121,"PbEGTA-2",0,16.3,0,0,-2,0,0,0,2
1,600,1,912
583.519,"DRP90",""
6009122,"PbHEGTA-1",0,21.9,0,0,-1,0,0,0,3
1,600,1,330,1,912
584.527,"DRP90",""
6009123,"Pb2EGTA-0",0,21.7,0,0,0,0,0,0,2
2,600,1,912
790.719,"DRP90",""
1829121,"CoEGTA-2",0,14.1,0,0,-2,0,0,0,2
1,182,1,912
435.252,"DRP90",""
1829122,"CoHEGTA-1",0,19.6,0,0,-1,0,0,0,3
1,182,1,330,1,912
436.26,"DRP90",""
1829123,"Co2EGTA-0",0,18.2,0,0,0,0,0,0,2
2,182,1,912
0,"",""
```

```
309121,"AlEGTA-1",0,17,0,0,-1,0,0,0,2
1,30,1,912
403.301,"DRP90",""
309122,"AlHEGTA-0",0,21.2,0,0,0,0,0,0,3
1,30,1,330,1,912
404.308,"DRP90",""
309123,"AlOHEGTA-2",0,11.3,0,0,-2,0,0,0,3
1,30,1,912,-1,330
420.308,"DRP90",""
309124,"AlOH2EGTA-3",0,2.1,0,0,-3,0,0,0,3
1,30,1,912,-2,330
437.386,"DRP90",""
3309691,"EDTAH-3",0,11.03,0,0,-3,0,0,0,2
1,330,1,969
289.22,"",""
3309692,"EDTAH2-2",0,17.78,0,0,-2,0,0,0,2
2,330,1,969
290.23,"",""
3309693,"EDTAH3-1",0,20.89,0,0,-1,0,0,0,2
3,330,1,969
291.24,"",""
3309694,"EDTAH4-0",0,23.1,0,0,0,0,0,0,2
4,330,1,969
292.25,"",""
1509691,"CaEDTA-2",0,12.32,0,0,-2,0,0,0,2
1,150,1,969
328.29,"",""
1509692,"CaHEDTA-1",0,15.93,0,0,-1,0,0,0,3
1,150,1,330,1,969
329.3,"",""
4609691,"MgEDTA-2",0,10.54,0,0,-2,0,0,0,2
1,460,1,969
312.52,"",""
4609692,"MgHEDTA-1",0,14.71,0,0,-1,0,0,0,3
1,460,1,330,1,969
313.53,"",""
2819691,"FeEDTA-1",0,27.57,0,0,-1,0,0,0,2
1,281,1,969
344.06,"",""
2819692,"FeHEDTA-0",0,29.08,0,0,0,0,0,0,3
1,281,1,330,1,969
345.07,"",""
2819693,"Fe(OH)EDTA-2",0,19.29,0,0,-2,0,0,0,3
1,281,-1,330,1,969
361.07,"",""
2819694,"Fe(OH2EDTA-3",0,9.6,0,0,-3,0,0,0,3
1,281,-2,330,1,969
378.08,"",""
2809691,"FeIIEDTA-2",0,15.98,0,0,-2,0,0,0,2
1,280,1,969
344.06,"",""
2809692,"FeHEDTA-1",0,19.11,0,0,-1,0,0,0,3
1,280,1,33,1,969
345.07,"",""
2809693,"FeIIOHEDTA-3",0,6.27,0,0,-3,0,0,0,3
1,280,-1,330,1,969
361.07,"",""
4709691,"MnEDTA-2",0,15.52,0,0,-2,0,0,0,2
1,470,1,969
343.15,"",""
4709692,"MnHEDTA-1",0,19.1,0,0,-1,0,0,0,3
1,470,1,330,1,969
344.16,"",""
1829691,"CoEDTA-2",0,17.97,0,0,-2,0,0,0,2
1,182,1,969
347.15,"",""
1829692,"CoHEDTA-1",0,21.4,0,0,-1,0,0,0,3
```

```
1,182,1,330,1,969
348.15,"",""
1829693,"CoH2EDTA-0",0,24.1,0,0,0,0,0,0,3
1,182,1,969,2,330
349.162,"SM 89",""
1839691,"CoIIIEDTA-1",0,39.8,0,0,-1,0,0,0,2
1,183,1,969
347.146,"SPO 80",""
1839692,"CoIIIHEDTA-0",0,41.2,0,0,0,0,0,0,3
1,183,1,969,1,330
348.154,"SPO 80",""
3629691,"HgEDTA-2",0,23.21,0,0,-2,0,0,0,2
1,362,1,969
488.8,"",""
3629692,"HgHEDTA-1",0,26.74,0,0,-1,0,0,0,3
1,362,1,330,1,969
489.81,"",""
3629693,"HgOHEDTA-3",0,13.5,0,0,-3,0,0,0,3
1,362,1,696,-1,330
505.81,"MS 82",""
309691,"AlEDTA-1",0,19.07,0,0,-1,0,0,0,2
1,30,1,969
315.2,"",""
309692,"AlHEDTA-0",0,21.78,0,0,0,0,0,0,3
1,30,1,330,1,969
316.2,"",""
309693,"Al(OH)EDTA-2",0,12.82,0,0,-2,0,0,0,3
1,30,-1,330,1,969
332.2,"",""
309694,"Al(OH2EDTA-3",0,1.7,0,0,-3,0,0,0,3
1,30,1,969,-2,330
349.209,"MS74",""
3309111,"HHEDTA-2",0,10.5,0,0,-2,0,0,0,2
1,330,1,911
276.246,"DRP90",""
3309112,"H2HEDTA-1",0,16.3,0,0,-1,0,0,0,2
2,330,1,911
277.254,"DRP90",""
3309113,"H3HEDTA-0",0,19.2,0,0,0,0,0,0,2
3,330,1,911
278.262,"DRP90",""
1509111,"CaHEDTA-1",0,9.5,0,0,-1,0,0,0,2
1,150,1,911
315.318,"DRP90",""
4609111,"MgHEDTA-1",0,8.3,0,0,-1,0,0,0,2
1,460,1,911
299.543,"DRP90",""
8009111,"SrHEDTA-1",0,8.1,0,0,-1,0,0,0,2
1,800,1,911
362.858,"DRP90",""
2819111,"FeHEDTA-0",0,21.8,0,0,0,0,0,0,2
1,281,1,911
331.085,"DRP90",""
2819112,"FeOHHEDTA-1",0,17.6,0,0,-1,0,0,0,3
1,281,1,911,-1,330
348.163,"DRP90",""
2819113,"FeOH2HEDTA-2",0,8.4,0,0,-2,0,0,0,3
1,281,1,911,-2,330
365.241,"DRP90",""
2819114,"Fe2OH2HEDT-2",0,32.9,0,0,-2,0,0,0,3
2,281,2,911,-2,330
696.326,"DRP90",""
2819115,"FeOH3HEDTA-3",0,-2.2,0,0,-3,0,0,0,3
1,281,1,911,-3,330
382.319,"DRP90",""
2809111,"FeIIHEDTA-1",0,13.5,0,0,-1,0,0,0,2
1,280,1,911
```

```
331.085,"DRP90",""
2809112,"FeIIHHEDTA-0",0,16.5,0,0,0,0,0,0,3
1,280,1,330,1,911
332.093,"DRP90",""
2809113,"FeIIOHHEDT-2",0,4.3,0,0,-2,0,0,0,3
1,280,1,911,-1,330
348.092,"DRP90",""
2809114,"FeIIOH2HED-3",0,-6.1,0,0,-3,0,0,0,3
1,280,1,911,-2,330
365.17,"DRP90",""
4709111,"MnHEDTA-1",0,12.7,0,0,-1,0,0,0,2
1,470,1,911
330.176,"DRP90",""
2319111,"CuHEDTA-1",0,18.7,0,0,-1,0,0,0,2
1,231,1,911
338.784,"DRP90",""
2319112,"CuHHEDTA-0",0,21.4,0,0,0,0,0,0,3
1,231,1,330,1,911
339.792,"DRP90",""
1009111,"BaHEDTA-1",0,7.5,0,0,-1,0,0,0,2
1,100,1,991
412.568,"DRP90",""
1609111,"CdHEDTA-1",0,15.48,0,0,-1,0,0,0,2
1,160,1,911
387.648,"SM89 8/1",""
1609112,"CdHHEDTA-0",0,16.88,0,0,0,0,0,0,3
1,160,1,330,1,911
388.656,"WAN 90, ",""
9509111,"ZnHEDTA-1",0,15.9,0,0,-1,0,0,0,2
1,950,1,911
340.618,"DRP90",""
5409111,"NiHEDTA-1",0,18.4,0,0,-1,0,0,0,2
1,540,1,991
333.938,"DRP90",""
5409112,"NiHHEDTA-0",0,21.7,0,0,0,0,0,0,3
1,540,1,330,1,911
334.946,"DRP90",""
3629111,"HgHEDTA-1",0,21.4,0,0,-1,0,0,0,2
1,362,1,911
475.828,"DRP90",""
3629112,"HgOHHEDTA-2",0,12.6,0,0,-2,0,0,0,3
1,362,1,911,-1,330
492.906,"DRP90",""
6009111,"PbHEDTA-1",0,16.88,0,0,-1,0,0,0,2
1,600,1,911
482.438,"SM89 8/1",""
6009112,"PbHHEDTA-0",0,19.08,0,0,0,0,0,0,3
1,600,1,330,1,911
483.446,"WAN90 8/",""
1829111,"CoHEDTA-1",0,15.8,0,0,-1,0,0,0,2
1,182,1,911
334.171,"DRP90",""
1829112,"CoHHEDTA-0",0,18.3,0,0,0,0,0,0,3
1,182,1,330,1,911
335.179,"DRP90",""
309111,"AlHEDTA-0",0,16.4,0,0,0,0,0,0,2
1,30,1,911
302.22,"DRP90",""
309112,"AlHHEDTA+1",0,18.5,0,0,1,0,0,0,3
1,30,1,330,1,911
303.227,"DRP90",""
309113,"AlOHHEDTA-1",0,11.2,0,0,-1,0,0,0,3
1,30,1,911,-1,330
319.227,"DRP90",""
309114,"AlOH2HEDTA-2",0,1.5,0,0,-2,0,0,0,3
1,30,1,911,-2,330
336.305,"DRP90",""
```

```
3309531,"DTPAH-4",0,11.52,0,0,-4,0,0,0,2
1,330,1,953
388.21,"",""
3309532,"DTPAH2-3",0,20.91,0,0,-3,0,0,0,2
2,330,1,953
389.22,"",""
3309533,"DTPAH3-2",0,25.83,0,0,-2,0,0,0,2
3,330,1,953
390.22,"",""
3309534,"DTPAH4-1",0,28.91,0,0,-1,0,0,0,2
4,330,1,953
391.23,"",""
3309535,"DTPAH5-0",0,31.22,0,0,0,0,0,0,2
5,330,1,953
392.24,"",""
1509531,"CaDTPA-3",0,12.89,0,0,-3,0,0,0,2
1,150,1,953
427.28,"",""
1509532,"CaHDTPA-2",0,19.64,0,0,-2,0,0,0,3
1,150,1,330,1,953
428.29,"",""
1509533,"Ca2DTPA-1",0,15.83,0,0,-1,0,0,0,2
2,150,1,953
467.36,"",""
4609531,"MgDTPA-3",0,11.48,0,0,-3,0,0,0,2
1,460,1,953
411.51,"",""
4609532,"MgHDTPA-2",0,18.97,0,0,-2,0,0,0,3
1,460,1,330,1,953
412.51,"",""
2819531,"FeDTPA-2",0,30.51,0,0,-2,0,0,0,2
1,281,1,953
444.157,"WLL79",""
2819532,"FeHDTPA-1",0,34.5,0,0,-1,0,0,0,3
1,281,1,330,1,953
445.165,"WLL79",""
2819533,"Fe(OH)DTPA-3",0,19.43,0,0,-3,0,0,0,3
1,281,-1,330,1,953
461.164,"WLL79",""
2809531,"FeIIDTPA-3",0,18.54,0,0,-3,0,0,0,2
1,280,1,953
443.05,"",""
2809532,"FeIIHDTPA-2",0,24.48,0,0,-2,0,0,0,3
1,280,1,330,1,953
444.06,"",""
2809533,"FeIIOHDTPA-4",0,8.88,0,0,-4,0,0,0,3
1,280,-1,330,1,953
460.05,"",""
2809534,"FeII2DTPA-1",0,22.8,0,0,-1,0,0,0,2
2,280,1,953
498.89,"",""
2809535,"FeOH)2DTPA-5",0,-1.62,0,0,-5,0,0,0,3
1,280,-2,330,1,953
477.06,"",""
9509531,"ZnDTPA-3",0,20.43,0,0,-3,0,0,0,2
1,950,1,953
452.58,"",""
9509532,"ZnHDTPA-2",0,26.67,0,0,-2,0,0,0,3
1,950,1,330,1,953
453.59,"",""
9509533,"ZnH2DTPA-1",0,30.15,0,0,-1,0,0,0,3
1,950,2,330,1,953
454.74,"",""
9509534,"Zn2DTPA-1",0,26.09,0,0,-1,0,0,0,2
2,950,1,953
517.96,"",""
1009531,"BaDTPA-3",0,10.9,0,0,-3,0,0,0,2
```

```
1,100,1,953
525.64,"DRP 90",""
1009532,"BaHDTPA-2",0,16.9,0,0,-2,0,0,0,3
1,100,1,330,1,953
526.448,"DRP 90",""
2319531,"CuDTPA-3",0,23.52,0,0,-3,0,0,0,2
1,231,1,953
450.75,"",""
2319532,"CuHDTPA-2",0,28.97,0,0,-2,0,0,0,3
1,231,1,330,1,953
451.76,"",""
2319533,"CuH2DTPA-1",0,32.17,0,0,-1,0,0,0,3
1,231,2,330,1,953
454.6,"",""
2319534,"CuH3DTPA-0",0,35.15,0,0,0,0,0,0,3
1,231,3,330,1,953
453.77,"",""
2319535,"Cu2DTPA-1",0,31.59,0,0,-1,0,0,0,2
2,231,1,953
514.29,"",""
4709531,"MnDTPA-3",0,17.65,0,0,-3,0,0,0,2
1,470,1,953
442.14,"",""
4709532,"MnHDTPA-2",0,22.69,0,0,-2,0,0,0,3
1,470,1,330,1,953
443.15,"",""
4709533,"Mn2DTPA-1",0,21.02,0,0,-1,0,0,0,2
2,470,1,953
497.08,"",""
1609531,"CdDTPA-3",0,21.14,0,0,-3,0,0,0,2
1,160,1,953
499.61,"",""
1609532,"CdHDTPA-2",0,25.95,0,0,-2,0,0,0,3
1,160,1,330,1,953
500.62,"",""
1609533,"CdH2DTPA-1",0,29.74,0,0,-1,0,0,0,3
1,160,2,330,1,953
501.63,"",""
1609534,"Cd2DTPA-1",0,24.72,0,0,-1,0,0,0,2
2,160,1,953
612.02,"",""
6009531,"PbDTPA-3",0,20.8,0,0,-3,0,0,0,2
1,600,1,953
594.4,"",""
6009532,"PbHDTPA-2",0,25.96,0,0,-2,0,0,0,3
1,600,1,330,1,953
595.41,"",""
6009533,"Pb2DTPA-1",0,25.49,0,0,-1,0,0,0,2
2,600,1,953
801.6,"",""
5409531,"NiDTPA-3",0,22.31,0,0,-3,0,0,0,2
1,540,1,953
445.9,"",""
5409532,"NiHDTPA-2",0,28.62,0,0,-2,0,0,0,3
1,540,1,330,1,953
446.91,"",""
5409533,"NiH2DTPA-1",0,32.05,0,0,-1,0,0,0,3
1,540,2,330,1,953
447.92,"",""
5409534,"Ni2DTPA-1",0,29.18,0,0,-1,0,0,0,2
2,540,1,953
504.6,"",""
1829531,"CoDTPA-3",0,21.29,0,0,-3,0,0,0,2
1,182,1,953
446.13,"",""
1829532,"CoHDTPA-2",0,26.87,0,0,-2,0,0,0,3
1,182,1,330,1,953
```

```
447.14,"",""
1829533,"CoH2DTPA-1",0,30.45,0,0,-1,0,0,0,3
1,182,2,330,1,953
448.15,"",""
1829534,"Co2DTPA-1",0,26.31,0,0,-1,0,0,0,2
2,182,1,953
505.07,"",""
3629531,"HgDTPA-3",0,28.54,0,0,-3,0,0,0,2
1,362,1,953
587.79,"",""
3629532,"HgHDTPA-2",0,33.42,0,0,-2,0,0,0,3
1,362,1,330,1,953
588.8,"",""
309531,"AlDTPA-2",0,21.91,0,0,-2,0,0,0,2
1,30,1,953
414.18,"",""
309532,"AlHDTPA-1",0,26.64,0,0,-1,0,0,0,3
1,30,1,330,1,953
415.19,"",""
309533,"AlOHDTPA-3",0,13.87,0,0,-3,0,0,0,3
1,30,-1,330,1,953
431.19,"",""
3309101,"HCDTA-3",0,13.2,0,0,-3,0,0,0,2
1,330,1,910
289.221,"DRP 90",""
3309102,"H2CDTA-2",0,19.9,0,0,-2,0,0,0,2
2,330,1,910
290.229,"DRP 90",""
3309103,"H3CDTA-1",0,23.9,0,0,-1,0,0,0,2
3,330,1,910
291.237,"DRP 90",""
3309104,"H4CDTA-0",0,26.6,0,0,0,0,0,0,2
4,330,1,910
292.245,"DRP 90",""
1509101,"CaCDTA-2",0,12.4,0,0,-2,0,0,0,2
1,150,1,910
328.293,"DRP 90",""
1509102,"CaHCDTA-1",0,15.9,0,0,-1,0,0,0,3
1,150,1,330,1,910
329.301,"DRP 90",""
4609101,"MgCDTA-2",0,12.8,0,0,-2,0,0,0,2
1,460,1,910
312.518,"DRP 90",""
2819101,"FeCDTA-1",0,32.6,0,0,-1,0,0,0,2
1,281,1,910
344.06,"DRP 90",""
2819102,"FeOHCDTA-2",0,22.5,0,0,-2,0,0,0,3
1,281,1,910,-1,30
361.138,"DRP 90",""
2809101,"FeIICDTA-2",0,20.6,0,0,-2,0,0,0,2
1,280,1,910
344.06,"DRP 90",""
2809102,"FeIIHCDTA-1",0,23.8,0,0,-1,0,0,0,3
1,280,1,330,1,910
345.068,"DRP 90",""
4709101,"MnCDTA-2",0,19.2,0,0,-2,0,0,0,2
1,470,1,910
343.151,"DRP 90",""
4709102,"MnHCDTA-1",0,22.4,0,0,-1,0,0,0,3
1,470,1,330,1,910
344.159,"DRP 90",""
2319101,"CuCDTA-2",0,23.6,0,0,-2,0,0,0,2
1,231,1,910
351.759,"DRP 90",""
2319102,"CuHCDTA-1",0,27.2,0,0,-1,0,0,0,3
1,231,1,330,1,910
352.767,"DRP 90",""
```

```
1009101,"BaCDTA-2",0,10.3,0,0,-2,0,0,0,2
1,100,1,910
425.543,"DRP 90",""
1009102,"BaHCDTA-1",0,17.6,0,0,-1,0,0,0,3
1,100,1,330,1,910
426.551,"DRP 90",""
1609101,"CdCDTA-2",0,21.6,0,0,-2,0,0,0,2
1,160,1,910
400.623,"DRP 90",""
1609102,"CdHCDTA-1",0,25,0,0,-1,0,0,0,3
1,160,1,330,1,910
401.631,"DRP 90",""
9509101,"ZnCDTA-2",0,21.07,0,0,-2,0,0,0,2
1,950,1,910
353.593,"DRP 90",""
9509102,"ZnHCDTA-1",0,24.4,0,0,-1,0,0,0,3
1,950,1,330,1,910
354.601,"DRP 90",""
5409101,"NiCDTA-2",0,21.9,0,0,-2,0,0,0,2
1,540,1,910
346.913,"DRP 90",""
5409102,"NiHCDTA-1",0,25.3,0,0,-1,0,0,0,3
1,540,1,330,1,910
347.921,"DRP 90",""
3629101,"HgCDTA-2",0,26.5,0,0,-2,0,0,0,2
1,362,1,910
488.803,"",""
3629102,"HgHCDTA-1",0,30,0,0,-1,0,0,0,3
1,362,1,330,1,910
489.811,"DRP 90",""
3629103,"HgOHCDTA-3",0,15.4,0,0,-3,0,0,0,3
1,362,1,910,-1,330
505.81,"DRP 90",""
6009101,"PbCDTA-2",0,22,0,0,-2,0,0,0,2
1,600,1,910
495.413,"DRP 90",""
6009102,"PbHCDTA-1",0,25.2,0,0,-1,0,0,0,3
1,600,1,330,1,910
496.421,"DRP 90",""
1829101,"CoCDTA-2",0,21.3,0,0,-2,0,0,0,2
1,182,1,910
347.146,"DRP 90",""
1829102,"CoHCDTA-1",0,24.6,0,0,-1,0,0,0,3
1,182,1,330,1,910
348.154,"DRP 90",""
309101,"AlCDTA-1",0,22.2,0,0,-1,0,0,0,2
1,30,1,910
315.195,"DRP 90",""
309102,"AlHCDTA-0",0,24.8,0,0,0,0,0,0,3
1,30,1,330,1,910
316.202,"DRP 90",""
309103,"AlOHCDTA+1",0,13.9,0,0,1,0,0,0,3
1,30,1,910,-1,330
332.202,"DRP 90",""
3309371,"DCHAH-2",0,11.8,0,0,-2,0,0,0,2
1,330,1,937
314.34,"SLR07",""
3309372,"DCHAH2-1",0,21.56,0,0,-1,0,0,0,2
2,330,1,937
315.34,"SLR07",""
3309373,"DCHAH3-0",0,29.66,0,0,0,0,0,0,2
3,330,1,937
316.35,"SLR07",""
3309374,"DCHAH4-1",0,35.64,0,0,1,0,0,0,2
4,330,1,937
317.36,"SLR07",""
1509371,"CaDCHA-1",0,6.16,0,0,-1,0,0,0,2
```

```
1,150,1,937
353.41,"SLR07",""
1509372,"CaHDCHA-0",0,16.01,0,0,0,0,0,0,3
1,150,1,330,1,937
354.41,"SLR07",""
1509373,"CaH2DCHA-1",0,25.37,0,0,1,0,0,0,3
1,150,2,330,1,937
355.42,"SLR07",""
4609371,"MgDCHA-1",0,6.29,0,0,-1,0,0,0,2
1,460,1,937
337.63,"SLR07",""
4609371,"MgOHDCHA-2",0,-3.45,0,0,-2,0,0,0,3
1,460,-1,330,1,937
354.64,"SLR07",""
2819371,"FeDCHA-0",0,29.86,0,0,0,0,0,0,2
1,281,1,937
369.17,"SLR07",""
2819372,"FeHDCHA-1",0,32.09,0,0,1,0,0,0,3
1,281,1,330,1,937
370.18,"SLR07",""
2819373,"FeOHDCHA-1",0,21.89,0,0,-1,0,0,0,3
1,281,-1,330,1,937
386.18,"SLR07",""
2319371,"CuDCHA-1",0,23.66,0,0,-1,0,0,0,2
1,231,1,937
376.41,"SLR07",""
2319372,"CuHDCHA-0",0,29.02,0,0,0,0,0,0,3
1,231,1,330,1,937
377.88,"SLR07",""
2319373,"CuH2DCHA-1",0,33.38,0,0,1,0,0,0,3
1,231,2,330,1,937
378.89,"SLR07",""
3309381,"HJB-3",0,13.21,0,0,-3,0,0,0,2
1,330,1,938
413.47,"SLR07",""
3309382,"HJBH2-2",0,23.71,0,0,-2,0,0,0,2
2,330,1,938
414.47,"SLR07",""
3309383,"HJBH3-1",0,32.08,0,0,-1,0,0,0,2
3,330,1,938
415.47,"SLR07",""
3309384,"HJBH4-0",0,36.9,0,0,0,0,0,0,2
4,330,1,938
414.47,"SLR07",""
1509381,"CaHJB-2",0,9.34,0,0,-2,0,0,0,2
1,150,1,938
452.51,"SLR07",""
1509382,"CaHHJB-1",0,17.9,0,0,-1,0,0,0,3
1,150,1,330,1,938
453.52,"SLR07",""
1509383,"CaH2HJB-0",0,25.05,0,0,0,0,0,0,3
1,150,2,330,1,938
454.53,"SLR07",""
4609381,"MgHJB-2",0,10.43,0,0,-2,0,0,0,2
1,460,1,938
436.74,"SLR07",""
4609382,"MgHHJB-1",0,19.59,0,0,-1,0,0,0,3
1,460,1,330,1,938
437.75,"SLR07",""
4609383,"MgH2HJB-0",0,27.47,0,0,0,0,0,0,3
1,460,2,330,1,938
438.76,"SLR07",""
2819381,"FeHJB-1",0,36.43,0,0,-1,0,0,0,2
1,281,1,938
468.28,"SLR07",""
2819382,"FeHHJB-0",0,37.46,0,0,0,0,0,0,3
1,281,1,330,1,938
```

```
469.29,"SLR07",""
2319381,"CuHJB-2",0,23.22,0,0,-2,0,0,0,2
1,231,1,938
475.98,"SLR07",""
2319382,"CuHHJB-1",0,32.46,0,0,-1,0,0,0,3
1,231,1,330,1,938
476.99,"SLR07",""
2319383,"CuH2HJB-0",0,37.93,0,0,0,0,0,0,3
1,231,2,330,1,938
492.99,"SLR07",""
3309351,"HBEDH-3",0,13.32,0,0,-3,0,0,0,2
1,330,1,935
385.4,"FYM02",""
3309352,"HBEDH2-2",0,24.96,0,0,-2,0,0,0,2
2,330,1,935
386.4,"FYM02",""
3309353,"HBEDH3-1",0,33.71,0,0,-1,0,0,0,2
3,330,1,935
387.4,"FYM02",""
3309354,"HBEDH4-0",0,38.56,0,0,0,0,0,0,2
4,330,1,935
388.4,"FYM02",""
1509351,"CaHBED-2",0,11,0,0,-2,0,0,0,2
1,150,1,935
424.4,"FYM02",""
1509352,"CaHHBED-1",0,20.12,0,0,-1,0,0,0,3
1,150,1,330,1,935
425.4,"FYM02",""
1509353,"CaH2HBED-0",0,27.83,0,0,0,0,0,0,3
1,150,2,330,1,935
426.4,"FYM02",""
4609351,"MgHBED-2",0,12.22,0,0,-2,0,0,0,2
1,460,1,935
408.7,"FYM02",""
4609352,"MgHHBED-1",0,20.8,0,0,-1,0,0,0,3
1,460,1,330,1,935
409.7,"FYM02",""
4609353,"MgH2HBED-0",0,28.02,0,0,0,0,0,0,3
1,460,2,330,1,935
410.7,"FYM02",""
2819351,"FeHBED-1",0,42.25,0,0,-1,0,0,0,2
1,281,1,935
440.25,"FYM02",""
2319351,"CuHBED-2",0,23.09,0,0,-2,0,0,0,2
1,231,1,935
447.95,"FYM02",""
2319352,"CuHHBED-1",0,32.15,0,0,-1,0,0,0,3
1,231,1,330,1,935
448.95,"FYM02",""
2319353,"CuH2HBED-0",0,37.54,0,0,0,0,0,0,3
1,231,2,330,1,935
449.95,"FYM02",""
3309361,"IDHAH-3",0,11.38,0,0,-3,0,0,0,2
1,330,1,936
246.1,"SLR11",""
3309362,"IDHAH2-2",0,16.57,0,0,-2,0,0,0,2
2,330,1,936
247.1,"SLR11",""
3309363,"IDHAH3-1",0,20.53,0,0,-1,0,0,0,2
3,330,1,936
248.1,"SLR11",""
3309364,"IDHAH40",0,23.17,0,0,0,0,0,0,2
4,330,1,936
249.1,"SLR11",""
3309365,"IDHAH5+1",0,24.69,0,0,1,0,0,0,2
5,330,1,936
250.1,"SLR11",""
```

```
2819361,"FeIDHA-1",0,16.43,0,0,-1,0,0,0,2
1,281,1,936
300.947,"SLR11",""
2819362,"FeHIDHA",0,20.53,0,0,0,0,0,0,3
1,281,1,330,1,936
301.947,"SLR11",""
2819363,"FeOHIDHA-2",0,10.7,0,0,-2,0,0,0,3
1,281,-1,330,1,936
299.947,"SLR11",""
2319361,"CuIDHA-2",0,14.59,0,0,-2,0,0,0,2
1,231,1,936
308.646,"SLR11",""
2319362,"CuHIDHA-1",0,19.41,0,0,-1,0,0,0,3
1,231,1,330,1,936
309.646,"SLR11",""
2319363,"CuH2IDHA",0,22.75,0,0,0,0,0,0,3
1,231,2,330,1,936
310.646,"SLR11",""
2319364,"CuOHIDHA-3",0,3.55,0,0,-3,0,0,0,3
1,231,-1,330,1,936
307.646,"SLR11",""
4709361,"MnIDHA-2",0,8.97,0,0,-2,0,0,0,2
1,470,1,936
300.038,"SLR11",""
9509361,"ZnIDHA-2",0,11.86,0,0,-2,0,0,0,2
1,950,1,936
310.47,"SLR11",""
9509362,"ZnHIDHA-1",0,16.7,0,0,-1,0,0,0,3
1,950,1,330,1,936
311.47,"SLR11",""
9509363,"ZnOHIDHA-3",0,0.82,0,0,-3,0,0,0,3
1,950,-1,330,1,936
309.47,"SLR11",""
1509361,"CaIDHA-2",0,6.01,0,0,-2,0,0,0,2
1,150,1,936
285.18,"SLR11",""
4609361,"MgIDHA-2",0,7.16,0,0,-2,0,0,0,2
1,460,1,936
269.412,"SLR11",""
3309391,"EDDSH-3",0,10.87,0,0,-3,0,0,0,2
1,330,1,939
293.02,"SLR11",""
3309392,"EDDSH2-2",0,18.33,0,0,-2,0,0,0,2
2,330,1,939
294.02,"SLR11",""
3309393,"EDDSH3-1",0,22.5,0,0,-1,0,0,0,2
3,330,1,939
295.02,"SLR11",""
3309394,"EDDSH40",0,25.66,0,0,0,0,0,0,2
4,330,1,939
296.02,"SLR11",""
3309395,"EDDSH5+1",0,26.95,0,0,1,0,0,0,2
5,330,1,939
297.02,"SLR11",""
3309396,"EDDSH6+2",0,28.72,0,0,2,0,0,0,2
6,330,1,939
298.02,"SLR11",""
2819391,"FeEDDS-1",0,23.68,0,0,-1,0,0,0,2
1,281,1,939
347.86,"SLR11",""
2319391,"CuEDDS-2",0,20.46,0,0,-2,0,0,0,2
1,231,1,939
355.56,"SLR11",""
2319392,"CuHEDDS-1",0,24.39,0,0,-1,0,0,0,3
1,231,1,330,1,939
356.56,"SLR11",""
3309393,"CuH2EDDS",0,26.8,0,0,0,0,0,0,3
```

```
1,231,1,330,1,939
357.56,"SLR11",""
2319394,"CuOHEDDS-3",0,8.81,0,0,-3,0,0,0,3
1,231,-1,330,1,939
354.56,"SLR11",""
4709391,"MnEDDS-2",0,10.77,0,0,-2,0,0,0,2
1,470,1,939
346.96,"SLR11",""
9509391,"ZnEDDS-2",0,15.34,0,0,-2,0,0,0,2
1,950,1,939
357.42,"SLR11",""
9509392,"ZnHEDDS-1",0,19.34,0,0,-1,0,0,0,3
1,950,1,330,1,939
358.42,"SLR11",""
1509391,"CaEDDS-2",0,6.34,0,0,-2,0,0,0,2
1,150,1,939
332.32,"SLR11",""
4609391,"MgEDDS-2",0,7.77,0,0,-2,0,0,0,2
1,460,1,939
316.56,"SLR11",""
3309201,"EDDHAH-3",0,12.8,0,0,-3,0,0,0,2
1,330,1,920
357.4,"FYM02",""
3309202,"EDDHAH2-2",0,24.17,0,0,-2,0,0,0,2
2,330,1,920
358.4,"FYM02",""
3309203,"EDDHAH3-1",0,33.26,0,0,-1,0,0,0,2
3,330,1,920
359.4,"FYM02",""
3309204,"EDDHAH4-0",0,39.66,0,0,0,0,0,0,2
4,330,1,920
360.4,"FYM02",""
1509201,"CaEDDHA-2",0,9,0,0,-2,0,0,0,2
1,150,1,920
396.5,"FYM02",""
1509202,"CaHEDDHA-1",0,18.91,0,0,-1,0,0,0,3
1,150,1,330,1,920
397.5,"FYM02",""
1509203,"CaH2EDDHA-0",0,28.3,0,0,0,0,0,0,3
1,150,2,330,1,920
398.5,"FYM02",""
4609201,"MgEDDHA-2",0,11.47,0,0,-2,0,0,0,2
1,460,1,920
380.7,"FYM02",""
4609202,"MgHEDDHA-1",0,20.32,0,0,-1,0,0,0,3
1,460,1,330,1,920
381.7,"FYM02",""
4609203,"MgH2EDDHA-0",0,27.71,0,0,0,0,0,0,3
1,460,2,330,1,920
382.7,"FYM02",""
2819201,"FeEDDHA-1",0,37.66,0,0,-1,0,0,0,2
1,281,1,920
412.25,"FYM02",""
2819202,"FeHEDDHA-0",0,39.67,0,0,0,0,0,0,3
1,281,1,330,1,920
413.25,"FYM02",""
2819203,"FeOHEDDHA-2",0,25.8,0,0,-2,0,0,0,3
1,281,-1,330,1,920
429.25,"FYM02",""
2319201,"CuEDDHA-2",0,26.84,0,0,-2,0,0,0,2
1,231,1,920
419.9,"FYM02",""
2319202,"CuHEDDHA-1",0,34.75,0,0,-1,0,0,0,3
1,231,1,330,1,920
420.908,"FYM02",""
2319203,"CuH2EDDHA-0",0,39.66,0,0,0,0,0,0,3
1,231,2,330,1,920
```

```
421.9,"FYM02",""
4709201,"MnEDDHA-2",0,11.28,0,0,-2,0,0,0,2
1,470,1,920
415.07,"CCL08",""
4709202,"MnHEDDHA-1",0,22.03,0,0,-1,0,0,0,3
1,470,1,330,1,920
416.07,"CCL08",""
4709203,"MnH2EDDHA-0",0,29.46,0,0,0,0,0,0,3
1,470,2,330,1,920
417.07,"CCL08",""
9509201,"ZnEDDHA-2",0,20.46,0,0,-2,0,0,0,2
1,950,1,920
425.5,"CCL08",""
3309211,"rac-EDDHAH-3",0,12.74,0,0,-3,0,0,0,2
1,330,1,921
357.4,"FYM02",""
3309212,"rac-EDDHAH2-2",0,24.18,0,0,-2,0,0,0,2
2,330,1,921
358.4,"FYM02",""
3309213,"rac-EDDHAH3-1",0,33.29,0,0,-1,0,0,0,2
3,330,1,921
359.4,"FYM02",""
3309214,"rac-EDDHAH4-0",0,39.78,0,0,0,0,0,0,2
4,330,1,921
360.4,"FYM02",""
1509211,"Carac-EDDHA-2",0,9.7,0,0,-2,0,0,0,2
1,150,1,921
396.5,"FYM02",""
1509212,"CaHrac-EDDHA-1",0,19.56,0,0,-1,0,0,0,3
1,150,1,330,1,921
397.5,"FYM02",""
1509213,"CaH2rac-EDDHA-0",0,29.23,0,0,0,0,0,0,3
1,150,2,330,1,921
398.5,"FYM02",""
4609211,"Mgrac-EDDHA-2",0,11.84,0,0,-2,0,0,0,2
1,460,1,921
380.7,"FYM02",""
2819211,"Ferac-EDDHA-1",0,38.43,0,0,-1,0,0,0,2
1,281,1,921
412.25,"FYM02",""
2819212,"FeOHrac-EDDHA-2",0,25.26,0,0,-2,0,0,0,3
1,281,-1,330,1,921
429.25,"FYM02",""
2319211,"Curac-EDDHA-2",0,26.65,0,0,-2,0,0,0,2
1,231,1,921
419.95,"FYM02",""
2319212,"CuHrac-EDDHA-1",0,35.01,0,0,-1,0,0,0,3
1,231,1,330,1,921
420.95,"FYM02",""
2319213,"CuH2rac-EDDHA-0",0,39.69,0,0,0,0,0,0,3
1,231,2,330,1,921
421.95,"FYM02",""
3309221,"mes-EDDHAH-3",0,12.76,0,0,-3,0,0,0,2
1,330,1,922
357.4,"FYM02",""
3309222,"mes-EDDHAH2-2",0,24.29,0,0,-2,0,0,0,2
2,330,1,922
358.4,"FYM02",""
3309223,"mes-EDDHAH3-1",0,33.3,0,0,-1,0,0,0,2
3,330,1,922
359.4,"FYM02",""
3309224,"mes-EDDHAH4-0",0,39.68,0,0,0,0,0,0,2
4,330,1,922
360.4,"FYM02",""
1509221,"Cames-EDDHA-2",0,9.27,0,0,-2,0,0,0,2
1,150,1,922
396.5,"FYM02",""
```

```
1509222,"CaHmes-EDDHA-1",0,19.24,0,0,-1,0,0,0,3
1,150,1,330,1,922
397.5,"FYM02",""
1509223,"CaH2mes-EDDHA-0",0,28.76,0,0,0,0,0,0,3
1,150,2,330,1,922
398.5,"FYM02",""
4609221,"Mgmes-EDDHA-2",0,11.16,0,0,-2,0,0,0,2
1,460,1,922
380.7,"FYM02",""
4609222,"MgHmes-EDDHA-1",0,19.65,0,0,-1,0,0,0,3
1,460,1,330,1,922
381.7,"FYM02",""
4609223,"MgH2mes-EDDHA-0",0,28.91,0,0,0,0,0,0,3
1,460,2,330,1,922
382.7,"FYM02",""
2819221,"Femes-EDDHA-1",0,36.71,0,0,-1,0,0,0,2
1,281,1,922
412.25,"FYM02",""
2819222,"FeHmes-EDDHA-0",0,39.35,0,0,0,0,0,0,3
1,281,1,330,1,922
413.25,"FYM02",""
2819223,"FeOHmes-EDDHA-2",0,24.95,0,0,-2,0,0,0,3
1,281,-1,330,1,922
429.25,"FYM02",""
2319221,"Cumes-EDDHA-2",0,25.39,0,0,-2,0,0,0,2
1,231,1,922
419.95,"FYM02",""
2319222,"CuHmes-EDDHA-1",0,34.44,0,0,-1,0,0,0,3
1,231,1,330,1,922
420.95,"FYM02",""
2319223,"CuH2mes-EDDHA-0",0,39.6,0,0,0,0,0,0,3
1,231,2,330,1,922
421.95,"FYM02",""
3309231,"p,pEDDHAH-3",0,10.85,0,0,-3,0,0,0,2
1,330,1,923
357.4,"FYM02",""
3309232,"p,pEDDHAH2-2",0,20.6,0,0,-2,0,0,0,2
2,330,1,923
358.4,"FYM02",""
3309233,"p,pEDDHAH3-1",0,27.88,0,0,-1,0,0,0,2
3,330,1,923
359.4,"FYM02",""
3309234,"p,pEDDHAH4-0",0,32.46,0,0,0,0,0,0,2
4,330,1,923
360.4,"FYM02",""
1509231,"Cap,pEDDHA-2",0,5.25,0,0,-2,0,0,0,2
1,150,1,923
396.5,"FYM02",""
1509232,"CaHp,pEDDHA-1",0,15.07,0,0,-1,0,0,0,3
1,150,1,330,1,923
397.5,"FYM02",""
1509233,"CaH2p,pEDDHA-0",0,23.56,0,0,0,0,0,0,3
1,150,2,330,1,923
398.5,"FYM02",""
4609231,"Mgp,pEDDHA-2",0,5.45,0,0,-2,0,0,0,2
1,460,1,923
380.7,"FYM02",""
4609232,"MgHp,pEDDHA-1",0,15.03,0,0,-1,0,0,0,3
1,460,1,330,1,923
381.7,"FYM02",""
4609233,"MgH2p,pEDDHA-0",0,23.14,0,0,0,0,0,0,3
1,460,2,330,1,923
382.7,"FYM02",""
2319231,"Cup,pEDDHA-2",0,16.46,0,0,-2,0,0,0,2
1,231,1,923
419.95,"FYM02",""
2319232,"CuHp,pEDDHA-1",0,24.53,0,0,-1,0,0,0,3
```

```
1,231,1,330,1,923
420.95,"FYM02",""
2319233,"CuH2p,pEDDHA-0",0,30.85,0,0,0,0,0,0,3
1,231,2,330,1,923
421.95,"FYM02",""
2319234,"CuH3p,pEDDHA+1",0,33.45,0,0,1,0,0,0,3
1,231,3,330,1,923
422.95,"FYM02",""
3309311,"o,pEDDHAH-3",0,12.04,0,0,-3,0,0,0,2
1,330,1,931
357.4,"FYM02",""
3309312,"o,pEDDHAH2-2",0,22.86,0,0,-2,0,0,0,2
2,330,1,931
358.4,"FYM02",""
3309313,"o,pEDDHAH3-1",0,31.94,0,0,-1,0,0,0,2
3,330,1,931
359.4,"FYM02",""
3309314,"o,pEDDHAH4-0",0,38.35,0,0,0,0,0,0,2
4,330,1,931
360.4,"FYM02",""
3309315,"o,pEDDHAH5+1",0,40.92,0,0,1,0,0,0,2
5,330,1,931
361.4,"FYM02",""
3309316,"o,pEDDHAH6+2",0,42.2,0,0,2,0,0,0,2
6,330,1,931
362.4,"FYM02",""
1509311,"Cao,pEDDHA-2",0,5.83,0,0,-2,0,0,0,2
1,150,1,931
396.4,"FYM02",""
1509312,"CaHo,pEDDHA-1",0,16.41,0,0,-1,0,0,0,3
1,150,1,330,1,931
397.4,"FYM02",""
1509313,"CaH2o,pEDDHA",0,25.59,0,0,0,0,0,0,3
1,150,2,330,1,931
398.4,"FYM02",""
4609311,"Mgo,pEDDHA-2",0,7.36,0,0,-2,0,0,0,2
1,460,1,931
380.7,"FYM02",""
4609312,"MgHo,pEDDHA-1",0,17.69,0,0,-1,0,0,0,3
1,460,1,330,1,931
381.7,"FYM02",""
4609313,"MgH2o,pEDDHA",0,26.18,0,0,0,0,0,0,3
1,460,2,330,1,931
382.7,"FYM02",""
4709311,"Mno,pEDDHA-2",0,9.81,0,0,-2,0,0,0,2
1,470,1,931
415.07,"CCL08",""
4709312,"MnHo,pEDDHA-1",0,20.5,0,0,-1,0,0,0,3
1,470,1,330,1,931
416.07,"CCL08",""
9509311,"Zno,pEDDHA-2",0,14.15,0,0,-2,0,0,0,2
1,950,1,931
425.5,"CCL08",""
9509312,"ZnHo,pEDDHA-1",0,24.81,0,0,-1,0,0,0,3
1,950,1,330,1,931
426.5,"CCL08",""
9509313,"ZnH2o,pEDDHA",0,32.46,0,0,0,0,0,0,3
1,950,2,330,1,931
427.5,"CCL08",""
2819311,"Feo,pEDDHA-1",0,31.29,0,0,-1,0,0,0,2
1,281,1,931
412.25,"FYM02",""
2819312,"FeHo,pEDDHA-0",0,37.81,0,0,0,0,0,0,3
1,281,1,330,1,931
413.25,"FYM02",""
2819313,"FeH2o,pEDDHA+1",0,40.13,0,0,1,0,0,0,3
1,281,2,330,1,931
```

```
414.25,"FYM02",""
2819314,"FeOHo,pEDDHA-2",0,21.59,0,0,-2,0,0,0,3
1,281,-1,330,1,931
429.25,"FYM02",""
2319311,"Cuo,pEDDHA-2",0,23.45,0,0,-2,0,0,0,2
1,231,1,931
419.9,"FYM02",""
2319312,"CuHo,pEDDHA-1",0,33.1,0,0,-1,0,0,0,3
1,231,1,330,1,931
420.9,"FYM02",""
2319313,"CuH2o,pEDDHA-0",0,38.52,0,0,0,0,0,0,3
1,231,2,330,1,931
421.9,"FYM02",""
2319314,"CuH3o,pEDDHA+1",0,40.5,0,0,1,0,0,0,3
1,231,3,330,1,931
422.9,"FYM02",""
3309241,"EDDH4MAH-3",0,12.49,0,0,-3,0,0,0,2
1,330,1,924
385.4,"FYM02",""
3309242,"EDDH4MAH2-2",0,23.61,0,0,-2,0,0,0,2
2,330,1,924
386.4,"FYM02",""
3309243,"EDDH4MAH3-1",0,32.78,0,0,-1,0,0,0,2
3,330,1,924
387.4,"FYM02",""
3309244,"EDDH4MAH4-0",0,39.39,0,0,0,0,0,0,2
4,330,1,924
388.4,"FYM02",""
1509241,"CaEDDH4MA-2",0,7.55,0,0,-2,0,0,0,2
1,150,1,924
424.5,"FYM02",""
1509242,"CaHEDDH4MA-1",0,18,0,0,-1,0,0,0,3
1,150,1,330,1,924
425.5,"FYM02",""
1509243,"CaH2EDDH4MA-0",0,26.93,0,0,0,0,0,0,3
1,150,2,330,1,924
426.5,"FYM02",""
4609241,"MgEDDH4MA-2",0,9.71,0,0,-2,0,0,0,2
1,460,1,924
408.7,"FYM02",""
4609242,"MgHEDDH4MA-1",0,19.2,0,0,-1,0,0,0,3
1,460,1,330,1,924
409.7,"FYM02",""
4609243,"MgH2EDDH4MA-0",0,27.17,0,0,0,0,0,0,3
1,460,2,330,1,924
410.7,"FYM02",""
2819241,"FeEDDH4MA-1",0,37.01,0,0,-1,0,0,0,2
1,281,1,924
440.25,"FYM02",""
2819242,"FeHEDDH4MA-0",0,39.38,0,0,0,0,0,0,3
1,281,1,330,1,924
441.25,"FYM02",""
2819243,"FeOHEDDH4MA-2",0,24.95,0,0,-2,0,0,0,3
1,281,-1,330,1,924
457.25,"FYM02",""
2319241,"CuEDDH4MA-2",0,25.65,0,0,-2,0,0,0,2
1,231,1,924
447.95,"FYM02",""
2319242,"CuHEDDH4MA-1",0,33.2,0,0,-1,0,0,0,3
1,231,1,330,1,924
448.95,"FYM02",""
2319243,"CuH2EDDH4MA-0",0,38.43,0,0,0,0,0,0,3
1,231,2,330,1,924
449.95,"FYM02",""
3309251,"racEDDH4MAH-3",0,12.69,0,0,-3,0,0,0,2
1,330,1,925
385.4,"FYM02",""
```

```
3309252,"racEDDH4MAH2-2",0,24.04,0,0,-2,0,0,0,2
2,330,1,925
386.4,"FYM02",""
3309253,"racEDDH4MAH3-1",0,33.05,0,0,-1,0,0,0,2
3,330,1,925
387.4,"FYM02",""
3309254,"racEDDH4MAH4-0",0,39.44,0,0,0,0,0,0,2
4,330,1,925
388.4,"FYM02",""
1509251,"CaracEDDH4MA-2",0,8.89,0,0,-2,0,0,0,2
1,150,1,925
424.5,"FYM02",""
1509252,"CaHracEDDH4MA-1",0,18.8,0,0,-1,0,0,0,3
1,150,1,330,1,925
425.5,"FYM02",""
1509253,"CaH2racEDDH4MA-0",0,28.66,0,0,0,0,0,0,3
1,150,2,330,1,925
426.5,"FYM02",""
4609251,"MgracEDDH4MA-2",0,9.53,0,0,-2,0,0,0,2
1,460,1,925
408.7,"FYM02",""
4609252,"MgHracEDDH4MA-1",0,19.15,0,0,-1,0,0,0,3
1,460,1,330,1,925
409.7,"FYM02",""
4609253,"MgH2racEDDH4MA-0",0,27.78,0,0,0,0,0,0,3
1,460,2,330,1,925
410.7,"FYM02",""
2819251,"FeracEDDH4MA-1",0,36.31,0,0,-1,0,0,0,2
1,281,1,925
440.25,"FYM02",""
2819252,"FeHracEDDH4MA-0",0,39.09,0,0,0,0,0,0,3
1,281,1,330,1,925
441.25,"FYM02",""
2819253,"FeOHracEDDH4MA-2",0,24.48,0,0,-2,0,0,0,3
1,281,-1,330,1,925
457.25,"FYM02",""
2319251,"CuracEDDH4MA-2",0,24.38,0,0,-2,0,0,0,2
1,231,1,925
447.95,"FYM02",""
2319252,"CuHracEDDH4MA-1",0,33.63,0,0,-1,0,0,0,3
1,231,1,330,1,925
448.95,"FYM02",""
2319253,"CuH2racEDDH4MA-0",0,38.98,0,0,0,0,0,0,3
1,231,2,330,1,925
449.95,"FYM02",""
3309261,"mesEDDH4MAH-3",0,12.83,0,0,-3,0,0,0,2
1,330,1,926
385.4,"FYM02",""
3309262,"mesEDDH4MAH2-2",0,24.22,0,0,-2,0,0,0,2
2,330,1,926
386.4,"FYM02",""
3309263,"mesEDDH4MAH3-1",0,33.37,0,0,-1,0,0,0,2
3,330,1,926
387.4,"FYM02",""
3309264,"mesEDDH4MAH4-0",0,39.94,0,0,0,0,0,0,2
4,330,1,926
388.4,"FYM02",""
1509261,"CamesEDDH4MA-2",0,8.56,0,0,-2,0,0,0,2
1,150,1,926
424.5,"FYM02",""
1509262,"CaHmesEDDH4MA-1",0,19.03,0,0,-1,0,0,0,3
1,150,1,330,1,926
425.5,"FYM02",""
1509263,"CaH2mesEDDH4MA-0",0,28.67,0,0,0,0,0,0,3
1,150,2,330,1,926
426.5,"FYM02",""
4609261,"MgmesEDDH4MA-2",0,11.37,0,0,-2,0,0,0,2
```

```
1,460,1,926
408.7,"FYM02",""
4609262,"MgHmesEDDH4MA-1",0,20.02,0,0,-1,0,0,0,3
1,460,1,330,1,926
409.7,"FYM02",""
4609263,"MgH2mesEDDH4MA-0",0,28.69,0,0,0,0,0,0,3
1,460,2,330,1,926
410.7,"FYM02",""
2819261,"FemesEDDH4MA-1",0,38.1,0,0,-1,0,0,0,2
1,281,1,926
440.25,"FYM02",""
2819262,"FeHmesEDDH4MA-0",0,39.63,0,0,0,0,0,0,3
1,281,1,330,1,926
441.25,"FYM02",""
2819263,"FeOHmesEDDH4MA-2",0,25.59,0,0,-2,0,0,0,3
1,281,-1,330,1,926
457.25,"FYM02",""
2319261,"CumesEDDH4MA-2",0,26.18,0,0,-2,0,0,0,2
1,231,1,926
447.95,"FYM02",""
2319262,"CuHmesEDDH4MA-1",0,34.52,0,0,-1,0,0,0,3
1,231,1,330,1,926
447.95,"FYM02",""
2319263,"CuH2mesEDDH4MA-0",0,39.56,0,0,0,0,0,0,3
1,231,2,330,1,926
448.95,"FYM02",""
3309271,"EDDH5MAH-3",0,12.75,0,0,-3,0,0,0,2
1,330,1,927
385.4,"FYM02",""
3309272,"EDDH5MAH2-2",0,24.17,0,0,-2,0,0,0,2
2,330,1,927
386.4,"FYM02",""
3309273,"EDDH5MAH3-1",0,33.31,0,0,-1,0,0,0,2
3,330,1,927
387.4,"FYM02",""
3309274,"EDDH5MAH4-0",0,40.08,0,0,0,0,0,0,2
4,330,1,927
388.4,"FYM02",""
1509271,"CaEDDH5MA-2",0,8.36,0,0,-2,0,0,0,2
1,150,1,927
424.5,"FYM02",""
1509272,"CaHEDDH5MA-1",0,18.9,0,0,-1,0,0,0,3
1,150,1,330,1,927
425.5,"FYM02",""
1509273,"CaH2EDDH5MA-0",0,28.58,0,0,0,0,0,0,3
1,150,2,330,1,927
426.5,"FYM02",""
4609271,"MgEDDH5MA-2",0,9.54,0,0,-2,0,0,0,2
1,460,1,927
408.7,"FYM02",""
4609272,"MgHEDDH5MA-1",0,19.02,0,0,-1,0,0,0,3
1,460,1,330,1,927
409.7,"FYM02",""
4609273,"MgH2EDDH5MA-0",0,27.64,0,0,0,0,0,0,3
1,460,2,330,1,927
410.7,"FYM02",""
2819271,"FeEDDH5MA-1",0,36.23,0,0,-1,0,0,0,2
1,281,1,927
440.25,"FYM02",""
2819272,"FeHEDDH5MA-0",0,39.19,0,0,0,0,0,0,3
1,281,1,330,1,927
441.25,"FYM02",""
2819273,"FeOHEDDH5MA-2",0,24.12,0,0,-2,0,0,0,3
1,281,-1,330,1,927
457.25,"FYM02",""
2319271,"CuEDDH5MA-2",0,25.17,0,0,-2,0,0,0,2
1,231,1,927
```

```
447.95,"FYM02",""
2319272,"CuHEDDH5MA-1",0,34.35,0,0,-1,0,0,0,3
1,231,1,330,1,927
448.95,"FYM02",""
2319273,"CuH2EDDH5MA-0",0,39.72,0,0,0,0,0,0,3
1,231,2,330,1,927
449.95,"FYM02",""
3309281,"PDDHAH-3",0,13.03,0,0,-3,0,0,0,2
1,330,1,928
371.4,"FYM02",""
3309282,"PDDHAH2-2",0,24.75,0,0,-2,0,0,0,2
2,330,1,928
372.4,"FYM02",""
3309283,"PDDHAH3-1",0,33.97,0,0,-1,0,0,0,2
3,330,1,928
373.4,"FYM02",""
3309284,"PDDHAH4-0",0,41.25,0,0,0,0,0,0,2
4,330,1,928
374.4,"FYM02",""
1509281,"CaPDDHA-2",0,7.88,0,0,-2,0,0,0,2
1,150,1,928
410.5,"FYM02",""
1509282,"CaHPDDHA-1",0,18.57,0,0,-1,0,0,0,3
1,150,1,330,1,928
411.5,"FYM02",""
1509283,"CaH2PDDHA-0",0,28.22,0,0,0,0,0,0,3
1,150,2,330,1,928
412.5,"FYM02",""
4609281,"MgPDDHA-2",0,10.52,0,0,-2,0,0,0,2
1,460,1,928
394.7,"FYM02",""
4609282,"MgHPDDHA-1",0,19.47,0,0,-1,0,0,0,3
1,460,1,330,1,928
395.7,"FYM02",""
4609283,"MgH2PDDHA-0",0,27.92,0,0,0,0,0,0,3
1,460,2,330,1,928
396.7,"FYM02",""
2819281,"FePDDHA-1",0,36.11,0,0,-1,0,0,0,2
1,281,1,928
426.25,"FYM02",""
2819282,"FeHPDDHA-0",0,38.62,0,0,0,0,0,0,3
1,281,1,330,1,928
427.25,"FYM02",""
2819283,"FeOHPDDHA-2",0,23.88,0,0,-2,0,0,0,3
1,281,-1,330,1,928
443.25,"FYM02",""
2319281,"CuPDDHA-2",0,24.02,0,0,-2,0,0,0,2
1,231,1,928
433.95,"FYM02",""
2319282,"CuHPDDHA-1",0,33.87,0,0,-1,0,0,0,3
1,231,1,330,1,928
434.95,"FYM02",""
2319283,"CuH2PDDHA-0",0,41.23,0,0,0,0,0,0,3
1,231,2,330,1,928
435.95,"FYM02",""
3309291,"XDDHAH-3",0,12.56,0,0,-3,0,0,0,2
1,330,1,929
433.5,"FYM02",""
3309292,"XDDHAH2-2",0,24.06,0,0,-2,0,0,0,2
2,330,1,929
434.5,"FYM02",""
3309293,"XDDHAH3-1",0,32.99,0,0,-1,0,0,0,2
3,330,1,929
435.5,"FYM02",""
3309294,"XDDHAH4-0",0,40.1,0,0,0,0,0,0,2
4,330,1,929
436.5,"FYM02",""
```

```
1509291,"CaXDDHA-2",0,7.76,0,0,-2,0,0,0,2
1,150,1,929
472.6,"FYM02",""
1509292,"CaHXDDHA-1",0,18.69,0,0,-1,0,0,0,3
1,150,1,330,1,929
473.6,"FYM02",""
1509293,"CaH2XDDHA",0,27.42,0,0,0,0,0,0,3
1,150,2,330,1,929
474.6,"FYM02",""
4609291,"MgXDDHA-2",0,9.06,0,0,-2,0,0,0,2
1,460,1,929
456.8,"FYM02",""
4609292,"MgHXDDHA-1",0,18.73,0,0,-1,0,0,0,3
1,460,1,330,1,929
457.8,"FYM02",""
4609293,"MgH2XDDHA",0,27.21,0,0,0,0,0,0,3
1,460,2,330,1,929
458.8,"FYM02",""
2819291,"FeXDDHA-1",0,32.7,0,0,-1,0,0,0,2
1,281,1,929
488.35,"FYM02",""
2819292,"FeHXDDHA-0",0,36.9,0,0,0,0,0,0,3
1,281,1,330,1,929
489.35,"FYM02",""
2319291,"CuXDDHA-2",0,19.23,0,0,-2,0,0,0,2
1,231,1,929
496.05,"FYM02",""
2319292,"CuHXDDHA-1",0,28.73,0,0,-1,0,0,0,3
1,231,1,330,1,929
497.05,"FYM02",""
3309301,"BDDHAH-3",0,12.82,0,0,-3,0,0,0,2
1,330,1,930
385.4,"FYM02",""
3309302,"BDDHAH2-2",0,24.35,0,0,-2,0,0,0,2
2,330,1,930
386.4,"FYM02",""
3309303,"BDDHAH3-1",0,33.51,0,0,-1,0,0,0,2
3,330,1,930
387.4,"FYM02",""
3309304,"BDDHAH4-0",0,41.22,0,0,0,0,0,0,2
4,330,1,930
388.4,"FYM02",""
1509301,"CaBDDHA-2",0,8.87,0,0,-2,0,0,0,2
1,150,1,930
424.5,"FYM02",""
1509302,"CaHBDDHA-1",0,18.45,0,0,-1,0,0,0,3
1,150,1,330,1,930
425.6,"FYM02",""
1509303,"CaH2BDDHA",0,27.82,0,0,0,0,0,0,3
1,150,2,330,1,930
426.6,"FYM02",""
4609301,"MgBDDHA-2",0,9.23,0,0,-2,0,0,0,2
1,460,1,930
408.7,"FYM02",""
4609302,"MgHBDDHA-1",0,18.29,0,0,-1,0,0,0,3
1,460,1,330,1,930
409.7,"FYM02",""
4609303,"MgH2BDDHA",0,27.49,0,0,0,0,0,0,3
1,460,2,330,1,930
410.7,"FYM02",""
2819301,"FeBDDHA-1",0,32.25,0,0,-1,0,0,0,2
1,281,1,930
440.25,"FYM02",""
2819302,"FeHBDDHA-0",0,36.44,0,0,0,0,0,0,3
1,281,1,330,1,930
441.25,"FYM02",""
2819303,"FeOHBDDHA-2",0,20.89,0,0,-2,0,0,0,3
```

```
1,281,-1,330,1,930
457.25,"FYM02",""
2319301,"CuBDDHA-2",0,21.23,0,0,-2,0,0,0,2
1,231,1,930
447.99,"FYM02",""
2319302,"CuHBDDHA-1",0,30.82,0,0,-1,0,0,0,3
1,231,1,330,1,930
448.99,"FYM02",""
2319303,"CuH2BDDHA",0,37.74,0,0,0,0,0,0,3
1,231,2,330,1,930
449.99,"FYM02",""
3309321,"EDDMetxAH-1",0,8.04,0,0,-1,0,0,0,2
1,330,1,932
387.5,"FYM02",""
3309322,"EDDMetxAH2-0",0,13.18,0,0,0,0,0,0,2
2,330,1,932
388.5,"FYM02",""
1509321,"CaEDDMetxA-0",0,4.05,0,0,0,0,0,0,2
1,150,1,932
426.6,"FYM02",""
1509322,"CaHEDDMetxA+1",0,11.5,0,0,1,0,0,0,3
1,150,1,330,1,932
427.6,"FYM02",""
4609321,"MgEDDMetxA-0",0,4.79,0,0,0,0,0,0,2
1,460,1,932
410.8,"FYM02",""
4609322,"MgHEDDMetxA+1",0,11.72,0,0,1,0,0,0,3
1,460,1,330,1,932
411.8,"FYM02",""
4609323,"MgOHEDDMetxA-1",0,-3.92,0,0,-1,0,0,0,3
1,460,-1,330,1,932
426.8,"FYM02",""
2319321,"CuEDDMetxA-0",0,16.15,0,0,0,0,0,0,2
1,231,1,932
426.6,"FYM02",""
2319322,"CuHEDDMetxA+1",0,24.51,0,0,1,0,0,0,3
1,231,1,330,1,932
450.05,"FYM02",""
2319323,"CuH2EDDMetxA+2",0,30.98,0,0,2,0,0,0,3
1,231,2,330,1,932
451.05,"FYM02",""
2319324,"CuH3EDDMetxA+3",0,33.45,0,0,3,0,0,0,3
1,231,3,330,1,932
452.05,"FYM02",""
3309331,"PDDHAbisH-3",0,12.81,0,0,-3,0,0,0,2
1,330,1,933
353.05,"FYM02",""
3309332,"PDDHAbisH2-2",0,24.18,0,0,-2,0,0,0,2
2,330,1,933
372.4,"FYM02",""
3309333,"PDDHAbisH3-1",0,33.39,0,0,-1,0,0,0,2
3,330,1,933
373.4,"FYM02",""
3309334,"PDDHAbisH4-0",0,40.69,0,0,0,0,0,0,2
4,330,1,933
374.4,"FYM02",""
1509331,"CaPDDHAbis-2",0,7.2,0,0,-2,0,0,0,2
1,150,1,933
410.5,"FYM02",""
1509332,"CaHPDDHAbis-1",0,18.1,0,0,-1,0,0,0,3
1,150,1,330,1,933
411.5,"FYM02",""
1509333,"CaH2PDDHAbis-0",0,27.77,0,0,0,0,0,0,3
1,150,2,330,1,933
412.5,"FYM02",""
4609331,"MgPDDHAbis-2",0,9.46,0,0,-2,0,0,0,2
1,460,1,933
```

```
394.7,"FYM02",""
4609332,"MgHPDDHAbis-1",0,18.37,0,0,-1,0,0,0,3
1,460,1,330,1,933
395.7,"FYM02",""
4609333,"MgH2PDDHAbis-0",0,27.13,0,0,0,0,0,0,3
1,460,2,330,1,933
396.7,"FYM02",""
2819331,"FePDDHAbis-1",0,35.45,0,0,-1,0,0,0,2
1,281,1,933
426.25,"FYM02",""
2819332,"FeHPDDHAbis-0",0,37.66,0,0,0,0,0,0,3
1,281,1,330,1,933
427.25,"FYM02",""
2819333,"FeOHPDDHAbis-2",0,23.27,0,0,-2,0,0,0,3
1,281,-1,330,1,933
443.25,"FYM02",""
2319331,"CuPDDHAbis-2",0,23.21,0,0,-2,0,0,0,2
1,231,1,933
433.95,"FYM02",""
2319332,"CuHPDDHAbis-1",0,33.46,0,0,-1,0,0,0,3
1,231,1,330,1,933
434.95,"FYM02",""
2319333,"CuH2PDDHAbis-0",0,40.88,0,0,0,0,0,0,3
1,231,2,330,1,933
435.95,"FYM02",""
3309341,"EDDHSAH-5",0,11.71,0,0,-5,0,0,0,2
1,330,1,934
515.4,"FYM02",""
3309342,"EDDHSAH2-4",0,21.68,0,0,-4,0,0,0,2
2,330,1,934
516.4,"FYM02",""
3309343,"EDDHSAH3-3",0,29.99,0,0,-3,0,0,0,2
3,330,1,934
517.4,"FYM02",""
3309344,"EDDHSAH4-2",0,36.52,0,0,-2,0,0,0,2
4,330,1,934
518.4,"FYM02",""
3309345,"EDDHSAH5-1 ",0,39.58,0,0,-1,0,0,0,2
5,330,1,934
519.4,"FYM02",""
3309346,"EDDHSAH6+0",0,41.3,0,0,0,0,0,0,2
6,330,1,934
520.4,"FYM02",""
1509341,"CaEDDHSA-4",0,7.97,0,0,-4,0,0,0,2
1,150,1,934
554.48,"FYM02",""
1509342,"CaHEDDHSA-3",0,16.57,0,0,-3,0,0,0,3
1,150,1,330,1,934
555.48,"FYM02",""
1509343,"CaH2EDDHSA-2",0,25.82,0,0,-2,0,0,0,3
1,150,2,330,1,934
556.48,"FYM02",""
1509344,"Ca2EDDHSA-2",0,9.56,0,0,-2,0,0,0,2
2,150,1,934
594.56,"FYM02",""
4609341,"MgEDDHSA-4",0,9.52,0,0,-4,0,0,0,2
1,460,1,934
538.7,"FYM02",""
4609342,"MgHEDDHSA-3",0,17.71,0,0,-3,0,0,0,3
1,460,1,330,1,934
539.7,"FYM02",""
4609343,"MgH2EDDHSA-2",0,25.5,0,0,-2,0,0,0,3
1,460,2,330,1,934
540.7,"FYM02",""
4609344,"Mg2EDDHSA-2",0,11.36,0,0,-2,0,0,0,2
2,460,1,934
563,"FYM02",""
```

```
2819341,"FeEDDHSA-3",0,36.64,0,0,-3,0,0,0,2
1,281,1,934
570.25,"FYM02",""
2819342,"FeHEDDHSA-2",0,39.13,0,0,-2,0,0,0,3
1,281,1,330,1,934
571.25,"FYM02",""
2819343,"FeH2EDDHSA-1",0,41.07,0,0,-1,0,0,0,3
1,281,2,330,1,934
572.25,"FYM02",""
2819344,"FeOHEDDHSA-4",0,24.91,0,0,-4,0,0,0,3
1,281,-1,330,1,934
587.25,"FYM02",""
2319341,"CuEDDHSA-4",0,24.19,0,0,-4,0,0,0,2
1,231,1,934
577.95,"FYM02",""
2319342,"CuHEDDHSA-3",0,33.04,0,0,-3,0,0,0,3
1,231,1,330,1,934
578.95,"FYM02",""
2319343,"CuH2EDDHSA-2",0,38.05,0,0,-2,0,0,0,3
1,231,2,330,1,934
579.95,"FYM02",""
2319344,"CuH3EDDHSA-1",0,39.98,0,0,-1,0,0,0,3
1,231,3,330,1,934
580.95,"FYM02",""
3309541,"EDDHAH-3(Lindsay)",0,12.54,0,0,-3,0,0,0,2
1,330,1,954
357.34,"",""
3309542,"EDDHAH2-2(Lindsay)",0,23.42,0,0,-2,0,0,0,2
2,330,1,954
358.35,"",""
3309543,"EDDHAH3-1(Lindsay)",0,32.49,0,0,-1,0,0,0,2
3,330,1,954
359.36,"",""
3309544,"EDDHAH4-0(Lindsay)",0,39.02,0,0,0,0,0,0,2
4,330,1,954
360.37,"",""
1509541,"CaEDDHA-2(Lindsay)",0,8.91,0,0,-2,0,0,0,2
1,150,1,954
396.41,"",""
1509542,"CaHEDDHA-1(Lindsay)",0,18.62,0,0,-1,0,0,0,3
1,150,1,330,1,954
397.42,"",""
1509543,"CaH2EDDHA-0(Lindsay)",0,26,0,0,0,0,0,0,3
1,150,2,330,1,954
398.43,"",""
4609541,"MgEDDHA-2(Lindsay)",0,9.71,0,0,-2,0,0,0,2
1,460,1,954
380.64,"",""
4609542,"MgHEDDHA-1(Lindsay)",0,19.02,0,0,-1,0,0,0,3
1,460,1,330,1,954
381.65,"",""
4609543,"MgH2EDDHA-0(Lindsay)",0,27.2,0,0,0,0,0,0,3
1,460,2,330,1,954
382.66,"",""
2819541,"FeEDDHA-1(Lindsay)",0,36.47,0,0,-1,0,0,0,2
1,281,1,954
412.18,"",""
2809541,"FeIIEDDHA-2(Lindsay)",0,16.01,0,0,-2,0,0,0,2
1,280,1,954
412.18,"",""
9509541,"ZnEDDHA-2(Lindsay)",0,18.51,0,0,-2,0,0,0,2
1,950,1,954
421.71,"",""
9509542,"ZnHEDDHA-1(Lindsay)",0,26.68,0,0,-1,0,0,0,3
1,950,1,330,1,954
422.72,"",""
9509543,"ZnH2EDDHA-0(Lindsay)",0,33.6,0,0,0,0,0,0,3
```

```
1,950,2,330,1,954
423.73,"",""
1609541,"CdEDDHA-2(Lindsay)",0,14.84,0,0,-2,0,0,0,2
1,160,1,954
468.74,"",""
1609542,"CdHEDDHA-1(Lindsay)",0,23.97,0,0,-1,0,0,0,3
1,160,1,330,1,954
469.75,"",""
1609543,"CdH2EDDHA-0(Lindsay)",0,32.1,0,0,0,0,0,0,3
1,160,2,330,1,954
470.76,"",""
1829541,"CoEDDHA-2(Lindsay)",0,21.6,0,0,-2,0,0,0,2
1,182,1,954
414.267,"DRP 90 E",""
1829542,"CoHEDDHA-1(Lindsay)",0,29.8,0,0,-1,0,0,0,3
1,182,1,330,1,954
416.275,"DRP 90 E",""
1829543,"CoH2EDDHA-0(Lindsay)",0,35.6,0,0,0,0,0,0,3
1,182,2,330,1,954
417.283,"DRP 99 E",""
2319541,"CuEDDHA-2(Lindsay)",0,24,0,0,-2,0,0,0,2
1,231,1,954
419.88,"",""
2319542,"CuHEDDHA-1(Lindsay)",0,32.5,0,0,-1,0,0,0,3
1,231,1,330,1,954
420.888,"DRP 90",""
2319543,"CuH2EDDHA-0(Lindsay)",0,37.7,0,0,0,0,0,0,3
1,231,2,330,1,954
421.896,"DRP 90",""
4709541,"MnEDDHA-2(Lindsay)",0,19.5,0,0,-2,0,0,0,2
1,470,1,954
411.272,"DRP 90 E",""
4709542,"MnHEDDHA-1(Lindsay)",0,27.6,0,0,-1,0,0,0,3
1,470,1,330,1,954
412.28,"DRP 90 E",""
4709543,"MnH2EDDHA-0(Lindsay)",0,11.2,0,0,0,0,0,0,3
1,470,2,330,1,954
413.288,"DRP 90 E",""
6009541,"PbEDDHA-2(Lindsay)",0,16.82,0,0,-2,0,0,0,2
1,600,1,954
563.53,"",""
6009542,"PbHEDDHA-1(Lindsay)",0,26.85,0,0,-1,0,0,0,3
1,600,1,330,1,954
564.54,"",""
6009543,"PbH2EDDHA-0(Lindsay)",0,34.4,0,0,0,0,0,0,3
1,600,2,330,1,954
565.55,"",""
5409541,"NiEDDHA-2(Lindsay)",0,21.37,0,0,-2,0,0,0,2
1,540,1,954
415.03,"",""
5409542,"NiHEDDHA-1(Lindsay)",0,29.43,0,0,-1,0,0,0,3
1,540,1,330,1,954
416.04,"",""
5409543,"NiH2EDDHA-0(Lindsay)",0,35.7,0,0,0,0,0,0,3
1,540,2,330,1,954
417.05,"",""
3309131,"HBPDS-1",0,5.5,0,0,-1,0,0,0,2
1,330,1,913
491.528,"DRP90",""
3309132,"H(BPDS)2-3",0,7.4,0,0,-3,0,0,0,2
1,330,2,913
982.048,"DRP90",""
3309133,"H(BPDS)3-5",0,9.3,0,0,-5,0,0,0,2
1,330,3,913
1472.568,"DRP90",""
3309134,"H2BPDS-0",0,6.7,0,0,0,0,0,0,2
2,330,1,913
```

```
492.536,"DRP90",""
3309135,"H3BPDS+1",0,7.7,0,0,1,0,0,0,2
3,330,1,913
493.544,"DRP90",""
1509131,"CaBPDS-0",0,1.9,0,0,0,0,0,0,2
1,150,1,913
530.6,"DRP90 ap",""
1509132,"Ca(BPDS)3-3",0,18.79,0,0,-4,0,0,0,2
1,150,3,913
1511.64,"Schwab &",""
4609131,"MgBPDS-0",0,2.1,0,0,0,0,0,0,2
1,460,1,913
514.825,"DRP90 es",""
2819131,"Fe(BPDS)3-3",0,15,0,0,-3,0,0,0,2
1,281,3,913
1527.407,"DRP90 es",""
2809131,"FeIIBPDS-0",0,7.3,0,0,0,0,0,0,2
1,280,1,913
546.367,"DRP90",""
2809132,"FeII(BPDS3-4",0,23.45,0,0,-4,0,0,0,2
1,280,3,913
1527.407,"Schwab &",""
4709131,"MnBPDS-0",0,5,0,0,0,0,0,0,2
1,470,1,913
545.458,"DRP90 es",""
4709132,"Mn(BPDS)2-2",0,8.2,0,0,-2,0,0,0,2
1,470,2,913
1035.978,"DRP90 es",""
4709133,"Mn(BPDS)3-4",0,10.4,0,0,-4,0,0,0,2
1,470,3,913
1526.498,"DRP90 es",""
2319131,"CuBPDS-0",0,10.6,0,0,0,0,0,0,2
1,231,1,913
554.066,"DRP90",""
2319132,"Cu(BPDS)2-2",0,16.8,0,0,-2,0,0,0,2
1,231,2,913
1044.586,"DRP90",""
2319133,"Cu(BPDS)3-4",0,20.9,0,0,-4,0,0,0,2
1,231,3,913
1535.106,"DRP90",""
1609131,"CdBPDS-0",0,6.7,0,0,0,0,0,0,2
1,160,1,913
602.93,"DRP90 es",""
1609132,"Cd(BPDS)2-2",0,11.5,0,0,-2,0,0,0,2
1,160,2,913
1093.45,"DRP90 es",""
1609133,"Cd(BPDS)3-4",0,14.8,0,0,-4,0,0,0,2
1,160,3,913
1583.97,"DRP90 es",""
9509131,"ZnBPDS -0",0,7.3,0,0,0,0,0,0,2
1,950,1,913
555.9,"DRP90 es",""
9509132,"Zn(BPDS)2-2",0,12.1,0,0,-2,0,0,0,2
1,950,2,913
1046.42,"DRP90 es",""
9509133,"Zn(BPDS)3-4",0,17.2,0,0,-4,0,0,0,2
1,950,3,913
1536.94,"DRP90 es",""
5409131,"NiBPDS-0",0,9.6,0,0,0,0,0,0,2
1,540,1,913
549.22,"DRP90 es",""
5409132,"Ni(BPDS)2-2",0,17.8,0,0,-2,0,0,0,2
1,540,2,913
1039.74,"DRP90 es",""
5409133,"Ni(BPDS)3-4",0,24.7,0,0,-4,0,0,0,2
1,540,3,913
1530.26,"DRP90",""
```

```
1829131,"CoBPDS-0",0,8.1,0,0,0,0,0,0,2
1,182,1,913
549.453,"DRP90 es",""
1829132,"Co(BPDS)2-2",0,14.8,0,0,-2,0,0,0,2
1,182,2,913
1039.973,"DRP90 es",""
1829133,"Co(BPDS)3-4",0,19.9,0,0,-4,0,0,0,2
1,182,3,913
1530.493,"DRP90 es",""
3309711,"PROPANOTH",0,4.61,0,0,0,0,0,0,2
1,330,1,971
74.03,"",""
3309581,"METHYLAM H",0,10.72,0,0,1,0,0,0,2
1,330,1,958
32.06,"",""
3309611,"HEXYLAM H",0,10.63,0,0,1,0,0,0,2
1,330,1,961
101.17,"",""
3309721,"BUTANOAT H",0,4.73,0,0,0,0,0,0,2
1,330,1,972
88.04,"",""
3309684,"NTAH4",0,16.224,0,0,1,0,0,0,2
4,330,1,968
192.06,"",""
3309551,"DIETHYLAM H",0,10.774,0,0,1,0,0,0,2
1,330,1,955
74.14,"",""
3309661,"TMETHAM H",0,9.8,0,0,1,0,0,0,2
1,330,1,966
60.04,"",""
3309801,"2METPYR H",0,5.95,0,0,1,0,0,0,2
1,330,1,980
94.12,"",""
3309811,"3METPYR H",0,5.7,0,0,1,0,0,0,2
1,330,1,981
94.12,"",""
3309821,"4METPYR H",0,6,0,0,1,0,0,0,2
1,330,1,982
94.12,"",""
3309641,"NPROPYLAMH",0,10.8,0,0,1,0,0,0,2
1,330,1,964
60.44,"",""
3309963,"GLUTAM H3",0,16.6,0,0,1,0,0,0,2
3,330,1,996
148.13,"",""
3309831,"FORMATE H",0,3.745,0,0,0,0,0,0,2
1,330,1,983
46.02,"",""
3309841,"ISOVALERIC H",0,4.781,0,0,0,0,0,0,2
1,330,1,984
102.13,"",""
3309731,"ISOBUTRYIC H",0,4.849,0,0,0,0,0,0,2
1,330,1,973
88.043,"",""
3309851,"VALERIC H",0,4.843,0,0,0,0,0,0,2
1,330,1,985
102.13,"",""
1609691,"CdEDTA-2",0,18.21,0,0,-2,0,0,0,2
1,160,1,969
400.62,"M89 8/10",""
1609681,"CDNTA",0,9.4,0,0,-1,0,0,0,2
1,160,1,968
300.46,"",""
1609682,"CDNTA2",0,14.3,0,0,-4,0,0,0,2
1,160,2,968
488.52,"",""
4609631,"MGEN",0,0.37,0,0,2,0,0,0,2
```

```
1,460,1,963
84.43,"",""
1509631,"CAEN",0,0.1,0,0,2,0,0,0,2
1,150,1,963
100.2,"",""
4609671,"MGCITRATE",0,3.37,0,0,-1,0,0,0,2
1,460,1,967
223.37,"",""
4609672,"MGCITRATEH",0,8.17,0,0,0,0,0,0,3
1,460,1,967,1,330
224.37,"",""
4609673,"MGCITRATEH2",0,11.59,0,0,1,0,0,0,3
1,460,1,967,2,330
225.37,"",""
5009920,"NaACETATE",0,-0.18,0,0,0,0,0,0,2
1,500,1,992
82.0398,"",""
4609920,"MgACETATE",0,1.14,0,0,1,0,0,0,2
1,460,1,992
83.362,"",""
1509920,"CaACETATE",0,1.18,0,0,1,0,0,0,2
1,150,1,992
99.13,"",""
4709920,"MnACETATE",0,1.31,0,0,1,0,0,0,2
1,470,1,992
93.312,"",""
2809920,"FeACETATE",0,1.82,0,0,1,0,0,0,2
1,280,1,992
114.897,"",""
3619920,"HgACETATE",0,12.23,0,0,1,0,0,0,4
1,361,1,992,2,330,-2,2
259.66,"",""
3619921,"HgACETATE2",0,16.2,0,0,0,0,0,0,4
1,361,2,992,2,330,-2,2
318.71,"",""
3619922,"HgACETATE3",0,20.18,0,0,-1,0,0,0,4
1,361,3,992,2,330,-2,2
377.76,"",""
3619923,"HgACETATE4",0,23.96,0,0,-2,0,0,0,4
1,361,4,992,2,330,-2,2
436.81,"",""
2819920,"FeACETATE",0,3.21,0,0,2,0,0,0,2
1,281,1,992
114.897,"",""
2819921,"FeACETATE2",0,6.3,0,0,1,0,0,0,2
1,281,2,992
174.3971,"",""
2819922,"FeACETATE3",0,8.2,0,0,0,0,0,0,2
1,281,3,992
233.447,"",""
5009690,"Na EDTA",0,1.66,0,0,-3,0,0,0,2
1,500,1,969
298.9898,"",""
0,"",0,0,0,0,0,0,0,0,0
0,"",""
0,"",0,0,0,0,0,0,0,0,0
0,"",""
0,"",0,0,0,0,0,0,0,0,0
0,"",""
2089100,"URANINITE",77.948,4.7,0,0,0,0,0,0,3
-4,330,1,891,2,2
270.0278,"",""
2089101,"UO2 (AM)",109.746,-0.93,0,0,0,0,0,0,3
-4,330,1,891,2,2
270.0278,"",""
3089100,"U4O9 (C)",423.546,3.38,0,-3.08,0,0,0,0,4
-18,330,-2,1,4,891,9,2
```

```
1096.1106,"",""
3089101,"U3O8 (C)",485.428,-21.1,0,-34.589,0,0,0,0,4
-16,330,-4,1,3,891,8,2
842.0822,"",""
8089100,"USIO4 (C)",60.835,7.62,0,0,0,0,0,0,3
-4,330,1,891,1,770
330.1121,"",""
4289100,"UF4 (C)",79.078,18.6,0,0,0,0,0,0,2
1,891,4,270
314.0226,"",""
4289101,"UF4.2.5H2O",2.427,27.57,0,0,0,0,0,0,3
1,891,4,270,2.5,2
359.0606,"",""
7089100,"UHPO4)2,4H2O",-16.067,51.58,0,0,0,0,0,0,4
1,891,2,580,2,330,4,2
502.0486,"",""
7015000,"NINGYOITE",9.498,53.9,0,0,0,0,0,0,4
1,891,1,150,2,580,2,2
504.0822,"",""
2089300,"UO3 (C)",80.793,-7.71,0,0,0,0,0,0,3
-2,330,1,893,1,2
286.0272,"",""
2089301,"GUMMITE",96.274,-10.4,0,0,0,0,0,0,3
-2,330,1,893,1,2
286.0272,"",""
2089302,"B-UO2(OH)2",57.446,-5.54,0,0,0,0,0,0,3
-2,330,1,893,2,2
304.0424,"",""
2089303,"SCHOEPITE",50.375,-5.4,0,0,0,0,0,0,3
-2,330,1,893,3,2
322.0576,"",""
5089300,"RUTHERFORDIN",6.025,14.43,0,0,0,0,0,0,2
1,893,1,140
330.037,"",""
7089300,"(UO2)3(PO4)2",-397.062,49.03,129.134,0,0,0,0,0,2
3,893,2,580
1000.0262,"",""
7089301,"H-AUTUNITE",15.062,47.93,0,0,0,0,0,0,3
2,330,2,893,2,580
732.0144,"",""
7050000,"NA-AUTUNITE",1.925,47.4,0,0,0,0,0,0,3
2,500,2,893,2,580
775.978,"",""
7041000,"K-AUTUNITE",-24.518,48.24,0,0,0,0,0,0,3
2,410,2,893,2,580
808.2024,"",""
7049000,"URAMPHITE",-40.585,51.74,0,0,0,0,0,0,3
2,893,2,490,2,580
766.0756,"",""
7046000,"SALEEITE",84.433,43.64,0,0,0,0,0,0,3
2,893,1,460,2,580
754.3104,"",""
7015001,"AUTUNITE",59.999,43.92,0,0,0,0,0,0,3
2,893,1,150,2,580
770.0784,"",""
7080000,"SR-AUTUNITE",54.601,44.45,0,0,0,0,0,0,3
2,893,1,800,2,580
817.6184,"",""
7010000,"URANOCIRCITE",42.258,44.63,0,0,0,0,0,0,3
2,893,1,100,2,580
867.3384,"",""
7028000,"BASSETITE",83.262,44.48,0,0,0,0,0,0,3
2,893,1,280,2,580
785.8454,"",""
7023102,"TORBERNITE",66.526,45.27,0,0,0,0,0,0,3
2,893,1,231,2,580
793.5444,"",""
```

```
7060000,"PRZHEVALSKIT",46.024,44.36,0,0,0,0,0,0,3
2,893,1,600,2,580
937.1883,"",""
8015000,"URANOPHANE",0,-17.49,0,0,0,0,0,0,4
-6,330,2,893,1,150,2,770
766.5176,"",""
5189300,"UO2NO3)2",84.266,-12.36,0,0,0,0,0,0,2
1,893,2,492
394.038,"",""
5189301,"UO2NO3.2H2O",25.355,-4.85,0,0,0,0,0,0,3
1,893,2,492,2,2
430.069,"",""
5189302,"UO2NO3.3H2O",10.042,-3.64,0,0,0,0,0,0,3
1,893,2,492,3,2
448.084,"",""
5189303,"UO2NO3.6H2O",-19.958,-2.3,0,0,0,0,0,0,3
1,893,2,492,6,2
502.13,"",""
2003000,"AlOH3 amorp",113.135,-9.66,-9.69,0,0,0,0,0,3
1,30,3,2,-3,330
78.003,"WLL790",""
6003000,"ALOHSO4",0,3.23,3.39,3.07,0,0,0,0,4
-1,330,1,30,1,732,1,2
140.0505,"",""
6003001,"AL4(OH)10SO4",0,-22.7,0,0,0,0,0,0,4
-10,330,4,30,1,732,10,2
374.0616,"",""
6041000,"ALUM K",-30.208,5.17,0,0,0,0,0,0,4
1,410,1,30,2,732,12,2
438.3597,"",""
6041001,"ALUNITE",-16.359,1.34,0,0,0,0,0,0,5
1,410,3,30,2,732,6,2,-6,330
414.2141,"",""
6015000,"ANHYDRITE",15.732,4.63,0,0,0,0,0,0,2
1,150,1,732
136.1416,"",""
5015000,"ARAGONITE",10.92,8.36,0,0,0,0,0,0,2
1,150,1,140
100.0894,"",""
5046000,"ARTINITE",120.248,-9.6,0,0,0,0,0,0,4
-2,330,2,460,1,140,5,2
196.6941,"",""
4210000,"BAF2",-4.184,5.76,6.74,4.65,0,0,0,0,2
1,100,2,270
175.3368,"",""
6010000,"BARITE",-26.276,9.97,0,9.773,0,0,0,0,2
1,100,1,732
233.4016,"",""
2003001,"BOEHMITE",117.696,-8.13,-8.065,0,0,0,0,0,3
-3,330,1,30,2,2
59.9884,"WLL79",""
2003004,"BAYERITE",0,-8.51,0,0,0,0,0,0,3
1,30,3,2,-3,330
78.003,"WLL79",""
2046000,"BRUCITE",108.115,-16.79,0,0,0,0,0,0,3
1,460,2,2,-2,330
58.3268,"",""
5015001,"CALCITE",10.795,8.48,8.56,0,0,0,0,0,2
1,150,1,140
100.0894,"P&B82",""
6080000,"CELESTITE",1.966,6.46,0,6.349,0,0,0,0,2
1,800,1,732
183.6816,"",""
2077000,"CHALCEDONY",-19.288,3.52,0,0,0,0,0,0,2
-2,2,1,770
60.0848,"",""
8646000,"CHRYSOTILE",219.576,-32.18,0,0,0,0,0,0,4
```

```
-6,330,3,460,2,770,1,2
277.1349,"",""
8246000,"CLINOENSTITE",83.722,-11.33,-10.972,-11.632,0,0,0,0,4
-1,2,1,460,1,770,-2,330
100.3964,"",""
2077001,"CRISTOBALITE",-23.012,3.58,0,0,0,0,0,0,2
-2,2,1,770
60.0848,"",""
8215000,"DIOPSIDE",135.06,-19.88,0,0,0,0,0,0,5
-2,2,1,150,1,460,2,770,-4,330
216.5608,"",""
5015002,"DOLOMITE",34.685,17,0,0,0,0,0,0,3
1,150,1,460,2,140
184.4108,"",""
6046000,"EPSOMITE",-11.799,2.14,0,0,0,0,0,0,3
1,460,1,732,7,2
246.4807,"",""
8646003,"SEPIOLITE(C)",114.056,-15.91,0,0,0,0,0,0,4
-0.5,2,2,460,3,770,-4,330
323.9313,"",""
2028100,"Ferrihydrite",100.4,-3.2,0,0,0,0,0,0,3
1,281,3,2,-3,330
106.8692,"LiuMill99","LiuMill99"
2028104,"Fe(OH)3amorp",0,-3.54,0,0,0,0,0,0,3
-3,330,1,281,3,2
106.9,"",""
2028103,"Ferrihydrite (aged)",100.4,-2.69,0,0,0,0,0,0,3
1,281,-3,330,3,2
106.8689,"NIST 46.7","LiuMill99"
2028107,"Soil-Fe WLL",0,-2.7,0,0,0,0,0,0,3
1,281,3,2,-3,330
106.9,"",""
2028101,"FE3(OH)8 FH",0,-17.67,-17.112,-24.105,0,0,0,0,4
-8,330,2,281,1,280,8,2
297.6002,"",""
2028105,"FeOOH Lepido",0,-1.39,0,0,0,0,0,0,3
-3,330,1,281,2,2
88.85,"",""
4128100,"FEOH)2.7CL.3",0,3.04,0,0,0,0,0,0,4
-2.7,330,1,281,2.7,2,0.3,180
110.4029,"",""
1028000,"FES PPT",0,3.91,0,0,0,0,0,0,3
-1,330,1,280,1,730
85.911,"",""
6028100,"FE2(SO4)3",247.358,-3.58,0.65,0,0,0,0,0,2
2,281,3,732
395.8788,"",""
7015002,"FCO3APATITE",-164.808,114.4,0,0,0,0,0,0,6
9.496,150,0.36,500,0.144,460,4.8,580,1.2,140,2.48,270
967.367,"",""
7015003,"CaHPO4.2H20",0,18.92,0,0,0,0,0,0,4
1,150,1,330,1,580,2,2
172.09,"WLL79",""
7015004,"CaHPO4 monet",0,19.25,0,0,0,0,0,0,3
1,150,1,330,1,580
136.06,"WLL79",""
7015005,"OCTACAPHOS",0,46.89,0,0,0,0,0,0,4
4,150,1,330,3,580,2.5,2
491.28,"WLL79",""
7015006,"B-TRICAL P",0,28.92,0,0,0,0,0,0,2
3,140,2,580
310.183,"WLL79",""
7015007,"HYDROXYAPATI",0,44.19,0,0,0,0,0,0,4
5,150,3,580,1,2,-1,330
502.322,"WLL79",""
7015008,"FLUORAPATITE",0,59.59,0,0,0,0,0,0,3
5,140,3,580,1,270
```

```
504.313,"WLL79",""
4215000,"FLUORITE",-19.707,10.41,0,0,0,0,0,0,2
1,150,2,270
78.0768,"WLL79",""
8046000,"FORSTERITE",202.966,-28.29,0,0,0,0,0,0,3
-4,330,2,460,1,770
236.8234,"",""
7003000,"VARISCITE",0,22.05,0,0,0,0,0,0,3
1,30,1,580,2,2
157.983,"WLL79",""
2003003,"GIBBSITE (c",95.395,-8.04,-8.487,-9.44,0,0,0,0,3
-3,330,1,30,3,2
78.0037,"WLL79",""
2003005,"NORSTRANDIT",0,-8.13,0,0,0,0,0,0,3
1,30,3,2,-3,330
78.003,"WLL79",""
3003000,"Al2O3",0,-22.98,0,0,0,0,0,0,3
2,30,3,2,-6,330
101.9504,"",""
2028102,"GOETHITE",60.584,0.02,0,0,0,0,0,0,3
-3,330,1,281,2,2
86.8536,"",""
8628000,"GREENALITE",0,-20.81,0,0,0,0,0,0,4
-6,330,3,280,2,770,1,2
365.7393,"",""
1028001,"GREIGITE",0,45.03,0,0,0,0,0,0,4
-4,330,2,281,1,280,4,730
289.797,"",""
6015001,"GYPSUM",-1.088,4.66,0,0,0,0,0,0,3
1,150,1,732,2,2
172.1722,"",""
4150000,"HALITE",-3.807,-1.58,0,0,0,0,0,0,2
1,500,1,180
58.4428,"",""
3028100,"HEMATITE",129.035,-0.18,0,0,0,0,0,0,3
-6,330,2,281,3,2
155.6919,"",""
5015003,"HUNTITE",107.78,29.96,0,0,0,0,0,0,3
3,460,1,150,4,140
353.0536,"",""
5046001,"HYDRMAGNESIT",218.447,8.76,0,0,0,0,0,0,4
5,460,4,140,-2,330,6,2
467.6736,"",""
6050000,"JAROSITE NA",151.377,11.2,0,0,0,0,0,0,5
-6,330,1,500,3,281,2,732,6,2
478.6978,"",""
6041002,"JAROSITE K",130.876,14.8,0,0,0,0,0,0,5
-6,330,1,410,3,281,2,732,6,2
494.81,"",""
6028101,"JAROSITE H",230.748,12.1,0,0,0,0,0,0,4
-5,330,3,281,2,732,7,2
480.732,"",""
1028002,"MACKINAWITE",0,4.64,0,0,0,0,0,0,3
-1,330,1,280,1,730
87.911,"",""
8450000,"MAGADIITE",0,14.3,0,0,0,0,0,0,4
-1,330,-9,2,1,500,7,770
532.6521,"",""
3028101,"MAGHEMITE",0,-3.18,0,0,0,0,0,0,3
-6,330,2,281,3,2
159.6922,"",""
5046002,"MAGNESITE",25.773,8.02,8.279,7.779,0,0,0,0,2
1,460,1,140
84.3214,"",""
3028000,"MAGNETITE",211.125,-9.61,-3.367,-6.595,0,0,0,0,4
-8,330,2,281,1,280,4,2
231.5386,"",""
```

```
6028000,"MELANTERITE",-11.966,2.47,0,0,0,0,0,0,3
1,280,1,732,7,2
278.0157,"",""
6050001,"MIRABILITE",-79.412,1.11,0,0,0,0,0,0,3
2,500,1,732,10,2
322.1942,"",""
3050000,"NATRON",-65.856,1.31,0,0,0,0,0,0,3
2,500,1,140,10,2
286.142,"",""
5046003,"NESQUEHONITE",24.184,5.62,5.133,4.546,0,0,0,0,3
1,460,1,140,3,2
138.3673,"",""
8646001,"PHLOGOPITE",361.33,-66.3,0,0,0,0,0,0,5
-10,330,1,410,3,460,1,30,3,770
417.2863,"",""
1028003,"PYRITE",-47.279,18.47,0,0,0,0,0,0,4
-2,330,-2,1,1,280,2,730
119.975,"",""
2077002,"QUARTZ",-26.024,4,0,0,0,0,0,0,2
-2,2,1,770
60.0848,"",""
8646004,"SEPIOLITE(A)",0,-18.78,0,0,0,0,0,0,4
-0.5,2,2,460,3,770,-4,330
323.9308,"",""
5028000,"SIDERITE",22.259,10.55,12.104,0,0,0,0,0,2
1,280,1,140
115.8564,"",""
2077003,"SIO2(A,GL)",-18.577,3.01,0,0,0,0,0,0,2
-2,2,1,770
60.0848,"",""
2077004,"SIO2(A,PT)",-16.359,2.71,0,0,0,0,0,0,2
-2,2,1,770
60.0848,"",""
4280000,"SRF2",-5.23,8.54,9.12,0,0,0,0,0,2
1,800,2,270
125.6168,"",""
7028100,"STRENGITE",8.494,26.4,29.123,26.235,0,0,0,0,3
1,281,1,580,2,2
186.849,"WLL79",""
5080000,"STRONTIANITE",2.887,9.25,11.789,0,0,0,0,0,2
1,800,1,140
147.6294,"",""
8646002,"TALC",146.44,-23.05,-18.988,-23.088,0,0,0,0,4
-4,2,3,460,4,770,-6,330
379.2888,"",""
6050002,"THENARDITE",2.385,0.17,0,0,0,0,0,0,2
2,500,1,732
142.0412,"",""
5050001,"THERMONATR",11.715,-0.12,0,0,0,0,0,0,3
2,500,1,140,1,2
124.0043,"",""
8215001,"TREMOLITE",404.216,-56.54,0,0,0,0,0,0,5
-8,2,2,150,5,460,8,770,-14,330
812.4096,"",""
7028001,"VIVIANITE",0,35.99,0,0,0,0,0,0,3
3,280,2,580,8,2
501.6062,"WLL79",""
5010000,"WITHERITE",-1.506,8.58,13.335,0,0,0,0,0,2
1,100,1,140
197.3494,"",""
2047000,"PYROLUSITE",0,-41.89,0,0,0,0,0,0,4
1,470,2,2,-4,330,-2,1
86.936,"",""
2047001,"BIRNESSITE",0,-18.09,0,0,0,0,0,0,4
-4,330,-1,1,1,471,2,2
86.9368,"",""
2047002,"NSUTITE",0,-17.5,0,0,0,0,0,0,4
```

```
-4,330,-1,1,1,471,2,2
86.9368,"",""
3047100,"BIXBYITE",63.764,0.61,2.226,0.43,0,0,0,0,3
-6,330,2,471,3,2
157.8742,"",""
3047000,"HAUSMANNITE",335.306,-61.54,0,0,0,0,0,0,4
-8,330,-2,1,3,470,4,2
228.8116,"",""
2047003,"PYROCROITE",94.517,-15.08,0,-15.381,0,0,0,0,3
-2,330,1,470,2,2
88.9528,"",""
2047004,"MANGANITE",0,-25.2,0,0,0,0,0,0,4
-3,330,1,470,2,2,-1,1
87.944,"",""
5047000,"RHODOCHROSIT",0,10,11.01,99.99,3,0,0,0,2
1,470,1,140
114.946,"",""
4147000,"MNCL2, 4H2O",-72.718,-2.71,0,0,0,0,0,0,3
1,470,2,180,4,2
197.9052,"",""
1047000,"MNS GREEN",24.225,-3.8,0,0,0,0,0,0,3
-1,330,1,470,1,730
87.002,"",""
6047000,"MNSO4",64.768,-2.66,0,0,0,0,0,0,2
1,470,1,732
150.9996,"",""
6047100,"MN2(SO4)3",163.427,5.71,0,0,0,0,0,0,2
2,471,3,732
398.0608,"",""
7047000,"MN3(PO4)2Tri",0,30.7,0,0,0,0,0,0,3
3,470,2,580,3,2
408.799,"",""
7047002,"Mn5H2(PO4)4",0,73.44,0,0,0,0,0,0,4
5,470,4,580,2,330,4,2
712.902,"",""
7047003,"MnPO4.1.5H20",0,9.27,0,0,0,0,0,0,4
1,470,1,580,1.5,2,-1,1
176.931,"",""
3041000,"A-CRYPTOMELN",0,0,0,0,0,0,0,0,5
-34,330,16,471,0.8,410,17,2,-7.4,470
775.7382,"",""
3010000,"HOLLANDITE",0,0,0,0,0,0,0,0,6
-32,330,14,471,0.82,100,0.57,280,16,2,-6.41,470
817.4214,"",""
3015000,"TODOROKITE",0,0,0,0,0,0,0,0,6
-24,330,0.393,150,0.473,460,10,471,14,2,-3.866,470
592.4641,"",""
3044000,"LITHIOPHORIT",0,0,0,0,0,0,0,0,6
-70,330,2,440,8,30,20,471,49,2,-8,470
1953.3934,"",""
3015001,"RANCIEITE",0,0,0,0,0,0,0,0,5
-18,330,0.44,150,8,471,12,2,-3.44,470
466.193,"",""
23000,"CU METAL I",-71.672,8.76,0,8.8,0,0,0,0,2
1,230,1,1
63.546,"",""
2023100,"Soil-Cu WLL",0,-2.8,0,0,0,0,0,0,3
1,231,2,2,-2,330
97.561,"",""
4123000,"NANTOKITE",-41.756,6.76,0,6.63,0,0,0,0,2
1,230,1,180
98.999,"",""
4223000,"CUF",51.756,-7.08,0,0,0,0,0,0,2
1,230,1,270
82.5444,"",""
2023000,"CUPRITE",-26.108,1.55,1.87,0.7,0,0,0,0,3
-2,330,2,230,1,2
```

```
143.0914,"","",
1023000,"CHALCOCITE",-206.48,34.61,34.92,30.9,0,0,0,0,3
-1,330,2,230,1,730
159.156,"","",
1023001,"DJURLEITE",-200.33,33.92,0,0,0,0,0,0,4
-1,330,0.066,231,1.868,230,1,730
154.962,"","",
1023002,"ANILITE",-182.13,31.87,0,0,0,0,0,0,4
-1,330,0.25,231,1.5,230,1,730
143.2695,"","",
1023003,"BLAUBLEI II",0,27.27,0,0,0,0,0,0,4
-1,330,0.6,231,0.8,230,1,730
121.0284,"","",
1023100,"BLAUBLEI I",0,24.16,0,0,0,0,0,0,4
-1,330,0.9,231,0.2,230,1,730
101.9646,"","",
1023101,"COVELLITE",-100.458,23.03,0,22.17,0,0,0,0,3
-1,330,1,231,1,730
95.61,"","",
6023000,"CU2SO4",19.079,1.95,0,0,0,0,0,0,2
2,230,1,732
223.1536,"","",
3023000,"CUPROUSFERIT",0,13.53,0,6.88,0,0,0,0,4
-8,330,2,230,2,281,4,2
151.3918,"WLL79",""
4123100,"MELANOTHALLI",51.547,-3.73,0,-4.45,0,0,0,0,2
1,231,2,180
134.452,"","",
5023100,"CUCO3",0,9.63,9.65,9.61,0,0,0,0,2
1,231,1,140
123.5552,"","",
4223100,"CUF2",55.731,0.62,0,0,0,0,0,0,2
1,231,2,270
101.5428,"","",
4223101,"CUF2, 2H2O",15.272,4.55,0,0,0,0,0,0,3
1,231,2,270,2,2
137.5732,"","",
2023100,"CU(OH)2",63.806,-8.64,0,-9.2,0,0,0,0,3
-2,330,1,231,2,2
97.5606,"","",
4123101,"ATACAMITE",78.199,-7.34,-7.24,-7.49,0,0,0,0,4
-3,330,2,231,3,2,1,180
213.5669,"","",
5123100,"CU2(OH)3NO3",72.592,-9.24,0,-9.31,0,0,0,0,4
-3,330,2,231,3,2,1,492
240.1188,"","",
6023100,"ANTLERITE",0,-8.29,0,-8.9,0,0,0,0,4
-4,330,3,231,4,2,1,732
354.7248,"","",
6023101,"BROCHANTITE",0,-15.34,-15.15,-15.5,0,0,0,0,4
-6,330,4,231,6,2,1,732
452.2854,"","",
6023102,"LANGITE",165.728,-16.79,0,-17.4,0,0,0,0,4
-6,330,4,231,7,2,1,732
470.3006,"","",
2023101,"TENORITE",63.764,-7.66,-7.35,-7.89,0,0,0,0,3
-2,330,1,231,1,2
79.5454,"WLL79",""
6023103,"CUOCUSO4",148.825,-11.53,0,0,0,0,0,0,4
-2,330,2,231,1,2,1,732
239.149,"","",
7023100,"CU3(PO4)2",0,36.85,0,36.9,0,0,0,0,2
3,231,2,580
380.5808,"","",
7023101,"CU3(PO4)2,3W",0,35.12,0,0,0,0,0,0,3
3,231,2,580,3,2
434.6264,"","",
```

```
6023104,"CUSO4",75.898,-3.01,-2.63,-3.42,0,0,0,0,2
1,231,1,732
159.6036,"",""
6023105,"CHALCANTHITE",-6.025,2.64,2.96,2.135,0,0,0,0,3
1,231,1,732,5,2
249.6796,"",""
2023102,"DIOPTASE",37.489,-6.5,0,0,0,0,0,0,3
-2,330,1,231,1,770
157.6449,"",""
3023100,"FERRITE CuII",161.879,-10.13,-5.35,0,0,0,0,0,4
-8,330,1,231,2,281,4,2
239.2376,"WLL79",""
1023102,"CHALCOPYRITE",-148.448,35.27,0,30.79,0,0,0,0,4
-2,330,1,231,1,280,2,730
183.513,"",""
4023000,"CUBR",-54.727,8.21,0,0,0,0,0,0,2
1,230,1,130
143.45,"",""
4323000,"CUI",-84.266,11.89,0,0,0,0,0,0,2
1,230,1,380
190.4505,"",""
95000,"ZN METAL",153.888,-25.75,0,-25.79,0,0,0,0,2
1,950,2,1
65.38,"",""
4195000,"ZNCL2",73.136,-7.03,0,-7.06,0,0,0,0,2
1,950,2,180
136.286,"",""
5095000,"SMITHSONITE",18.242,10,10.81,9.82,0,0,0,0,2
1,950,1,140
125.3892,"",""
5095001,"ZNCO3.H20",0,10.26,0,0,0,0,0,0,3
1,950,1,140,1,2
143.4044,"",""
4295000,"ZNF2",54.727,1.52,0,1.08,0,0,0,0,2
1,950,2,270
103.3768,"",""
2095000,"ZN(OH)2 (A)",0,-12.45,-12.26,-12.48,0,0,0,0,3
-2,330,1,950,2,2
99.3946,"",""
2095001,"ZN(OH)2 (C)",0,-12.2,0,0,0,0,0,0,3
-2,330,1,950,2,2
99.3946,"",""
2095002,"ZN(OH)2 (B)",0,-11.75,-11.32,-11.89,0,0,0,0,3
-2,330,1,950,2,2
99.3946,"",""
2095003,"ZN(OH)2 (G)",0,-11.71,-11.19,-11.84,0,0,0,0,3
-2,330,1,950,2,2
99.3946,"",""
2095004,"ZN(OH)2 (E)",0,-11.5,-10.95,-11.62,0,0,0,0,3
-2,330,1,950,2,2
99.3946,"",""
2095007,"Soil-Zn WLL",0,-5.8,0,0,0,0,0,0,3
1,950,2,2,-2,330
99.384,"",""
4195001,"ZN2(OH)3CL",0,-15.2,0,0,0,0,0,0,4
-3,330,2,950,3,2,1,180
217.2349,"",""
4195002,"ZN5(OH)8CL2",0,-38.5,0,0,0,0,0,0,4
-8,330,5,950,8,2,2,180
533.8644,"",""
6095000,"ZN2(OH)2SO4",0,-7.5,0,0,0,0,0,0,4
-2,330,2,950,2,2,1,732
260.8322,"",""
6095001,"ZN4(OH)6SO4",0,-28.4,0,0,0,0,0,0,4
-6,330,4,950,6,2,1,732
459.6214,"",""
5195000,"ZNNO3)2,6H2O",-23.054,-3.44,0,0,0,0,0,0,3
```

```
1,950,2,492,6,2
297.481,"",""
2095005,"ZNO(ACTIVE)",0,-11.31,-11.57,-11.86,0,0,0,0,3
-2,330,1,950,1,2
81.3794,"",""
2095006,"ZINCITE",91.462,-11.14,-10.99,-11.54,0,0,0,0,3
-2,330,1,950,1,2
81.3794,"",""
6095002,"ZN3O(SO4)2",259.408,-19.02,0,0,0,0,0,0,4
-2,330,3,950,2,732,1,2
404.2546,"",""
7095000,"ZN3(PO4),4W",0,32.04,0,0,0,0,0,0,3
3,950,2,580,4,2
458.1436,"",""
1095000,"ZNS (A)",-15.355,9.05,0,0,0,0,0,0,3
-1,330,1,950,1,730
97.44,"",""
1095001,"SPHALERITE",-34.518,11.61,13.212,5.952,0,0,0,0,3
-1,330,1,950,1,730
97.44,"",""
1095002,"WURTZITE",-21.171,9.68,10.182,8.552,0,0,0,0,3
-1,330,1,950,1,730
97.44,"",""
8295000,"ZNSIO3",76.442,-2.93,0,0,0,0,0,0,4
-2,330,-1,2,1,950,1,770
141.4637,"",""
8095000,"WILLEMITE",139.62,-15.33,-13.35,0,0,0,0,0,3
-4,330,2,950,1,770
220.8431,"",""
6095003,"ZINCOSITE",80.333,-3.01,0,-3.93,0,0,0,0,2
1,950,1,732
161.4376,"",""
6095004,"ZNSO4, 1H2O",44.518,0.57,0,0.5,0,0,0,0,3
1,950,1,732,1,2
179.4528,"",""
6095005,"BIANCHITE",0.669,1.76,0,1.02,0,0,0,0,3
1,950,1,732,6,2
269.5288,"",""
6095006,"GOSLARITE",-13.807,1.96,0,1.87,0,0,0,0,3
1,950,1,732,7,2
287.544,"",""
4095000,"ZNBR2, 2H2O",31.422,-5.21,0,0,0,0,0,0,3
1,950,2,130,2,2
261.2184,"",""
4395000,"ZNI2",56.233,-7.23,0,0,0,0,0,0,2
1,950,2,380
319.189,"",""
16000,"CD METAL",75.312,-13.49,0,-13.64,0,0,0,0,2
1,160,2,1
112.41,"",""
16001,"GAMMA CD",75.898,-13.59,0,0,0,0,0,0,2
1,160,2,1
112.41,"",""
5016000,"CdCO3 otavit",2.427,11.99,13.81,11.21,0,0,0,0,2
1,160,1,140
172.4192,"WLL79",""
4116000,"CDCL2",18.702,0.68,0,0.47,0,0,0,0,2
1,160,2,180
183.316,"",""
4116001,"CDCL2, 1H2O",7.615,1.71,0,0,0,0,0,0,3
1,160,2,180,1,2
201.3312,"",""
4116002,"CDCL2,2.5H2O",-7.155,1.94,0,0,0,0,0,0,3
1,160,2,180,2.5,2
228.3536,"",""
4216000,"CDF2",40.668,2.98,0,0,0,0,0,0,2
1,160,2,270
```

```
150.4068,"",""
2016000,"Cd(OH)2 (A)",86.902,-13.65,-13.61,-14.3,0,0,0,0,3
-2,330,1,160,2,2
146.4246,"WLL79",""
2016001,"Cd(OH)2 (C)",0,-13.65,0,0,0,0,0,0,3
-2,330,1,160,2,2
146.4246,"",""
2016003,"Soil-Cd FLK",0,-6.5,0,0,0,0,0,0,3
1,160,2,2,-2,330
146.425,"FLK91",""
4116003,"CDOHCL",30.962,-3.52,-3.3,0,0,0,0,0,4
-1,330,1,160,1,2,1,180
164.8703,"",""
6016000,"CD3(OH)4SO4",0,-22.56,0,0,0,0,0,0,4
-4,330,3,160,4,2,1,732
501.3168,"",""
6016001,"CD3OH2(SO4)2",0,-6.71,0,0,0,0,0,0,4
-2,330,3,160,2,2,2,732
563.3598,"",""
6016002,"CD4(OH)6SO4",0,-28.4,0,0,0,0,0,0,4
-6,330,4,160,6,2,1,732
647.7414,"",""
2016002,"MONTEPONITE",103.596,-15.12,0,-15.74,0,0,0,0,3
-2,330,1,160,1,2
128.4094,"",""
7016000,"Cd3(PO4)2",0,38.1,0,0,0,0,0,0,2
3,160,2,580
527.1728,"WLL79",""
8216000,"CdSIO3",69.58,-7.63,-7.96,0,0,0,0,0,4
-1,2,1,160,1,770,-2,330
188.4937,"WLL79",""
6016003,"CDSO4",61.672,0.1,0.13,0.05,0,0,0,0,2
1,160,1,732
208.4676,"",""
6016004,"CDSO4, 1H2O",31.464,1.65,1.68,1.63,0,0,0,0,3
1,160,1,732,1,2
226.4828,"",""
6016005,"CDSO4,2.7H2O",17.991,1.87,1.89,1.86,0,0,0,0,3
1,160,1,732,2.67,2
256.3879,"",""
1016000,"GREENOCKITE",-68.45,14.17,0,13.112,0,0,0,0,3
-1,330,1,160,1,730
144.47,"WLL79",""
4016000,"CDBR2, 4H2O",-30.25,2.42,0,0,0,0,0,0,3
1,160,2,130,4,2
344.2788,"",""
4316000,"CDI2",-17.071,3.61,0,0,0,0,0,0,2
1,160,2,380
366.219,"",""
60000,"PB METAL",-1.674,-4.27,-4.07,-4.31,0,0,0,0,2
1,600,2,1
207.2,"",""
4160000,"COTUNNITE",-23.43,4.77,4.976,4.67,0,0,0,0,2
1,600,2,180
278.106,"",""
4160001,"MATLOCKITE",-33.263,9.43,0,8.6,0,0,0,0,3
1,600,1,180,1,270
261.6514,"",""
4160002,"PHOSGENITE",0,19.81,19.94,0,0,0,0,0,3
2,600,2,180,1,140
545.3152,"",""
5060000,"PbCO3 cerusi",-20.334,13.5,13.44,12.83,0,0,0,0,2
1,600,1,140
267.2092,"WLL79",""
4260000,"PBF2",2.929,7.44,7.57,0,0,0,0,0,2
1,600,2,270
245.1968,"",""
```

```
2060000,"Pb(OH)2 (c)",0,-8.16,0,0,0,0,0,0,3
-2,330,1,600,1,2
223.1994,"WLL79",""
2060001,"LITHARGE",68.534,-12.72,-12.64,-13.07,0,0,0,0,3
-2,330,1,600,1,2
223.1994,"",""
2060002,"PBO, .3H2O",0,-12.98,0,0,0,0,0,0,3
-2,330,1,600,1.33,2
229.1444,"",""
5060001,"PB2OCO3",47.949,0.5,0.78,0,0,0,0,0,4
-2,330,2,600,1,2,1,140
490.4086,"",""
6060000,"LARNAKITE",26.945,0.28,6.3,0,0,0,0,0,4
-2,330,2,600,1,732,1,2
526.457,"",""
6060001,"PB3O2SO4",86.818,-10.4,0,0,0,0,0,0,4
-4,330,3,600,1,732,2,2
749.6564,"",""
6060002,"PB4O3SO4",146.733,-22.1,0,0,0,0,0,0,4
-6,330,4,600,1,732,3,2
972.8558,"",""
7060001,"Pb5(PO4)3Cl",0,83.7,0,34.51,0,0,0,0,3
5,600,3,580,1,180
1356.3672,"WLL79",""
7060002,"HXYPYROMORPH",0,62.79,0,0,0,0,0,0,4
-1,330,5,600,3,580,1,2
1337.9215,"",""
5060002,"PB3O2CO3",110.583,-11.02,0,0,0,0,0,0,4
-4,330,3,600,1,140,2,2
713.608,"",""
7060003,"PLUMBGUMMITE",0,32.79,0,0,0,0,0,0,5
-5,330,1,600,3,30,2,580,6,2
581.1391,"",""
7060004,"HINSDALITE",0,2.5,0,0,0,0,0,0,6
-6,330,1,600,3,30,1,580,1,732,6,2
581.2174,"",""
7060005,"TSUMEBITE",0,9.79,0,0,0,0,0,0,5
-3,330,2,600,1,231,1,580,6,2
677.9849,"",""
8260000,"PbSiO3",38.744,-5.94,-6.12,-7.64,0,0,0,0,4
-1,2,-2,330,1,600,1,770
283.2837,"WLL79",""
8060000,"PB2SIO4",108.784,-19.76,-19.22,-20.05,0,0,0,0,3
-4,330,2,600,1,770
506.4831,"",""
6060003,"PbSO4 angls",-8.996,7.79,7.87,0,0,0,0,0,2
1,600,1,732
303.2576,"WLL79",""
1060001,"PbS galena",-81.17,14.61,16.452,13.682,0,0,0,0,3
-1,330,1,600,1,730
239.26,"WLL79",""
2060003,"PLATTNERITE",295.934,-49.3,-49,0,0,0,0,0,4
-4,330,-2,1,1,600,2,2
239.1988,"",""
3060000,"PB2O3",0,-61.04,0,0,0,0,0,0,4
-6,330,-2,1,2,600,3,2
462.3982,"",""
3060001,"MINIUM",429.948,-73.69,-70.8,0,0,0,0,0,4
-8,330,-2,1,3,600,4,2
685.5976,"",""
160003,"LAURIONITE",0,-0.62,-0.175,0,0,0,0,0,4
-1,330,1,600,1,180,1,2
259.6603,"",""
4160004,"PB2(OH)3CL",0,-8.79,0,0,0,0,0,0,4
-3,330,2,600,3,2,1,180
500.8749,"",""
5060003,"HYDCERRUSITE",0,17.46,0,0,0,0,0,0,4
```

```
-2,330,3,600,2,140,2,2
775.633,"",""
2060005,"PB2O(OH)2",0,-26.2,0,-27.1,0,0,0,0,3
-4,330,2,600,3,2
464.414,"",""
4060000,"PBBR2",-33.89,5.18,5.34,4.41,0,0,0,0,2
1,600,2,130
367.008,"",""
4060001,"PBBRF",0,8.49,0,0,0,0,0,0,3
1,600,1,130,1,270
306.1024,"",""
4360000,"PBI2",-63.429,8.07,0,0,0,0,0,0,2
1,600,2,380
461.009,"",""
6060004,"PB4(OH)6SO4",0,-21.1,0,0,0,0,0,0,4
-6,330,4,600,1,732,6,2
1026.9014,"",""
5054000,"NICO3",41.589,6.84,0,0,0,0,0,0,2
1,540,1,140
118.7092,"",""
2054000,"NI(OH)2",-127.403,-10.8,-10.59,-13.3,0,0,0,0,3
-2,330,1,540,2,2
92.7146,"",""
2054002,"Soil-Ni ABL",0,-6.95,0,0,0,0,0,0,3
1,540,2,2,-2,330
92.704,"",""
6054000,"NI4(OH)6SO4",0,-32,0,0,0,0,0,0,4
-6,330,4,540,1,732,6,2
432.9014,"",""
2054001,"BUNSENITE",100.081,-12.45,0,-12.39,0,0,0,0,3
-2,330,1,540,1,2
74.6994,"",""
7054000,"NI3(PO4)2",0,31.3,0,0,0,0,0,0,2
3,540,2,580
366.0428,"",""
1054000,"MILLERITE",-10.46,8.04,8.132,0,0,0,0,0,3
-1,330,1,540,1,730
90.76,"",""
6054001,"RETGERSITE",-4.602,2.04,0,0,0,0,0,0,3
1,540,1,732,6,2
262.8488,"",""
6054002,"MORENOSITE",-12.301,2.36,0,0,0,0,0,0,3
1,540,1,732,7,2
280.864,"",""
8054000,"NI2SIO4",139.578,-14.54,0,0,0,0,0,0,3
-4,330,2,540,1,770
209.4831,"",""
2000,"AG METAL",-105.562,13.51,0,0,0,0,0,0,2
1,20,1,1
107.868,"",""
4002000,"BROMYRITE",-84.391,12.27,0,0,0,0,0,0,2
1,20,1,130
187.772,"",""
4102000,"CERARGYRITE",-65.48,9.75,0,0,0,0,0,0,2
1,20,1,180
143.321,"",""
5002000,"AG2CO3",-39.874,11.07,0,0,0,0,0,0,2
2,20,1,140
275.7452,"",""
4202000,"AGF.4H2O",-17.866,-0.55,0,0,0,0,0,0,3
1,20,1,270,4,2
198.9272,"",""
4302000,"IODYRITE",-112.215,16.07,0,0,0,0,0,0,2
1,20,1,380
234.7725,"",""
2002000,"AG2O",43.639,-12.58,0,0,0,0,0,0,3
-2,330,2,20,1,2
```

```
231.7354,"",""
7002000,"AG3PO4",0,17.55,0,0,0,0,0,0,2
3,20,1,580
418.5754,"",""
1002000,"ACANTHITE",-223.007,36.05,0,0,0,0,0,0,3
-1,330,2,20,1,730
247.796,"",""
6002000,"AG2SO4",-17.782,4.92,0,0,0,0,0,0,2
2,20,1,732
311.7936,"",""
8450001,"ANALCIME",95.563,-8.15,0,0,0,0,0,0,5
1,500,1,30,2,770,-1,2,-4,330
220.155,"WLL79",""
8603000,"HALLOYSITE",166.23,-8.72,0,0,0,0,0,0,4
2,30,2,770,1,2,-6,330
258.162,"WLL79",""
8603001,"KAOLINITE",147.612,-5.45,0,0,0,0,0,0,4
2,30,2,770,1,2,-6,330
258.162,"WLL79",""
8415000,"LEONHARDITE",357.146,-17.29,0,0,0,0,0,0,5
-1,2,-16,330,2,150,8,770,4,30
922.867,"WLL79",""
8450002,"LOW ALBITE",72.802,-2.74,0,0,0,0,0,0,5
1,500,1,30,3,770,-4,330,-4,2
262.225,"WLL79",""
8450003,"ANALBITE",83.68,-3.67,0,0,0,0,0,0,5
1,500,1,30,3,770,-4,330,-4,2
262.225,"WLL79",""
8641000,"MUSCOVITE",248.279,-13.44,0,0,0,0,0,0,4
1,410,3,30,3,770,-10,330
398.311,"WLL79",""
8641001,"ANNITE",274.972,-23.29,0,0,0,0,0,0,5
1,410,3,280,1,30,3,770,-10,330
511.89,"",""
8415001,"ANORTHITE",295.641,-26.1,0,0,0,0,0,0,4
1,150,2,30,2,770,-8,330
278.211,"WLL79",""
8603002,"PYROPHYLLITE",0,1.92,0,0,0,0,0,0,4
2,30,4,770,-4,2,-6,330
360.3138,"WLL79",""
8415002,"LAUMONTITE",211.083,-14.46,0,0,0,0,0,0,4
1,150,2,30,4,770,-8,330
470.441,"",""
8415003,"WAIRAKITE",264.22,-16.25,0,0,0,0,0,0,5
1,150,2,30,4,770,-8,330,-2,2
434.411,"WLL79",""
5023101,"MALACHITE",65.312,5.18,0,3.94,0,0,0,0,4
2,231,2,2,1,140,-2,330
221.1162,"",""
5023102,"AZURITE",99.454,16.92,0,0,0,0,0,0,4
3,231,2,2,2,140,-2,330
344.6716,"",""
3006000,"ARSENOLITE",-59.957,2.8,2.859,2.728,0,0,0,0,2
4,60,-6,2
395.6824,"",""
3006001,"CLAUDETITE",-55.605,3.06,0,3.021,0,0,0,0,2
4,60,-6,2
395.6824,"",""
4306000,"ASI3",-7.824,-4.15,0,0,0,0,0,0,4
1,60,3,380,3,330,-3,2
455.6347,"",""
1006000,"ORIPMENT",-346.812,60.97,0,46.004,0,0,0,0,4
2,60,3,730,3,330,-6,2
246.035,"",""
1006001,"REALGAR",-127.779,19.74,26.574,0,0,0,0,0,5
1,60,1,730,2,330,1,1,-3,2
106.9855,"",""
```

```
3006100,"AS2O5",22.594,-6.69,0,-9.478,0,0,0,0,2
2,61,-3,2
229.84,"",""
74001,"Sb",-83.868,11.7058,0,0,0,0,0,0,4
1,740,3,330,3,1,-3,2
121.75," ",""
1074000,"Sb2S3 Stib",-289.909,60.156,0,0,0,0,0,0,4
2,740,3,730,3,330,-6,2
339.698," ",""
1274000,"Sb2Se3",-343.046,67.7571,0,0,0,0,0,0,4
2,740,3,760,3,330,-6,2
480.38," ",""
1474001,"NiSb Breitha",-96.002,18.5225,0,0,0,0,0,0,5
1,740,5,1,3,330,1,540,-3,2
180.44," ",""
1474002,"ZnSb",54.877,-11.0138,0,0,0,0,0,0,5
1,740,5,1,1,950,3,330,-3,2
187.14," ",""
1474003,"AlSb",0,-65.6241,0,0,0,0,0,0,5
1,740,6,1,1,30,3,330,-3,2
148.7315," ",""
1474004,"CdSb",-22.363,0.3943,0,0,0,0,0,0,5
1,740,5,1,3,330,1,160,-3,2
234.161," ",""
1474005,"Mg2Sb3",0,-74.6838,0,0,0,0,0,0,5
2,460,3,740,9,330,13,1,-9,2
413.86," ",""
1474006,"Ag3Sb",0,56.1818,0,0,0,0,0,0,5
1,740,6,1,3,20,3,330,-3,2
445.3546," ",""
1474007,"Na3Sb",431.977,-94.4084,0,0,0,0,0,0,5
3,500,1,740,3,330,6,1,-3,2
190.7193," ",""
1474008,"NaSb",93.659,-23.177,0,0,0,0,0,0,5
1,500,1,740,3,330,4,1,-3,2
144.7398," ",""
1474009,"Mn2Sb",0,-61.0796,0,0,0,0,0,0,5
2,470,1,740,7,1,3,330,-3,2
231.6261," ",""
1474010,"Ca3Sb2",732.744,-142.9738,0,0,0,0,0,0,5
3,150,2,740,6,330,12,1,-6,2
363.734," ",""
1474011,"USb2",103.261,-29.5246,0,0,0,0,0,0,5
1,893,2,740,12,1,10,330,-8,2
481.5289," ",""
1474012,"Cu2Sb",-233.237,34.8827,0,0,0,0,0,0,5
1,740,6,1,3,330,1,230,1,231
248.842," ",""
1474013,"MnSb",-21.108,2.9099,0,0,0,0,0,0,5
1,471,1,740,6,1,3,330,-3,2
176.6881," ",""
1474014,"Cu3Sb",-308.131,42.5937,0,0,0,0,0,0,5
1,740,6,1,3,330,3,230,-3,2
312.388," ",""
1474015,"U3Sb4",986.252,-152.3288,0,0,0,0,0,0,5
3,891,4,740,24,1,12,330,-12,2
1201.0867," ",""
2074001,"Sb2O4",68.074,-3.4597,0,0,0,0,0,0,4
2,740,-2,2,-2,330,-2,1
307.4976," ",""
2074002,"Sb4O6 II,CUB",-61.086,19.6586,0,0,0,0,0,0,2
4,740,-6,2
582.9964," ",""
2074003,"Sb4O6 I,ORTH",-37.614,17.0346,0,0,0,0,0,0,2
4,740,-6,2
582.9964,"",""
2074004,"Sb(OH)3 (s)",-30.125,7.1099,0,0,0,0,0,0,1
```

```
1,740
172.7719," ",""
2074005,"Cu(SbO3)2",0,-45.2105,0,0,0,0,0,0,4
2,740,1,231,-6,330,-4,1
403.0424," ",""
2074006,"Sb2O3 SENARM",-30.648,12.3654,0,0,0,0,0,0,2
2,740,-3,2
291.4982," ",""
2074007,"Sb2O3 VALENT",-19.016,8.4806,0,0,0,0,0,0,2
2,740,-3,2
291.4982," ",""
2074100,"Sb2O5",0,12.4827,0,0,0,0,0,0,3
2,741,2,330,-7,2
323.497," ",""
2074102,"SbO2",0,27.8241,0,0,0,0,0,0,4
1,741,1,1,2,330,-4,2
153.7488," ",""
4074000,"SbBr3",21.221,-1.0562,0,0,0,0,0,0,4
1,740,3,130,3,330,-3,2
361.462," ",""
4174000,"SbCl3",35.204,-0.5915,0,0,0,0,0,0,4
1,740,3,180,3,330,-3,2
228.1081," ",""
4274000,"SbF3",6.728,10.2251,0,0,0,0,0,0,4
1,740,3,330,3,270,-3,2
178.7452," ",""
4374000,"SbI3",-13.59,0.538,0,0,0,0,0,0,4
1,740,3,330,3,380,-3,2
502.4634," ",""
5295000,"ZN(BO2)2",0,-8.29,0,0,0,0,0,0,4
-2,2,-2,330,1,950,2,90
150.9893,"",""
5216000,"CD(BO2)2",0,-9.84,0,0,0,0,0,0,4
-2,2,-2,330,1,160,2,90
198.0188,"",""
5260000,"PB(BO2)2",24.267,-7.61,0,0,0,0,0,0,4
-2,2,-2,330,1,600,2,90
292.8093,"",""
7047001,"MNHPO43H2O",0,19.79,0,0,0,0,0,0,4
1,470,1,580,1,330,3,2
204.961,"",""
7060006,"PbHPO4 (c)",0,23.8,0,0,0,0,0,0,3
1,600,1,580,1,330
303.1693,"WLL79",""
7060007,"PB3(PO4)2",0,44.5,0,0,0,0,0,0,2
3,600,2,580
811.5125,"",""
73100,"SULFUR",17.573,2.11,0,0,0,0,0,0,3
1,730,-1,330,-2,1
32.064,"",""
7203000,"ALASO4.2W",0,-4.8,0,0,0,0,0,0,4
1,30,1,61,2,2,-3,330
165.9006,"",""
7215000,"CA3(ASO4)26W",0,-22.3,0,0,0,0,0,0,4
3,150,2,61,4,2,-6,330
506.17,"",""
7223100,"CU3(ASO4)26W",0,-6.1,0,0,0,0,0,0,4
3,231,2,61,2,2,-6,330
576.568,"",""
7228100,"FEASO4.2W",0,-0.4,0,0,0,0,0,0,4
1,281,1,61,2,2,-3,330
230.7967,"",""
7247000,"MN3ASO428W",0,-12.5,0,0,0,0,0,0,4
3,470,2,61,8,2,-6,330
586.7746,"",""
7254000,"NI3(ASO4)28W",0,-15.7,0,0,0,0,0,0,4
3,540,2,61,8,2,-6,330
```

```
459.1707,"",""
7260000,"PB3(ASO4)2",0,-5.8,0,0,0,0,0,0,3
3,600,2,61,-6,330
899.4079,"",""
7295000,"ZN3ASO422.5W",0,-13.65,0,0,0,0,0,0,4
3,950,2,61,2.5,2,-6,330
518.9862,"",""
7210000,"BA(ASO4)2",-11.046,8.91,0,0,0,0,0,0,3
3,100,2,61,-6,330
689.8582,"",""
90000,"V METAL",263.174,-42.35,0,0,0,0,0,0,2
1,901,3,1
50.94,"",""
2090000,"VO",117.236,-13.08,0,0,0,0,0,0,4
-2,330,1,901,1,2,1,1
66.939,"",""
4190000,"VCL2",149.787,-17.97,0,0,0,0,0,0,3
1,901,2,180,1,1
121.846,"",""
3090100,"V2O3",82.508,-4.9,0,0,0,0,0,0,3
-3,330,1,901,1.5,2
149.878,"",""
2090100,"V(OH)3",0,-7.65,0,0,0,0,0,0,3
-3,330,1,901,3,2
101.962,"",""
4190100,"VCL3",183.929,-21.73,0,0,0,0,0,0,2
1,901,3,180
157.299,"",""
4190101,"VOCL",109.495,-9.41,0,0,0,0,0,0,4
1,901,1,180,1,2,-2,330
137.845,"",""
3090200,"V2O4",58.869,-4.27,0,0,0,0,0,0,3
-2,330,1,902,1,2
165.878,"",""
2090200,"VO(OH)2",0,-5.85,0,0,0,0,0,0,3
-2,330,1,902,2,2
100.954,"",""
4290200,"VF4",199.117,-14.93,0,0,0,0,0,0,4
-1,2,1,902,4,270,2,330
126.932,"",""
6090200,"VOSO4 (C)",86.692,-3.57,0,0,0,0,0,0,2
1,902,1,732
162.997,"",""
7090200,"(VO)3(PO4)2",0,8.37,0,0,0,0,0,0,2
1,902,0.667,580
390.753,"",""
4190200,"VOCL2",117.989,-12.79,0,0,0,0,0,0,2
1,902,2,180
137.845,"",""
3090300,"V2O5",17.405,0.72,0,0,0,0,0,0,3
-1,330,1,903,0.5,2
181.877,"",""
7315000,"TYUYAMUNITE",76.567,-2.04,0,0,0,0,0,0,5
-4,330,0.5,150,1,893,1,903,2,2
810.013,"",""
7315001,"CA-VANADATE",42.384,-2.83,0,0,0,0,0,0,4
-2,330,0.5,150,1,903,1,2
237.956,"",""
7315002,"CA3(VO4)2",146.733,-19.48,0,0,0,0,0,0,4
-4,330,1.5,150,1,903,2,2
350.115,"",""
7315003,"CA2V2O7",79.747,-8.75,0,0,0,0,0,0,4
-3,330,1,150,1,903,1.5,2
294.036,"",""
7328000,"FE-VANADATE",30.836,1.86,0,0,0,0,0,0,4
-2,330,0.5,280,1,903,1,2
508.431,"",""
```

```
7346000,"MG-VANADATE",68.325,-5.64,0,0,0,0,0,0,4
-2,330,0.5,460,1,903,1,2
222.186,"",""
7346001,"MG2V2O7",127.612,-13.18,0,0,0,0,0,0,4
-3,330,1,460,1,903,1.5,2
262.496,"",""
7347000,"MN-VANADATE",46.233,-2.45,0,0,0,0,0,0,4
-2,330,0.5,470,1,903,1,2
252.816,"",""
7349000,"NH4VO3",15.774,-2.69,0,0,0,0,0,0,4
-2,330,1,490,1,903,1,2
116.977,"",""
7350000,"NA-VANADATE",29.33,-3.71,0,0,0,0,0,0,4
-2,330,1,500,1,903,1,2
121.928,"",""
7350001,"NA3VO4",185.853,-36.94,0,0,0,0,0,0,4
-4,330,3,500,1,903,2,2
183.908,"",""
7350002,"NA4V2O7",100.542,-18.7,0,0,0,0,0,0,4
-3,330,2,500,1,903,1.5,2
305.836,"",""
7360000,"PB3(VO4)2",36.317,-3.07,0,0,0,0,0,0,4
-4,330,1.5,600,1,903,2,2
851.475,"",""
7360001,"PB2V2O7",13.472,0.95,0,0,0,0,0,0,4
-3,330,1,600,1,903,1.5,2
628.276,"",""
7346002,"CARNOTITE",36.401,-0.23,0,0,0,0,0,0,5
-4,330,1,410,1,893,1,903,2,2
848.133,"",""
7302000,"AG-VANADATE",0,-0.77,0,0,0,0,0,0,4
-2,330,1,20,1,903,1,2
206.808,"",""
7302001,"AG2HVO4",0,-1.48,0,0,0,0,0,0,4
-3,330,2,20,1,903,2,2
331.686,"",""
7302002,"AG3H2VO5",0,-5.18,0,0,0,0,0,0,4
-4,330,3,20,1,903,3,2
456.563,"",""
4190300,"VO2CL",40.376,-2.81,0,0,0,0,0,0,2
1,903,1,180
118.392,"",""
3090101,"V3O5",98.45,-1.87,0,0,0,0,0,0,4
-4,330,3,902,2,2,2,1
232.817,"",""
3090201,"V4O7",163.804,-7.14,0,0,0,0,0,0,4
-6,330,4,902,3,2,2,1
315.756,"",""
3090202,"V6O13",-271.5,60.86,0,0,0,0,0,0,4
-2,330,6,903,1,2,4,1
513.632,"",""
2015000,"LIME",193.552,-32.79,0,0,0,0,0,0,3
-2,330,1,150,1,2
56.08,"",""
2015001,"PORTLANDITE",128.407,-22.67,0,0,0,0,0,0,3
-2,330,1,150,2,2
73.088,"",""
2015002,"Soil-Ca",0,2.5,0,0,0,0,0,0,2
1,150,2,2
40.08,"WLL79",""
2046002,"Soil-Mg",0,3,0,0,0,0,0,0,2
1,460,2,2
24.305,"WLL79",""
2028000,"WUSTITE",103.931,-11.68,0,0,0,0,0,0,3
-2,330,0.947,280,1,2
71.85,"",""
2046001,"PERICLASE",151.168,-21.51,0,0,0,0,0,0,3
```

```
-2,330,1,460,1,2
40.32,"",""
3028001,"HERCYNITE",327.858,-27.16,0,0,0,0,0,0,4
-8,330,1,280,2,30,4,2
173.81,"",""
3046000,"SPINEL",372.711,-36.33,0,0,0,0,0,0,4
-8,330,1,460,2,30,4,2
142.28,"",""
3046001,"MAG-FERRITE",278.78,-16.76,0,0,0,0,0,0,4
-8,330,1,460,2,281,4,2
200.02,"",""
4250000,"CRYOLITE",-45.606,31.49,0,0,0,0,0,0,3
1,30,3,500,6,270
209.953,"",""
8215002,"WOLLASTONITE",81.546,-12.99,0,0,0,0,0,0,4
-1,2,-2,330,1,770,1,150
116.17,"",""
8215003,"P-WOLLSTANIT",88.115,-13.84,0,0,0,0,0,0,4
-1,2,-2,330,1,770,1,150
116.17,"",""
8015001,"CA-OLIVINE",228.823,-37.64,0,0,0,0,0,0,3
-4,330,1,770,2,150
172.25,"",""
8015002,"LARNITE",239.45,-39.14,0,0,0,0,0,0,3
-4,330,1,770,2,150
172.25,"",""
8015007,"CA3SIO5",444.885,-73.86,0,0,0,0,0,0,4
-6,330,1,770,3,150,1,2
228.33,"",""
8015003,"MONTICELLITE",206.773,-30.27,0,0,0,0,0,0,4
-4,330,1,770,1,150,1,460
156.49,"",""
8015005,"AKERMINITE",319.825,-47.47,0,0,0,0,0,0,5
-1,2,-6,330,2,770,2,150,1,460
272.66,"",""
8015004,"MERWINITE",448.148,-68.54,0,0,0,0,0,0,4
-8,330,2,770,1,460,3,150
328.74,"",""
8441000,"KALSILITE",120.959,-12.83,0,0,0,0,0,0,4
-4,330,1,770,1,30,1,410
158.17,"",""
8441001,"LEUCITE",92.383,-6.42,0,0,0,0,0,0,5
-2,2,-4,330,2,770,1,30,1,410
278.26,"",""
8441002,"MICROCLINE",51.463,-0.61,0,0,0,0,0,0,5
-4,2,-4,330,3,770,1,30,1,410
378.35,"",""
8441003,"H SANIDINE",59.622,-1.06,0,0,0,0,0,0,5
-4,2,-4,330,3,770,1,30,1,410
378.35,"",""
8450004,"NEPHELINE",138.909,-14.21,0,0,0,0,0,0,4
-4,330,1,770,1,30,1,500
142.061,"",""
8015006,"GEHLENITE",485.846,-56.82,0,0,0,0,0,0,5
-10,330,2,30,1,770,2,150,3,2
374.21,"",""
8650000,"NA-NONTRONIT",0,14.5,12.122,16.886,0,0,0,0,6
-7.32,330,-2.68,2,0.33,30,2,281,0.33,500,3.67,770
425.269,"",""
8641002,"K-NONTRONITE",0,15.54,12.763,18.334,0,0,0,0,6
-7.32,330,-2.68,2,0.33,30,2,281,0.33,410,3.67,770
430.585,"",""
8615000,"CA-NONTRONIT",0,20.88,19.057,22.722,0,0,0,0,6
-7.32,330,-2.68,2,0.33,30,2,281,0.167,150,3.67,770
424.375,"",""
8646005,"MG-NONTRONIT",0,20.58,19.013,22.165,0,0,0,0,6
-7.32,330,-2.68,2,0.33,30,2,281,0.167,460,3.67,770
```

```
408.615,"",""
8646006,"Montmorillon",0,-2.68,0,0,0,0,0,0,6
3.81,770,0.49,460,-6.76,330,-3.24,2,0.22,281,1.71,30
371.349,"WLL79",""
8646007,"Chlorite",0,-60.3,0,0,0,0,0,0,5
5,460,2,30,3,770,6,2,-16,330
555.797,"WLL79",""
8646008,"Flurphlogopt",0,-7.85,0,0,0,0,0,0,7
1,410,3,460,1,30,3,770,2,270,-8,330,-2,2
421.242,"WLL79",""
87000,"Tl metal",-5.356,-5.6733,0,0,0,0,0,0,2
1,870,1,1
204.37,"",""
2087000,"Tl2O",96.462,-27.0984,0,0,0,0,0,0,3
2,870,1,2,-2,330
424.7394,"",""
2087001,"TlOH",41.568,-12.9225,0,0,0,0,0,0,3
1,870,1,2,-1,330
221.3773,"",""
4187000,"TlCl",-42.413,3.7243,0,0,0,0,0,0,2
1,870,1,180
239.823,"",""
4087000,"TlBr",-57.074,5.419,0,0,0,0,0,0,2
1,870,1,130
284.274,"",""
4387000,"TlI",-72.304,7.1964,0,0,0,0,0,0,2
1,870,1,380
331.2745,"",""
1087000,"Tl2S",-90.207,7.1832,0,0,0,0,0,0,3
2,870,1,730,-1,330
440.8,"",""
6087000,"Tl2SO4",-33.221,3.6942,0,0,0,0,0,0,2
2,870,1,732
504.7976,"",""
1287000,"Tl2Se",-85.186,6.6848,0,0,0,0,0,0,3
2,870,1,760,-1,330
487.7,"",""
6187000,"Tl2SeO4",-40.836,4.0168,0,0,0,0,0,0,2
2,870,1,762
551.6976,"",""
5187000,"TlNO3",-41.924,1.5319,0,0,0,0,0,0,2
1,870,1,492
266.3749,"",""
5087000,"Tl2CO3",-33.556,3.8482,0,0,0,0,0,0,2
2,870,1,140
468.7492,"",""
2087101,"Tl(OH)3",0,6.4503,0,0,0,0,0,0,1
1,871
255.3919,"",""
2087100,"Avicennite",0,16.3236,0,0,0,0,0,0,2
2,871,-3,2
456.7382,"",""
76000,"Se hex,blac",-15.899,7.6963,0,0,0,0,0,0,3
1,760,-1,330,-2,1
78.96,"",""
76001,"Se (A)",-10.878,7.1099,0,0,0,0,0,0,3
1,760,-1,330,-2,1
78.96,"",""
1228001,"Ferroselite",-47.279,18.5959,0,0,0,0,0,0,4
2,760,1,280,-2,330,-2,1
213.767,"",""
1260000,"Clausthalit",-117.152,21.2162,0,0,0,0,0,0,3
1,760,1,600,-1,330
286.16,"",""
1202000,"Ag2Se",-271.751,43.6448,0,0,0,0,0,0,3
1,760,2,20,-1,330
294.696,"",""
```

```
1216000,"CdSe",-75.981,18.0739,0,0,0,0,0,0,3
1,760,1,160,-1,330
191.37,"",""
1223100,"CuSe",-121.127,26.5121,0,0,0,0,0,0,3
1,760,1,231,-1,330
142.506,"",""
1223000,"Cu2Se alpha",-214.263,36.0922,0,0,0,0,0,0,3
1,760,2,230,-1,330
206.052,"",""
1223101,"CuSe2",-140.582,33.3655,0,0,0,0,0,0,4
2,760,1,231,-2,330,-2,1
221.466,"",""
1223001,"Cu3Se2",-340.327,63.4911,0,0,0,0,0,0,4
2,760,2,230,1,231,-2,330
348.558,"",""
1228000,"FeSe",-2.092,7.1466,0,0,0,0,0,0,3
1,760,1,280,-1,330
134.807,"",""
1247000,"MnSe",56.317,-5.3508,0,0,0,0,0,0,3
1,760,1,470,-1,330
133.898,"",""
1295000,"ZnSe",-26.941,11.3642,0,0,0,0,0,0,3
1,760,1,950,-1,330
144.34,"",""
1220000,"CoSe",0,16.2723,0,0,0,0,0,0,3
1,760,1,200,-1,330
137.8932,"",""
1254000,"NiSe",0,17.7382,0,0,0,0,0,0,3
1,760,1,540,-1,330
137.66,"",""
2076100,"SeO2",-1.402,-0.1246,0,0,0,0,0,0,3
1,761,1,330,-1,2
110.9588,"",""
6110000,"BaSeO3",26.276,-4.1634,0,0,0,0,0,0,3
1,761,1,100,-1,330
264.2882,"",""
6115000,"CaSeO3:2H2O",19.456,-2.8139,0,0,0,0,0,0,4
1,761,1,150,2,2,-1,330
203.0686,"",""
6123100,"CuSeO3:2H2O",36.861,-0.4838,0,0,0,0,0,0,4
1,761,1,231,2,2,-1,330
226.5346,"",""
6128100,"Fe2(SeO3)3:",0,20.6262,0,0,0,0,0,0,4
3,761,2,281,2,2,-3,330
528.599,"",""
6128101,"Fe2(OH)4SeO",0,-1.5539,0,0,0,0,0,0,4
1,761,2,281,4,2,-5,330
306.6814,"",""
6146000,"MgSeO3:6H2O",-5.23,-4.0314,0,0,0,0,0,0,4
1,761,1,460,6,2,-1,330
259.3544,"",""
6147001,"MnSEO3:2H2O",-8.494,-0.9822,0,0,0,0,0,0,4
1,761,1,470,2,2,-1,330
217.9266,"",""
6154000,"NiSeO3:2H2O",31.003,-2.8147,0,0,0,0,0,0,4
1,761,1,540,2,2,-1,330
221.6886,"",""
6180000,"SrSeO3",0,-0.1034,0,0,0,0,0,0,3
1,761,1,800,-1,330
214.5782,"",""
6147000,"MnSeO3",0,-0.044,0,0,0,0,0,0,3
1,761,1,470,-1,330
181.8962,"",""
6120000,"CoSeO3",0,-0.1906,0,0,0,0,0,0,3
1,761,1,200,-1,330
185.8914,"",""
6102000,"Ag2SeO3",-39.622,8.1977,0,0,0,0,0,0,3
```

```
1,761,2,20,-1,330
342.6942,"",""
2076200,"SeO3",146.377,-21.044,0,0,0,0,0,0,3
1,762,2,330,-1,2
126.9582,"",""
6102001,"Ag2SeO4",-43.723,8.9014,0,0,0,0,0,0,2
1,762,2,20
358.6936,"",""
6110001,"BaSeO4",-8.368,5.1895,0,0,0,0,0,0,2
1,762,1,100
280.2876,"",""
6115001,"CaSeO4:2H2O",-3.682,2.9473,0,0,0,0,0,0,3
1,762,1,150,2,2
219.068,"",""
6160000,"PbSeO4",-15.899,6.8387,0,0,0,0,0,0,2
1,762,1,600
350.1576,"",""
6180001,"SrSeO4",-11.255,6.8747,0,0,0,0,0,0,2
1,762,1,800
230.5776,"",""
36000,"Hg metal (l",-83.408,13.4552,0,0,0,0,0,0,2
0.5,360,1,1
200.59,"",""
4036000,"Hg2Br2",-130.758,22.2091,0,0,0,0,0,0,2
1,360,2,130
560.988,"",""
5036000,"Hg2CO3",0,13.9586,0,0,0,0,0,0,2
1,360,1,140
461.1892,"",""
4136000,"Calomel",-98.09,17.8427,0,0,0,0,0,0,2
1,360,2,180
472.086,"",""
4236000,"Hg2F2",18.543,3.0811,0,0,0,0,0,0,2
1,360,2,270
439.1768,"",""
4336000,"Hg2I2",0,28.2782,0,0,0,0,0,0,2
1,360,2,380
654.989,"",""
2036000,"Hg2(OH)2",0,-5.2603,0,0,0,0,0,0,3
1,360,2,2,-2,330
435.1946,"",""
7036000,"Hg2HPO4",0,25.9795,0,0,0,0,0,0,3
1,360,1,330,1,580
497.1593,"",""
1036000,"Hg2S",-69.747,11.6765,0,0,0,0,0,0,3
1,360,1,730,-1,330
433.24,"",""
6036000,"Hg2SO4",-0.962,6.1593,0,0,0,0,0,0,2
1,360,1,732
497.2376,"",""
6136000,"Hg2SeO3",0,4.657,0,0,0,0,0,0,3
1,360,1,761,-1,330
528.1382,"",""
4036100,"HgBr2",-144.147,25.373,0,0,0,0,0,0,4
1,361,2,130,2,330,-2,2
360.398,"",""
5036100,"HgCO3",-92.592,28.6817,0,0,0,0,0,0,4
1,361,1,140,2,330,-2,2
260.5992,"",""
4136100,"HgCl2",-114.073,21.7858,0,0,0,0,0,0,4
1,361,2,180,2,330,-2,2
271.496,"",""
4336100,"Coccinite",-208.079,34.6599,0,0,0,0,0,0,4
1,361,2,380,2,330,-2,2
454.399,"",""
2036100,"Montroydite",-21.401,3.6503,0,0,0,0,0,0,2
1,361,-1,2
```

```
216.5894,"",""
2036101,"Hg(OH)2",0,3.4963,0,0,0,0,0,0,1
1,361
234.6046,"",""
1036100,"Cinnabar",-252.839,45.1885,0,0,0,0,0,0,4
1,361,1,730,1,330,-2,2
232.65,"",""
1036101,"Metacinnaba",-249.074,44.822,0,0,0,0,0,0,4
1,361,1,730,1,330,-2,2
232.65,"",""
6036100,"HgSO4",-14.686,9.4189,0,0,0,0,0,0,4
1,361,1,732,2,330,-2,2
296.6476,"",""
6136100,"HgSeO3",0,12.6953,0,0,0,0,0,0,4
1,361,1,761,1,330,-2,2
327.5482,"",""
4336102,"HgI2:2NH3",-136.532,16.1066,0,0,0,0,0,0,4
1,361,2,380,2,490,-2,2
488.4598,"",""
4336103,"HgI2:6NH3",86.057,-33.8566,0,0,0,0,0,0,5
1,361,2,380,6,490,-2,2,-4,330
556.5814,"",""
2021100,"CR(OH)2",35.606,-10.8189,0,0,0,0,0,0,3
1,210,2,2,-2,330
86.0106,"",""
4021100,"CRBR3",141.323,-19.9086,0,0,0,0,0,0,4
1,211,3,130,2,330,-2,2
291.708,"",""
4121100,"CRCL3",115.098,-13.5067,0,0,0,0,0,0,4
1,211,3,180,2,330,-2,2
158.355,"",""
4221100,"CRF3",18.255,13.2597,0,0,0,0,0,0,4
1,211,3,270,2,330,-2,2
108.9912,"",""
4321100,"CRI3",134.419,-20.4767,0,0,0,0,0,0,4
1,211,3,380,2,330,-2,2
432.7095,"",""
3021100,"FECR2O4",104.014,0.9016,0,0,0,0,0,0,3
2,211,1,280,-4,330
223.8366,"",""
3021101,"MGCR2O4",166.774,-12.0796,0,0,0,0,0,0,3
2,211,1,460,-4,330
192.2946,"",""
21000,"CR METAL",143.511,-32.244,0,0,0,0,0,0,2
1,210,2,1
51.996,"",""
3021102,"CR2O3",50.731,3.3937,0,0,0,0,0,0,3
2,211,-2,330,-1,2
151.9902,"",""
2021102,"CR(OH)3 (A)",0,0.75,0,0,0,0,0,0,3
1,211,1,2,-1,330
103.0179,"",""
2021101,"CR(OH)3 (C)",29.769,-1.7005,0,0,0,0,0,0,3
1,211,1,2,-1,330
103.0179,"",""
4121000,"CRCL2",82.283,-15.8676,0,0,0,0,0,0,2
1,210,2,180
122.902,"",""
3021200,"AG2CRO4",-58.743,11.5548,0,0,0,0,0,0,2
1,212,2,20
331.7296,"",""
3021201,"BACRO4",-26.736,9.6681,0,0,0,0,0,0,2
1,212,1,100
253.3236,"",""
3021202,"CS2CRO4",-31.397,0.5541,0,0,0,0,0,0,2
1,212,2,220
381.8044,"",""
```

```
3021203,"CS2CR2O7",-95.809,17.7793,0,0,0,0,0,0,4
2,212,2,220,2,330,-1,2
481.7986,"",""
3021204,"CUCRO4",0,5.4754,0,0,0,0,0,0,2
1,212,1,231
179.5396,"",""
3021205,"K2CRO4",-17.782,-0.0073,0,0,0,0,0,0,2
1,212,2,410
194.1902,"",""
3021206,"K2CR2O7",-75.835,15.6712,0,0,0,0,0,0,4
2,212,2,410,2,330,-1,2
294.1844,"",""
3021207,"LI2CRO4",45.279,-4.8568,0,0,0,0,0,0,2
1,212,2,440
129.8756,"",""
3021208,"MGCRO4",88.952,-5.3801,0,0,0,0,0,0,2
1,212,1,460
140.2986,"",""
3021209,"(NH4)2CRO4",-9.163,-0.4046,0,0,0,0,0,0,2
1,212,2,490
152.0702,"",""
3021210,"NA2CRO4",19.288,-3.2618,0,0,0,0,0,0,2
1,212,2,500
161.9731,"",""
3021211,"NA2CR2O7",-22.196,9.8953,0,0,0,0,0,0,4
2,212,2,500,2,330,-1,2
261.9673,"",""
3021212,"PBCRO4",-42.802,13.6848,0,0,0,0,0,0,2
1,212,1,600
323.1936,"",""
3021213,"RB2CRO4",-24.652,0.0968,0,0,0,0,0,0,2
1,212,2,680
286.9292,"",""
3021214,"SRCRO4",10.125,4.8443,0,0,0,0,0,0,2
1,212,1,800
203.6136,"",""
2021200,"CrO3",5.209,3.2105,0,0,0,0,0,0,3
1,212,2,330,-1,2
99.9942,"",""
3015000,"CaCrO4",26.945,2.2657,0,0,0,0,0,0,2
1,150,1,212
156.0736,"",""
3036000,"Hg2CrO4",0,8.7031,0,0,0,0,0,0,2
1,360,1,212
517.1736,"",""
3087000,"Tl2CrO4",-105.897,12.0136,0,0,0,0,0,0,2
2,870,1,212
524.7336,"",""
1102001,"Ag4FeCN)6.H2",0,89.69,0,0,0,0,0,0,4
6,143,4,20,1,280,1,2
661.4415," ",""
1102002,"AgCN",-110.395,16.218,0,0,0,0,0,0,2
1,143,1,20
133.8859," ",""
1116001,"Cd2FeCN)6.7H",0,62.982,0,0,0,0,0,0,4
6,143,2,160,1,280,7,2
562.8824," ",""
1121001,"CrCN",0,-23.888,0,0,0,0,0,0,3
1,143,1,210,1,1
78.0138," ",""
1121002,"Cr2CN",0,-56.645,0,0,0,0,0,0,3
1,143,2,210,3,1
130.0099," ",""
1123001,"CuCN",-126.357,19.497,0,0,0,0,0,0,2
1,143,1,230
89.5637," ",""
1123102,"Cu2FeCN)6",0,61.416,0,0,0,0,0,0,3
```

```
6,143,2,231,1,280
339.0454," ",""
1138001,"CNI",72.421,-11.311,0,0,0,0,0,0,3
1,143,1,380,-2,1
152.9222," ",""
1141001,"K12Ni8FeCN67",0,431.09,0,0,0,0,0,0,4
42,143,12,410,8,540,7,280
2422.3737," ",""
1141002,"KCN i, cub",-11.464,-1.44,0,0,0,0,0,0,2
1,143,1,410
65.116," ",""
1141003,"K2CdFeCN)6",0,63.027,0,0,0,0,0,0,4
6,143,2,410,1,160,1,280
402.561," ",""
1141004,"K4Ni4FeCN63",0,183.546,0,0,0,0,0,0,4
18,143,4,410,4,540,3,280
1027.0135," ",""
1141005,"K4FeCN)6",-400.074,48.824,0,0,0,0,0,0,3
6,143,4,410,1,280
368.3466," ",""
1141006,"K2Mn3FeCN62",0,121.001,0,0,0,0,0,0,4
12,143,2,410,3,470,2,280
666.9176," ",""
1141007,"K2Ni3FeCN62",0,123.126,0,0,0,0,0,0,4
12,143,2,410,3,540,2,280
678.1735," ",""
1141008,"K4FeCN6.3H",-414.948,49.542,0,0,0,0,0,0,4
6,143,4,410,1,280,3,2
422.3925," ",""
1141009,"K12Cd8FeCN67",0,441.985,0,0,0,0,0,0,4
42,143,12,410,8,160,7,280
2852.1417," ",""
1141010,"KZn1.5FeCN)6",0,66.808,0,0,0,0,0,0,4
6,143,1,410,1.5,950,1,280
349.1367," ",""
1141011,"K3Fe(CN)6",-348.485,54.644,0,0,0,0,0,0,3
6,143,3,410,1,281
329.2483," ",""
1141012,"K8Mn6FeCN65",0,293.684,0,0,0,0,0,0,4
30,143,8,410,6,470,5,280
1702.1819," ",""
1141013,"K2Cu2FeCN)6",0,72.514,0,0,0,0,0,0,4
6,143,2,410,2,230,1,280
417.242," ",""
1147014,"Mn2Fe(CN)6",0,59.027,0,0,0,0,0,0,3
6,143,2,470,1,280
321.8295," ",""
1150001,"NaCN cri,cub",2.176,-2.286,0,0,0,0,0,0,2
1,143,1,500
49.0075," ",""
1160001,"Pb2FeCN6.3H",0,63.601,0,0,0,0,0,0,4
6,143,2,600,1,280,3,2
680.3993," ",""
1187001,"Tl4FeCN6.2H",0,56.916,0,0,0,0,0,0,4
6,143,4,870,1,280,2,2
1065.5172," ",""
1195001,"Zn2FeCN6.2H",0,61.232,0,0,0,0,0,0,4
6,143,2,950,1,280,2,2
378.764," ",""
7756001,"AgOCN",-55.124,6.615,0,0,0,0,0,0,2
1,560,1,20
149.8853," ",""
1102002,"Ag4Fe(CN)6",-1091.647,193.914,0,0,0,0,0,0,3
6,143,4,20,1,280
133.8859," ",""
1116002,"Cd2Fe(CN)6",0,28.224,0,0,0,0,0,0,3
6,143,2,160,1,280
```

```
436.7754," ",""
1136100,"Hg(CN)2",-254.094,45.379,0,0,0,0,0,0,4
1,361,2,143,2,330,-2,2
252.6255," ",""
1160002,"Pb2Fe(CN)6",0,27.589,0,0,0,0,0,0,3
6,143,2,600,1,280
626.3534," ",""
1195002,"Zn2Fe(CN)6",0,29.926,0,0,0,0,0,0,3
6,143,2,950,1,280
342.7334," ",""
0,"",0,0,0,0,0,0,0,0,0
0,"","",""
2812800,"Fe+3/Fe+2",-41.84,13.04,0,0,0,0,0,0,3
1,281,-1,280,1,1
0,"WLL79",""
4914920,"NO2/NO3",-183.092,28.57,0,0,0,0,0,0,5
1,492,-1,491,2,330,2,1,-1,2
0,"","",""
4904920,"NH4/NO3",-782.638,119.077,0,0,0,0,0,0,5
-1,490,1,492,-3,2,10,330,8,1
0,"","",""
600610,"ASO3/ASO4",-125.583,19.444,0,0,0,0,0,0,5
1,61,2,1,2,330,-1,60,-1,2
0,"","",""
7407410,"SbOH6-/SbOH3",0,25.7791,0,0,0,0,0,0,5
-1,740,1,741,2,1,3,330,-3,2
0,"","",""
8908930,"U+3/UO2+2",-41.966,0.42,0,0,0,0,0,0,5
1,893,3,1,4,330,-1,890,-2,2
0,"","",""
8918930,"U+4/UO2+2",-144.055,9.216,0,0,0,0,0,0,5
1,893,2,1,4,330,-1,891,-2,2
0,"","",""
8928930,"UO2+/UO2+2",-13.807,2.785,0,0,0,0,0,0,3
1,893,1,1,-1,892
0,"","",""
4714700,"Mn+3/Mn+2",107.78,25.55,0,0,0,0,0,0,3
1,471,1,1,-1,470
0,"WLL79",""
4724700,"Mn+4/Mn+2",0,51.06,0,0,0,0,0,0,3
1,472,2,1,-1,470
0,"WLL79",""
2312300,"Cu+2/Cu+1",6.904,2.62,0,0,0,0,0,0,3
1,231,1,1,-1,230
0,"WLL79",""
9009030,"V+2/VO2+1",-147.821,18.38,0,0,0,0,0,0,5
1,903,3,1,4,330,-1,900,-2,2
0,"","",""
9019030,"V+3/VO2+1",-185.058,22.61,0,0,0,0,0,0,5
1,903,2,1,4,330,-1,901,-2,2
0,"","",""
9029030,"VO+2/VO2+1",-122.675,16.93,0,0,0,0,0,0,5
1,903,1,1,2,330,-1,902,-1,2
0,"","",""
7307320,"HS-/SO4-2",-251.626,33.66,0,0,0,0,0,0,5
1,732,9,330,8,1,-1,730,-4,2
0,"","",""
8718700,"Tl(OH)3/Tl+",0,48.0178,0,0,0,0,0,0,5
1,871,2,1,3,330,-1,870,-3,2
0,"","",""
7617600,"HSeO3-/HSe-",-327.063,44.866,0,0,0,0,0,0,5
1,761,6,1,6,330,-1,760,-3,2
0,"","",""
7627600,"SeO4-2/HSe-",-528.439,81.185,0,0,0,0,0,0,5
1,762,8,1,9,330,-1,760,-4,2
0,"","",""
7627610,"SeO4/HSeO3-",-201.229,36.319,0,0,0,0,0,0,5
```

```
1,762,2,1,3,330,-1,761,-1,2
0,"","",""
3613600,"Hg(OH)2/Hg2",-266.061,42.987,0,0,0,0,0,0,5
2,361,4,330,2,1,-1,360,-4,2
0,"","",""
2102110,"CR+2/CR(OH)2",-26.61,-2.947,0,0,0,0,0,0,5
1,210,2,2,-1,211,-2,330,-1,1
0,"","",""
2122110,"CRO4/CR(OH)2",-430.952,67.376,0,0,0,0,0,0,5
1,212,6,330,3,1,-1,211,-2,2
0,"","",""
3301404,"CH4 (g)",-255.224,40.1,0,0,0,0,0,0,4
1,140,8,1,10,330,-3,2
16.0432,"","",""
3301403,"CO2 (g)",-2.218,18.15,0,0,0,0,0,0,3
1,140,2,330,-1,2
41.01,"WLL79","",""
3300021,"O2 (g)",559.945,-83.12,0,0,0,0,0,0,3
2,2,-4,330,-4,1
31.9988,"WLL79","",""
3600001,"Hg (g)",-22.029,7.8708,0,0,0,0,0,0,2
0.5,360,1,1
200.59,"","",""
3600002,"Hg2 (g)",-58.032,14.963,0,0,0,0,0,0,2
1,360,2,1
401.18,"","",""
3611400,"Hg(CH3)2(g)",-482.834,73.724,0,0,0,0,0,0,5
1,361,2,140,16,1,20,330,-8,2
230.6594,"","",""
3601300,"HgBr (g)",142.273,-16.79,0,0,0,0,0,0,2
0.5,360,1,130
280.494,"","",""
3601800,"HgCl (g)",167.77,-20.5,0,0,0,0,0,0,2
0.5,360,1,180
236.043,"","",""
3602700,"HgF (g)",254.873,-32.72,0,0,0,0,0,0,2
0.5,360,1,270
219.5884,"","",""
3603800,"HgI (g)",105.705,-11.15,0,0,0,0,0,0,2
0.5,360,1,380
327.4945,"","",""
3611300,"HgBr2 (g)",-60.04,18.47,0,0,0,0,0,0,4
1,361,2,130,2,330,-2,2
360.398,"","",""
3612700,"HgF2 (g)",0,-0.38,0,0,0,0,0,0,4
1,361,2,270,2,330,-2,2
238.5868,"","",""
3613800,"HgI2 (g)",-119.788,27.28,0,0,0,0,0,0,4
1,361,2,380,2,330,-2,2
454.399,"","",""
3300010,"H2 (g)",0,0,0,0,0,0,0,0,2
2,1,2,330
2.016,"CCL08","",""
0,"",0,0,0,0,0,0,0,0,0
0,"","",""
```