

528395



Sandia National Laboratories

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date: April 21, 2003

to: Laurence Brush, 6822

from: Sue Downes, 6821

Sue Downes

Technical Review NATHALIE A. WALL *AW* Date 4/21/03

QA Review Manio Crespo Date 4/28/03

subject: Spreadsheet Calculations of Actinide Solubilities for the WIPP Compliance Recertification Application

Larry,

This memo documents the method I used to perform the spreadsheet calculations of the summation of Molarities of thorium, neptunium, and americium from the FMT calculations in output files **ap098_fmt_run012**, **ap098_fmt_run018**, **ap098_fmt_run022**, and **ap098_fmt_run028**.

- Attachment 1 contains a printout of the original text output files.
- Attachment 2 contains the imported table for each run (Excel Format).
- Attachments 3, 4, and 5 contain the Molarity summations for thorium, neptunium, and americium, respectively, for each run.

The table below details the methodology.

Methodology for Determining Molarity Summations	
Step 1	Print out original text output file for reference
Step 2	Import table entitled <i>Table of Batch Concentrations for Batch System</i> into Microsoft Excel® 2000
Step 3	Label Worksheet as Original Data
Step 4	Create Sheets called Am, Np, and Th
Step 5	Copy Data (as values) to new sheet named Am
Step 6	In sheet "Am" Search Column Entitled <i>Species</i> for "Am" and mark row
Step 7	Sort Table based on marked row
Step 8	Delete rows that do not contain Am
Step 9	Separate the rows containing data for Am that is in solid form (place in separate table)
Step 10	Sort aqueous data based on descending order of Molarity
Step 11	Sum column titled Molarity
Step 12	Copy Original Data (as values) to sheet named Np
Step 13	In sheet "Np" Search Column Entitled <i>Species</i> for "Np" and mark row
Step 14	Sort Table based on marked row
Step 15	Delete rows that do not contain Np
Step 16	Separate the rows containing data for Np that is in solid form
Step 17	Sort aqueous data based on descending order of Molarity
Step 18	Sum column titled Molarity
Step 19	Copy Original Data (as values) to sheet named Th
Step 20	In sheet "Th" Search Column Entitled <i>Species</i> for "Th" and mark row
Step 21	Sort Table based on marked row
Step 22	Delete rows that do not contain Th
Step 23	Separate the rows containing data for Th that is in solid form (place in separate table)
Step 24	Sort aqueous data based on descending order of Molarity
Step 25	Sum column titled Molarity

File code: WIPP:1.3.5.1.2:PA:QA-L:527285

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ATTACHMENT 1

ap098-fmt_run012

INPUT file name is:AP098\$PROD:[000000]AP098_FMT_RUN012.IN;1
 INGUSS file name is:AP098\$PROD:[000000]AP098_FMT_RUN012.INGUSS;1
 OUTPUT file name is:AP098\$PROD:[000000]AP098_FMT_RUN012.OUT;1
 CHEMDAT file name is AP098\$PROD:[000000]AP098_FMT.CHEMDAT;1
 Temperature is Hard Coded as 298.15K
 CRA GWB recipe, calc
 FMT_021120.chemdat
 ERG update of FMT_970407.chemdat (PAVT db)

FMT V2.4

Accuracy of reactions is 1.0000E-06
 Minimum elemental abundance is 1.0000E-18
 Number of Aqueous Species is 126

PITZER Data Base NOT Echoed in this Run
 using PITZER ACTIVITY COEFFICIENT model
 Charge Balance replaces element Oxygen

Species CaCO3 _____ Aragonite prevented from forming in DISABLE
 Species CaNa2(CO3)2.5H2O _____ Gaylussite prevented from forming in DISABLE
 Species MgCO3 _____ Magnesite prevented from forming in DISABLE
 Species MgCO3.3H2O _____ Nesquehonite prevented from forming in DISABLE
 Species Na2Ca(CO3)2.2H2O _____ Pirssonite prevented from forming in DISABLE
 Species CaMg(CO3)2 _____ Dolomite prevented from forming in DISABLE
 Species Mg5(CO3)4(OH)2.4H2O_HydroMagne5424 prevented from forming in DISABLE
 Species Mg4(CO3)3(OH)2.3H2O_HydroMagne4323 prevented from forming in DISABLE
 fCO2(g) not specified in the INPUT file
 Target pH not specified in the INPUT file
 this is a BATCH problem

- FOR088 file name is AP098\$PROD:[000000]AP098_FMT_RUN012.DAT;1

Ideal Gas Constant is Unity (Dimensionless)
 Temperature = 298.15 [=] degree Kelvin

214 Species 27 Elements

Element Name	Molecular Weight
Hydrogen	1.00790
Oxygen	15.99940
Sodium	22.98977
Potassium	39.09830
Magnesium	24.30500
Calcium	40.08000
Chlorine	35.45300

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ap098_fmt_run012

Sulfur	32.06000
Carbon	12.01100
PosIon:EL	0.00000
NegIon:EL	0.00000
Oxalate:EL	28.84000
Boron	10.81000
Bromine	79.90400
Acetate:EL	59.04400
Th(IV)	232.03810
Am(III)	243.00000
Pu(III)	238.02900
Np(V)	237.04820
ClO4:EL	99.45060
Phosphorus	30.97400
U(IV)	242.00000
Lactate:EL	89.07000
EDTA:EL	888.88800
Citrate:EL	189.10000
Electron:E	0.00000
Charge:EL	0.00000

Species Name	Phase	Mol.Wt.	Std Chemical Potential, u/RT
1 H2O	WATER	18.015	-95.6635
2 Na+	Na+ aqueous	22.990	-105.6510
3 K+	K+ aqueous	39.098	-113.9570
4 Ca++	Ca++ aqueous	40.080	-223.3000
5 Mg++	Mg++ aqueous	24.305	-183.4680
6 MgOH+	MgOH+ aqueous	41.312	-251.9400
7 H+	H+ aqueous	1.008	0.0000
8 Cl-	Cl- aqueous	35.453	-52.9550
9 SO4=	SO4= aqueous	96.058	-300.3860
10 HSO4-	HSO4- aqueous	97.066	-304.9420
11 OH-	OH- aqueous	17.007	-63.4350
12 HCO3-	HCO3- aqueous	61.017	-236.7510
13 CO3=	CO3= aqueous	60.009	-212.9440
14 CO2 (aq)	CO2 (aq) aqueous	44.010	-155.6800
15 CaCO3 (aq)	CaCO3 (aq) aqueous	100.089	-443.5000
16 MgCO3 (aq)	MgCO3 (aq) aqueous	84.314	-403.1550
17 B(OH)3 (aq)	B(OH)3 (aq) aqueous	61.832	-390.8100
18 B(OH)4-	B(OH)4- aqueous	78.839	-465.2000
19 B3O3(OH)4-	B3O3(OH)4- aqueous	148.457	-963.7700
20 B4O5(OH)4=	B4O5(OH)4= aqueous	191.266	-1239.1000
21 CaB(OH)4+	CaB(OH)4+ aqueous	118.919	-692.3000
22 MgB(OH)4+	MgB(OH)4+ aqueous	103.144	-651.8900
23 Br-	Br- aqueous	79.904	-999.9900

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24	ClO4-	perchlorate	aqueous	99.451	-73.8100
25	NaOH(aq)	to.titrate.base.only	aqueous	39.997	500.0000
26	HCl(aq)	to.titrate.acid.only	aqueous	36.461	500.0000
27	HClO4(aq)	to.titrate.acid.only	aqueous	100.459	500.0000
28	PosIon	POSITIVE.ION	aqueous	0.000	0.0000
29	NegIon	NEGATIVE.ION	aqueous	0.000	0.0000
30	PosIon(OH)(aq)	to.titrate.base	aqueous	17.007	500.0000
31	HNegIon(aq)	to.titrate.acid	aqueous	1.008	500.0000
32	H3PO4(aq)	H3PO4(aq)	aqueous	97.995	-460.9000
33	H2PO4-	H2PO4-	aqueous	96.987	-455.9600
34	HPO4=	HPO4=	aqueous	95.980	-439.3670
35	PO4=-	PO4=-	aqueous	94.972	-410.9470
36	Am+++	Am+++	aqueous	243.000	-241.6940
37	AmCO3+	AmCO3+	aqueous	303.009	-473.2900
38	Am(CO3)2-	Am(CO3)2-	aqueous	363.018	-697.5200
39	Am(CO3)3=-	Am(CO3)3=-	aqueous	423.028	-915.5300
40	AmOH++	AmOH++	aqueous	260.007	-319.9600
41	Am(OH)2+	Am(OH)2+	aqueous	277.015	-396.8900
42	Am(OH)3(aq)	Am(OH)3(aq)	aqueous	294.022	-469.5300
43	AmCl++	AmCl++	aqueous	278.453	-295.2000
44	AmCl2+	AmCl2+	aqueous	313.906	-345.9000
45	Am(CO3)4=-	Am(CO3)4=-	aqueous	483.037	-1123.4000
46	Am(SO4)2-	Am(SO4)2-	aqueous	435.115	-850.9900
47	AmSO4+	AmSO4+	aqueous	339.058	-549.5600
48	Pu(OH)2+	deactivated	aqueous	272.044	999.9990
49	Pu(OH)3(aq)	deactivated	aqueous	289.051	999.9990
50	Th++++	Th++++	aqueous	232.038	-284.2270
51	Th(CO3)5===	Th(CO3)5===	aqueous	532.084	-1411.3780
52	Th(OH)3(CO3)-	Th(OH)3(CO3)-	aqueous	343.069	-775.6270
53	Th(OH)4(aq)	Th(OH)4(aq)	aqueous	300.067	-622.4700
54	Th(SO4)2(aq)	Th(SO4)2(aq)	aqueous	424.153	-911.6900
55	Th(SO4)3=	Th(SO4)3=	aqueous	520.211	-1214.0000
56	U++++	U++++	aqueous	242.000	-214.1900
57	UOH+++	UOH+++	aqueous	259.007	-308.7000
58	U(CO3)5===	U(CO3)5===	aqueous	542.046	-1345.3930
59	U(OH)2(CO3)2=	U(OH)2(CO3)2=	aqueous	396.033	-863.3830
60	U(OH)4(CO3)2==	U(OH)4(CO3)2==	aqueous	430.048	-998.6620
61	U(OH)4(aq)	deactivated	aqueous	310.029	999.9990
62	U(SO4)2(aq)	deactivated	aqueous	434.115	999.9990
63	U(SO4)3=	deactivated	aqueous	530.173	999.9990
64	NpO2+	NpO2+	aqueous	269.047	-369.1050
65	NpO2CO3-	NpO2CO3-	aqueous	329.056	-593.6010
66	NpO2(CO3)2=-	NpO2(CO3)2=-	aqueous	389.065	-809.8320
67	NpO2(CO3)3=-	NpO2(CO3)3=-	aqueous	449.075	-1020.2140
68	NpO2OH(aq)	NpO2OH(aq)	aqueous	286.054	-438.7300
69	NpO2(OH)2-	NpO2(OH)2-	aqueous	303.062	-506.2380

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70	HAc (aq)	AceticAcid	aqueous	60.052	-158.3000
71	Ac-	Acetate-	aqueous	59.044	-147.3470
72	H3Citrate(aq)	CitricAcid	aqueous	192.124	0.0000
73	H2Citrate-	H2Citrate-	aqueous	191.116	7.4760
74	HCitrate=	HCitrate=	aqueous	190.108	18.6200
75	Citrate=-	Citrate=-	aqueous	189.100	33.4100
76	H4EDTA(aq)	H4EDTA(aq)	aqueous	892.920	0.0000
77	H3EDTA-	H3EDTA-	aqueous	891.912	5.7610
78	H2EDTA=	H2EDTA=	aqueous	890.904	12.8700
79	HEDTA=-	HEDTA=-	aqueous	889.896	28.7100
80	EDTA==	EDTA==	aqueous	888.888	53.0500
81	H2Ox(aq)	OxalicAcid	aqueous	30.856	0.0000
82	HOx-	Bioxalate-	aqueous	29.848	3.2090
83	Ox=	Oxalate=	aqueous	28.840	13.0170
84	HLactate(aq)	LacticAcid	aqueous	90.078	0.0000
85	Lactate-	Lactate-	aqueous	89.070	8.7980
86	AmAc++	AmAcetate++	aqueous	302.044	-395.3560
87	AmCit(aq)	AmCitrate(aq)	aqueous	432.100	-228.5430
88	AmEDTA-	AmEDTA-	aqueous	1131.888	-232.3240
89	AmOx+	AmOxalate+	aqueous	271.840	-242.8530
90	AmLac++	AmLactate++	aqueous	332.070	-241.4360
91	ThAc2++	ThAcetate2++	aqueous	350.126	-604.8000
92	PuCit(aq)	deactivated	aqueous	427.129	999.9990
93	NpO2H2EDTA-	NpO2H2EDTA-	aqueous	1159.951	-364.0980
94	PuOx+	deactivated	aqueous	266.869	999.9990
95	ThLac2++	ThLactate2++	aqueous	410.178	-292.4000
96	ThAc+++	ThAc+++	aqueous	291.082	-448.5250
97	ThCit+	ThCit+	aqueous	421.138	-285.8980
98	ThEDTA(aq)	ThEDTA(aq)	aqueous	1120.926	-285.4190
99	ThOx++	Th(C2O4)++	aqueous	260.878	-297.4280
100	ThLac+++	ThLac+++	aqueous	321.108	-291.1520
101	UAc+++	deactivated	aqueous	301.044	999.9990
102	UCit+	deactivated	aqueous	431.100	999.9990
103	UEDTA(aq)	deactivated	aqueous	1130.888	999.9990
104	ULac+++	deactivated	aqueous	331.070	999.9990
105	UOx++	deactivated	aqueous	270.840	999.9990
106	NpO2Ac(aq)	NpO2Ac(aq)	aqueous	296.092	-519.6150
107	NpO2Cit=	NpO2Citrate=	aqueous	458.147	-343.7470
108	NpO2EDTA=-	NpO2EDTA=-	aqueous	1157.935	-335.7080
109	NpO2Ox-	NpO2Oxalate-	aqueous	297.887	-365.8510
110	NpO2Lac(aq)	NpO2Lactate(aq)	aqueous	358.117	-364.8370
111	MgAc+	MgAc+	aqueous	83.349	-333.3780
112	MgCit-	MgCit-	aqueous	213.405	-162.2610
113	MgEDTA=	MgEDTA=	aqueous	913.193	-153.7340
114	MgOx(aq)	MgOx(aq)	aqueous	53.145	-179.1850
115	MgLac+	MgLac+	aqueous	113.375	999.9990

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116	CaAc+	(Mg-analog)	aqueous	99.124	-373.2100
117	CaCit-	(Mg-analog)	aqueous	229.180	-202.0930
118	CaEDTA=	(Mg-analog)	aqueous	928.968	-193.5660
119	CaOx (aq)	(Mg-analog)	aqueous	68.920	-219.0170
120	CaLac+	(Mg-analog)	aqueous	129.150	999.9990
121	UnuCat #1+	UC#1+	aqueous	0.000	999.9990
122	NpO2HEDTA=	NpO2HEDTA=	aqueous	1158.943	-351.8520
123	UnuAn#2-	UA#2-	aqueous	0.000	999.9990
124	UnuAn#3-	UA#3-	aqueous	0.000	999.9990
125	UnuAn#4-	UA#4-	aqueous	0.000	999.9990
126	UnuNeu#1 (aq)	UN#1 (aq)	aqueous	0.000	999.9990
127	AmOHCO3 (c)	AmOHCO3 (c)	solid	320.017	-570.3400
128	Am(OH)3 (s)	Am(OH)3 (s)	solid	294.022	-495.3200
129	NaAm(CO3)2.6H2O (c)		solid	494.099	-1396.4700
130	AmPO4 (c)	AmPO4 (c)	solid	337.972	-709.7500
131	PuOHCO3 (c)	deactivated	solid	315.046	999.9990
132	Pu(OH)3 (s)	deactivated	solid	289.051	999.9990
133	NaPu(CO3)2.6H2O (c)	deactivated	solid	489.128	999.9990
134	PuPO4 (c)	deactivated	solid	333.001	999.9990
135	ThO2 (am)	Hydrous_Thorium_Oxide	solid	264.037	-451.4080
136	Th(SO4)2.9H2O (s)		solid	586.290	-1775.9000
137	Th(SO4)2.8H2O (s)		solid	568.275	-1680.0000
138	Th(SO4)2.Na2SO4.6H2O (16C, s)		solid	674.282	-2011.2900
139	Th(SO4)2.K2SO4.4H2O (16C, s)		solid	670.468	-1837.5700
140	Th(SO4)2.2K2SO4.2H2O (16C, s)		solid	808.692	-2181.8100
141	2[Th(SO4)2.7/2K2SO4 (16C, s)]		solid	2068.086	-5581.6600
142	UO2 (am)	Hydrous_U(IV)_Oxide	solid	273.999	-399.6700
143	NpO2OH (aged)	NpO2OH (aged)	solid	286.054	-454.3690
144	NpO2OH (amor)	NpO2OH (amor)	solid	286.054	-452.7570
145	2[NaNpO2CO3.7/2H2O (s)]		solid	830.198	-2096.1160
146	Na3NpO2 (CO3)2 (s)	Na3NpO2 (CO3)2 (s)	solid	458.035	-1144.5970
147	KNpO2CO3 (s)	KNpO2CO3 (s)	solid	368.155	-727.3300
148	K3NpO2 (CO3)2 (s)	K3NpO2 (CO3)2 (s)	solid	506.360	-1173.5460
149	H2Ox.2H2O (s)	H2C2O4.2H2O (s)	solid	66.886	-191.3460
150	NaHOx.H2O (s)	NaHC2O4.H2O (s)	solid	70.853	-202.2530
151	Na2Ox (s)	Na2C2O4 (s)	solid	74.820	-203.8230
152	CO2 ("solid", DISABLED)		solid	44.010	0.0000
153	CaSO4	Anhydrite	solid	136.138	-533.7300
154	NaK3(SO4)2	Aphthitalite/Glaserite	solid	332.400	-1057.0500
155	CaCl2.6H2O	Antarcticite	solid	219.077	-893.6500
156	CaCO3	Aragonite	solid	100.089	-455.1700
157	K2SO4	Arcanite	solid	174.254	-532.3900
158	MgCl2.6H2O	Bischofite	solid	203.302	-853.1000
159	Na2Mg(SO4)2.4H2O	Bloedite	solid	334.461	-1383.6000
160	Mg(OH)2	Brucite	solid	58.320	-335.4000
161	Na6CO3(SO4)2	Burkeite	solid	390.063	-1449.4000

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ATTACHMENT 1

ap098_fmt_run012

162	CaCO3	Calcite	solid	100.089	-455.6000
163	CaCl2.4H2O	CaCl2_Tetrahydrate	solid	183.047	-698.7000
164	Ca4Cl12(OH)6.13H2O	CaOxychloride_A	solid	567.467	-2658.4500
165	Ca2Cl12(OH)2.H2O	CaOxychloride_B	solid	203.096	-778.4100
166	KMgCl3.6H2O	Carnallite	solid	277.854	-1020.3000
167	MgSO4.7H2O	Epsomite	solid	246.469	-1157.8300
168	CaNa2(CO3)2.5H2O	Gaylussite	solid	296.154	-1360.5000
169	Na2Ca(SO4)2	Glauberite	solid	278.175	-1047.4500
170	CaSO4.2H2O	Gypsum	solid	172.168	-725.5600
171	NaCl	Halite	solid	58.443	-154.9900
172	MgSO4.6H2O	Hexahydrate	solid	228.454	-1061.6000
173	KMgClSO4.3H2O	Kainite	solid	248.960	-938.2000
174	KHCO3	Kallicinite	solid	100.115	-350.0600
175	MgSO4.H2O	Kieserite	solid	138.378	-579.8000
176	K2Mg(SO4)2.4H2O	Leonite	solid	366.678	-1403.9700
177	Na4Ca(SO4)3.2H2O	Labile_Salt	solid	456.242	-1751.4500
178	MgCO3	Magnesite	solid	84.314	-414.4500
179	Mg2Cl(OH)3.4H2O	MgOxychloride	solid	207.146	-1029.6000
180	KHSO4	Mercallite	solid	136.164	-417.5700
181	Na2SO4.10H2O	Mirabilite	solid	322.189	-1471.1500
182	K8H6(SO4)7	Misenite	solid	991.237	-3039.2400
183	NaHCO3	Nahcolite	solid	84.007	-343.3300
184	Na2CO3.10H2O	Natron	solid	286.141	-1382.7800
185	MgCO3.3H2O	Nesquehonite	solid	138.360	-695.3000
186	K2Mg(SO4)2.6H2O	Picromerite/Schoen	solid	402.708	-1596.1000
187	Na2Ca(CO3)2.2H2O	Pirssonite	solid	242.108	-1073.1000
188	K2MgCa2(SO4)4.2H2O	Polyhalite	solid	602.922	-2282.5000
189	Ca(OH)2	Portlandite	solid	74.095	-362.1200
190	K2CO3.3/2H2O	Potassium_Carbonate	solid	165.229	-577.3700
191	K8H4(CO3)6.3H2O	K-Sequicarbonate	solid	730.919	-2555.4000
192	KNaCO3.6H2O	K-Na-Carbonate	solid	230.188	-1006.8000
193	K2NaH(CO3)2.2H2O	Potassium_Trona	solid	258.243	-971.7400
194	K3H(SO4)2	Sesquipotassium_Sulfate	solid	310.418	-950.8000
195	Na3H(SO4)2	Sesquisodium_Sulfate	solid	262.092	-919.6000
196	Na2CO3.7H2O	Na2CO3-Heptahydrate	solid	232.095	-1094.9500
197	KCl	Sylvite	solid	74.551	-164.8400
198	K2Ca(SO4)2.H2O	Syngenite	solid	328.407	-1164.8000
199	Mg2CaCl6.12H2O	Tachyhydrate	solid	517.590	-2015.9000
200	Na2SO4	Thenardite	solid	142.037	-512.3500
201	Na2CO3.H2O	Thermonatrite	solid	124.004	-518.8000
202	Na3H(CO3)2.2H2O	Trona	solid	226.026	-960.3800
203	Na2B4O7.10H2O	Borax	solid	381.367	-2224.1600
204	B(OH)3	Borix_Acid_Solid	solid	61.832	-390.8800
205	KB5O8.4H2O	K-Pentaborate_(30_C)	solid	293.204	-1770.2600
206	K2B4O7.4H2O	K-Tetraborate_(30_C)	solid	305.493	-1663.4700
207	NaBO2.4H2O	Sodium_Metaborate	solid	137.859	-761.4200

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ATTACHMENT 1

ap098_fmt_run012

Preventing Formation of SOLID Species Mg4 (CO3)3 (OH)2.3H2O_HydroMagne4323
 Preventing Formation of SOLID Species OH-/H2O(solid)_____to.set.aH+

1 Solubility Product Violations, adding Mg2Cl(OH)3.4H2O_____MgOxychloride

AQ VIOLATION, Estimated Conc= 1.06E-24 Th++++ Th++++
 Preventing Formation of SOLID Species MgCO3_____Magnesite
 Preventing Formation of SOLID Species CaMg (CO3) 2_____Dolomite
 Preventing Formation of SOLID Species Mg5 (CO3) 4 (OH) 2.4H2O_HydroMagne5424
 Preventing Formation of SOLID Species OH-/H2O(solid)_____to.set.aH+

nonconvergent elemental abundances

MU(ttl)= 0.100223533973463 x 1
 134.500489367874 Hydrogen
 129.794726810469 Oxygen
 13.9046759199647 Sodium
 1.51389125613328 Potassium
 11.1220333103347 Magnesium
 11.0109652359741 Calcium
 16.1824035399441 Chlorine
 10.1916125989379 Sulfur
 2.000000000000000 Carbon
 0.000000000000000E+000 PosIon:EL
 0.000000000000000E+000 NegIon:EL
 2.423591950322903E-002 Oxalate:EL
 0.173915163101875 Boron
 2.917286606870161E-002 Bromine
 5.666268217190122E-003 Acetate:EL
 1.000000000000000 Th(IV)
 1.000000000000000 Am(III)
 0.000000000000000E+000 Pu(III)
 1.000000000000000 Np(V)
 0.000000000000000E+000 ClO4:EL
 0.000000000000000E+000 Phosphorus
 0.000000000000000E+000 U(IV)
 0.000000000000000E+000 Lactate:EL
 4.342268910995193E-006 EDTA:EL
 4.297387578581813E-004 Citrate:EL
 0.000000000000000E+000 Electron:E
 0.000000000000000E+000 Charge:EL

AQ VIOLATION, Estimated Conc= 1.21E-24 Th++++ Th++++
 Preventing Formation of SOLID Species OH-/H2O(solid)_____to.set.aH+
 Preventing Formation of SOLID Species Mg5 (CO3) 4 (OH) 2.4H2O_HydroMagne5424
 Preventing Formation of SOLID Species CaMg (CO3) 2_____Dolomite

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Preventing Formation of SOLID Species MgCO3 _____ Magnesite
 AQ VIOLATION, Estimated Conc= 1.09E-24 Th++++ Th++++
 Preventing Formation of SOLID Species MgCO3 _____ Magnesite
 Preventing Formation of SOLID Species CaMg(CO3)2 _____ Dolomite
 Preventing Formation of SOLID Species Mg5(CO3)4(OH)2.4H2O_HydroMagne5424
 Preventing Formation of SOLID Species OH-/H2O(solid) _____ to.set.aH+
 # inversions for batch pblm 301
 1CRA GWB recipe, calc FMT V2.4
 FMT_021120.chemdat
 ERG update of FMT_970407.chemdat (PAVT db)
 Pressure= 1.00000E+00 [=] ATM Temperature= 2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

Total Moles	Aq. Molality	Aq. Molarity	Aq. mg/liter	
Using NaCl Density	Correlation			
1.34500489E+02	1.11655043E+02	9.73570272E+01	9.81261477E+04	Hydrogen
1.29794727E+02	5.70212071E+01	4.97193415E+01	7.95479632E+05	Oxygen
1.39046759E+01	4.96821551E+00	4.33200937E+00	9.95918990E+04	Sodium
1.51389126E+00	5.58960962E-01	4.87383070E-01	1.90558495E+04	Potassium
1.11220333E+01	6.67089616E-01	5.81665280E-01	1.41373746E+04	Magnesium
1.10109652E+01	1.26711073E-02	1.10485053E-02	4.42824092E+02	Calcium
1.61824035E+01	6.22892730E+00	5.43128038E+00	1.92555183E+05	Chlorine
1.01916126E+01	2.08739878E-01	1.82009638E-01	5.83522900E+03	Sulfur
2.00000000E+00	4.22596170E-04	3.68480507E-04	4.42581936E+00	Carbon
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	PosIon:EL
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	NegIon:EL
2.42359195E-02	2.63614251E-02	2.29857059E-02	6.62907758E+02	Oxalate:EL
1.73915163E-01	1.89167634E-01	1.64943723E-01	1.78304164E+03	Boron
2.91728661E-02	3.17313450E-02	2.76679793E-02	2.21078222E+03	Bromine
5.66626822E-03	6.16320356E-03	5.37397291E-03	3.17300856E+02	Acetate:EL
1.00000000E+00	1.42528195E-08	1.24276709E-08	2.88369315E-03	Th(IV)
1.00000000E+00	3.52119748E-07	3.07028961E-07	7.46080376E-02	Am(III)
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Pu(III)
1.00000000E+00	1.11509268E-06	9.72299198E-07	2.30481775E-01	Np(V)
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	ClO4:EL
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Phosphorus
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	U(IV)
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Lactate:EL
4.34226891E-06	4.72308867E-06	4.11827231E-06	3.66068283E+00	EDTA:EL
4.29738758E-04	4.67427121E-04	4.07570618E-04	7.70716039E+01	Citrate:EL
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Electron:E
4.67422615E-15	5.08415876E-15	4.43310548E-15	0.00000000E+00	Charge:EL

Solution Parameters, Calculated

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SOLUTION MASS 1297.19989217616 grams
 H2O MASS 919.370610689967 grams
 TDS (g/kg) 410.965150607373 g/kgH2O

Specified Solution Density
 DENSITY 1230.28363765684 kg/m³ = g/l

Solution Parameters Based on Specified Density
 SOLUTION VOL 1.05439091642864 liters
 TDS 358.338900306493 g/l

Density based on TDS and NaCl solutions 1230.28 g/l
 % Relative difference vs NaCl density 0.00 %
 Calculated Ratio of molality to Molarity 1.147

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	8.12980E-01	7.32777E-01	0.9013	5.10331E+01	4.84005E+01	8.71945E+05
CaSO4	Anhydrite	1.08767E+01	1.00000E+00	1.000	9.99970E+00	9.48387E+00	1.29111E+06
NaCl	Halite	1.01559E+01	1.00000E+00	1.000	9.33704E+00	8.85539E+00	5.17534E+05
Mg(OH)2	Brucite	8.99681E+00	1.00000E+00	1.000	8.27140E+00	7.84472E+00	4.57501E+05
Cl-	Cl-	6.22893E+00	8.06472E+00	1.295	5.72669E+00	5.43128E+00	1.92555E+05
Mg2Cl(OH)3.4H2O	MgOxychloride	1.21677E+00	1.00000E+00	1.000	1.11867E+00	1.06096E+00	2.19773E+05
ThO2(am)	Hydrous_Thorium_Oxide	1.08770E+00	1.00000E+00	1.000	1.00000E+00	9.48415E-01	2.50417E+05
Am(OH)3(s)	Am(OH)3(s)	1.08770E+00	1.00000E+00	1.000	1.00000E+00	9.48415E-01	2.78855E+05
KNpO2CO3(s)	KNpO2CO3(s)	1.08770E+00	1.00000E+00	1.000	9.99999E-01	9.48414E-01	3.49163E+05
CaCO3	Calcite	1.08728E+00	1.00000E+00	1.000	9.99613E-01	9.48047E-01	9.48893E+04
K+	K+	5.58961E-01	2.41936E-01	0.4328	5.13892E-01	4.87383E-01	1.90558E+04
SO4=	SO4=	2.08740E-01	4.44960E-03	2.1316E-02	1.91909E-01	1.82010E-01	1.74834E+04
MgB(OH)4+	MgB(OH)4+	7.36072E-02	1.40655E-01	1.911	6.76723E-02	6.41814E-02	6.61994E+03
Br-	Br-	3.17313E-02	8.57994E-03	0.2704	2.91729E-02	2.76680E-02	2.21078E+03
MgOx(aq)	MgOx(aq)	2.58685E-02	3.27361E-02	1.265	2.37827E-02	2.25559E-02	1.19873E+03
Ac-	Acetate-	3.10867E-03	1.72726E-03	0.5556	2.85802E-03	2.71059E-03	1.60044E+02
MgCit-	MgCit-	4.53252E-04	7.80549E-05	0.1722	4.16707E-04	3.95211E-04	8.43400E+01
MgEDTA=	MgEDTA=	4.58557E-06	5.96992E-07	0.1302	4.21584E-06	3.99837E-06	3.65128E+00
Na+	Na+	4.96822E+00	4.61126E+00	0.9282	4.56763E+00	4.33201E+00	9.95919E+04
Mg++	Mg++	5.62017E-01	9.98313E-01	1.776	5.16702E-01	4.90048E-01	1.19106E+04
B(OH)4-	B(OH)4-	5.51524E-02	5.61813E-03	0.1019	5.07055E-02	4.80899E-02	3.79137E+03
B(OH)3(aq)	B(OH)3(aq)	2.53793E-02	2.71440E-02	1.070	2.33330E-02	2.21294E-02	1.36830E+03
Ca++	Ca++	1.02664E-02	9.76394E-03	0.9511	9.43860E-03	8.95171E-03	3.58785E+02
B4O5(OH)4=	B4O5(OH)4=	5.75024E-03	2.43095E-05	4.2276E-03	5.28660E-03	5.01389E-03	9.58989E+02
B3O3(OH)4-	B3O3(OH)4-	3.30520E-03	5.41203E-04	0.1637	3.03870E-03	2.88195E-03	4.27847E+02
							-3.80E-09
							-7.86E-09
							-9.11E-08
							-5.80E-08
							-5.64E-09
							1.67E-07
							-1.75E-07

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MgAc+	MgAc+	3.02471E-03	2.23728E-02	7.397	2.78083E-03	2.63738E-03	2.19823E+02	-1.56E-08
CaB(OH)4+	CaB(OH)4+	2.11211E-03	2.45209E-03	1.161	1.94181E-03	1.84164E-03	2.19006E+02	-5.98E-08
MgOH+	MgOH+	1.77392E-03	5.55943E-04	0.3134	1.63089E-03	1.54676E-03	6.39003E+01	1.52E-09
MgCO3(aq)	MgCO3(aq)	3.40318E-04	3.40318E-04	1.000	3.12879E-04	2.96739E-04	2.50193E+01	-6.43E-10
CaOx(aq)	(Mg-analog)	2.53005E-04	3.20174E-04	1.265	2.32606E-04	2.20607E-04	1.52042E+01	9.50E-10
Ox=	Oxalate=	2.39096E-04	5.27999E-06	2.2083E-02	2.19818E-04	2.08478E-04	6.01252E+00	1.71E-10
HCO3-	HCO3-	5.05431E-05	1.79271E-05	0.3553	4.63851E-05	4.39924E-05	2.68429E+00	2.17E-09
CaAc+	(Mg-analog)	2.95830E-05	2.18816E-04	7.397	2.71977E-05	2.57947E-05	2.55688E+00	-2.32E-08
CO3=	CO3=	2.60940E-05	4.01949E-07	1.5404E-02	2.39900E-05	2.27525E-05	1.36536E+00	4.48E-09
Citrate=-	Citrate=-	9.74126E-06	3.92137E-10	4.0255E-05	8.95583E-06	8.49384E-06	1.60618E+00	1.02E-09
OH-	OH-	8.14131E-06	3.61595E-06	0.4441	7.48488E-06	7.09877E-06	1.20731E-01	2.73E-09
CaCO3(aq)	CaCO3(aq)	5.55951E-06	5.55951E-06	1.000	5.11125E-06	4.84759E-06	4.85191E-01	3.33E-10
CaCit-	(Mg-analog)	4.43301E-06	7.63412E-07	0.1722	4.07558E-06	3.86534E-06	8.85858E-01	1.06E-09
NpO2Ox-	NpO2Oxalate-	8.13552E-07	2.34930E-08	2.8877E-02	7.47956E-07	7.09373E-07	2.11313E-01	1.79E-09
Am(OH)2+	Am(OH)2+	2.53918E-07	1.75244E-10	6.9016E-04	2.33444E-07	2.21402E-07	6.13316E-02	5.56E-09
HAc(aq)	AceticAcid	2.01500E-07	2.01500E-07	1.000	1.85253E-07	1.75696E-07	1.05509E-02	-1.16E-08
NpO2+	NpO2+	1.34592E-07	2.56029E-07	1.902	1.23740E-07	1.17356E-07	3.15744E-02	-2.29E-09
NpO2CO3-	NpO2CO3-	1.22337E-07	1.07011E-08	8.7473E-02	1.12473E-07	1.06671E-07	3.51007E-02	5.17E-09
AmEDTA-	AmEDTA-	9.26150E-08	2.79284E-09	3.0155E-02	8.51475E-08	8.07551E-08	9.14058E-02	4.11E-09
CaEDTA=	(Mg-analog)	4.48489E-08	5.83884E-09	0.1302	4.12328E-08	3.91058E-08	3.63280E-02	1.07E-09
NpO2Ac(aq)	NpO2Ac(aq)	3.81943E-08	1.04549E-08	0.2737	3.51147E-08	3.33033E-08	9.86085E-03	-7.27E-09
CO2(aq)	CO2(aq)	3.14974E-08	1.08660E-07	3.450	2.89577E-08	2.74640E-08	1.20868E-03	-4.58E-09
Th(OH)3(CO3)-	Th(OH)3(CO3)-	1.34037E-08	3.62427E-09	0.2704	1.23230E-08	1.16873E-08	4.00955E-03	2.14E-10
NpO2OH(aq)	NpO2OH(aq)	4.81688E-09	4.51642E-10	9.3762E-02	4.42805E-09	4.20005E-09	1.20144E-03	5.74E-09
AmOH++	AmOH++	2.71323E-09	6.67753E-11	2.4611E-02	2.49446E-09	2.36578E-09	6.15121E-04	-4.29E-09
NpO2(CO3)2=-	NpO2(CO3)2=-	1.49425E-09	1.15114E-13	7.7038E-05	1.37377E-09	1.30290E-09	5.06913E-04	4.13E-09
HSO4-	HSO4-	1.06268E-09	8.65080E-10	0.8141	9.76994E-10	9.26596E-10	8.99405E-05	-3.03E-09
Th(OH)4(aq)	Th(OH)4(aq)	8.49114E-10	8.49114E-10	1.000	7.80651E-10	7.40381E-10	2.22164E-04	-1.30E-09
HOx-	Bioxalate-	6.97436E-10	1.96012E-10	0.2810	6.41202E-10	6.08125E-10	1.81513E-05	-2.09E-09
Am(OH)3(aq)	Am(OH)3(aq)	6.94688E-10	6.30297E-12	9.0731E-03	6.38676E-10	6.05729E-10	1.78098E-04	8.34E-09
AmAc++	AmAcetate++	5.59406E-10	6.38702E-12	1.1418E-02	5.14301E-10	4.87771E-10	1.47328E-04	-4.07E-09
AmOx+	AmOxalate+	5.36269E-10	5.06481E-11	9.4445E-02	4.93030E-10	4.67597E-10	1.27111E-04	-1.67E-08
H+	H+	4.60460E-10	2.04216E-09	4.435	4.23333E-10	4.01495E-10	4.04667E-07	-5.88E-09
AmCO3+	AmCO3+	4.51352E-10	3.38847E-10	0.7507	4.14959E-10	3.93554E-10	1.19250E-04	-5.50E-09
HCitrate=	HCitrate=	3.17410E-10	2.12199E-12	6.6853E-03	2.91817E-10	2.76764E-10	5.26150E-05	-2.86E-09
AmCit(aq)	AmCitrate(aq)	2.59295E-10	1.64885E-12	6.3590E-03	2.38389E-10	2.26091E-10	9.76941E-05	7.84E-10
Am(CO3)2-	Am(CO3)2-	1.68307E-10	1.08548E-11	6.4494E-02	1.54736E-10	1.46754E-10	5.32744E-05	1.64E-09
AmSO4+	AmSO4+	1.14393E-10	5.27492E-11	0.4611	1.05169E-10	9.97441E-11	3.38190E-05	-6.74E-09
NpO2Cit=	NpO2Citrate=	8.06230E-11	3.15258E-13	3.9103E-03	7.41224E-11	7.02988E-11	3.22072E-05	-5.41E-09
EDTA==	EDTA==	4.63900E-11	4.47396E-17	9.6442E-07	4.26496E-11	4.04495E-11	3.59551E-05	6.50E-09
Am(CO3)3=-	Am(CO3)3=-	4.42527E-11	6.91717E-16	1.5631E-05	4.06847E-11	3.85859E-11	1.63229E-05	9.28E-09
NpO2(CO3)3=-	NpO2(CO3)3=-	1.87194E-11	3.56973E-21	1.9070E-10	1.72101E-11	1.63223E-11	7.32994E-06	-1.11E-08
Am+++	Am+++	1.66564E-11	6.68916E-12	0.4016	1.53134E-11	1.45234E-11	3.52919E-06	-1.19E-08
Am(SO4)2-	Am(SO4)2-	1.38315E-11	6.66715E-13	4.8203E-02	1.27163E-11	1.20603E-11	5.24763E-06	8.81E-10
Am(CO3)4=-	Am(CO3)4=-	1.34491E-11	1.73976E-24	1.2936E-13	1.23647E-11	1.17268E-11	5.66449E-06	2.26E-08
NpO2(OH)2-	NpO2(OH)2-	7.05331E-12	9.59175E-14	1.3599E-02	6.48460E-12	6.15009E-12	1.86386E-06	9.34E-09

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HEDTA--	HEDTA--	4.18042E-12	3.40024E-15	8.1337E-04	3.84336E-12	3.64510E-12	3.24376E-06	5.17E-09
AmCl++	AmCl++	1.83313E-12	9.35960E-11	51.06	1.68533E-12	1.59839E-12	4.45076E-07	-8.80E-09
NpO2EDTA--	NpO2EDTA--	2.30095E-13	3.92799E-15	1.7071E-02	2.11543E-13	2.00630E-13	2.32317E-07	1.49E-09
AmCl2+	AmCl2+	9.88172E-14	7.91612E-11	801.1	9.08496E-14	8.61631E-14	2.70471E-08	-4.72E-09
H2EDTA=	H2EDTA=	5.21574E-15	5.25803E-17	1.0081E-02	4.79520E-15	4.54784E-15	4.05168E-09	4.50E-10
H2Citrate-	H2Citrate-	2.32399E-15	2.99647E-16	0.1289	2.13661E-15	2.02639E-15	3.87275E-10	-6.58E-09
Th(CO3)5===	Th(CO3)5===	4.69721E-16	1.35264E-29	2.8797E-14	4.31848E-16	4.09571E-16	2.17926E-10	-3.38E-08
NpO2HEDTA=	NpO2HEDTA=	4.54989E-16	8.23208E-17	0.1809	4.18304E-16	3.96725E-16	4.59782E-10	-4.78E-09
H2Ox(aq)	OxalicAcid	9.90886E-18	9.90886E-18	1.000	9.10991E-18	8.63997E-18	2.66593E-13	-1.25E-09
Th(SO4)3=	Th(SO4)3=	9.18508E-18	2.33986E-19	2.5475E-02	8.44450E-18	8.00889E-18	4.16631E-12	1.77E-11
ThEDTA(aq)	ThEDTA(aq)	4.01319E-18	1.60170E-17	3.991	3.68961E-18	3.49928E-18	3.92243E-12	-6.25E-09
Th(SO4)2(aq)	Th(SO4)2(aq)	2.07146E-19	7.67867E-18	37.07	1.90444E-19	1.80620E-19	7.66105E-14	-9.69E-09
NpO2H2EDTA-	NpO2H2EDTA-	7.25011E-20	3.49921E-20	0.4826	6.66554E-20	6.32170E-20	7.33286E-14	-1.78E-08
ThCit+	ThCit+	3.32637E-20	6.69595E-19	20.13	3.05817E-20	2.90041E-20	1.22147E-14	-4.19E-08
ThOx++	Th(C2O4)++	2.58076E-21	1.27601E-18	494.4	2.37268E-21	2.25028E-21	5.87050E-16	-4.73E-08
ThAc2++	ThAcetate2++	1.75683E-21	5.13701E-19	292.4	1.61518E-21	1.53186E-21	5.36343E-16	-4.95E-08
H3Citrate(aq)	CitricAcid	1.08015E-21	1.08015E-21	1.000	9.93062E-22	9.41835E-22	1.80949E-16	-1.07E-08
H3EDTA-	H3EDTA-	5.83392E-22	1.31314E-22	0.2251	5.36353E-22	5.08686E-22	4.53703E-16	-5.31E-09
ThAc+++	ThAc+++	4.10538E-22	3.94432E-20	96.08	3.77436E-22	3.57966E-22	1.04198E-16	-4.32E-08
Th++++	Th++++	0.00000E+00	0.00000E+00	0.9093	0.00000E+00	0.00000E+00	0.00000E+00	-2.40E+01
AmOHC03(c)	AmOHC03(c)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.13E-01
NaAm(CO3)2.6H2O(c)		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.72E+00
Th(SO4)2.9H2O(s)		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.69E+01
Th(SO4)2.8H2O(s)		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.69E+01
Th(SO4)2.Na2SO4.6H2O(16C,s)		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.29E+01
Th(SO4)2.K2SO4.4H2O(16C,s)		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.48E+01
Th(SO4)2.2K2SO4.2H2O(16C,s)		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.49E+01
2[Th(SO4)2.7/2K2SO4(16C,s)]		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.32E+01
NpO2OH(aged)	NpO2OH(aged)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.55E+00
NpO2OH(amor)	NpO2OH(amor)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.25E+00
2[NaNpO2CO3.7/2H2O(s)]		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.41E+00
Na3NpO2(CO3)2(s)	Na3NpO2(CO3)2(s)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.21E+00
K3NpO2(CO3)2(s)	K3NpO2(CO3)2(s)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-5.30E+00
H2Ox.2H2O(s)	H2C2O4.2H2O(s)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.73E+01
NaHOx.H2O(s)	NaHC2O4.H2O(s)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.38E+00
Na2Ox(s)	Na2C2O4(s)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.54E+00
CO2("solid",DISABLED)		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.46E+01
NaK3(SO4)2_Aphtitalite/Glaserite		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.09E+00
CaCl2.6H2O	Antarcticite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-5.15E+00
CaCO3	Aragonite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.87E-01
K2SO4	Arcanite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.81E+00
MgCl2.6H2O	Bischofite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.45E+00
Na2Mg(SO4)2.4H2O	Bloedite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.57E+00
Na6CO3(SO4)2	Burkeite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-6.34E+00
CaCl2.4H2O	CaCl2_Tetrahydrate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-6.45E+00
Ca4Cl2(OH)6.13H2O_CaOxychloride_A		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.54E+01

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Ca2Cl2(OH)2.H2O	CaOxychloride_B	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-1.18E+01
KMgCl3.6H2O	Carnallite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-3.04E+00
MgSO4.7H2O	Epsomite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-1.42E+00
CaNa2(CO3)2.5H2O	Gaylussite	NAF	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.73E+00
Na2Ca(SO4)2	Glauberite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-1.42E-01
CaSO4.2H2O	Gypsum	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-5.16E-02
MgSO4.6H2O	Hexahydrate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-1.53E+00
KMgClSO4.3H2O	Kainite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-2.27E+00
KHCO3	Kalicinite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-5.64E+00
MgSO4.H2O	Kieserite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-2.36E+00
K2Mg(SO4)2.4H2O	Leonite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-2.50E+00
Na4Ca(SO4)3.2H2O	Labile_Salt	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-1.01E+00
MgCO3	Magnesite	NAF	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	1.44E+00
KHSO4	Mercallite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-1.03E+01
Na2SO4.10H2O	Mirabilite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-1.15E+00
K8H6(SO4)7	Misenite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-6.27E+01
NaHCO3	Nahcolite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-3.68E+00
Na2CO3.10H2O	Natron	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-5.59E+00
MgCO3.3H2O	Nesquehonite	NAF	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.63E+00
K2Mg(SO4)2.6H2O	Picromerite/Schoen	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-2.42E+00
Na2Ca(CO3)2.2H2O	Pirssonite	NAF	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.50E+00
K2MgCa2(SO4)4.2H2O	Polyhalite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-1.19E+00
Ca(OH)2	Portlandite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-7.70E+00
K2CO3.3/2H2O	Potassium_Carbonate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-1.09E+01
K8H4(CO3)6.3H2O	K-Sequicarbonate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-4.41E+01
KNaCO3.6H2O	K-Na-Carbonate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-7.04E+00
K2NaH(CO3)2.2H2O	Potassium_Trona	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-1.32E+01
K3H(SO4)2	Sesquipotassium_Sulfate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-1.17E+01
Na3H(SO4)2	Sesquisodium_Sulfate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-1.06E+01
Na2CO3.7H2O	Na2CO3-Heptahydrate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-5.55E+00
KCl	Sylvite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-6.10E-01
K2Ca(SO4)2.H2O	Syngenite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-6.33E-01
Mg2CaCl6.12H2O	Tachyhydrite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-1.56E+01
Na2SO4	Thenardite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-7.37E-01
Na2CO3.H2O	Thermonatrite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-5.69E+00
Na3H(CO3)2.2H2O	Trona	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-8.38E+00
Na2B4O7.10H2O	Borax	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-6.97E-01
B(OH)3	Borix_Acid_Solid	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-1.54E+00
KB5O8.4H2O	K-Pentaborate_(30_C)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-4.02E+00
K2B4O7.4H2O	K-Tetraborate_(30_C)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-3.89E+00
NaBO2.4H2O	Sodium_Metaborate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-2.19E+00
NaB5O8.5H2O	Sodium_Pentaborate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-4.10E+00
NaBO2.NaCl.2H2O	Teepleite_(20_C)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-1.62E+00
CaMg(CO3)2	Dolomite	NAF	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	2.28E+00
Mg5(CO3)4(OH)2.4H2O	HydroMagne5424	NAF	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	8.68E-02
Mg4(CO3)3(OH)2.3H2O	HydroMagne4323	NAF	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.78E-01

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H+(solid)	to.set.aH+	NAF	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-8.69E+00
OH-/H2O(solid)	to.set.aH+	NAF	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	8.69E+00
NaOH(aq)	to.titrate.base.only		0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-2.95E+02
HCl(aq)	to.titrate.acid.only		0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-2.48E+02
H4EDTA(aq)	H4EDTA(aq)		0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-2.81E+01

pH (-log[aH+]); pmH(-log[mH+]); pCH(-log[MH+]) 8.6899 9.3368 9.3963
 Osmotic Coefficient= 1.351548
 Equilibrium RH (%) = 73.277712
 Ionic Strength (m) = 7.539364
 Density, kg/m3 = 1230.28
 fCO2(g); log[fCO2(g)]= 3.295E-06 -5.482

- NOTES: - Water "molality" is mole fraction H2O in aqueous phase
 - "Descriptor" means:
 *dG/RT/ln10 for species with nonzero concs. (convergence criterion)
 *Saturation Index for minerals, SI=log10(IAP/Ksp)
 *log10(activity) for aqueous species with very small concentrations
 *log10(activity) for aqueous species Not Allowed to Form
 *NAF signifies that the species was Not Allowed to Form

Total G/RT= -1.88434219E+04

Total Diagonal Inversions 301

Total Stoichiometric Reoptimizations 27

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ATTACHMENT 1

ap098-fmt_run018

INPUT file name is:AP098\$PROD:[000000]AP098_FMT_RUN018.IN;1
 INGUSS file name is:AP098\$PROD:[000000]AP098_FMT_RUN018.INGUSS;1
 OUTPUT file name is:AP098\$PROD:[000000]AP098_FMT_RUN018.OUT;1
 CHEMDAT file name is AP098\$PROD:[000000]AP098_FMT.CHEMDAT;1
 Temperature is Hard Coded as 298.15K
 CRA GWB recipe, calc
 FMT_021120.chemdat
 ERG update of FMT_970407.chemdat (PAVT db)

FMT V2.4

Accuracy of reactions is 1.0000E-06
 Minimum elemental abundance is 1.0000E-18
 Number of Aqueous Species is 126

PITZER Data Base NOT Echoed in this Run
 using PITZER ACTIVITY COEFFICIENT model
 Charge Balance replaces element Oxygen

Species CaCO3 _____ Aragonite prevented from forming in DISABLE
 Species CaCO3 _____ Calcite prevented from forming in DISABLE
 Species CaNa2(CO3)2.5H2O _____ Gaylussite prevented from forming in DISABLE
 Species MgCO3 _____ Magnesite prevented from forming in DISABLE
 Species MgCO3.3H2O _____ Nesquehonite prevented from forming in DISABLE
 Species Na2Ca(CO3)2.2H2O _____ Pirssonite prevented from forming in DISABLE
 Species CaMg(CO3)2 _____ Dolomite prevented from forming in DISABLE
 Species Mg4(CO3)3(OH)2.3H2O_HydroMagne4323 prevented from forming in DISABLE
 fCO2(g) not specified in the INPUT file
 Target pH not specified in the INPUT file
 this is a BATCH problem

FOR088 file name is AP098\$PROD:[000000]AP098_FMT_RUN018.DAT;1

Ideal Gas Constant is Unity (Dimensionless)
 Temperature = 298.15 [=] degree Kelvin

214 Species 27 Elements

Element Name	Molecular Weight
Hydrogen	1.00790
Oxygen	15.99940
Sodium	22.98977
Potassium	39.09830
Magnesium	24.30500
Calcium	40.08000
Chlorine	35.45300

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ATTACHMENT 1

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Sulfur	32.06000
Carbon	12.01100
PosIon:EL	0.00000
NegIon:EL	0.00000
Oxalate:EL	28.84000
Boron	10.81000
Bromine	79.90400
Acetate:EL	59.04400
Th(IV)	232.03810
Am(III)	243.00000
Pu(III)	238.02900
Np(V)	237.04820
ClO4:EL	99.45060
Phosphorus	30.97400
U(IV)	242.00000
Lactate:EL	89.07000
EDTA:EL	888.88800
Citrate:EL	189.10000
Electron:E	0.00000
Charge:EL	0.00000

Species Name	Phase	Mol.Wt.	Std Chemical Potential, u/RT
1 H2O	WATER aqueous	18.015	-95.6635
2 Na+	Na+ aqueous	22.990	-105.6510
3 K+	K+ aqueous	39.098	-113.9570
4 Ca++	Ca++ aqueous	40.080	-223.3000
5 Mg++	Mg++ aqueous	24.305	-183.4680
6 MgOH+	MgOH+ aqueous	41.312	-251.9400
7 H+	H+ aqueous	1.008	0.0000
8 Cl-	Cl- aqueous	35.453	-52.9550
9 SO4=	SO4= aqueous	96.058	-300.3860
10 HSO4-	HSO4- aqueous	97.066	-304.9420
11 OH-	OH- aqueous	17.007	-63.4350
12 HCO3-	HCO3- aqueous	61.017	-236.7510
13 CO3=	CO3= aqueous	60.009	-212.9440
14 CO2 (aq)	CO2 (aq) aqueous	44.010	-155.6800
15 CaCO3 (aq)	CaCO3 (aq) aqueous	100.089	-443.5000
16 MgCO3 (aq)	MgCO3 (aq) aqueous	84.314	-403.1550
17 B(OH)3 (aq)	B(OH)3 (aq) aqueous	61.832	-390.8100
18 B(OH)4-	B(OH)4- aqueous	78.839	-465.2000
19 B3O3(OH)4-	B3O3(OH)4- aqueous	148.457	-963.7700
20 B4O5(OH)4=	B4O5(OH)4= aqueous	191.266	-1239.1000
21 CaB(OH)4+	CaB(OH)4+ aqueous	118.919	-692.3000
22 MgB(OH)4+	MgB(OH)4+ aqueous	103.144	-651.8900
23 Br-	Br- aqueous	79.904	-999.9900

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24 ClO4-	perchlorate	aqueous	99.451	-73.8100
25 NaOH(aq)	to.titrate.base.only	aqueous	39.997	500.0000
26 HCl(aq)	to.titrate.acid.only	aqueous	36.461	500.0000
27 HClO4(aq)	to.titrate.acid.only	aqueous	100.459	500.0000
28 PosIon	POSITIVE ION	aqueous	0.000	0.0000
29 NegIon	NEGATIVE ION	aqueous	0.000	0.0000
30 PosIon(OH)(aq)	to.titrate.base	aqueous	17.007	500.0000
31 HNegIon(aq)	to.titrate.acid	aqueous	1.008	500.0000
32 H3PO4(aq)	H3PO4(aq)	aqueous	97.995	-460.9000
33 H2PO4-	H2PO4-	aqueous	96.987	-455.9600
34 HPO4=	HPO4=	aqueous	95.980	-439.3670
35 PO4=-	PO4=-	aqueous	94.972	-410.9470
36 Am+++	Am+++	aqueous	243.000	-241.6940
37 AmCO3+	AmCO3+	aqueous	303.009	-473.2900
38 Am(CO3)2-	Am(CO3)2-	aqueous	363.018	-697.5200
39 Am(CO3)3=-	Am(CO3)3=-	aqueous	423.028	-915.5300
40 AmOH++	AmOH++	aqueous	260.007	-319.9600
41 Am(OH)2+	Am(OH)2+	aqueous	277.015	-396.8900
42 Am(OH)3(aq)	Am(OH)3(aq)	aqueous	294.022	-469.5300
43 AmCl++	AmCl++	aqueous	278.453	-295.2000
44 AmCl2+	AmCl2+	aqueous	313.906	-345.9000
45 Am(CO3)4=-	Am(CO3)4=-	aqueous	483.037	-1123.4000
46 Am(SO4)2-	Am(SO4)2-	aqueous	435.115	-850.9900
47 AmSO4+	AmSO4+	aqueous	339.058	-549.5600
48 Pu(OH)2+	deactivated	aqueous	272.044	999.9990
49 Pu(OH)3(aq)	deactivated	aqueous	289.051	999.9990
50 Th++++	Th++++	aqueous	232.038	-284.2270
51 Th(CO3)5===	Th(CO3)5===	aqueous	532.084	-1411.3780
52 Th(OH)3(CO3)-	Th(OH)3(CO3)-	aqueous	343.069	-775.6270
53 Th(OH)4(aq)	Th(OH)4(aq)	aqueous	300.067	-622.4700
54 Th(SO4)2(aq)	Th(SO4)2(aq)	aqueous	424.153	-911.6900
55 Th(SO4)3=	Th(SO4)3=	aqueous	520.211	-1214.0000
56 U++++	U++++	aqueous	242.000	-214.1900
57 UOH+++	UOH+++	aqueous	259.007	-308.7000
58 U(CO3)5===	U(CO3)5===	aqueous	542.046	-1345.3930
59 U(OH)2(CO3)2=	U(OH)2(CO3)2=	aqueous	396.033	-863.3830
60 U(OH)4(CO3)2==	U(OH)4(CO3)2==	aqueous	430.048	-998.6620
61 U(OH)4(aq)	deactivated	aqueous	310.029	999.9990
62 U(SO4)2(aq)	deactivated	aqueous	434.115	999.9990
63 U(SO4)3=	deactivated	aqueous	530.173	999.9990
64 NpO2+	NpO2+	aqueous	269.047	-369.1050
65 NpO2CO3-	NpO2CO3-	aqueous	329.056	-593.6010
66 NpO2(CO3)2=-	NpO2(CO3)2=-	aqueous	389.065	-809.8320
67 NpO2(CO3)3=-	NpO2(CO3)3=-	aqueous	449.075	-1020.2140
68 NpO2OH(aq)	NpO2OH(aq)	aqueous	286.054	-438.7300
69 NpO2(OH)2-	NpO2(OH)2-	aqueous	303.062	-506.2380

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70	HAc(aq)	AceticAcid	aqueous	60.052	-158.3000
71	Ac-	Acetate-	aqueous	59.044	-147.3470
72	H3Citrate(aq)	CitricAcid	aqueous	192.124	0.0000
73	H2Citrate-	H2Citrate-	aqueous	191.116	7.4760
74	HCitrate=	HCitrate=	aqueous	190.108	18.6200
75	Citrate=-	Citrate=-	aqueous	189.100	33.4100
76	H4EDTA(aq)	H4EDTA(aq)	aqueous	892.920	0.0000
77	H3EDTA-	H3EDTA-	aqueous	891.912	5.7610
78	H2EDTA=	H2EDTA=	aqueous	890.904	12.8700
79	HEDTA=-	HEDTA=-	aqueous	889.896	28.7100
80	EDTA==	EDTA==	aqueous	888.888	53.0500
81	H2Ox(aq)	OxalicAcid	aqueous	30.856	0.0000
82	HOx-	Bioxalate-	aqueous	29.848	3.2090
83	Ox=	Oxalate=	aqueous	28.840	13.0170
84	HLactate(aq)	LacticAcid	aqueous	90.078	0.0000
85	Lactate-	Lactate-	aqueous	89.070	8.7980
86	AmAc++	AmAcetate++	aqueous	302.044	-395.3560
87	AmCit(aq)	AmCitrate(aq)	aqueous	432.100	-228.5430
88	AmEDTA-	AmEDTA-	aqueous	1131.888	-232.3240
89	AmOx+	AmOxalate+	aqueous	271.840	-242.8530
90	AmLac++	AmLactate++	aqueous	332.070	-241.4360
91	ThAc2++	ThAcetate2++	aqueous	350.126	-604.8000
92	PuCit(aq)	deactivated	aqueous	427.129	999.9990
93	NpO2H2EDTA-	NpO2H2EDTA-	aqueous	1159.951	-364.0980
94	PuOx+	deactivated	aqueous	266.869	999.9990
95	ThLac2++	ThLactate2++	aqueous	410.178	-292.4000
96	ThAc+++	ThAc+++	aqueous	291.082	-448.5250
97	ThCit+	ThCit+	aqueous	421.138	-285.8980
98	ThEDTA(aq)	ThEDTA(aq)	aqueous	1120.926	-285.4190
99	ThOx++	Th(C2O4)++	aqueous	260.878	-297.4280
100	ThLac+++	ThLac+++	aqueous	321.108	-291.1520
101	UAc+++	deactivated	aqueous	301.044	999.9990
102	UCit+	deactivated	aqueous	431.100	999.9990
103	UEDTA(aq)	deactivated	aqueous	1130.888	999.9990
104	ULac+++	deactivated	aqueous	331.070	999.9990
105	UOx++	deactivated	aqueous	270.840	999.9990
106	NpO2Ac(aq)	NpO2Ac(aq)	aqueous	296.092	-519.6150
107	NpO2Cit=	NpO2Citrate=	aqueous	458.147	-343.7470
108	NpO2EDTA=-	NpO2EDTA=-	aqueous	1157.935	-335.7080
109	NpO2Ox-	NpO2Oxalate-	aqueous	297.887	-365.8510
110	NpO2Lac(aq)	NpO2Lactate(aq)	aqueous	358.117	-364.8370
111	MgAc+	MgAc+	aqueous	83.349	-333.3780
112	MgCit-	MgCit-	aqueous	213.405	-162.2610
113	MgEDTA=	MgEDTA=	aqueous	913.193	-153.7340
114	MgOx(aq)	MgOx(aq)	aqueous	53.145	-179.1850
115	MgLac+	MgLac+	aqueous	113.375	999.9990

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116	CaAc+	(Mg-analog)	aqueous	99.124	-373.2100
117	CaCit-	(Mg-analog)	aqueous	229.180	-202.0930
118	CaEDTA=	(Mg-analog)	aqueous	928.968	-193.5660
119	CaOx(aq)	(Mg-analog)	aqueous	68.920	-219.0170
120	CaLac+	(Mg-analog)	aqueous	129.150	999.9990
121	UnuCat#1+	UC#1+	aqueous	0.000	999.9990
122	NpO2HEDTA=	NpO2HEDTA=	aqueous	1158.943	-351.8520
123	UnuAn#2-	UA#2-	aqueous	0.000	999.9990
124	UnuAn#3-	UA#3-	aqueous	0.000	999.9990
125	UnuAn#4-	UA#4-	aqueous	0.000	999.9990
126	UnuNeu#1(aq)	UN#1(aq)	aqueous	0.000	999.9990
127	AmOHCO3(c)	AmOHCO3(c)	solid	320.017	-570.3400
128	Am(OH)3(s)	Am(OH)3(s)	solid	294.022	-495.3200
129	NaAm(CO3)2.6H2O(c)		solid	494.099	-1396.4700
130	AmPO4(c)	AmPO4(c)	solid	337.972	-709.7500
131	PuOHCO3(c)	deactivated	solid	315.046	999.9990
132	Pu(OH)3(s)	deactivated	solid	289.051	999.9990
133	NaPu(CO3)2.6H2O(c)	deactivated	solid	489.128	999.9990
134	PuPO4(c)	deactivated	solid	333.001	999.9990
135	ThO2(am)	Hydrous_Thorium_Oxide	solid	264.037	-451.4080
136	Th(SO4)2.9H2O(s)		solid	586.290	-1775.9000
137	Th(SO4)2.8H2O(s)		solid	568.275	-1680.0000
138	Th(SO4)2.Na2SO4.6H2O(16C,s)		solid	674.282	-2011.2900
139	Th(SO4)2.K2SO4.4H2O(16C,s)		solid	670.468	-1837.5700
140	Th(SO4)2.2K2SO4.2H2O(16C,s)		solid	808.692	-2181.8100
141	2[Th(SO4)2.7/2K2SO4(16C,s)]		solid	2068.086	-5581.6600
142	UO2(am)	Hydrous_U(IV)_Oxide	solid	273.999	-399.6700
143	NpO2OH(aged)	NpO2OH(aged)	solid	286.054	-454.3690
144	NpO2OH(amor)	NpO2OH(amor)	solid	286.054	-452.7570
145	2[NaNpO2CO3.7/2H2O(s)]		solid	830.198	-2096.1160
146	Na3NpO2(CO3)2(s)	Na3NpO2(CO3)2(s)	solid	458.035	-1144.5970
147	KNpO2CO3(s)	KNpO2CO3(s)	solid	368.155	-727.3300
148	K3NpO2(CO3)2(s)	K3NpO2(CO3)2(s)	solid	506.360	-1173.5460
149	H2Ox.2H2O(s)	H2C2O4.2H2O(s)	solid	66.886	-191.3460
150	NaHOx.H2O(s)	NaHC2O4.H2O(s)	solid	70.853	-202.2530
151	Na2Ox(s)	Na2C2O4(s)	solid	74.820	-203.8230
152	CO2("solid",DISABLED)		solid	44.010	0.0000
153	CaSO4	Anhydrite	solid	136.138	-533.7300
154	NaK3(SO4)2	Aphthitalite/Glaserite	solid	332.400	-1057.0500
155	CaCl2.6H2O	Antarcticite	solid	219.077	-893.6500
156	CaCO3	Aragonite	solid	100.089	-455.1700
157	K2SO4	Arcanite	solid	174.254	-532.3900
158	MgCl2.6H2O	Bischofite	solid	203.302	-853.1000
159	Na2Mg(SO4)2.4H2O	Bloedite	solid	334.461	-1383.6000
160	Mg(OH)2	Brucite	solid	58.320	-335.4000
161	Na6CO3(SO4)2	Burkeite	solid	390.063	-1449.4000

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162	CaCO3	Calcite	solid	100.089	-455.6000
163	CaCl2.4H2O	CaCl2_Tetrahydrate	solid	183.047	-698.7000
164	Ca4Cl2(OH)6.13H2O	CaOxychloride_A	solid	567.467	-2658.4500
165	Ca2Cl2(OH)2.H2O	CaOxychloride_B	solid	203.096	-778.4100
166	KMgCl3.6H2O	Carnallite	solid	277.854	-1020.3000
167	MgSO4.7H2O	Epsomite	solid	246.469	-1157.8300
168	CaNa2(CO3)2.5H2O	Gaylussite	solid	296.154	-1360.5000
169	Na2Ca(SO4)2	Glauberite	solid	278.175	-1047.4500
170	CaSO4.2H2O	Gypsum	solid	172.168	-725.5600
171	NaCl	Halite	solid	58.443	-154.9900
172	MgSO4.6H2O	Hexahydrate	solid	228.454	-1061.6000
173	KMgClSO4.3H2O	Kainite	solid	248.960	-938.2000
174	KHCO3	Kalocinrite	solid	100.115	-350.0600
175	MgSO4.H2O	Kieserite	solid	138.378	-579.8000
176	K2Mg(SO4)2.4H2O	Leonite	solid	366.678	-1403.9700
177	Na4Ca(SO4)3.2H2O	Labile_Salt	solid	456.242	-1751.4500
178	MgCO3	Magnesite	solid	84.314	-414.4500
179	Mg2Cl(OH)3.4H2O	MgOxychloride	solid	207.146	-1029.6000
180	KHSO4	Mercallite	solid	136.164	-417.5700
181	Na2SO4.10H2O	Mirabilite	solid	322.189	-1471.1500
182	K8H6(SO4)7	Misenite	solid	991.237	-3039.2400
183	NaHCO3	Nahcolite	solid	84.007	-343.3300
184	Na2CO3.10H2O	Natron	solid	286.141	-1382.7800
185	MgCO3.3H2O	Nesquehonite	solid	138.360	-695.3000
186	K2Mg(SO4)2.6H2O	Picromerite/Schoen	solid	402.708	-1596.1000
187	Na2Ca(CO3)2.2H2O	Pirssonite	solid	242.108	-1073.1000
188	K2MgCa2(SO4)4.2H2O	Polyhalite	solid	602.922	-2282.5000
189	Ca(OH)2	Portlandite	solid	74.095	-362.1200
190	K2CO3.3/2H2O	Potassium_Carbonate	solid	165.229	-577.3700
191	K8H4(CO3)6.3H2O	K-Sequicarbonate	solid	730.919	-2555.4000
192	KNaCO3.6H2O	K-Na-Carbonate	solid	230.188	-1006.8000
193	K2NaH(CO3)2.2H2O	Potassium_Trona	solid	258.243	-971.7400
194	K3H(SO4)2	Sesquipotassium_Sulfate	solid	310.418	-950.8000
195	Na3H(SO4)2	Sesquisodium_Sulfate	solid	262.092	-919.6000
196	Na2CO3.7H2O	Na2CO3-Heptahydrate	solid	232.095	-1094.9500
197	KCl	Sylvite	solid	74.551	-164.8400
198	K2Ca(SO4)2.H2O	Syngenite	solid	328.407	-1164.8000
199	Mg2CaCl6.12H2O	Tachyhydrate	solid	517.590	-2015.9000
200	Na2SO4	Thenardite	solid	142.037	-512.3500
201	Na2CO3.H2O	Thermonatrite	solid	124.004	-518.8000
202	Na3H(CO3)2.2H2O	Trona	solid	226.026	-960.3800
203	Na2B4O7.10H2O	Borax	solid	381.367	-2224.1600
204	B(OH)3	Borix_Acid_Solid	solid	61.832	-390.8800
205	KB5O8.4H2O	K-Pentaborate_(30_C)	solid	293.204	-1770.2600
206	K2B4O7.4H2O	K-Tetraborate_(30_C)	solid	305.493	-1663.4700
207	NaBO2.4H2O	Sodium_Metaborate	solid	137.859	-761.4200

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1 Solubility Product Violations, adding Mg2Cl(OH)3.4H2O _____ MgOxychloride

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AQ VIOLATION, Estimated Conc= 1.06E-24 Th++++ Th++++
Preventing Formation of SOLID Species MgCO3 _____ Magnesite
Preventing Formation of SOLID Species CaMg (CO3)2 _____ Dolomite
Preventing Formation of SOLID Species OH-/H2O(solid) _____ to.set.aH+
AQ VIOLATION, Estimated Conc= 1.06E-24 Th++++ Th++++
Preventing Formation of SOLID Species OH-/H2O(solid) _____ to.set.aH+
Preventing Formation of SOLID Species CaMg (CO3)2 _____ Dolomite
Preventing Formation of SOLID Species MgCO3 _____ Magnesite
AQ VIOLATION, Estimated Conc= 1.06E-24 Th++++ Th++++
Preventing Formation of SOLID Species MgCO3 _____ Magnesite
Preventing Formation of SOLID Species CaMg (CO3)2 _____ Dolomite
Preventing Formation of SOLID Species OH-/H2O(solid) _____ to.set.aH+

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inversions for batch pblm 75
 1CRA GWB recipe, calc
 FMT_021120.chemdat

FMT V2.4

ERG update of FMT_970407.chemdat (PAVT db)
 Pressure= 1.00000E+00 [=] ATM Temperature= 2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

Total Moles	Aq. Molality	Aq. Molarity	Aq. mg/liter	
Using NaCl Density	Correlation			
1.44500489E+02	1.11655071E+02	9.73560367E+01	9.81251494E+04	Hydrogen
1.44794727E+02	5.70228047E+01	4.97202162E+01	7.95493627E+05	Oxygen
1.39046759E+01	4.96843422E+00	4.33215492E+00	9.95952451E+04	Sodium
1.51389126E+00	5.58982614E-01	4.87396868E-01	1.90563890E+04	Potassium
1.61220333E+01	6.67200133E-01	5.81755581E-01	1.41395694E+04	Magnesium
1.00109652E+01	1.26493527E-02	1.10294216E-02	4.42059217E+02	Calcium
1.61824035E+01	6.22855810E+00	5.43090185E+00	1.92541763E+05	Chlorine
1.01916126E+01	2.09147198E-01	1.82362898E-01	5.84655450E+03	Sulfur
5.00000000E+00	4.02003686E-04	3.50521345E-04	4.21011187E+00	Carbon
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	PosIon:EL
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	NegIon:EL
0.00000000E+00	0.00000000E+00	0.00000000E+00	6.62926466E+02	Oxalate:EL
2.42359195E-02	2.63624438E-02	2.29863546E-02	1.78309196E+03	Boron
1.73915163E-01	1.89174944E-01	1.64948378E-01	2.21084461E+03	Bromine
2.91728661E-02	3.17325713E-02	2.76687601E-02	3.17309811E+02	Acetate:EL
5.66626822E-03	6.16344173E-03	5.37412456E-03	2.75157320E-03	Th(IV)
1.00000000E+00	1.35999508E-08	1.18582819E-08	7.45780059E-02	Am(III)
1.00000000E+00	3.51981680E-07	3.06905374E-07	0.00000000E+00	Pu(III)
0.00000000E+00	0.00000000E+00	0.00000000E+00		

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1.00000000E+00	1.16583455E-06	1.01653270E-06	2.40967248E-01	Np(V)
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	ClO4:EL
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Phosphorus
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	U(IV)
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Lactate:EL
4.34226891E-06	4.72327119E-06	4.11838853E-06	3.66078614E+00	EDTA:EL
4.29738758E-04	4.67445185E-04	4.07582120E-04	7.70737790E+01	Citrate:EL
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Electron:E
-1.24723925E-16	-1.35667535E-16	-1.18293360E-16	0.00000000E+00	Charge:EL

Solution Parameters, Calculated

SOLUTION MASS	1297.18031836799	grams
H2O MASS	919.335083608783	grams
TDS(g/kg)	410.998385132870	g/kgH2O

Specified Solution Density

DENSITY	1230.29979243581	kg/m ³ = g/l
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Solution Parameters Based on Specified Density

SOLUTION VOL	1.05436116168057	liters
TDS	358.364143608009	g/l

Density based on TDS and NaCl solutions	1230.30	g/l
% Relative difference vs NaCl density	0.00	%
Calculated Ratio of molality to Molarity	1.147	

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	8.12976E-01	7.32772E-01	0.9013	5.10311E+01	4.84000E+01	8.71936E+05	
CaSO4	1.08767E+01	1.00000E+00	1.000	9.99934E+00	9.48379E+00	1.29110E+06	Anhydrite
NaCl	1.01563E+01	1.00000E+00	1.000	9.33702E+00	8.85562E+00	5.17547E+05	Halite
Mg(OH)2	8.99630E+00	1.00000E+00	1.000	8.27061E+00	7.84419E+00	4.57470E+05	Brucite
Cl-	6.22856E+00	8.06466E+00	1.295	5.72613E+00	5.43090E+00	1.92542E+05	Cl-
Mg2Cl(OH)3.4H2O	1.21746E+00	1.00000E+00	1.000	1.11925E+00	1.06154E+00	2.19894E+05	MgOxychloride
ThO2(am)	1.08774E+00	1.00000E+00	1.000	1.00000E+00	9.48442E-01	2.50424E+05	Hydrous_Thorium_Oxide
Am(OH)3(s)	1.08774E+00	1.00000E+00	1.000	1.00000E+00	9.48441E-01	2.78863E+05	Am(OH)3(s)
KNpO2CO3(s)	1.08774E+00	1.00000E+00	1.000	9.99999E-01	9.48441E-01	3.49173E+05	KNpO2CO3(s)
Mg5(CO3)4(OH)2.4H2O	1.08764E+00	1.00000E+00	1.000	9.99908E-01	9.48354E-01	4.43486E+05	HydroMagne5424
K+	5.58983E-01	2.41930E-01	0.4328	5.13892E-01	4.87397E-01	1.90564E+04	K+
SO4=	2.09147E-01	4.45828E-03	2.1316E-02	1.92276E-01	1.82363E-01	1.75173E+04	SO4=
MgB(OH)4+	7.36204E-02	1.40660E-01	1.911	6.76818E-02	6.41923E-02	6.62106E+03	MgB(OH)4+
Br-	3.17326E-02	8.57972E-03	0.2704	2.91729E-02	2.76688E-02	2.21084E+03	Br-

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MgOx(aq)	MgOx(aq)	2.58700E-02	3.27376E-02	1.265	2.37832E-02	2.25570E-02	1.19879E+03	
Ac-	Acetate-	3.10870E-03	1.72732E-03	0.5556	2.85793E-03	2.71058E-03	1.60044E+02	
MgCit-	MgCit-	4.53282E-04	7.80384E-05	0.1722	4.16718E-04	3.95232E-04	8.43446E+01	
MgEDTA=	MgEDTA=	4.58582E-06	5.97031E-07	0.1302	4.21590E-06	3.99854E-06	3.65144E+00	
Na+	Na+	4.96843E+00	4.61129E+00	0.9281	4.56766E+00	4.33215E+00	9.95952E+04	-1.43E-09
Mg++	Mg++	5.62129E-01	9.98382E-01	1.776	5.16785E-01	4.90140E-01	1.19129E+04	-1.07E-09
B(OH)4-	B(OH)4-	5.51506E-02	5.61792E-03	0.1019	5.07019E-02	4.80878E-02	3.79120E+03	-3.47E-08
B(OH)3(aq)	B(OH)3(aq)	2.53794E-02	2.71439E-02	1.070	2.33322E-02	2.21292E-02	1.36829E+03	-5.57E-08
Ca++	Ca++	1.02494E-02	9.74494E-03	0.9508	9.42263E-03	8.93682E-03	3.58188E+02	-2.93E-10
B4O5(OH)4=	B4O5(OH)4=	5.75012E-03	2.43084E-05	4.2275E-03	5.28629E-03	5.01374E-03	4.27854E+02	-1.88E-07
B3O3(OH)4-	B3O3(OH)4-	3.30528E-03	5.41191E-04	0.1637	3.03866E-03	2.88200E-03	2.19840E+02	-5.99E-09
MgAc+	MgAc+	3.02498E-03	2.23751E-02	7.397	2.78097E-03	2.63759E-03	2.18596E+02	-3.85E-08
CaB(OH)4+	CaB(OH)4+	2.10817E-03	2.44722E-03	1.161	1.93811E-03	1.83819E-03	6.39132E+01	7.57E-10
MgOH+	MgOH+	1.77430E-03	5.55962E-04	0.3133	1.63117E-03	1.54707E-03	2.38000E+01	4.59E-10
MgCO3(aq)	MgCO3(aq)	3.23737E-04	3.23737E-04	1.000	2.97623E-04	2.82278E-04	1.51743E+01	1.96E-10
CaOx(aq)	(Mg-analog)	2.52510E-04	3.19543E-04	1.265	2.32142E-04	2.20173E-04	6.01153E+00	2.39E-09
Ox=	Oxalate=	2.39059E-04	5.27986E-06	2.2086E-02	2.19775E-04	2.08444E-04	2.55364E+00	1.61E-09
HCO3-	HCO3-	4.79980E-05	1.70529E-05	0.3553	4.41262E-05	4.18511E-05	2.55193E+00	-7.40E-09
CaAc+	(Mg-analog)	2.95260E-05	2.18398E-04	7.397	2.71443E-05	2.57448E-05	1.29879E+00	4.55E-09
CO3=	CO3=	2.48220E-05	3.82338E-07	1.5403E-02	2.28198E-05	2.16432E-05	1.60573E+00	4.97E-09
Citrate=-	Citrate=-	9.73857E-06	3.92027E-10	4.0255E-05	8.95301E-06	8.49141E-06	1.20727E-01	2.08E-09
OH-	OH-	8.14110E-06	3.61583E-06	0.4441	7.48440E-06	7.09852E-06	4.60616E-01	7.29E-10
CaCO3(aq)	CaCO3(aq)	5.27798E-06	5.27798E-06	1.000	4.85223E-06	4.60206E-06	8.84121E-01	-2.98E-11
CaCit-	(Mg-analog)	4.42436E-06	7.61712E-07	0.1722	4.06747E-06	3.85776E-06	2.22139E-01	-8.15E-10
NpO2Ox-	NpO2Oxalate-	8.55243E-07	2.46980E-08	2.8878E-02	7.86255E-07	7.45717E-07	6.13024E-02	-6.78E-11
Am(OH)2+	Am(OH)2+	2.53799E-07	1.75250E-10	6.9050E-04	2.33327E-07	2.21297E-07	1.05515E-02	-4.13E-09
HAc(aq)	AceticAcid	2.01512E-07	2.01512E-07	1.000	1.85257E-07	1.75706E-07	3.32002E-02	-7.39E-10
NpO2+	NpO2+	1.41523E-07	1.07014E-08	1.902	1.30107E-07	1.23399E-07	3.50963E-02	1.90E-09
NpO2CO3-	NpO2CO3-	1.22323E-07	2.79312E-09	8.7485E-02	1.12456E-07	1.06658E-07	9.14303E-02	-2.55E-09
AmEDTA-	AmEDTA-	9.26408E-08	5.82746E-09	3.0150E-02	8.51680E-08	8.07768E-08	3.62564E-02	5.74E-10
CaEDTA=	(Mg-analog)	4.47610E-08	1.09918E-08	0.1302	4.11503E-08	3.90287E-08	1.03663E-02	-3.73E-09
NpO2Ac(aq)	NpO2Ac(aq)	4.01527E-08	1.03365E-07	0.2737	3.69138E-08	3.50105E-08	1.14958E-03	-1.09E-09
CO2(aq)	CO2(aq)	2.99576E-08	1.03365E-07	3.450	2.75411E-08	2.61211E-08	3.81422E-03	1.47E-09
Th(OH)3(CO3)-	Th(OH)3(CO3)-	1.27508E-08	3.44752E-09	0.2704	1.17223E-08	1.11179E-08	3.81422E-03	7.57E-10
NpO2OH(aq)	NpO2OH(aq)	5.06319E-09	4.74803E-10	9.3775E-02	4.65476E-09	4.41477E-09	6.15325E-04	-1.30E-09
AmOH++	AmOH++	2.71415E-09	6.67799E-11	2.4604E-02	2.49522E-09	2.36657E-09	4.81978E-04	3.13E-09
NpO2(CO3)2=-	NpO2(CO3)2=-	1.42076E-09	1.09500E-13	7.7072E-05	1.30615E-09	1.23881E-09	9.01174E-05	-2.41E-09
HSO4-	HSO4-	1.06478E-09	8.66791E-10	0.8141	9.78889E-10	9.28419E-10	2.22159E-04	-1.92E-10
Th(OH)4(aq)	Th(OH)4(aq)	8.49103E-10	8.49103E-10	1.000	7.80610E-10	7.40363E-10	1.81497E-05	-2.04E-10
HOx-	Bioxalate-	6.97384E-10	1.96013E-10	0.2811	6.41129E-10	6.08074E-10	1.78087E-04	1.09E-09
Am(OH)3(aq)	Am(OH)3(aq)	6.94652E-10	6.30297E-12	9.0736E-03	6.38618E-10	6.05692E-10	1.47435E-04	-1.53E-09
AmAc++	AmAcetate++	5.59815E-10	6.38791E-12	1.1411E-02	5.14658E-10	4.88123E-10	1.27033E-04	-6.62E-09
AmOx+	AmOxalate+	5.35945E-10	5.06521E-11	9.4510E-02	4.92713E-10	4.67310E-10	4.04678E-07	-1.43E-09
H+	H+	4.60477E-10	2.04222E-09	4.435	4.23333E-10	4.01506E-10	1.13446E-04	-9.46E-10
AmCO3+	AmCO3+	4.29385E-10	3.22348E-10	0.7507	3.94749E-10	3.74397E-10	5.26057E-05	8.88E-11
HCitrate=	HCitrate=	3.17357E-10	2.12145E-12	6.6848E-03	2.91757E-10	2.76715E-10		

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AmCit(aq)	AmCitr(aq)	2.59172E-10	1.64856E-12	6.3609E-03	2.38266E-10	2.25981E-10	9.76464E-05	-2.09E-09
Am(CO3)2-	Am(CO3)2-	1.52312E-10	9.82246E-12	6.4489E-02	1.40025E-10	1.32806E-10	4.82110E-05	1.65E-09
AmSO4+	AmSO4+	1.14616E-10	5.28575E-11	0.4612	1.05370E-10	9.99374E-11	3.38845E-05	-2.28E-09
NpO2Cit=	NpO2Citr(aq)	8.47292E-11	3.31343E-13	3.9106E-03	7.78945E-11	7.38784E-11	3.38472E-05	-1.89E-09
EDTA==	EDTA==	4.63790E-11	4.47394E-17	9.6465E-07	4.26379E-11	4.04395E-11	3.59462E-05	1.21E-08
Am(CO3)3=-	Am(CO3)3=-	3.80931E-11	5.95393E-16	1.5630E-05	3.50203E-11	3.32147E-11	1.40508E-05	9.52E-09
NpO2(CO3)3=-	NpO2(CO3)3=-	1.69191E-11	3.22998E-21	1.9091E-10	1.55543E-11	1.47524E-11	6.62491E-06	-1.30E-09
Am+++	Am+++	1.66211E-11	6.68985E-12	0.4025	1.52804E-11	1.44926E-11	3.52169E-06	-1.95E-09
Am(SO4)2-	Am(SO4)2-	1.38876E-11	6.69386E-13	4.8200E-02	1.27674E-11	1.21091E-11	5.26887E-06	2.81E-10
Am(CO3)4=-	Am(CO3)4=-	1.10105E-11	1.42443E-24	1.2937E-13	1.01223E-11	9.60046E-12	4.63737E-06	2.89E-08
NpO2(OH)2-	NpO2(OH)2-	7.41392E-12	1.00833E-13	1.3600E-02	6.81588E-12	6.46446E-12	1.95913E-06	2.40E-09
HEDTA=-	HEDTA=-	4.18055E-12	3.40032E-15	8.1337E-04	3.84333E-12	3.64517E-12	3.24382E-06	5.45E-09
AmCl++	AmCl++	1.83511E-12	9.36050E-11	51.01	1.68708E-12	1.60010E-12	4.45552E-07	-1.93E-10
NpO2EDTA=-	NpO2EDTA=-	2.41870E-13	4.12954E-15	1.7073E-02	2.22359E-13	2.10895E-13	2.44203E-07	5.26E-09
AmCl2+	AmCl2+	9.88945E-14	7.91683E-11	800.5	9.09172E-14	8.62296E-14	2.70680E-08	1.76E-09
H2EDTA=	H2EDTA=	5.21612E-15	5.25830E-17	1.0081E-02	4.79536E-15	4.54812E-15	4.05194E-09	-8.61E-10
H2Citr(aq)	H2Citr(aq)	2.32367E-15	2.99580E-16	0.1289	2.13623E-15	2.02609E-15	3.87218E-10	-2.73E-09
NpO2HEDTA=	NpO2HEDTA=	4.78215E-16	8.65474E-17	0.1810	4.39640E-16	4.16973E-16	4.83247E-10	-2.75E-09
Th(CO3)5===	Th(CO3)5===	3.66325E-16	1.05347E-29	2.8758E-14	3.36776E-16	3.19412E-16	1.69954E-10	2.63E-08
H2Ox(aq)	OxalicAcid	9.90916E-18	9.90916E-18	1.000	9.10984E-18	8.64015E-18	2.66599E-13	-4.46E-10
Th(SO4)3=	Th(SO4)3=	9.23945E-18	2.35386E-19	2.5476E-02	8.49415E-18	8.05621E-18	4.19093E-12	2.19E-09
ThEDTA(aq)	ThEDTA(aq)	4.01400E-18	1.60190E-17	3.991	3.69021E-18	3.49995E-18	3.92319E-12	-4.82E-09
Th(SO4)2(aq)	Th(SO4)2(aq)	2.08025E-19	7.70960E-18	37.06	1.91245E-19	1.81384E-19	7.69347E-14	-1.88E-09
NpO2H2EDTA-	NpO2H2EDTA-	7.61829E-20	3.67897E-20	0.4829	7.00376E-20	6.64266E-20	7.70516E-14	-9.21E-09
ThCit+	ThCit+	3.32399E-20	6.69490E-19	20.14	3.05586E-20	2.89831E-20	1.22059E-14	-1.44E-08
ThOx++	Th(C2O4)++	2.58103E-21	1.27614E-18	494.4	2.37283E-21	2.25049E-21	5.87103E-16	-1.37E-08
ThAc2++	ThAcetate2++	1.75833E-21	5.13801E-19	292.2	1.61650E-21	1.53315E-21	5.36798E-16	-1.47E-08
H3Citr(aq)	CitricAcid	1.07994E-21	1.07994E-21	1.000	9.92827E-22	9.41639E-22	1.80911E-16	-4.34E-09
H3EDTA-	H3EDTA-	5.83411E-22	1.31325E-22	0.2251	5.36350E-22	5.08697E-22	4.53713E-16	-4.34E-09
ThAc+++	ThAc+++	4.11306E-22	3.94495E-20	95.91	3.78128E-22	3.58632E-22	1.04391E-16	-1.05E-08
Th+++	Th+++	0.00000E+00	0.00000E+00	0.9341	0.00000E+00	0.00000E+00	0.00000E+00	-2.40E+01
AmOHCO3(c)	AmOHCO3(c)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.35E-01
NaAm(CO3)2.6H2O(c)		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.76E+00
Th(SO4)2.9H2O(s)		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.69E+01
Th(SO4)2.8H2O(s)		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.69E+01
Th(SO4)2.Na2SO4.6H2O(16C,s)		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.29E+01
Th(SO4)2.K2SO4.4H2O(16C,s)		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.48E+01
Th(SO4)2.2K2SO4.2H2O(16C,s)		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.49E+01
2[Th(SO4)2.7/2K2SO4(16C,s)]		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.32E+01
NpO2OH(aged)	NpO2OH(aged)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.53E+00
NpO2OH(amor)	NpO2OH(amor)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.23E+00
2[NaNpO2CO3.7/2H2O(s)]		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.41E+00
Na3NpO2(CO3)2(s)	Na3NpO2(CO3)2(s)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.23E+00
K3NpO2(CO3)2(s)	K3NpO2(CO3)2(s)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-5.32E+00
H2Ox.2H2O(s)	H2C2O4.2H2O(s)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.73E+01
NaHOx.H2O(s)	NaHC2O4.H2O(s)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.38E+00

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Na2Ox(s)	Na2C2O4(s)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.54E+00
CO2("solid",DISABLED)		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.46E+01
NaK3(SO4)2	Aphthitalite/Glaserite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.08E+00
CaCl2.6H2O	Antarcticite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-5.15E+00
CaCO3	Aragonite	NAF	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	-2.09E-01
K2SO4	Arcanite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.81E+00
MgCl2.6H2O	Bischofite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.45E+00
Na2Mg(SO4)2.4H2O	Bloedite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.57E+00
Na6CO3(SO4)2	Burkeite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-6.36E+00
CaCO3	Calcite	NAF	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	-2.26E-02
CaCl2.4H2O	CaCl2_Tetrahydrate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-6.46E+00
Ca4Cl2(OH)6.13H2O	CaOxychloride_A	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.54E+01
Ca2Cl2(OH)2.H2O	CaOxychloride_B	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.18E+01
KMgCl3.6H2O	Carnallite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.04E+00
MgSO4.7H2O	Epsomite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.42E+00
CaNa2(CO3)2.5H2O	Gaylussite	NAF	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	-4.77E+00
Na2Ca(SO4)2	Glauberite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.41E-01
CaSO4.2H2O	Gypsum	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-5.16E-02
MgSO4.6H2O	Hexahydrate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.53E+00
KMgClSO4.3H2O	Kainite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.27E+00
KHCO3	Kalinite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-5.57E+00
MgSO4.H2O	Kieserite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.36E+00
K2Mg(SO4)2.4H2O	Leonite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.50E+00
Na4Ca(SO4)3.2H2O	Labile_Salt	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.01E+00
MgCO3	Magnesite	NAF	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	1.42E+00
KHSO4	Mercallite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.03E+01
Na2SO4.10H2O	Mirabilite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.15E+00
K8H6(SO4)7	Misenite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-6.27E+01
NaHCO3	Nahcolite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.70E+00
Na2CO3.10H2O	Natron	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-5.52E+00
MgCO3.3H2O	Nesquehonite	NAF	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	-1.66E+00
K2Mg(SO4)2.6H2O	Picromerite/Schoen	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.42E+00
Na2Ca(CO3)2.2H2O	Pirssonite	NAF	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	-4.55E+00
K2MgCa2(SO4)4.2H2O	Polyhalite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.19E+00
Ca(OH)2	Portlandite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.70E+00
K2CO3.3/2H2O	Potassium_Carbonate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.09E+01
K8H4(CO3)6.3H2O	K-Sequicarbonate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.43E+01
KNaCO3.6H2O	K-Na-Carbonate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.06E+00
K2NaH(CO3)2.2H2O	Potassium_Trona	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.33E+01
K3H(SO4)2	Sesquipotassium_Sulfate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.17E+01
Na3H(SO4)2	Sesquisodium_Sulfate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.06E+01
Na2CO3.7H2O	Na2CO3-Heptahydrate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-5.57E+00
KCl	Sylvite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-6.10E-01
K2Ca(SO4)2.H2O	Syngenite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-6.32E-01
Mg2CaCl6.12H2O	Tachyhydrate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.56E+01
Na2SO4	Thenardite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.36E-01

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Na2CO3.H2O	Thermonatrite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-5.71E+00
Na3H(CO3)2.2H2O	Trona	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-8.42E+00
Na2B4O7.10H2O	Borax	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-6.97E+01
B(OH)3	Borix_Acid_Solid	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-1.54E+00
KB5O8.4H2O	K-Pentaborate_(30_C)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-4.02E+00
K2B4O7.4H2O	K-Tetraborate_(30_C)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-3.89E+00
NaBO2.4H2O	Sodium_Metaborate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-2.19E+00
NaB5O8.5H2O	Sodium_Pentaborate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-4.10E+00
NaBO2.NaCl.2H2O	Teepleite_(20_C)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-1.62E+00
CaMg(CO3)2	Dolomite	NAF	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	2.24E+00
Mg4(CO3)3(OH)2.3H2O	HydroMagne4323	NAF	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-3.44E+01
H+(solid)	to.set.aH+	NAF	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-8.69E+00
OH-/H2O(solid)	to.set.aH+	NAF	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	8.69E+00
NaOH(aq)	to.titrate.base.only		0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-2.95E+02
HCl(aq)	to.titrate.acid.only		0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-2.48E+02
H4EDTA(aq)	H4EDTA(aq)		0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-2.81E+01

pH (-log[aH+]); pmH(-log[mH+]); pCH(-log[MH+]) 8.6899 9.3368 9.3963
 Osmotic Coefficient= 1.351539
 Equilibrium RH (%) = 73.277213
 Ionic Strength (m) = 7.540304
 Density, kg/m3 = 1230.30
 fCO2(g); log[fCO2(g)]= 3.135E-06 -5.504

NOTES: - Water "molality" is mole fraction H2O in aqueous phase
 - "Descriptor" means:
 *dG/RT/ln10 for species with nonzero concs. (convergence criterion)
 *Saturation Index for minerals, SI=log10(IAP/Ksp)
 *log10(activity) for aqueous species with very small concentrations
 *log10(activity) for aqueous species Not Allowed to Form
 *NAF signifies that the species was Not Allowed to Form

Total G/RT= -2.07518818E+04

Total Diagonal Inversions 75
 Total Stoichiometric Reoptimizations 9

Information Only

ATTACHMENT 1

ap098_fmt_run022

INPUT file name is:AP098\$PROD:[000000]AP098_FMT_RUN022.IN;1
 INGUESS file name is:AP098\$PROD:[000000]AP098_FMT_RUN022.INGUESS;1
 OUTPUT file name is:AP098\$PROD:[000000]AP098_FMT_RUN022.OUT;1
 CHEMDAT file name is AP098\$PROD:[000000]AP098_FMT.CHEMDAT;1
 Temperature is Hard Coded as 298.15K
 CRA ERDA-6 recipe, calc
 FMT_021120.chemdat
 ERG update of FMT_970407.chemdat (PAVT db)

FMT V2.4

Accuracy of reactions is 1.0000E-06
 Minimum elemental abundance is 1.0000E-18
 Number of Aqueous Species is 126

PITZER Data Base NOT Echoed in this Run
 using PITZER ACTIVITY COEFFICIENT model
 Charge Balance replaces element Oxygen

Species CaCO3 _____ Aragonite prevented from forming in DISABLE
 Species CaNa2(CO3)2.5H2O _____ Gaylussite prevented from forming in DISABLE
 Species MgCO3 _____ Magnesite prevented from forming in DISABLE
 Species MgCO3.3H2O _____ Nesquehonite prevented from forming in DISABLE
 Species Na2Ca(CO3)2.2H2O _____ Pirssonite prevented from forming in DISABLE
 Species CaMg(CO3)2 _____ Dolomite prevented from forming in DISABLE
 Species Mg5(CO3)4(OH)2.4H2O_HydroMagne5424 prevented from forming in DISABLE
 Species Mg4(CO3)3(OH)2.3H2O_HydroMagne4323 prevented from forming in DISABLE
 fCO2(g) not specified in the INPUT file
 Target pH not specified in the INPUT file
 this is a BATCH problem

FOR088 file name is AP098\$PROD:[000000]AP098_FMT_RUN022.DAT;1

Ideal Gas Constant is Unity (Dimensionless)
 Temperature = 298.15 [=] degree Kelvin

214 Species

27 Elements

Element Name	Molecular Weight
Hydrogen	1.00790
Oxygen	15.99940
Sodium	22.98977
Potassium	39.09830
Magnesium	24.30500
Calcium	40.08000
Chlorine	35.45300
Sulfur	32.06000

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ATTACHMENT 1

ap098_fmt_run022

Carbon	12.01100
PosIon:EL	0.00000
NegIon:EL	0.00000
Oxalate:EL	28.84000
Boron	10.81000
Bromine	79.90400
Acetate:EL	59.04400
Th(IV)	232.03810
Am(III)	243.00000
Pu(III)	238.02900
Np(V)	237.04820
ClO4:EL	99.45060
Phosphorus	30.97400
U(IV)	242.00000
Lactate:EL	89.07000
EDTA:EL	888.88800
Citrate:EL	189.10000
Electron:E	0.00000
Charge:EL	0.00000

Species Name	Phase	Mol.Wt.	Std Chemical Potential, u/RT
1 H2O	WATER aqueous	18.015	-95.6635
2 Na+	Na+ aqueous	22.990	-105.6510
3 K+	K+ aqueous	39.098	-113.9570
4 Ca++	Ca++ aqueous	40.080	-223.3000
5 Mg++	Mg++ aqueous	24.305	-183.4680
6 MgOH+	MgOH+ aqueous	41.312	-251.9400
7 H+	H+ aqueous	1.008	0.0000
8 Cl-	Cl- aqueous	35.453	-52.9550
9 SO4=	SO4= aqueous	96.058	-300.3860
10 HSO4-	HSO4- aqueous	97.066	-304.9420
11 OH-	OH- aqueous	17.007	-63.4350
12 HCO3-	HCO3- aqueous	61.017	-236.7510
13 CO3=	CO3= aqueous	60.009	-212.9440
14 CO2 (aq)	CO2 (aq) aqueous	44.010	-155.6800
15 CaCO3 (aq)	CaCO3 (aq) aqueous	100.089	-443.5000
16 MgCO3 (aq)	MgCO3 (aq) aqueous	84.314	-403.1550
17 B(OH)3 (aq)	B(OH)3 (aq) aqueous	61.832	-390.8100
18 B(OH)4-	B(OH)4- aqueous	78.839	-465.2000
19 B3O3(OH)4-	B3O3(OH)4- aqueous	148.457	-963.7700
20 B4O5(OH)4=	B4O5(OH)4= aqueous	191.266	-1239.1000
21 CaB(OH)4+	CaB(OH)4+ aqueous	118.919	-692.3000
22 MgB(OH)4+	MgB(OH)4+ aqueous	103.144	-651.8900
23 Br-	Br- aqueous	79.904	-999.9900
24 ClO4-	perchlorate aqueous	99.451	-73.8100
25 NaOH(aq)	to.titrate.base.only aqueous	39.997	500.0000

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26	HCl(aq)	to.titrate.acid.only	aqueous	36.461	500.0000
27	HClO4(aq)	to.titrate.acid.only	aqueous	100.459	500.0000
28	PosIon	POSITIVE.ION	aqueous	0.000	0.0000
29	NegIon	NEGATIVE.ION	aqueous	0.000	0.0000
30	PosIon(OH)(aq)	to.titrate.base	aqueous	17.007	500.0000
31	HNegIon(aq)	to.titrate.acid	aqueous	1.008	500.0000
32	H3PO4(aq)	H3PO4(aq)	aqueous	97.995	-460.9000
33	H2PO4-	H2PO4-	aqueous	96.987	-455.9600
34	HPO4=	HPO4=	aqueous	95.980	-439.3670
35	PO4=-	PO4=-	aqueous	94.972	-410.9470
36	Am+++	Am+++	aqueous	243.000	-241.6940
37	AmCO3+	AmCO3+	aqueous	303.009	-473.2900
38	Am(CO3)2-	Am(CO3)2-	aqueous	363.018	-697.5200
39	Am(CO3)3=-	Am(CO3)3=-	aqueous	423.028	-915.5300
40	AmOH++	AmOH++	aqueous	260.007	-319.9600
41	Am(OH)2+	Am(OH)2+	aqueous	277.015	-396.8900
42	Am(OH)3(aq)	Am(OH)3(aq)	aqueous	294.022	-469.5300
43	AmCl++	AmCl++	aqueous	278.453	-295.2000
44	AmCl2+	AmCl2+	aqueous	313.906	-345.9000
45	Am(CO3)4=-	Am(CO3)4=-	aqueous	483.037	-1123.4000
46	Am(SO4)2-	Am(SO4)2-	aqueous	435.115	-850.9900
47	AmSO4+	AmSO4+	aqueous	339.058	-549.5600
48	Pu(OH)2+	deactivated	aqueous	272.044	999.9990
49	Pu(OH)3(aq)	deactivated	aqueous	289.051	999.9990
50	Th++++	Th++++	aqueous	232.038	-284.2270
51	Th(CO3)5===	Th(CO3)5===	aqueous	532.084	-1411.3780
52	Th(OH)3(CO3)-	Th(OH)3(CO3)-	aqueous	343.069	-775.6270
53	Th(OH)4(aq)	Th(OH)4(aq)	aqueous	300.067	-622.4700
54	Th(SO4)2(aq)	Th(SO4)2(aq)	aqueous	424.153	-911.6900
55	Th(SO4)3=	Th(SO4)3=	aqueous	520.211	-1214.0000
56	U++++	U++++	aqueous	242.000	-214.1900
57	UOH+++	UOH+++	aqueous	259.007	-308.7000
58	U(CO3)5===	U(CO3)5===	aqueous	542.046	-1345.3930
59	U(OH)2(CO3)2=	U(OH)2(CO3)2=	aqueous	396.033	-863.3830
60	U(OH)4(CO3)2==	U(OH)4(CO3)2==	aqueous	430.048	-998.6620
61	U(OH)4(aq)	deactivated	aqueous	310.029	999.9990
62	U(SO4)2(aq)	deactivated	aqueous	434.115	999.9990
63	U(SO4)3=	deactivated	aqueous	530.173	999.9990
64	NpO2+	NpO2+	aqueous	269.047	-369.1050
65	NpO2CO3-	NpO2CO3-	aqueous	329.056	-593.6010
66	NpO2(CO3)2=-	NpO2(CO3)2=-	aqueous	389.065	-809.8320
67	NpO2(CO3)3=-	NpO2(CO3)3=-	aqueous	449.075	-1020.2140
68	NpO2OH(aq)	NpO2OH(aq)	aqueous	286.054	-438.7300
69	NpO2(OH)2-	NpO2(OH)2-	aqueous	303.062	-506.2380
70	HAc(aq)	AceticAcid	aqueous	60.052	-158.3000
71	Ac-	Acetate-	aqueous	59.044	-147.3470
72	H3Citrate(aq)	CitricAcid	aqueous	192.124	0.0000

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ATTACHMENT 1

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73	H2Citrate-	H2Citrate-	aqueous	191.116	7.4760
74	HCitrate=	HCitrate=	aqueous	190.108	18.6200
75	Citrate=-	Citrate=-	aqueous	189.100	33.4100
76	H4EDTA (aq)	H4EDTA (aq)	aqueous	892.920	0.0000
77	H3EDTA-	H3EDTA-	aqueous	891.912	5.7610
78	H2EDTA=	H2EDTA=	aqueous	890.904	12.8700
79	HEDTA=-	HEDTA=-	aqueous	889.896	28.7100
80	EDTA=-	EDTA=-	aqueous	888.888	53.0500
81	H2Ox (aq)	OxalicAcid	aqueous	30.856	0.0000
82	HOx-	Bioxalate-	aqueous	29.848	3.2090
83	Ox=	Oxalate=	aqueous	28.840	13.0170
84	HLactate (aq)	LacticAcid	aqueous	90.078	0.0000
85	Lactate-	Lactate-	aqueous	89.070	8.7980
86	AmAc++	AmAcetate++	aqueous	302.044	-395.3560
87	AmCit (aq)	AmCitrate (aq)	aqueous	432.100	-228.5430
88	AmEDTA-	AmEDTA-	aqueous	1131.888	-232.3240
89	AmOx+	AmOxalate+	aqueous	271.840	-242.8530
90	AmLac++	AmLactate++	aqueous	332.070	-241.4360
91	ThAc2++	ThAcetate2++	aqueous	350.126	-604.8000
92	PuCit (aq)	deactivated	aqueous	427.129	999.9990
93	NpO2H2EDTA-	NpO2H2EDTA-	aqueous	1159.951	-364.0980
94	PuOx+	deactivated	aqueous	266.869	999.9990
95	ThLac2++	ThLactate2++	aqueous	410.178	-292.4000
96	ThAc+++	ThAc+++	aqueous	291.082	-448.5250
97	ThCit+	ThCit+	aqueous	421.138	-285.8980
98	ThEDTA (aq)	ThEDTA (aq)	aqueous	1120.926	-285.4190
99	ThOx++	Th (C2O4)++	aqueous	260.878	-297.4280
100	ThLac+++	ThLac+++	aqueous	321.108	-291.1520
101	UAc+++	deactivated	aqueous	301.044	999.9990
102	UCit+	deactivated	aqueous	431.100	999.9990
103	UEDTA (aq)	deactivated	aqueous	1130.888	999.9990
104	ULac+++	deactivated	aqueous	331.070	999.9990
105	UOx++	deactivated	aqueous	270.840	999.9990
106	NpO2Ac (aq)	NpO2Ac (aq)	aqueous	296.092	-519.6150
107	NpO2Cit=	NpO2Citrate=	aqueous	458.147	-343.7470
108	NpO2EDTA=-	NpO2EDTA=-	aqueous	1157.935	-335.7080
109	NpO2Ox-	NpO2Oxalate-	aqueous	297.887	-365.8510
110	NpO2Lac (aq)	NpO2Lactate (aq)	aqueous	358.117	-364.8370
111	MgAc+	MgAc+	aqueous	83.349	-333.3780
112	MgCit-	MgCit-	aqueous	213.405	-162.2610
113	MgEDTA=	MgEDTA=	aqueous	913.193	-153.7340
114	MgOx (aq)	MgOx (aq)	aqueous	53.145	-179.1850
115	MgLac+	MgLac+	aqueous	113.375	999.9990
116	CaAc+	(Mg-analog)	aqueous	99.124	-373.2100
117	CaCit-	(Mg-analog)	aqueous	229.180	-202.0930
118	CaEDTA=	(Mg-analog)	aqueous	928.968	-193.5660
119	CaOx (aq)	(Mg-analog)	aqueous	68.920	-219.0170

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ATTACHMENT 1

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120	CaLac+	(Mg-analog)	aqueous	129.150	999.9990
121	UnuCat#1+	UC#1+	aqueous	0.000	999.9990
122	NpO2HEDTA=	NpO2HEDTA=	aqueous	1158.943	-351.8520
123	UnuAn#2-	UA#2-	aqueous	0.000	999.9990
124	UnuAn#3-	UA#3-	aqueous	0.000	999.9990
125	UnuAn#4-	UA#4-	aqueous	0.000	999.9990
126	UnuNeu#1(aq)	UN#1(aq)	aqueous	0.000	999.9990
127	AmOHCO3(c)	AmOHCO3(c)	solid	320.017	-570.3400
128	Am(OH)3(s)	Am(OH)3(s)	solid	294.022	-495.3200
129	NaAm(CO3)2.6H2O(c)		solid	494.099	-1396.4700
130	AmPO4(c)	AmPO4(c)	solid	337.972	-709.7500
131	PuOHCO3(c)	deactivated	solid	315.046	999.9990
132	Pu(OH)3(s)	deactivated	solid	289.051	999.9990
133	NaPu(CO3)2.6H2O(c)	deactivated	solid	489.128	999.9990
134	PuPO4(c)	deactivated	solid	333.001	999.9990
135	ThO2(am)	Hydrous_Thorium_Oxide	solid	264.037	-451.4080
136	Th(SO4)2.9H2O(s)		solid	586.290	-1775.9000
137	Th(SO4)2.8H2O(s)		solid	568.275	-1680.0000
138	Th(SO4)2.Na2SO4.6H2O(16C,s)		solid	674.282	-2011.2900
139	Th(SO4)2.K2SO4.4H2O(16C,s)		solid	670.468	-1837.5700
140	Th(SO4)2.2K2SO4.2H2O(16C,s)		solid	808.692	-2181.8100
141	2[Th(SO4)2.7/2K2SO4(16C,s)]		solid	2068.086	-5581.6600
142	UO2(am)	Hydrous_U(IV)_Oxide	solid	273.999	-399.6700
143	NpO2OH(aged)	NpO2OH(aged)	solid	286.054	-454.3690
144	NpO2OH(amor)	NpO2OH(amor)	solid	286.054	-452.7570
145	2[NaNpO2CO3.7/2H2O(s)]		solid	830.198	-2096.1160
146	Na3NpO2(CO3)2(s)	Na3NpO2(CO3)2(s)	solid	458.035	-1144.5970
147	KNpO2CO3(s)	KNpO2CO3(s)	solid	368.155	-727.3300
148	K3NpO2(CO3)2(s)	K3NpO2(CO3)2(s)	solid	506.360	-1173.5460
149	H2Ox.2H2O(s)	H2C2O4.2H2O(s)	solid	66.886	-191.3460
150	NaHOx.H2O(s)	NaHC2O4.H2O(s)	solid	70.853	-202.2530
151	Na2Ox(s)	Na2C2O4(s)	solid	74.820	-203.8230
152	CO2("solid",DISABLED)		solid	44.010	0.0000
153	CaSO4	Anhydrite	solid	136.138	-533.7300
154	NaK3(SO4)2	Aphthitalite/Glaserite	solid	332.400	-1057.0500
155	CaCl2.6H2O	Antarcticite	solid	219.077	-893.6500
156	CaCO3	Aragonite	solid	100.089	-455.1700
157	K2SO4	Arcanite	solid	174.254	-532.3900
158	MgCl2.6H2O	Bischofite	solid	203.302	-853.1000
159	Na2Mg(SO4)2.4H2O	Bloedite	solid	334.461	-1383.6000
160	Mg(OH)2	Brucite	solid	58.320	-335.4000
161	Na6CO3(SO4)2	Burkeite	solid	390.063	-1449.4000
162	CaCO3	Calcite	solid	100.089	-455.6000
163	CaCl2.4H2O	CaCl2_Tetrahydrate	solid	183.047	-698.7000
164	Ca4Cl2(OH)6.13H2O	CaOxychloride_A	solid	567.467	-2658.4500
165	Ca2Cl2(OH)2.H2O	CaOxychloride_B	solid	203.096	-778.4100
166	KMgCl3.6H2O	Carnallite	solid	277.854	-1020.3000

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167	MgSO4.7H2O	Epsomite	solid	246.469	-1157.8300
168	CaNa2(CO3)2.5H2O	Gaylussite	solid	296.154	-1360.5000
169	Na2Ca(SO4)2	Glauberite	solid	278.175	-1047.4500
170	CaSO4.2H2O	Gypsum	solid	172.168	-725.5600
171	NaCl	Halite	solid	58.443	-154.9900
172	MgSO4.6H2O	Hexahydrite	solid	228.454	-1061.6000
173	KMgClSO4.3H2O	Kainite	solid	248.960	-938.2000
174	KHCO3	Kalicinite	solid	100.115	-350.0600
175	MgSO4.H2O	Kieserite	solid	138.378	-579.8000
176	K2Mg(SO4)2.4H2O	Leonite	solid	366.678	-1403.9700
177	Na4Ca(SO4)3.2H2O	Labile_Salt	solid	456.242	-1751.4500
178	MgCO3	Magnesite	solid	84.314	-414.4500
179	Mg2Cl(OH)3.4H2O	MgOxychloride	solid	207.146	-1029.6000
180	KHSO4	Mercallite	solid	136.164	-417.5700
181	Na2SO4.10H2O	Mirabilite	solid	322.189	-1471.1500
182	K8H6(SO4)7	Misenite	solid	991.237	-3039.2400
183	NaHCO3	Nahcolite	solid	84.007	-343.3300
184	Na2CO3.10H2O	Natron	solid	286.141	-1382.7800
185	MgCO3.3H2O	Nesquehonite	solid	138.360	-695.3000
186	K2Mg(SO4)2.6H2O	Picromerite/Schoen	solid	402.708	-1596.1000
187	Na2Ca(CO3)2.2H2O	Pirssonite	solid	242.108	-1073.1000
188	K2MgCa2(SO4)4.2H2O	Polyhalite	solid	602.922	-2282.5000
189	Ca(OH)2	Portlandite	solid	74.095	-362.1200
190	K2CO3.3/2H2O	Potassium_Carbonate	solid	165.229	-577.3700
191	K8H4(CO3)6.3H2O	K-Sequicarbonate	solid	730.919	-2555.4000
192	KNaCO3.6H2O	K-Na-Carbonate	solid	230.188	-1006.8000
193	K2NaH(CO3)2.2H2O	Potassium_Trona	solid	258.243	-971.7400
194	K3H(SO4)2	Sesquipotassium_Sulfate	solid	310.418	-950.8000
195	Na3H(SO4)2	Sesquisodium_Sulfate	solid	262.092	-919.6000
196	Na2CO3.7H2O	Na2CO3-Heptahydrate	solid	232.095	-1094.9500
197	KCl	Sylvite	solid	74.551	-164.8400
198	K2Ca(SO4)2.H2O	Syngenite	solid	328.407	-1164.8000
199	Mg2CaCl6.12H2O	Tachyhydrite	solid	517.590	-2015.9000
200	Na2SO4	Thenardite	solid	142.037	-512.3500
201	Na2CO3.H2O	Thermonatrite	solid	124.004	-518.8000
202	Na3H(CO3)2.2H2O	Trona	solid	226.026	-960.3800
203	Na2B4O7.10H2O	Borax	solid	381.367	-2224.1600
204	B(OH)3	Borix_Acid_Solid	solid	61.832	-390.8800
205	KB5O8.4H2O	K-Pentaborate_(30_C)	solid	293.204	-1770.2600
206	K2B4O7.4H2O	K-Tetraborate_(30_C)	solid	305.493	-1663.4700
207	NaBO2.4H2O	Sodium_Metaborate	solid	137.859	-761.4200
208	NaB5O8.5H2O	Sodium_Pentaborate	solid	295.111	-1854.8000
209	NaBO2.NaCl.2H2O	Teepelite_(20_C)	solid	160.272	-725.7700
210	CaMg(CO3)2	Dolomite	solid	184.403	-871.9900
211	Mg5(CO3)4(OH)2.4H2O	HydroMagne5424	solid	467.637	-2364.0600
212	Mg4(CO3)3(OH)2.3H2O	HydroMagne4323	solid	365.308	-1856.1040
213	H+(solid)	to.set.aH+	solid	1.008	0.0000

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214 OH-/H2O(solid) _____ to.set.aH+ solid -1.008 0.0000

Truncated Name	Formula	Matrix																				
1	H2O	2 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0																				
2	Na+	0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0																				
3	K+	0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0																				
4	Ca++	0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0																				
5	Mg++	0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0																				
6	MgOH+	1 1 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0																				
7	H+	1 0																				
8	Cl-	0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0																				
9	SO4=	0 4 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0																				
10	HSO4-	1 4 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0																				
11	OH-	1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0																				
12	HCO3-	1 3 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0																				
13	CO3=	0 3 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0																				
14	CO2(aq)	0 2 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0																				
15	CaCO3(aq)	0 3 0 0 0 1 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0																				
16	MgCO3(aq)	0 3 0 0 1 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0																				
17	B(OH)3(aq)	3 3 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0																				
18	B(OH)4-	4 4 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0																				
19	B3O3(OH)4-	4 7 0 0 0 0 0 0 0 0 0 0 3 0 0 0 0 0 0 0 0																				
20	B4O5(OH)4=	4 9 0 0 0 0 0 0 0 0 0 0 4 0 0 0 0 0 0 0 0																				
21	CaB(OH)4+	4 4 0 0 0 1 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0																				
22	MgB(OH)4+	4 4 0 0 1 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0																				
23	Br-	0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0																				
24	ClO4-	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0																				
25	NaOH(aq) to.ti	1 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0																				
26	HCl(aq) to.ti	1 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0																				
27	HClO4(aq) to.ti	1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0																				
28	PosIon	0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0																				
29	NegIon	0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0																				
30	PosIon(OH)(aq)	1 1 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0																				
31	HNegIon(aq)	1 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0																				
32	H3PO4(aq)	3 4 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0																				
33	H2PO4-	2 4 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0																				
34	HPO4=	1 4 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0																				
35	PO4=-	0 4 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0																				
36	Am+++	0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0																				
37	AmCO3+	0 3 0 0 0 0 0 0 1 0 0 0 0 0 1 0 0 0 0 0 0																				
38	Am(CO3)2-	0 6 0 0 0 0 0 0 2 0 0 0 0 0 1 0 0 0 0 0 0																				
39	Am(CO3)3=-	0 9 0 0 0 0 0 0 3 0 0 0 0 0 1 0 0 0 0 0 0																				
40	AmOH++	1 1 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0																				
41	Am(OH)2+	2 2 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0																				
42	Am(OH)3(aq)	3 3 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0																				
43	AmCl++	0 0 0 0 0 0 1 0 0 0 0 0 0 0 1 0 0 0 0 0 0																				

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44	AmCl2+	0	0	0	0	0	2	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
45	Am(CO3)4===	0	12	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	-5	
46	Am(SO4)2-	0	8	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1		
47	AmSO4+	0	4	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1		
48	Pu(OH)2+	2	2	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	1	
49	Pu(OH)3(aq)	3	3	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	
50	Th++++	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	4	
51	Th(CO3)5===	0	15	0	0	0	0	0	0	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-6	
52	Th(OH)3(CO3)-	3	6	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1	
53	Th(OH)4(aq)	4	4	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	
54	Th(SO4)2(aq)	0	8	0	0	0	0	0	2	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	
55	Th(SO4)3=	0	12	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-2	
56	U++++	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	4	
57	UOH+++	1	1	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	3	
58	U(CO3)5===	0	15	0	0	0	0	0	0	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-6	
59	U(OH)2(CO3)2=	2	8	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-2	
60	U(OH)4(CO3)2=	4	10	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-4	
61	U(OH)4(aq)	4	4	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	
62	U(SO4)2(aq)	0	8	0	0	0	0	0	2	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	
63	U(SO4)3=	0	12	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-2	
64	NpO2+	0	2	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	1	
65	NpO2CO3-	0	5	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1	
66	NpO2(CO3)2=-	0	8	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-3	
67	NpO2(CO3)3=-	0	11	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-5	
68	NpO2OH(aq)	1	3	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	
69	NpO2(OH)2-	2	4	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	-1	
70	HAc(aq)	1	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	
71	Ac-	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	-1	
72	H3Citrate(aq)	3	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	
73	H2Citrate-	2	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	-1	
74	HCitrate=	1	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	-2	
75	Citrate=-	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	-3	
76	H4EDTA(aq)	4	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	
77	H3EDTA-	3	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	-1	
78	H2EDTA=	2	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	-2	
79	HEDTA=-	1	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	-3	
80	EDTA==	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	-4	
81	H2Ox(aq)	2	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	
82	HOx-	1	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	-1	
83	Ox=	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	-2	
84	HLactate(aq)	1	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	
85	Lactate-	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	-1	
86	AmAc++	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	
87	AmCit(aq)	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	
88	AmEDTA-	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	-1	
89	AmOx+	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	1
90	AmLac++	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	2

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91	ThAc2++	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2
92	PuCit(aq)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	1	0	0	0	
93	NpO2H2EDTA-	2	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	1	0	0	-1		
94	PuOx+	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	1		
95	ThLac2++	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	2	0	0	0	0	0	2			
96	ThAc+++	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0	3		
97	ThCit+	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	1	0	1		
98	ThEDTA(aq)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	1	0	0	0			
99	ThOx++	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	2		
100	ThLac+++	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1	0	0	0	0	3			
101	UAc+++	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	1	0	0	0	0	0	3			
102	UCit+	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	1	0	0	1	0	1				
103	UEDTA(aq)	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	1	0	1	0	0	0	0				
104	ULac+++	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	1	1	0	0	0	0	3				
105	UOx++	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	2			
106	NpO2Ac(aq)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	1	0	0	0	0	0	0	0	0	0			
107	NpO2Cit=	0	2	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	1	0	-2			
108	NpO2EDTA=-	0	2	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	-3			
109	NpO2Ox-	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	-1			
110	NpO2Lac(aq)	0	2	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			
111	MgAc+	0	0	0	0	1	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	1			
112	MgCit-	0	0	0	0	1	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	-1			
113	MgEDTA=	0	0	0	0	1	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	-2			
114	MgOx(aq)	0	0	0	0	1	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			
115	MgLac+	0	0	0	0	1	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	1			
116	CaAc+	0	0	0	0	0	1	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	1		
117	CaCit-	0	0	0	0	0	1	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	-1			
118	CaEDTA=	0	0	0	0	0	1	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	-2			
119	CaOx(aq)	0	0	0	0	0	1	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		
120	CaLac+	0	0	0	0	0	1	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	1		
121	UnuCat#1+	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	0	0	1		
122	NpO2HEDTA=	1	2	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	-2			
123	UnuAn#2-	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	0	-1			
124	UnuAn#3-	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	0	-1			
125	UnuAn#4-	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	0	-1			
126	UnuNeu#1(aq)	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	0	0			
127	AmOHCO3(c)	1	4	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			
128	Am(OH)3(s)	3	3	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			
129	NaAm(CO3)2.6H2O(c)	12	12	1	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			
130	AmPO4(c)	0	4	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			
131	PuOHCO3(c)	1	4	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			
132	Pu(OH)3(s)	3	3	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			
133	NaPu(CO3)2.6H2O(c)	12	12	1	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			
134	PuPO4(c)	0	4	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			
135	ThO2(am)Hydrou	0	2	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			
136	Th(SO4)2.9H2O(s)	18	17	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			
137	Th(SO4)2.8H2O(s)	16	16	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			

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185 MgCO3.3H2O	6	6	0	0	1	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
186 K2Mg(SO4)2.6H2O_Pic	12	14	0	2	1	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
187 Na2Ca(CO3)2.2H2O	4	8	2	0	0	1	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
188 K2MgCa2(SO4)4.2H2O	4	18	0	2	1	2	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
189 Ca(OH)2	2	2	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
190 K2CO3.3/2H2O_Pota	3	4	0	2	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
191 K8H4(CO3)6.3H2O_K	10	21	0	8	0	0	0	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
192 KNaCO3.6H2O	12	9	1	1	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
193 K2NaH(CO3)2.2H2O	5	8	1	2	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
194 K3H(SO4)2_Sesquipo	1	8	0	3	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
195 Na3H(SO4)2_Sesqu	1	8	3	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
196 Na2CO3.7H2O_Na2C	14	10	2	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
197 KCl	0	0	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
198 K2Ca(SO4)2.H2O	2	9	0	2	0	1	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
199 Mg2CaCl6.12H2O	24	12	0	0	2	1	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
200 Na2SO4	0	4	2	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
201 Na2CO3.H2O	2	4	2	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
202 Na3H(CO3)2.2H2O	5	8	3	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
203 Na2B4O7.10H2O	20	17	2	0	0	0	0	0	0	0	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
204 B(OH)3_B	3	3	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
205 KB5O8.4H2O_K-Pen	8	12	0	1	0	0	0	0	0	0	0	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
206 K2B4O7.4H2O_K-Tet	8	11	0	2	0	0	0	0	0	0	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
207 NaBO2.4H2O_So	8	6	1	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
208 NaB5O8.5H2O_Sod	10	13	1	0	0	0	0	0	0	0	0	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
209 NaBO2.NaCl.2H2O_T	4	4	2	0	0	0	1	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
210 CaMg(CO3)2	0	6	0	0	1	1	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
211 Mg5(CO3)4(OH)2.4H2O	10	18	0	0	5	0	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
212 Mg4(CO3)3(OH)2.3H2O	8	14	0	0	4	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
213 H+(solid)	1	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	1	
214 OH-/H2O(solid)	-1	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	-1	

Preventing Formation of SOLID Species OH-/H2O(solid)_____to.set.aH+
 Preventing Formation of SOLID Species CaMg(CO3)2_____Dolomite
 Preventing Formation of SOLID Species MgCO3_____Magnesite
 *****SOLUBILITY PRODUCT VIOLATED***** Na2Ca(SO4)2_____Glauberite 4.2903E-02

1 Solubility Product Violations, adding Na2Ca(SO4)2_____Glauberite

Preventing Formation of SOLID Species MgCO3_____Magnesite
 Preventing Formation of SOLID Species CaMg(CO3)2_____Dolomite
 Preventing Formation of SOLID Species OH-/H2O(solid)_____to.set.aH+
 AQ VIOLATION, Estimated Conc= 8.63E-23 ThAc+++ ThAc+++
 AQ VIOLATION, Estimated Conc= 8.63E-23 ThAc+++ ThAc+++
 Preventing Formation of SOLID Species OH-/H2O(solid)_____to.set.aH+

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Preventing Formation of SOLID Species CaMg(CO3)2 Dolomite
 Preventing Formation of SOLID Species MgCO3 Magnesite
 AQ VIOLATION, Estimated Conc= 8.63E-23 ThAc+++ ThAc+++
 Preventing Formation of SOLID Species MgCO3 Magnesite
 Preventing Formation of SOLID Species CaMg(CO3)2 Dolomite
 Preventing Formation of SOLID Species OH-/H2O(solid) to.set.aH+
 # inversions for batch pblm 97

LCRA ERDA-6 recipe, calc

FMT V2.4

FMT_021120.chemdat

ERG update of FMT_970407.chemdat (PAVT db)

Pressure= 1.00000E+00 [=] ATM Temperature= 2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

Total Moles	Aq. Molality	Aq. Molarity	Aq. mg/liter	
Using NaCl Density Correlation				
1.34424796E+02	1.11282674E+02	9.78179042E+01	9.85906657E+04	Hydrogen
1.29527220E+02	5.65788325E+01	4.97330142E+01	7.95698388E+05	Oxygen
1.55053126E+01	6.02272719E+00	5.29400068E+00	1.21707858E+05	Sodium
1.10965407E+00	1.09254520E-01	9.60351491E-02	3.75481107E+03	Potassium
1.00214786E+01	1.65631567E-01	1.45590793E-01	3.53858421E+03	Magnesium
1.10135655E+01	1.34049714E-02	1.17830221E-02	4.72263528E+02	Calcium
1.54261808E+01	5.96191571E+00	5.24054714E+00	1.85793118E+05	Chlorine
1.01921772E+01	2.00244911E-01	1.76016057E-01	5.64307478E+03	Sulfur
2.01808727E+00	1.15925711E-04	1.01899151E-04	1.22391071E+00	Carbon
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	PosIon:EL
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	NegIon:EL
2.44178136E-02	2.43234525E-02	2.13804096E-02	6.16611012E+02	Oxalate:EL
7.12186231E-02	7.09434032E-02	6.23595279E-02	6.74106497E+02	Boron
1.24349977E-02	1.23869434E-02	1.08881715E-02	8.70008459E+02	Bromine
5.70879439E-03	5.68673311E-03	4.99866057E-03	2.95140915E+02	Acetate:EL
1.00000000E+00	6.64773844E-09	5.84338800E-09	1.35588865E-03	Th(IV)
1.00000000E+00	2.01468583E-07	1.77091669E-07	4.30332757E-02	Am(III)
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Pu(III)
1.00000000E+00	2.42009955E-05	2.12727694E-05	5.04267170E+00	Np(V)
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	ClO4:EL
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Phosphorus
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	U(IV)
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Lactate:EL
4.37485827E-06	4.35795191E-06	3.83065671E-06	3.40502479E+00	EDTA:EL
4.32964010E-04	4.31290848E-04	3.79106336E-04	7.16890082E+01	Citrate:EL
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Electron:E
5.15880085E-16	5.13886499E-16	4.51708235E-16	0.00000000E+00	Charge:EL

Solution Parameters, Calculated

SOLUTION MASS 1390.73348656624 grams

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H2O MASS	1003.87942839125	grams
TDS(g/kg)	385.359085199040	g/kgH2O
Specified Solution Density		
DENSITY	1217.73603507538	kg/m ³ = g/l
Solution Parameters Based on Specified Density		
SOLUTION VOL	1.14206482070652	liters
TDS	338.732137757003	g/l
Density based on TDS and NaCl solutions 1217.74 g/l		
% Relative difference vs NaCl density 0.00 %		
Calculated Ratio of molality to Molarity 1.138		

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	8.15675E-01	7.47722E-01	0.9167	5.57240E+01	4.87923E+01	8.79004E+05
CaSO4	Anhydrite	9.93453E+00	1.00000E+00	1.000	9.97307E+00	8.73249E+00	1.18882E+06
Mg(OH)2	Brucite	9.81712E+00	1.00000E+00	1.000	9.85520E+00	8.62929E+00	5.03257E+05
NaCl	Halite	9.40465E+00	1.00000E+00	1.000	9.44114E+00	8.26673E+00	4.83130E+05
Na+	Na+	6.02273E+00	5.82887E+00	0.9678	6.04609E+00	5.29400E+00	1.21708E+05
CaCO3	Calcite	1.01406E+00	1.00000E+00	1.000	1.01800E+00	8.91364E-01	8.92159E+04
ThO2(am)	Hydrous_Thorium_Oxide	9.96136E-01	1.00000E+00	1.000	1.00000E+00	8.75607E-01	2.31193E+05
Am(OH)3(s)	Am(OH)3(s)	9.96135E-01	1.00000E+00	1.000	1.00000E+00	8.75607E-01	2.57448E+05
KNpO2CO3(s)	KNpO2CO3(s)	9.96111E-01	1.00000E+00	1.000	9.99976E-01	8.75586E-01	3.22351E+05
SO4=	SO4=	2.00245E-01	3.85784E-03	1.9266E-02	2.01022E-01	1.76016E-01	1.69077E+04
Mg++	Mg++	1.26674E-01	2.42161E-01	1.912	1.27165E-01	1.11347E-01	2.70629E+03
K+	K+	1.09255E-01	5.22453E-02	0.4782	1.09678E-01	9.60351E-02	3.75481E+03
B(OH)4-	B(OH)4-	4.20899E-02	4.20581E-03	9.9925E-02	4.22531E-02	3.69971E-02	2.91683E+03
MgOx(aq)	MgOx(aq)	2.26344E-02	2.83557E-02	1.253	2.27222E-02	1.98957E-02	1.05736E+03
Br-	Br-	1.23869E-02	3.46312E-03	0.2796	1.24350E-02	1.08882E-02	8.70008E+02
Ac-	Acetate-	3.99031E-03	3.01745E-03	0.7562	4.00579E-03	3.50750E-03	2.07097E+02
MgCit-	MgCit-	4.01358E-04	8.01307E-05	0.1996	4.02915E-04	3.52795E-04	7.52883E+01
MgEDTA=	MgEDTA=	4.07175E-06	1.05201E-06	0.2584	4.08755E-06	3.57908E-06	3.26839E+00
Cl-	Cl-	5.96192E+00	6.38005E+00	1.070	5.98504E+00	5.24055E+00	1.85793E+05
MgB(OH)4+	MgB(OH)4+	1.34611E-02	2.55418E-02	1.897	1.35133E-02	1.18324E-02	1.22044E+03
B(OH)3(aq)	B(OH)3(aq)	1.05362E-02	1.00081E-02	0.9499	1.05771E-02	9.26136E-03	5.72648E+02
Ca++	Ca++	1.04548E-02	1.12616E-02	1.077	1.04954E-02	9.18981E-03	3.68328E+02
Na2Ca(SO4)2	Glauberite	9.00726E-03	1.00000E+00	1.000	9.04220E-03	7.91742E-03	2.20243E+03
CaB(OH)4+	CaB(OH)4+	1.79779E-03	2.11724E-03	1.178	1.80476E-03	1.58026E-03	1.87923E+02
MgAc+	MgAc+	1.62055E-03	9.48074E-03	5.850	1.62683E-03	1.42447E-03	1.18728E+02
CaOx(aq)	(Mg-analog)	1.05260E-03	1.31868E-03	1.253	1.05669E-03	9.25243E-04	6.37678E+01
MgOH+	MgOH+	7.64482E-04	2.73810E-04	0.3582	7.67447E-04	6.71982E-04	2.77611E+01

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Ox=	Oxalate=	6.13835E-04	1.88542E-05	3.0715E-02	6.16216E-04	5.39563E-04	1.55610E+01	1.74E-08
B3O3 (OH) 4-	B3O3 (OH) 4-	4.47392E-04	5.18404E-05	0.1159	4.49127E-04	3.93259E-04	5.83822E+01	9.17E-09
B4O5 (OH) 4=	B4O5 (OH) 4=	4.29068E-04	1.67419E-06	3.9019E-03	4.30733E-04	3.77153E-04	7.21366E+01	2.16E-08
CaAc+	(Mg-analog)	7.53631E-05	4.40899E-04	5.850	7.56555E-05	6.62445E-05	6.56642E+00	-3.24E-08
MgCO3 (aq)	MgCO3 (aq)	7.15726E-05	7.15726E-05	1.000	7.18503E-05	6.29126E-05	5.30442E+00	3.32E-08
NpO2Ox-	NpO2Oxalate-	2.26486E-05	4.48068E-07	1.9783E-02	2.27365E-05	1.99082E-05	5.93040E+00	-2.34E-08
HCO3-	HCO3-	2.25305E-05	7.81124E-06	0.3467	2.26179E-05	1.98044E-05	1.20840E+00	4.17E-08
CaCit-	(Mg-analog)	1.86650E-05	3.72646E-06	0.1996	1.87375E-05	1.64066E-05	3.76008E+00	-3.28E-08
CO3=	CO3=	1.57891E-05	3.48493E-07	2.2072E-02	1.58503E-05	1.38787E-05	8.32847E-01	4.19E-08
OH-	OH-	1.40375E-05	7.34182E-06	0.5230	1.40920E-05	1.23390E-05	2.09854E-01	3.40E-09
Citrate=-	Citrate=-	1.12654E-05	1.65958E-09	1.4732E-04	1.13091E-05	9.90235E-06	1.87253E+00	7.87E-09
CaCO3 (aq)	CaCO3 (aq)	5.55951E-06	5.55951E-06	1.000	5.58108E-06	4.88683E-06	4.89119E-01	3.09E-12
NpO2+	NpO2+	7.07352E-07	1.36747E-06	1.933	7.10096E-07	6.21765E-07	1.67284E-01	-3.63E-08
NpO2CO3-	NpO2CO3-	4.56370E-07	4.95544E-08	0.1086	4.58140E-07	4.01151E-07	1.32001E-01	-7.06E-09
NpO2Ac (aq)	NpO2Ac (aq)	3.37126E-07	9.75512E-08	0.2894	3.38433E-07	2.96335E-07	8.77424E-02	-4.69E-08
CaEDTA=	(Mg-analog)	1.89355E-07	4.89236E-08	0.2584	1.90090E-07	1.66444E-07	1.54621E-01	-3.44E-08
HAc (aq)	AceticAcid	1.76907E-07	1.76907E-07	1.000	1.77593E-07	1.55502E-07	9.33819E-03	-3.59E-09
Am(OH) 2+	Am(OH) 2+	1.02595E-07	8.63100E-11	8.4127E-04	1.02993E-07	9.01813E-08	2.49815E-02	-2.63E-08
AmEDTA-	AmEDTA-	9.68343E-08	2.42392E-09	2.5032E-02	9.72100E-08	8.51178E-08	9.63438E-02	4.24E-09
NpO2OH (aq)	NpO2OH (aq)	4.71966E-08	4.89784E-09	0.1038	4.73797E-08	4.14860E-08	1.18673E-02	-4.63E-08
CO2 (aq)	CO2 (aq)	6.71361E-09	2.33184E-08	3.473	6.73965E-09	5.90129E-09	2.59714E-04	3.27E-08
Th(OH) 3 (CO3) -	Th(OH) 3 (CO3) -	5.76364E-09	1.61139E-09	0.2796	5.78600E-09	5.06626E-09	1.73808E-03	4.11E-08
NpO2 (CO3) 2=-	NpO2 (CO3) 2=-	2.56036E-09	4.62171E-13	1.8051E-04	2.57029E-09	2.25056E-09	8.75616E-04	2.56E-08
NpO2Cit=	NpO2Citrate=	1.62788E-09	7.12617E-12	4.3776E-03	1.63420E-09	1.43092E-09	6.55570E-04	-2.40E-08
HOx-	Bioxalate-	1.34888E-09	3.51759E-10	0.2608	1.35412E-09	1.18567E-09	3.53899E-05	1.48E-08
Th(OH) 4 (aq)	Th(OH) 4 (aq)	8.84102E-10	8.84102E-10	1.000	8.87532E-10	7.77129E-10	2.33191E-04	1.64E-09
Am(OH) 3 (aq)	Am(OH) 3 (aq)	7.95189E-10	6.30297E-12	7.9264E-03	7.98274E-10	6.98974E-10	2.05514E-04	-9.07E-09
AmOH++	AmOH++	6.48687E-10	1.61977E-11	2.4970E-02	6.51204E-10	5.70199E-10	1.48256E-04	-2.43E-09
HSO4-	HSO4-	6.36376E-10	3.76936E-10	0.5923	6.38845E-10	5.59377E-10	5.42962E-05	4.14E-08
HCitrate=	HCitrate=	4.83192E-10	4.51327E-12	9.3405E-03	4.85067E-10	4.24728E-10	8.07441E-05	1.24E-08
AmOx+	AmOxalate+	3.21375E-10	2.16071E-11	6.7233E-02	3.22622E-10	2.82490E-10	7.67921E-05	1.26E-09
H+	H+	2.31769E-10	1.02631E-09	4.428	2.32668E-10	2.03726E-10	2.05336E-07	1.29E-09
NpO2 (OH) 2-	NpO2 (OH) 2-	1.32134E-10	2.11198E-12	1.5984E-02	1.32647E-10	1.16147E-10	3.51996E-05	-4.21E-08
AmCit (aq)	AmCitrate (aq)	1.05548E-10	8.33680E-13	7.8986E-03	1.05958E-10	9.27775E-11	4.00891E-05	-1.56E-08
AmAc++	AmAcetate++	8.55651E-11	1.33303E-12	1.5579E-02	8.58971E-11	7.52121E-11	2.27174E-05	-1.20E-08
AmCO3+	AmCO3+	4.72195E-11	3.50981E-11	0.7433	4.74027E-11	4.15062E-11	1.25767E-05	3.21E-08
Am (CO3) 2-	Am (CO3) 2-	1.77685E-11	9.74823E-13	5.4862E-02	1.78375E-11	1.56186E-11	5.66984E-06	7.33E-08
AmSO4+	AmSO4+	1.27336E-11	5.46381E-12	0.4291	1.27830E-11	1.11929E-11	3.79503E-06	3.01E-08
EDTA==	EDTA==	9.21112E-12	3.25018E-16	3.5285E-05	9.24685E-12	8.09661E-12	7.19698E-06	-9.14E-09
NpO2 (CO3) 3=-	NpO2 (CO3) 3=-	4.49177E-12	1.24261E-20	2.7664E-09	4.50919E-12	3.94828E-12	1.77307E-06	4.27E-08
HEDTA=-	HEDTA=-	2.68774E-12	1.24140E-14	4.6188E-03	2.69817E-12	2.36253E-12	2.10241E-06	1.80E-09
Am+++	Am+++	2.44867E-12	7.99150E-13	0.3264	2.45817E-12	2.15239E-12	5.23030E-07	-5.42E-08
Am (SO4) 2-	Am (SO4) 2-	1.55447E-12	5.98748E-14	3.8518E-02	1.56050E-12	1.36638E-12	5.94534E-07	7.39E-08
NpO2EDTA=-	NpO2EDTA=-	1.12414E-12	1.52410E-13	0.1356	1.12850E-12	9.88125E-13	1.14418E-06	-3.56E-08
Am (CO3) 3=-	Am (CO3) 3=-	1.03120E-12	5.38587E-17	5.2229E-05	1.03520E-12	9.06427E-13	3.83444E-07	1.04E-07
AmCl++	AmCl++	1.90901E-13	8.84605E-12	46.34	1.91642E-13	1.67803E-13	4.67252E-08	2.20E-08
AmCl2+	AmCl2+	7.25113E-15	5.91888E-12	816.3	7.27926E-15	6.37377E-15	2.00077E-09	1.83E-08

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H2EDTA=	H2EDTA=	6.80505E-15	9.64746E-17	1.4177E-02	6.83145E-15	5.98166E-15	5.32908E-09	7.86E-09
NpO2HEDTA=	NpO2HEDTA=	5.59755E-15	1.60525E-15	0.2868	5.61926E-15	4.92026E-15	5.70231E-09	-3.26E-08
H2Citrate-	H2Citrate-	2.60985E-15	3.20292E-16	0.1227	2.61997E-15	2.29407E-15	4.38433E-10	1.09E-08
Am(CO3)4===	Am(CO3)4===	2.23664E-15	1.17447E-25	5.2510E-11	2.24531E-15	1.96601E-15	9.49657E-10	1.02E-07
H2Ox(aq)	OxalicAcid	8.93662E-18	8.93662E-18	1.000	8.97129E-18	7.85533E-18	2.42382E-13	7.28E-09
ThEDTA(aq)	ThEDTA(aq)	1.89533E-18	7.12870E-18	3.761	1.90268E-18	1.66600E-18	1.86746E-12	3.16E-09
NpO2H2EDTA-	NpO2H2EDTA-	1.05668E-18	3.42917E-19	0.3245	1.06078E-18	9.28830E-19	1.07740E-12	-2.61E-08
Th(SO4)3=	Th(SO4)3=	5.60534E-19	9.34270E-21	1.6667E-02	5.62709E-19	4.92712E-19	2.56314E-13	1.09E-07
ThCit+	ThCit+	1.75195E-20	1.73614E-19	9.910	1.75875E-20	1.53997E-20	6.48541E-15	2.03E-08
Th(CO3)5===	Th(CO3)5===	1.14356E-20	4.05988E-31	3.5502E-11	1.14800E-20	1.00519E-20	5.34848E-15	2.29E-07
Th(SO4)2(aq)	Th(SO4)2(aq)	1.11376E-20	3.53627E-19	31.75	1.11809E-20	9.79004E-21	4.15248E-15	8.07E-08
ThOx++	Th(C2O4)++	1.56831E-21	2.79153E-19	178.0	1.57439E-21	1.37855E-21	3.59633E-16	4.66E-08
H3EDTA-	H3EDTA-	5.83347E-22	1.21085E-22	0.2076	5.85610E-22	5.12764E-22	4.57341E-16	7.07E-09
H3Citrate(aq)	CitricAcid	5.80241E-22	5.80241E-22	1.000	5.82492E-22	5.10034E-22	9.79896E-17	4.95E-09
ThAc2++	ThAcetate2++	5.44279E-22	9.60484E-20	176.5	5.46391E-22	4.78424E-22	1.67509E-16	2.53E-08
ThAc+++	ThAc+++	0.00000E+00	0.00000E+00	48.92	0.00000E+00	0.00000E+00	0.00000E+00	-2.04E+01
HCl(aq)	to.titrate.acid.only	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.48E+02
NaOH(aq)	to.titrate.base.only	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.95E+02
AmOHCO3(c)	AmOHCO3(c)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-9.90E-01
NaAm(CO3)2.6H2O(c)		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.61E+00
Th(SO4)2.9H2O(s)		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.82E+01
Th(SO4)2.8H2O(s)		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.82E+01
Th(SO4)2.Na2SO4.6H2O(16C,s)		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.40E+01
Th(SO4)2.K2SO4.4H2O(16C,s)		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.75E+01
Th(SO4)2.2K2SO4.2H2O(16C,s)		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.90E+01
2[Th(SO4)2.7/2K2SO4(16C,s)]		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.56E+01
NpO2OH(aged)	NpO2OH(aged)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.52E+00
NpO2OH(amor)	NpO2OH(amor)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.22E+00
2[NaNpO2CO3.7/2H2O(s)]		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.82E+00
Na3NpO2(CO3)2(s)	Na3NpO2(CO3)2(s)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.30E+00
K3NpO2(CO3)2(s)	K3NpO2(CO3)2(s)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-6.69E+00
H2Ox.2H2O(s)	H2C2O4.2H2O(s)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.73E+01
NaHOx.H2O(s)	NaHC2O4.H2O(s)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.01E+00
Na2Ox(s)	Na2C2O4(s)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.88E+01
CO2("solid",DISABLED)		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.52E+01
NaK3(SO4)2	Aphthitalite/Glaserite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.10E+00
CaCl2.6H2O	Antarcticite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-5.24E+00
CaCO3	Aragonite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.87E-01
K2SO4	Arcanite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.20E+00
MgCl2.6H2O	Bischofite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.22E+00
Na2Mg(SO4)2.4H2O	Bloedite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.07E+00
Na6CO3(SO4)2	Burkeite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-5.92E+00
CaCl2.4H2O	CaCl2_Tetrahydrite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-6.56E+00
Ca4Cl2(OH)6.13H2O	CaOxychloride_A	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.34E+01
Ca2Cl2(OH)2.H2O	CaOxychloride_B	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.12E+01
KMgCl3.6H2O	Carnallite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.57E+00
MgSO4.7H2O	Epsomite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.03E+00

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CaNa2 (CO3) 2.5H2O	Gaylussite	NAF	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.54E+00
CaSO4.2H2O	Gypsum		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.41E+02
MgSO4.6H2O	Hexahydrate		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.15E+00
KMgClSO4.3H2O	Kainite		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.69E+00
KHCO3	Kalicinite		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-6.67E+00
MgSO4.H2O	Kieserite		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.03E+00
K2Mg (SO4) 2.4H2O	Leonite		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.53E+00
Na4Ca (SO4) 3.2H2O	Labile_Salt		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.07E-01
MgCO3	Magnesite	NAF	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	7.60E-01
Mg2Cl (OH) 3.4H2O	MgOxychloride		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.74E-01
KHSO4	Mercallite		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.13E+01
Na2SO4.10H2O	Mirabilite		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-9.17E-01
K8H6 (SO4) 7	Misenite		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.03E+01
NaHCO3	Nahcolite		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.94E+00
Na2CO3.10H2O	Natron		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-5.36E+00
MgCO3.3H2O	Nesquehonite	NAF	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.29E+00
K2Mg (SO4) 2.6H2O	Picromerite/Schoen		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.44E+00
Na2Ca (CO3) 2.2H2O	Pirssonite	NAF	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.34E+00
K2MgCa2 (SO4) 4.2H2O	Polyhalite		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.24E+00
Ca (OH) 2	Portlandite		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.03E+00
K2CO3.3/2H2O	Potassium_Carbonate		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.22E+01
K8H4 (CO3) 6.3H2O	K-Sequicarbonate		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-5.10E+01
KNaCO3.6H2O	K-Na-Carbonate		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.62E+00
K2NaH (CO3) 2.2H2O	Potassium_Trona		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.49E+01
K3H (SO4) 2	Sesquipotassium_Sulfate		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.41E+01
Na3H (SO4) 2	Sesquisodium_Sulfate		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.07E+01
Na2CO3.7H2O	Na2CO3-Heptahydrate		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-5.35E+00
KCl	Sylvite		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.38E+00
K2Ca (SO4) 2.H2O	Syngenite		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.02E+00
Mg2CaCl6.12H2O	Tachyhydrite		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.73E+01
Na2SO4	Thenardite		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-5.95E-01
Na2CO3.H2O	Thermonatrite		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-5.53E+00
Na3H (CO3) 2.2H2O	Trona		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-8.48E+00
Na2B4O7.10H2O	Borax		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.59E+00
B (OH) 3	Borix_Acid_Solid		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.97E+00
KB5O8.4H2O	K-Pentaborate_(30_C)		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-6.58E+00
K2B4O7.4H2O	K-Tetraborate_(30_C)		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-6.37E+00
NaBO2.4H2O	Sodium_Metaborate		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.19E+00
NaB5O8.5H2O	Sodium_Pentaborate		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-5.89E+00
NaBO2.NaCl.2H2O	Teepelite_(20_C)		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.64E+00
CaMg (CO3) 2	Dolomite	NAF	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	1.60E+00
Mg5 (CO3) 4 (OH) 2.4H2O	HydroMagne5424	NAF	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.59E+00
Mg4 (CO3) 3 (OH) 2.3H2O	HydroMagne4323	NAF	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.28E+00
H+(solid)	to.set.aH+	NAF	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-8.99E+00
OH-/H2O(solid)	to.set.aH+	NAF	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	8.99E+00
H4EDTA(aq)	H4EDTA(aq)		0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.84E+01
Th++++	Th++++		0.00000E+00	0.00000E+00	0.5366	0.00000E+00	0.00000E+00	0.00000E+00	-2.52E+01

Information Only

ATTACHMENT 1

ap098_fmt_run022

pH (-log[aH+]); pmH(-log[mH+]); pcH(-log[MH+]) 8.9887 9.6349 9.6910
Osmotic Coefficient= 1.286513
Equilibrium RH (%) = 74.772191
Ionic Strength (m) = 6.762430
Density, kg/m3 = 1217.74
fCO2(g); log[fCO2(g)]= 7.071E-07 -6.150

NOTES: - Water "molality" is mole fraction H2O in aqueous phase
- "Descriptor" means:
*dG/RT/ln10 for species with nonzero concs. (convergence criterion)
*Saturation Index for minerals, SI=log10(IAP/Ksp)
*log10(activity) for aqueous species with very small concentrations
*log10(activity) for aqueous species Not Allowed to Form
*NAF signifies that the species was Not Allowed to Form

Total G/RT= -1.86736780E+04

Total Diagonal Inversions 97

Total Stoichiometric Reoptimizations 11

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ATTACHMENT 1

ap098_fmt_run028

INPUT file name is:AP098\$PROD:[000000]AP098_FMT_RUN028.IN;1
INGUESS file name is:AP098\$PROD:[000000]AP098_FMT_RUN028.INGUESS;1
OUTPUT file name is:AP098\$PROD:[000000]AP098_FMT_RUN028.OUT;1
CHEMDAT file name is AP098\$PROD:[000000]AP098_FMT.CHEMDAT;1
Temperature is Hard Coded as 298.15K
CRA ERDA-6 recipe, calc
FMT_021120.chemdat
ERG update of FMT_970407.chemdat (PAVT db)

FMT V2.4

Accuracy of reactions is 1.0000E-06
Minimum elemental abundance is 1.0000E-18
Number of Aqueous Species is 126

PITZER Data Base NOT Echoed in this Run
using PITZER ACTIVITY COEFFICIENT model
Charge Balance replaces element Oxygen

Species CaCO3_____Aragonite prevented from forming in DISABLE
Species CaCO3_____Calcite prevented from forming in DISABLE
Species CaNa2(CO3)2.5H2O_____Gaylussite prevented from forming in DISABLE
Species MgCO3_____Magnesite prevented from forming in DISABLE
Species MgCO3.3H2O_____Nesquehonite prevented from forming in DISABLE
Species Na2Ca(CO3)2.2H2O_____Pirssonite prevented from forming in DISABLE
Species CaMg(CO3)2_____Dolomite prevented from forming in DISABLE
Species Mg4(CO3)3(OH)2.3H2O_HydroMagne4323 prevented from forming in DISABLE
fCO2(g) not specified in the INPUT file
Target pH not specified in the INPUT file
this is a BATCH problem

FOR088 file name is AP098\$PROD:[000000]AP098_FMT_RUN028.DAT;1

Ideal Gas Constant is Unity (Dimensionless)
Temperature = 298.15 [=] degree Kelvin

214 Species

27 Elements

Element Name	Molecular Weight
Hydrogen	1.00790
Oxygen	15.99940
Sodium	22.98977
Potassium	39.09830
Magnesium	24.30500
Calcium	40.08000
Chlorine	35.45300
Sulfur	32.06000

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ATTACHMENT 1

ap098_fmt_run028

Carbon	12.01100
PosIon:EL	0.00000
NegIon:EL	0.00000
Oxalate:EL	28.84000
Boron	10.81000
Bromine	79.90400
Acetate:EL	59.04400
Th(IV)	232.03810
Am(III)	243.00000
Pu(III)	238.02900
Np(V)	237.04820
ClO4:EL	99.45060
Phosphorus	30.97400
U(IV)	242.00000
Lactate:EL	89.07000
EDTA:EL	888.88800
Citrate:EL	189.10000
Electron:E	0.00000
Charge:EL	0.00000

Species Name	Phase	Mol.Wt.	Std Chemical Potential, u/RT
1 H2O	WATER aqueous	18.015	-95.6635
2 Na+	Na+ aqueous	22.990	-105.6510
3 K+	K+ aqueous	39.098	-113.9570
4 Ca++	Ca++ aqueous	40.080	-223.3000
5 Mg++	Mg++ aqueous	24.305	-183.4680
6 MgOH+	MgOH+ aqueous	41.312	-251.9400
7 H+	H+ aqueous	1.008	0.0000
8 Cl-	Cl- aqueous	35.453	-52.9550
9 SO4=	SO4= aqueous	96.058	-300.3860
10 HSO4-	HSO4- aqueous	97.066	-304.9420
11 OH-	OH- aqueous	17.007	-63.4350
12 HCO3-	HCO3- aqueous	61.017	-236.7510
13 CO3=	CO3= aqueous	60.009	-212.9440
14 CO2(aq)	CO2(aq) aqueous	44.010	-155.6800
15 CaCO3(aq)	CaCO3(aq) aqueous	100.089	-443.5000
16 MgCO3(aq)	MgCO3(aq) aqueous	84.314	-403.1550
17 B(OH)3(aq)	B(OH)3(aq) aqueous	61.832	-390.8100
18 B(OH)4-	B(OH)4- aqueous	78.839	-465.2000
19 B3O3(OH)4-	B3O3(OH)4- aqueous	148.457	-963.7700
20 B4O5(OH)4=	B4O5(OH)4= aqueous	191.266	-1239.1000
21 CaB(OH)4+	CaB(OH)4+ aqueous	118.919	-692.3000
22 MgB(OH)4+	MgB(OH)4+ aqueous	103.144	-651.8900
23 Br-	Br- aqueous	79.904	-999.9900
24 ClO4-	perchlorate aqueous	99.451	-73.8100

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ATTACHMENT 1

ap098_fmt_run028

25	NaOH(aq)	to.titrate.base.only	aqueous	39.997	500.0000
26	HCl(aq)	to.titrate.acid.only	aqueous	36.461	500.0000
27	HClO4(aq)	to.titrate.acid.only	aqueous	100.459	500.0000
28	PosIon	POSITIVE.ION	aqueous	0.000	0.0000
29	NegIon	NEGATIVE.ION	aqueous	0.000	0.0000
30	PosIon(OH)(aq)	to.titrate.base	aqueous	17.007	500.0000
31	HNegIon(aq)	to.titrate.acid	aqueous	1.008	500.0000
32	H3PO4(aq)	H3PO4(aq)	aqueous	97.995	-460.9000
33	H2PO4-	H2PO4-	aqueous	96.987	-455.9600
34	HPO4=	HPO4=	aqueous	95.980	-439.3670
35	PO4=-	PO4=-	aqueous	94.972	-410.9470
36	Am+++	Am+++	aqueous	243.000	-241.6940
37	AmCO3+	AmCO3+	aqueous	303.009	-473.2900
38	Am(CO3)2-	Am(CO3)2-	aqueous	363.018	-697.5200
39	Am(CO3)3=-	Am(CO3)3=-	aqueous	423.028	-915.5300
40	AmOH++	AmOH++	aqueous	260.007	-319.9600
41	Am(OH)2+	Am(OH)2+	aqueous	277.015	-396.8900
42	Am(OH)3(aq)	Am(OH)3(aq)	aqueous	294.022	-469.5300
43	AmCl++	AmCl++	aqueous	278.453	-295.2000
44	AmCl2+	AmCl2+	aqueous	313.906	-345.9000
45	Am(CO3)4=-	Am(CO3)4=-	aqueous	483.037	-1123.4000
46	Am(SO4)2-	Am(SO4)2-	aqueous	435.115	-850.9900
47	AmSO4+	AmSO4+	aqueous	339.058	-549.5600
48	Pu(OH)2+	deactivated	aqueous	272.044	999.9990
49	Pu(OH)3(aq)	deactivated	aqueous	289.051	999.9990
50	Th++++	Th++++	aqueous	232.038	-284.2270
51	Th(CO3)5===	Th(CO3)5===	aqueous	532.084	-1411.3780
52	Th(OH)3(CO3)-	Th(OH)3(CO3)-	aqueous	343.069	-775.6270
53	Th(OH)4(aq)	Th(OH)4(aq)	aqueous	300.067	-622.4700
54	Th(SO4)2(aq)	Th(SO4)2(aq)	aqueous	424.153	-911.6900
55	Th(SO4)3=	Th(SO4)3=	aqueous	520.211	-1214.0000
56	U++++	U++++	aqueous	242.000	-214.1900
57	UOH+++	UOH+++	aqueous	259.007	-308.7000
58	U(CO3)5===	U(CO3)5===	aqueous	542.046	-1345.3930
59	U(OH)2(CO3)2=	U(OH)2(CO3)2=	aqueous	396.033	-863.3830
60	U(OH)4(CO3)2==	U(OH)4(CO3)2==	aqueous	430.048	-998.6620
61	U(OH)4(aq)	deactivated	aqueous	310.029	999.9990
62	U(SO4)2(aq)	deactivated	aqueous	434.115	999.9990
63	U(SO4)3=	deactivated	aqueous	530.173	999.9990
64	NpO2+	NpO2+	aqueous	269.047	-369.1050
65	NpO2CO3-	NpO2CO3-	aqueous	329.056	-593.6010
66	NpO2(CO3)2=-	NpO2(CO3)2=-	aqueous	389.065	-809.8320
67	NpO2(CO3)3=-	NpO2(CO3)3=-	aqueous	449.075	-1020.2140
68	NpO2OH(aq)	NpO2OH(aq)	aqueous	286.054	-438.7300
69	NpO2(OH)2-	NpO2(OH)2-	aqueous	303.062	-506.2380
70	HAc(aq)	AceticAcid	aqueous	60.052	-158.3000

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ATTACHMENT 1

ap098_fmt_run028

71	Ac-	Acetate-	aqueous	59.044	-147.3470
72	H3Citrate(aq)	CitricAcid	aqueous	192.124	0.0000
73	H2Citrate-	H2Citrate-	aqueous	191.116	7.4760
74	HCitrate=	HCitrate=	aqueous	190.108	18.6200
75	Citrate=-	Citrate=-	aqueous	189.100	33.4100
76	H4EDTA (aq)	H4EDTA (aq)	aqueous	892.920	0.0000
77	H3EDTA-	H3EDTA-	aqueous	891.912	5.7610
78	H2EDTA=	H2EDTA=	aqueous	890.904	12.8700
79	HEDTA=-	HEDTA=-	aqueous	889.896	28.7100
80	EDTA==	EDTA==	aqueous	888.888	53.0500
81	H2Ox(aq)	OxalicAcid	aqueous	30.856	0.0000
82	HOx-	Bioxalate-	aqueous	29.848	3.2090
83	Ox=	Oxalate=	aqueous	28.840	13.0170
84	HLactate(aq)	LacticAcid	aqueous	90.078	0.0000
85	Lactate-	Lactate-	aqueous	89.070	8.7980
86	AmAc++	AmAcetate++	aqueous	302.044	-395.3560
87	AmCit (aq)	AmCitrate(aq)	aqueous	432.100	-228.5430
88	AmEDTA-	AmEDTA-	aqueous	1131.888	-232.3240
89	AmOx+	AmOxalate+	aqueous	271.840	-242.8530
90	AmLac++	AmLactate++	aqueous	332.070	-241.4360
91	ThAc2++	ThAcetate2++	aqueous	350.126	-604.8000
92	PuCit (aq)	deactivated	aqueous	427.129	999.9990
93	NpO2H2EDTA-	NpO2H2EDTA-	aqueous	1159.951	-364.0980
94	PuOx+	deactivated	aqueous	266.869	999.9990
95	ThLac2++	ThLactate2++	aqueous	410.178	-292.4000
96	ThAc+++	ThAc+++	aqueous	291.082	-448.5250
97	ThCit+	ThCit+	aqueous	421.138	-285.8980
98	ThEDTA (aq)	ThEDTA (aq)	aqueous	1120.926	-285.4190
99	ThOx++	Th (C2O4)++	aqueous	260.878	-297.4280
100	ThLac+++	ThLac+++	aqueous	321.108	-291.1520
101	UAc+++	deactivated	aqueous	301.044	999.9990
102	UCit+	deactivated	aqueous	431.100	999.9990
103	UEDTA (aq)	deactivated	aqueous	1130.888	999.9990
104	ULac+++	deactivated	aqueous	331.070	999.9990
105	UOx++	deactivated	aqueous	270.840	999.9990
106	NpO2Ac (aq)	NpO2Ac (aq)	aqueous	296.092	-519.6150
107	NpO2Cit=	NpO2Citrate=	aqueous	458.147	-343.7470
108	NpO2EDTA=-	NpO2EDTA=-	aqueous	1157.935	-335.7080
109	NpO2Ox-	NpO2Oxalate-	aqueous	297.887	-365.8510
110	NpO2Lac (aq)	NpO2Lactate (aq)	aqueous	358.117	-364.8370
111	MgAc+	MgAc+	aqueous	83.349	-333.3780
112	MgCit-	MgCit-	aqueous	213.405	-162.2610
113	MgEDTA=	MgEDTA=	aqueous	913.193	-153.7340
114	MgOx (aq)	MgOx (aq)	aqueous	53.145	-179.1850
115	MgLac+	MgLac+	aqueous	113.375	999.9990
116	CaAc+	(Mg-analog)	aqueous	99.124	-373.2100

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ATTACHMENT 1

ap098_fmt_run028

117	CaCit-	(Mg-analog)	aqueous	229.180	-202.0930
118	CaEDTA=	(Mg-analog)	aqueous	928.968	-193.5660
119	CaOx (aq)	(Mg-analog)	aqueous	68.920	-219.0170
120	CaLac+	(Mg-analog)	aqueous	129.150	999.9990
121	UnuCat#1+	UC#1+	aqueous	0.000	999.9990
122	NpO2HEDTA=	NpO2HEDTA=	aqueous	1158.943	-351.8520
123	UnuAn#2-	UA#2-	aqueous	0.000	999.9990
124	UnuAn#3-	UA#3-	aqueous	0.000	999.9990
125	UnuAn#4-	UA#4-	aqueous	0.000	999.9990
126	UnuNeu#1 (aq)	UN#1 (aq)	aqueous	0.000	999.9990
127	AmOHCO3 (c)	AmOHCO3 (c)	solid	320.017	-570.3400
128	Am (OH) 3 (s)	Am (OH) 3 (s)	solid	294.022	-495.3200
129	NaAm (CO3) 2.6H2O (c)		solid	494.099	-1396.4700
130	AmPO4 (c)	AmPO4 (c)	solid	337.972	-709.7500
131	PuOHC03 (c)	deactivated	solid	315.046	999.9990
132	Pu (OH) 3 (s)	deactivated	solid	289.051	999.9990
133	NaPu (CO3) 2.6H2O (c)	deactivated	solid	489.128	999.9990
134	PuPO4 (c)	deactivated	solid	333.001	999.9990
135	ThO2 (am)	Hydrous_Thorium_Oxide	solid	264.037	-451.4080
136	Th (SO4) 2.9H2O (s)		solid	586.290	-1775.9000
137	Th (SO4) 2.8H2O (s)		solid	568.275	-1680.0000
138	Th (SO4) 2.Na2SO4.6H2O (16C, s)		solid	674.282	-2011.2900
139	Th (SO4) 2.K2SO4.4H2O (16C, s)		solid	670.468	-1837.5700
140	Th (SO4) 2.2K2SO4.2H2O (16C, s)		solid	808.692	-2181.8100
141	2[Th (SO4) 2.7/2K2SO4 (16C, s)]		solid	2068.086	-5581.6600
142	UO2 (am)	Hydrous_U (IV)_Oxide	solid	273.999	-399.6700
143	NpO2OH (aged)	NpO2OH (aged)	solid	286.054	-454.3690
144	NpO2OH (amor)	NpO2OH (amor)	solid	286.054	-452.7570
145	2 [NaNpO2CO3.7/2H2O (s)]		solid	830.198	-2096.1160
146	Na3NpO2 (CO3) 2 (s)	Na3NpO2 (CO3) 2 (s)	solid	458.035	-1144.5970
147	KNpO2CO3 (s)	KNpO2CO3 (s)	solid	368.155	-727.3300
148	K3NpO2 (CO3) 2 (s)	K3NpO2 (CO3) 2 (s)	solid	506.360	-1173.5460
149	H2Ox.2H2O (s)	H2C2O4.2H2O (s)	solid	66.886	-191.3460
150	NaHOx.H2O (s)	NaHC2O4.H2O (s)	solid	70.853	-202.2530
151	Na2Ox (s)	Na2C2O4 (s)	solid	74.820	-203.8230
152	CO2 ("solid", DISABLED)		solid	44.010	0.0000
153	CaSO4	Anhydrite	solid	136.138	-533.7300
154	NaK3 (SO4) 2	Aphthitalite/Glaserite	solid	332.400	-1057.0500
155	CaCl2.6H2O	Antarcticite	solid	219.077	-893.6500
156	CaCO3	Aragonite	solid	100.089	-455.1700
157	K2SO4	Arcanite	solid	174.254	-532.3900
158	MgCl2.6H2O	Bischofite	solid	203.302	-853.1000
159	Na2Mg (SO4) 2.4H2O	Bloedite	solid	334.461	-1383.6000
160	Mg (OH) 2	Brucite	solid	58.320	-335.4000
161	Na6CO3 (SO4) 2	Burkeite	solid	390.063	-1449.4000
162	CaCO3	Calcite	solid	100.089	-455.6000

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ATTACHMENT 1

ap098_fmt_run028

163	CaCl2.4H2O	CaCl2_Tetrahydrate	solid	183.047	-698.7000
164	Ca4Cl2(OH)6.13H2O	CaOxychloride_A	solid	567.467	-2658.4500
165	Ca2Cl2(OH)2.H2O	CaOxychloride_B	solid	203.096	-778.4100
166	KMgCl3.6H2O	Carnallite	solid	277.854	-1020.3000
167	MgSO4.7H2O	Epsomite	solid	246.469	-1157.8300
168	CaNa2(CO3)2.5H2O	Gaylussite	solid	296.154	-1360.5000
169	Na2Ca(SO4)2	Glauberite	solid	278.175	-1047.4500
170	CaSO4.2H2O	Gypsum	solid	172.168	-725.5600
171	NaCl	Halite	solid	58.443	-154.9900
172	MgSO4.6H2O	Hexahydrate	solid	228.454	-1061.6000
173	KMgClSO4.3H2O	Kainite	solid	248.960	-938.2000
174	KHCO3	Kalicerite	solid	100.115	-350.0600
175	MgSO4.H2O	Kieserite	solid	138.378	-579.8000
176	K2Mg(SO4)2.4H2O	Leonite	solid	366.678	-1403.9700
177	Na4Ca(SO4)3.2H2O	Labile_Salt	solid	456.242	-1751.4500
178	MgCO3	Magnesite	solid	84.314	-414.4500
179	Mg2Cl(OH)3.4H2O	MgOxychloride	solid	207.146	-1029.6000
180	KHSO4	Mercallite	solid	136.164	-417.5700
181	Na2SO4.10H2O	Mirabilite	solid	322.189	-1471.1500
182	K8H6(SO4)7	Misenite	solid	991.237	-3039.2400
183	NaHCO3	Nahcolite	solid	84.007	-343.3300
184	Na2CO3.10H2O	Natron	solid	286.141	-1382.7800
185	MgCO3.3H2O	Nesquehonite	solid	138.360	-695.3000
186	K2Mg(SO4)2.6H2O	Picromerite/Schoen	solid	402.708	-1596.1000
187	Na2Ca(CO3)2.2H2O	Pirssonite	solid	242.108	-1073.1000
188	K2MgCa2(SO4)4.2H2O	Polyhalite	solid	602.922	-2282.5000
189	Ca(OH)2	Portlandite	solid	74.095	-362.1200
190	K2CO3.3/2H2O	Potassium_Carbonate	solid	165.229	-577.3700
191	K8H4(CO3)6.3H2O	K-Sequicarbonate	solid	730.919	-2555.4000
192	KNaCO3.6H2O	K-Na-Carbonate	solid	230.188	-1006.8000
193	K2NaH(CO3)2.2H2O	Potassium_Trona	solid	258.243	-971.7400
194	K3H(SO4)2	Sesquipotassium_Sulfate	solid	310.418	-950.8000
195	Na3H(SO4)2	Sesquisodium_Sulfate	solid	262.092	-919.6000
196	Na2CO3.7H2O	Na2CO3-Heptahydrate	solid	232.095	-1094.9500
197	KCl	Sylvite	solid	74.551	-164.8400
198	K2Ca(SO4)2.H2O	Syngenite	solid	328.407	-1164.8000
199	Mg2CaCl6.12H2O	Tachyhydrite	solid	517.590	-2015.9000
200	Na2SO4	Thenardite	solid	142.037	-512.3500
201	Na2CO3.H2O	Thermonatrite	solid	124.004	-518.8000
202	Na3H(CO3)2.2H2O	Trona	solid	226.026	-960.3800
203	Na2B4O7.10H2O	Borax	solid	381.367	-2224.1600
204	B(OH)3	Borix_Acid_Solid	solid	61.832	-390.8800
205	KB5O8.4H2O	K-Pentaborate_(30_C)	solid	293.204	-1770.2600
206	K2B4O7.4H2O	K-Tetraborate_(30_C)	solid	305.493	-1663.4700
207	NaBO2.4H2O	Sodium_Metaborate	solid	137.859	-761.4200
208	NaB5O8.5H2O	Sodium_Pentaborate	solid	295.111	-1854.8000

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ATTACHMENT 1

ap098_fmt_run028

209	NaBO2.NaCl.2H2O_____Teepelite_(20_C)	solid	160.272	-725.7700
210	CaMg(CO3)2_____Dolomite	solid	184.403	-871.9900
211	Mg5(CO3)4(OH)2.4H2O_HydroMagne5424	solid	467.637	-2364.0600
212	Mg4(CO3)3(OH)2.3H2O_HydroMagne4323	solid	365.308	-1856.1040
213	H+(solid)_____to.set.aH+	solid	1.008	0.0000
214	OH-/H2O(solid)_____to.set.aH+	solid	-1.008	0.0000

Truncated Name		Formula Matrix																																									
1	H2O	2	1	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	0	0	0				
2	Na+	0	0	1	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	0	0	0	1		
3	K+	0	0	0	1	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	0	0	0	1	
4	Ca++	0	0	0	0	0	1	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	0	2	
5	Mg++	0	0	0	0	1	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	0	0	2	
6	MgOH+	1	1	0	0	1	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	0	0	0	1
7	H+	1	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	0	0	0	0	0	0	1	
8	Cl-	0	0	0	0	0	0	1	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	-1	
9	SO4=	0	4	0	0	0	0	0	1	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	-2	
10	HSO4-	1	4	0	0	0	0	0	1	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	-1		
11	OH-	1	1	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	0	0	0	0	-1		
12	HCO3-	1	3	0	0	0	0	0	0	1	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	-1		
13	CO3=	0	3	0	0	0	0	0	0	1	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	-2		
14	CO2(aq)	0	2	0	0	0	0	0	0	1	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		
15	CaCO3(aq)	0	3	0	0	0	1	0	0	1	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		
16	MgCO3(aq)	0	3	0	0	1	0	0	0	1	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		
17	B(OH)3(aq)	3	3	0	0	0	0	0	0	0	0	0	1	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		
18	B(OH)4-	4	4	0	0	0	0	0	0	0	0	0	1	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	-1			
19	B3O3(OH)4-	4	7	0	0	0	0	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1			
20	B4O5(OH)4=	4	9	0	0	0	0	0	0	0	0	0	0	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-2			
21	CaB(OH)4+	4	4	0	0	0	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1			
22	MgB(OH)4+	4	4	0	0	1	0	0	0	0	0	0	0	1	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	1			
23	Br-	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1			
24	ClO4-	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1			
25	NaOH(aq)	to.ti	1	1	1	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	0	0			
26	HCl(aq)	to.ti	1	0	0	0	0	0	1	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			
27	HClO4(aq)	to.ti	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
28	PosIon		0	0	0	0	0	0	0	0	0	1	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	1			
29	NegIon		0	0	0	0	0	0	0	0	0	0	1	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	-1			
30	PosIon(OH)(aq)		1	1	0	0	0	0	0	0	1	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			
31	HNegIon(aq)		1	0	0	0	0	0	0	0	0	0	1	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			
32	H3PO4(aq)		3	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
33	H2PO4-		2	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1			
34	HPO4=		1	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-2			
35	PO4=-		0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-3			
36	Am+++		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3			
37	AmCO3+		0	3	0	0	0	0	0	1	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1			

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38 Am(CO3)2-	0	6	0	0	0	0	0	0	2	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	-1
39 Am(CO3)3--	0	9	0	0	0	0	0	0	3	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	-3
40 AmOH++	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	2
41 Am(OH)2+	2	2	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	1
42 Am(OH)3(aq)	3	3	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
43 AmCl++	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	2
44 AmCl2+	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	1
45 Am(CO3)4===	0	12	0	0	0	0	0	0	4	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	-5
46 Am(SO4)2-	0	8	0	0	0	0	2	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	-1
47 AmSO4+	0	4	0	0	0	0	1	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	1
48 Pu(OH)2+	2	2	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	1
49 Pu(OH)3(aq)	3	3	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
50 Th++++	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	4
51 Th(CO3)5===	0	15	0	0	0	0	0	5	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	-6
52 Th(OH)3(CO3)-	3	6	0	0	0	0	0	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	-1
53 Th(OH)4(aq)	4	4	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
54 Th(SO4)2(aq)	0	8	0	0	0	0	2	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
55 Th(SO4)3=	0	12	0	0	0	0	3	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	-2
56 U++++	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	4
57 UOH+++	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	3
58 U(CO3)5===	0	15	0	0	0	0	0	5	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	-6
59 U(OH)2(CO3)2=	2	8	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	-2
60 U(OH)4(CO3)2==	4	10	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	-4
61 U(OH)4(aq)	4	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
62 U(SO4)2(aq)	0	8	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
63 U(SO4)3=	0	12	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	-2
64 NpO2+	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	1
65 NpO2CO3-	0	5	0	0	0	0	0	1	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	-1
66 NpO2(CO3)2--	0	8	0	0	0	0	0	2	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	-3
67 NpO2(CO3)3===	0	11	0	0	0	0	0	3	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	-5
68 NpO2OH(aq)	1	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
69 NpO2(OH)2-	2	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	-1
70 HAc(aq)	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
71 Ac-	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	-1
72 H3Citrate(aq)	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
73 H2Citrate-	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	-1
74 HCitrate=	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	-2
75 Citrate=-	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	-3
76 H4EDTA(aq)	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
77 H3EDTA-	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	-1
78 H2EDTA=	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	-2
79 HEDTA=-	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	-3
80 EDTA==	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	-4
81 H2Ox(aq)	2	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
82 HOx-	1	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1
83 Ox=	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-2

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84 HLactate(aq)	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
85 Lactate-	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	-1
86 AmAc++	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	1	0	0	0	0	0	0	0	0	0	0	2
87 AmCit(aq)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	1	0	0
88 AmEDTA-	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	1	0	-1
89 AmOx+	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	1	0	0	0	0	0	0	0	0	1
90 AmLac++	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1	0	0	0	2
91 ThAc2++	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	1	0	0	0	0	0	0	0	0	0	0	2
92 PuCit(aq)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1	0	0
93 NpO2H2EDTA-	2	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	1	0	0	-1
94 PuOx+	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	1	0	0	0	0	0	0	0	0	0	1
95 ThLac2++	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	2	0	0	2
96 ThAc+++	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	0	0	0	3
97 ThCit+	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	1	0	1
98 ThEDTA(aq)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	1	0	0
99 ThOx++	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	1	0	0	0	0	0	0	0	0	0	0	2
100 ThLac+++	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	1	0	0	0	3
101 UAc+++	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1	0	0	0	3
102 UCit+	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1	1
103 UEDTA(aq)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	1	0	0
104 ULac+++	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	3
105 UOx++	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	1	0	0	0	2
106 NpO2Ac(aq)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	1	0	0	0	0	0	0	0	0
107 NpO2Cit=	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	1	0	0	-2
108 NpO2EDTA==	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	1	0	0	-3
109 NpO2Ox-	0	2	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	1	0	0	0	-1
110 NpO2Lac(aq)	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	1	0	0	0	0
111 MgAc+	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	1
112 MgCit-	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	-1
113 MgEDTA=	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	-2
114 MgOx(aq)	0	0	0	0	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
115 MgLac+	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1
116 CaAc+	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	1
117 CaCit-	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	-1
118 CaEDTA=	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	-2
119 CaOx(aq)	0	0	0	0	0	1	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
120 CaLac+	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1
121 UnuCat#1+	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
122 NpO2HEDTA=	1	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	1	0	0	-2
123 UnuAn#2-	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1
124 UnuAn#3-	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1
125 UnuAn#4-	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	-1
126 UnuNeu#1(aq)	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
127 AmOHCO3(c)	1	4	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
128 Am(OH)3(s)	3	3	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
129 NaAm(CO3)2.6H2O(c)	12	12	1	0	0	0	0	0	2	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0

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ATTACHMENT 1

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H2O MASS 1003.56133696475 grams
 TDS(g/kg) 384.938790995855 g/kgH2O

Specified Solution Density
 DENSITY 1217.52838558997 kg/m³ = g/l

Solution Parameters Based on Specified Density
 SOLUTION VOL 1.14155122883042 liters
 TDS 338.407666677552 g/l

Density based on TDS and NaCl solutions 1217.53 g/l
 % Relative difference vs NaCl density 0.00 %
 Calculated Ratio of molality to Molarity 1.138

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	8.15610E-01	7.48023E-01	0.9171	5.57064E+01	4.87988E+01	8.79121E+05	
CaSO4	Anhydrite	9.96388E+00	1.00000E+00	1.000	9.99937E+00	8.75946E+00	1.19249E+06	
Mg(OH)2	Brucite	9.81579E+00	1.00000E+00	1.000	9.85075E+00	8.62926E+00	5.03255E+05	
NaCl	Halite	9.40421E+00	1.00000E+00	1.000	9.43770E+00	8.26743E+00	4.83172E+05	
Na+	Na+	6.04608E+00	5.86556E+00	0.9701	6.06761E+00	5.31524E+00	1.22196E+05	
Mg5(CO3)4(OH)2.4H2O	HydroMagne5424	1.00083E+00	1.00000E+00	1.000	1.00439E+00	8.79846E-01	4.11449E+05	
ThO2(am)	Hydrous_Thorium_Oxide	9.96451E-01	1.00000E+00	1.000	1.00000E+00	8.76001E-01	2.31297E+05	
Am(OH)3(s)	Am(OH)3(s)	9.96451E-01	1.00000E+00	1.000	1.00000E+00	8.76001E-01	2.57563E+05	
KNpO2CO3(s)	KNpO2CO3(s)	9.96446E-01	1.00000E+00	1.000	9.99994E-01	8.75996E-01	3.22502E+05	
SO4=	SO4=	1.92124E-01	3.68404E-03	1.9175E-02	1.92808E-01	1.68900E-01	1.62241E+04	
Mg++	Mg++	1.10758E-01	2.12856E-01	1.922	1.11152E-01	9.73696E-02	2.36657E+03	
K+	K+	1.09271E-01	5.25180E-02	0.4806	1.09660E-01	9.60622E-02	3.75587E+03	
B(OH)4-	B(OH)4-	4.35256E-02	4.35008E-03	9.9943E-02	4.36806E-02	3.82642E-02	3.01672E+03	
MgOx(aq)	MgOx(aq)	2.24031E-02	2.80716E-02	1.253	2.24828E-02	1.96950E-02	1.04669E+03	
Br-	Br-	1.23909E-02	3.47180E-03	0.2802	1.24350E-02	1.08931E-02	8.70400E+02	
Ac-	Acetate-	4.12133E-03	3.14997E-03	0.7643	4.13601E-03	3.62315E-03	2.13925E+02	
MgCit-	MgCit-	3.97229E-04	7.97748E-05	0.2008	3.98644E-04	3.49213E-04	7.45237E+01	
MgEDTA=	MgEDTA=	4.04226E-06	1.07241E-06	0.2653	4.05666E-06	3.55364E-06	3.24516E+00	
Cl-	Cl-	5.96723E+00	6.34014E+00	1.062	5.98848E+00	5.24592E+00	1.85983E+05	-7.36E-10
MgB(OH)4+	MgB(OH)4+	1.21800E-02	2.32209E-02	1.906	1.22233E-02	1.07077E-02	1.10443E+03	1.76E-09
Ca++	Ca++	1.08320E-02	1.17929E-02	1.089	1.08706E-02	9.52266E-03	3.81668E+02	-1.08E-09
B(OH)3(aq)	B(OH)3(aq)	1.02774E-02	9.70483E-03	0.9443	1.03140E-02	9.03510E-03	5.58657E+02	-1.92E-09
CaB(OH)4+	CaB(OH)4+	1.93877E-03	2.29318E-03	1.183	1.94568E-03	1.70442E-03	2.02688E+02	-1.76E-09
MgAc+	MgAc+	1.48470E-03	8.69937E-03	5.859	1.48999E-03	1.30523E-03	1.08790E+02	-1.53E-09
CaOx(aq)	(Mg-analog)	1.24121E-03	1.55526E-03	1.253	1.24563E-03	1.09117E-03	7.52034E+01	-8.97E-10
MgOH+	MgOH+	7.11798E-04	2.56708E-04	0.3606	7.14333E-04	6.25756E-04	2.58514E+01	9.89E-10

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Preventing Formation of SOLID Species CaCO3 _____ Aragonite
 Preventing Formation of SOLID Species CaCO3 _____ Calcite
 Preventing Formation of SOLID Species MgCO3 _____ Magnesite
 Preventing Formation of SOLID Species CaMg(CO3)2 _____ Dolomite
 Preventing Formation of SOLID Species OH-/H2O(solid) _____ to.set.aH+

inversions for batch pblm 84

1CRA ERDA-6 recipe, calc

FMT V2.4

FMT_021120.chemdat

ERG update of FMT_970407.chemdat (PAVT db)

Pressure= 1.00000E+00 [=] ATM Temperature= 2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

Total Moles	Aq. Molality	Aq. Molarity	Aq. mg/liter	
Using NaCl Density Correlation				
1.44424796E+02	1.11283090E+02	9.78312701E+01	9.86041371E+04	Hydrogen
1.44527221E+02	5.65478793E+01	4.97124123E+01	7.95368769E+05	Oxygen
1.55053126E+01	6.04608136E+00	5.31523540E+00	1.22196039E+05	Sodium
1.10965407E+00	1.09270720E-01	9.60621539E-02	3.75586691E+03	Potassium
1.50214786E+01	1.48255804E-01	1.30334749E-01	3.16778608E+03	Magnesium
1.00135655E+01	1.41458510E-02	1.24359107E-02	4.98431300E+02	Calcium
1.54261808E+01	5.96723038E+00	5.24591586E+00	1.85983455E+05	Chlorine
1.01921772E+01	1.92123796E-01	1.68900010E-01	5.41493432E+03	Sulfur
5.01808727E+00	5.31825667E-04	4.67538963E-04	5.61561049E+00	Carbon
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	PosIon:EL
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	NegIon:EL
2.44178136E-02	2.43311622E-02	2.13900288E-02	6.16888430E+02	Oxalate:EL
7.12186231E-02	7.09658896E-02	6.23875839E-02	6.74409782E+02	Boron
1.24349977E-02	1.23908696E-02	1.08930702E-02	8.70399881E+02	Bromine
5.70879439E-03	5.68853560E-03	5.00090950E-03	2.95273701E+02	Acetate:EL
1.00000000E+00	2.80870855E-08	2.46919388E-08	5.72947057E-03	Th(IV)
1.00000000E+00	1.92451269E-07	1.69187898E-07	4.11126592E-02	Am(III)
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Pu(III)
1.00000000E+00	5.77881302E-06	5.08027426E-06	1.20426987E+00	Np(V)
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	ClO4:EL
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Phosphorus
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	U(IV)
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Lactate:EL
4.37485827E-06	4.35933322E-06	3.83238015E-06	3.40655673E+00	EDTA:EL
4.32964010E-04	4.31427551E-04	3.79276899E-04	7.17212616E+01	Citrate:EL
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	Electron:EL
2.34659593E-15	2.33826857E-15	2.05562035E-15	0.00000000E+00	Charge:EL

Solution Parameters, Calculated

SOLUTION MASS 1389.87102470614 grams

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Ox=	Oxalate=	6.81803E-04	2.12351E-05	3.1145E-02	6.84231E-04	5.99387E-04	1.72863E+01	-2.37E-09
B3O3 (OH) 4-	B3O3 (OH) 4-	4.39557E-04	5.03578E-05	0.1146	4.41122E-04	3.86424E-04	5.73674E+01	-2.50E-09
B4O5 (OH) 4-	B4O5 (OH) 4-	4.31373E-04	1.68074E-06	3.8963E-03	4.32909E-04	3.79229E-04	7.25337E+01	-5.05E-09
MgCO3 (aq)	MgCO3 (aq)	3.17137E-04	3.17137E-04	1.000	3.18266E-04	2.78801E-04	2.35069E+01	1.78E-10
HCO3-	HCO3-	1.06529E-04	3.69321E-05	0.3467	1.06909E-04	9.36522E-05	5.71439E+00	-1.90E-10
CaAc+	(Mg-analog)	8.22576E-05	4.81975E-04	5.859	8.25505E-05	7.23144E-05	7.16809E+00	-2.34E-09
CO3=	CO3=	7.82755E-05	1.75676E-06	2.2443E-02	7.85543E-05	6.88136E-05	4.12945E+00	-7.65E-10
CaCO3 (aq)	CaCO3 (aq)	2.93478E-05	2.93478E-05	1.000	2.94524E-05	2.58003E-05	2.58233E+00	-6.70E-10
CaCit-	(Mg-analog)	2.20079E-05	4.41980E-06	0.2008	2.20862E-05	1.93476E-05	4.43408E+00	-9.96E-10
OH-	OH-	1.48628E-05	7.83093E-06	0.5269	1.49157E-05	1.30662E-05	2.22220E-01	-5.38E-10
Citrate=-	Citrate=-	1.21894E-05	1.87969E-09	1.5421E-04	1.22328E-05	1.07159E-05	2.02638E+00	-2.39E-09
NpO2Ox-	NpO2Oxalate-	5.09495E-06	9.95885E-08	1.9546E-02	5.11310E-06	4.47908E-06	1.33426E+00	-7.42E-10
NpO2CO3-	NpO2CO3-	4.52521E-07	4.92971E-08	0.1089	4.54133E-07	3.97821E-07	1.30905E-01	6.42E-10
CaEDTA=	(Mg-analog)	2.23955E-07	5.94154E-08	0.2653	2.24753E-07	1.96884E-07	1.82899E-01	-6.95E-10
HAc (aq)	AceticAcid	1.73211E-07	1.73211E-07	1.000	1.73828E-07	1.52273E-07	9.14430E-03	5.65E-10
NpO2+	NpO2+	1.38778E-07	2.69860E-07	1.945	1.39272E-07	1.22003E-07	3.28245E-02	6.64E-11
Am (OH) 2+	Am (OH) 2+	9.68178E-08	8.09192E-11	8.3579E-04	9.71626E-08	8.51146E-08	2.35780E-02	2.25E-09
AmEDTA-	AmEDTA-	9.31020E-08	2.31659E-09	2.4882E-02	9.34336E-08	8.18479E-08	9.26426E-02	2.29E-09
NpO2Ac (aq)	NpO2Ac (aq)	6.95275E-08	2.00964E-08	0.2890	6.97751E-08	6.11231E-08	1.80981E-02	1.57E-09
CO2 (aq)	CO2 (aq)	2.98386E-08	1.03365E-07	3.464	2.99448E-08	2.62317E-08	1.15445E-03	-4.99E-10
Th (OH) 3 (CO3) -	Th (OH) 3 (CO3) -	2.72023E-08	7.62181E-09	0.2802	2.72991E-08	2.39141E-08	8.20418E-03	-5.68E-10
NpO2 (CO3) 2=-	NpO2 (CO3) 2=-	1.25826E-08	2.31772E-12	1.8420E-04	1.26275E-08	1.10617E-08	4.30371E-03	-1.66E-10
NpO2OH (aq)	NpO2OH (aq)	9.95445E-09	1.03094E-09	0.1036	9.98990E-09	8.75117E-09	2.50331E-03	1.29E-09
Hox-	Bioxalate-	1.42593E-09	3.71583E-10	0.2606	1.43101E-09	1.25356E-09	3.74163E-05	-1.87E-09
Th (OH) 4 (aq)	Th (OH) 4 (aq)	8.84814E-10	8.84814E-10	1.000	8.87965E-10	7.77858E-10	2.33410E-04	-3.57E-10
Am (OH) 3 (aq)	Am (OH) 3 (aq)	8.04366E-10	6.30297E-12	7.8360E-03	8.07230E-10	7.07135E-10	2.07913E-04	2.14E-09
HSO4-	HSO4-	5.76779E-10	3.37607E-10	0.5853	5.78833E-10	5.07058E-10	4.92178E-05	3.13E-10
AmOH++	AmOH++	5.65882E-10	1.42375E-11	2.5160E-02	5.67897E-10	4.97478E-10	1.29348E-04	5.79E-10
HCitrate=	HCitrate=	5.06620E-10	4.79449E-12	9.4637E-03	5.08424E-10	4.45380E-10	8.46702E-05	-2.13E-09
Am (CO3) 2-	Am (CO3) 2-	3.73861E-10	2.04143E-11	5.4604E-02	3.75192E-10	3.28669E-10	1.19313E-04	2.81E-10
NpO2Cit=	NpO2Citrate=	3.61777E-10	1.59280E-12	4.4027E-03	3.63065E-10	3.18045E-10	1.45712E-04	-2.69E-09
AmOx+	AmOxalate+	3.01428E-10	2.00545E-11	6.6532E-02	3.02502E-10	2.64992E-10	7.20353E-05	-2.97E-09
H+	H+	2.16767E-10	9.62591E-10	4.441	2.17538E-10	1.90564E-10	1.92069E-07	-6.80E-10
AmCO3+	AmCO3+	1.95503E-10	1.45805E-10	0.7458	1.96199E-10	1.71871E-10	5.20784E-05	-1.81E-10
NpO2 (CO3) 3=-	NpO2 (CO3) 3=-	1.05595E-10	3.14131E-19	2.9749E-09	1.05971E-10	9.28305E-11	4.16878E-05	-1.29E-09
Am (CO3) 3=-	Am (CO3) 3=-	1.04453E-10	5.68570E-15	5.4433E-05	1.04825E-10	9.18272E-11	3.88454E-05	8.03E-11
AmCit (aq)	AmCitrate (aq)	9.89426E-11	7.78138E-13	7.8645E-03	9.92949E-11	8.69825E-11	3.75851E-05	8.26E-10
AmAc++	AmAcetate++	7.25408E-11	1.14677E-12	1.5809E-02	7.27991E-11	6.37721E-11	1.92620E-05	3.64E-09
NpO2 (OH) 2-	NpO2 (OH) 2-	2.96765E-11	4.74164E-13	1.5978E-02	2.97822E-11	2.60892E-11	7.90664E-06	1.17E-09
AmSO4+	AmSO4+	1.00272E-11	4.29978E-12	0.4288	1.00629E-11	8.81514E-12	2.98884E-06	3.43E-10
EDTA==	EDTA==	9.42535E-12	3.76936E-16	3.9992E-05	9.45892E-12	8.28602E-12	7.36535E-06	-1.68E-09
HEDTA=-	HEDTA=-	2.74810E-12	1.35032E-14	4.9136E-03	2.75789E-12	2.41591E-12	2.14991E-06	-2.53E-10
Am+++	Am+++	2.11708E-12	6.58566E-13	0.3111	2.12462E-12	1.86117E-12	4.52263E-07	-3.70E-10
Am (SO4) 2-	Am (SO4) 2-	1.17596E-12	4.49960E-14	3.8263E-02	1.18015E-12	1.03381E-12	4.49827E-07	1.46E-09
Am (CO3) 4=-	Am (CO3) 4=-	9.75203E-13	6.25010E-23	6.4090E-11	9.78676E-13	8.57321E-13	4.14118E-07	1.75E-10
NpO2EDTA=-	NpO2EDTA=-	2.38462E-13	3.48814E-14	0.1463	2.39311E-13	2.09637E-13	2.42746E-07	-1.52E-09

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AmCl++	AmCl++	1.52818E-13	7.24428E-12	47.40	1.53362E-13	1.34345E-13	3.74088E-08	-1.53E-08
H2EDTA=	H2EDTA=	6.84860E-15	9.84245E-17	1.4371E-02	6.87299E-15	6.02075E-15	5.36391E-09	2.65E-10
AmCl2+	AmCl2+	5.77023E-15	4.81682E-12	834.8	5.79078E-15	5.07273E-15	1.59236E-09	-3.35E-09
H2Citrate-	H2Citrate-	2.60174E-15	3.19126E-16	0.1227	2.61101E-15	2.28725E-15	4.37129E-10	-1.86E-09
NpO2HEDTA=	NpO2HEDTA=	1.18427E-15	3.44577E-16	0.2910	1.18849E-15	1.04111E-15	1.20659E-09	-1.01E-09
Th (CO3)5===	Th (CO3)5===	2.12661E-17	1.02192E-27	4.8054E-11	2.13418E-17	1.86955E-17	9.94756E-12	-1.44E-08
H2Ox (aq)	OxalicAcid	8.85419E-18	8.85419E-18	1.000	8.88572E-18	7.78390E-18	2.40179E-13	-6.62E-10
ThEDTA (aq)	ThEDTA (aq)	1.69762E-18	6.39265E-18	3.766	1.70367E-18	1.49242E-18	1.67289E-12	7.64E-10
Th (SO4)3=	Th (SO4)3=	3.74092E-19	6.29103E-21	1.6817E-02	3.75424E-19	3.28872E-19	1.71083E-13	1.17E-09
NpO2H2EDTA-	NpO2H2EDTA-	2.14981E-19	6.90396E-20	0.3211	2.15746E-19	1.88994E-19	2.19224E-13	-2.97E-09
ThCit+	ThCit+	1.54954E-20	1.52049E-19	9.813	1.55505E-20	1.36223E-20	5.73687E-15	-7.76E-09
Th (SO4)2 (aq)	Th (SO4)2 (aq)	7.82933E-21	2.49353E-19	31.85	7.85721E-21	6.88293E-21	2.91942E-15	-2.12E-10
ThOx++	Th (C2O4)++	1.36734E-21	2.43108E-19	177.8	1.37221E-21	1.20206E-21	3.13591E-16	-9.13E-09
H3EDTA-	H3EDTA-	5.58798E-22	1.15863E-22	0.2073	5.60788E-22	4.91251E-22	4.38153E-16	4.01E-11
H3Citrate (aq)	CitricAcid	5.42237E-22	5.42237E-22	1.000	5.44168E-22	4.76692E-22	9.15838E-17	-1.89E-09
ThAc2++	ThAcetate2++	4.52948E-22	8.09340E-20	178.7	4.54561E-22	3.98196E-22	1.39419E-16	-3.29E-09
ThAc+++	ThAc+++	6.77820E-23	3.40756E-21	50.27	6.80234E-23	5.95886E-23	1.73452E-17	-4.29E-09
HCl (aq)	to.titrate.acid.only	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.48E+02
NaOH (aq)	to.titrate.base.only	0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.95E+02
AmOHCO3 (c)	AmOHCO3 (c)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.44E-01
NaAm (CO3) 2. 6H2O (c)		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.29E+00
Th (SO4) 2. 9H2O (s)		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.83E+01
Th (SO4) 2. 8H2O (s)		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.83E+01
Th (SO4) 2. Na2SO4. 6H2O (16C, s)		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.42E+01
Th (SO4) 2. K2SO4. 4H2O (16C, s)		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.76E+01
Th (SO4) 2. 2K2SO4. 2H2O (16C, s)		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.92E+01
2 [Th (SO4) 2. 7/2K2SO4 (16C, s)]		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.60E+01
NpO2OH (aged)	NpO2OH (aged)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.19E+00
NpO2OH (amor)	NpO2OH (amor)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.89E+00
2 [NaNpO2CO3. 7/2H2O (s)]		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.81E+00
Na3NpO2 (CO3) 2 (s)	Na3NpO2 (CO3) 2 (s)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.59E+00
K3NpO2 (CO3) 2 (s)	K3NpO2 (CO3) 2 (s)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-5.99E+00
H2Ox. 2H2O (s)	H2C2O4. 2H2O (s)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.73E+01
NaHOx. H2O (s)	NaHC2O4. H2O (s)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-6.99E+00
Na2Ox (s)	Na2C2O4 (s)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.31E-01
CO2 ("solid", DISABLED)		0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.46E+01
NaK3 (SO4) 2	Aphthitalite/Glaserite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.14E+00
CaCl2. 6H2O	Antarcticite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-5.22E+00
CaCO3	Aragonite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	5.36E-01
K2SO4	Arcanite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.22E+00
MgCl2. 6H2O	Bischofite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.28E+00
Na2Mg (SO4) 2. 4H2O	Bloedit	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.16E+00
Na6CO3 (SO4) 2	Burkeite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-5.24E+00
CaCO3	Calcite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	7.23E-01
CaCl2. 4H2O	CaCl2_Tetrahydrate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-6.55E+00
Ca4Cl2 (OH) 6. 13H2O	CaOxychloride_A	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.31E+01

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Ca2Cl2(OH)2.H2O	CaOxychloride_B	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.11E+01
KMgCl3.6H2O	Carnallite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.63E+00
MgSO4.7H2O	Epsomite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.11E+00
CaNa2(CO3)2.5H2O	Gaylussite	NAF 0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.11E+00
Na2Ca(SO4)2	Glauberite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.46E-02
CaSO4.2H2O	Gypsum	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.37E-02
MgSO4.6H2O	Hexahydrate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.23E+00
KMgClSO4.3H2O	Kainite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.77E+00
KHCO3	Kalicinite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-5.99E+00
MgSO4.H2O	Kieserite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.11E+00
K2Mg(SO4)2.4H2O	Leonite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.62E+00
Na4Ca(SO4)3.2H2O	Labile_Salt	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.36E-01
MgCO3	Magnesite	NAF 0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	1.41E+00
Mg2Cl(OH)3.4H2O	MgOxychloride	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.04E-01
KHSO4	Mercallite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.13E+01
Na2SO4.10H2O	Mirabilite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-9.30E-01
K8H6(SO4)7	Misenite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.06E+01
NaHCO3	Nahcolite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.26E+00
Na2CO3.10H2O	Natron	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.65E+00
MgCO3.3H2O	Nesquehonite	NAF 0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.64E+00
K2Mg(SO4)2.6H2O	Picromerite/Schoen	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.53E+00
Na2Ca(CO3)2.2H2O	Pirssonite	NAF 0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.91E+00
K2MgCa2(SO4)4.2H2O	Polyhalite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.33E+00
Ca(OH)2	Portlandite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-6.95E+00
K2CO3.3/2H2O	Potassium_Carbonate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.15E+01
K8H4(CO3)6.3H2O	K-Sequicarbonate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.69E+01
KNaCO3.6H2O	K-Na-Carbonate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-6.91E+00
K2NaH(CO3)2.2H2O	Potassium_Trona	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.35E+01
K3H(SO4)2	Sesquipotassium_Sulfate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.42E+01
Na3H(SO4)2	Sesquisodium_Sulfate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.08E+01
Na2CO3.7H2O	Na2CO3-Heptahydrate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.64E+00
KCl	Sylvite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.38E+00
K2Ca(SO4)2.H2O	Syngenite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.03E+00
Mg2CaCl6.12H2O	Tachyhydrite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.74E+01
Na2SO4	Thenardite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-6.10E-01
Na2CO3.H2O	Thermonatrite	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-4.83E+00
Na3H(CO3)2.2H2O	Trona	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-7.09E+00
Na2B4O7.10H2O	Borax	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.58E+00
B(OH)3	Borix_Acid_Solid	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.98E+00
KB5O8.4H2O	K-Pentaborate_(30_C)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-6.62E+00
K2B4O7.4H2O	K-Tetraborate_(30_C)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-6.36E+00
NaBO2.4H2O	Sodium_Metaborate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.17E+00
NaB5O8.5H2O	Sodium_Pentaborate	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-5.92E+00
NaBO2.NaCl.2H2O	Teepelite_(20_C)	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-1.62E+00
CaMg(CO3)2	Dolomite	NAF 0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	2.97E+00
Mg4(CO3)3(OH)2.3H2O	HydroMagne4323	NAF 0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-3.44E-01

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H+(solid)	to.set.aH+	NAF	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-9.02E+00
OH-/H2O(solid)	to.set.aH+	NAF	0.00000E+00	1.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	9.02E+00
H4EDTA(aq)	H4EDTA(aq)		0.00000E+00	0.00000E+00	1.000	0.00000E+00	0.00000E+00	0.00000E+00	-2.85E+01
Th++++	Th++++		0.00000E+00	0.00000E+00	0.5481	0.00000E+00	0.00000E+00	0.00000E+00	-2.53E+01

pH (-log[aH+]); pmH(-log[mH+]); pCH(-log[MH+]) 9.0166 9.6640 9.7200
 Osmotic Coefficient= 1.284178
 Equilibrium RH (%) = 74.802264
 Ionic Strength (m) = 6.729876
 Density, kg/m3 = 1217.53
 fCO2(g); log[fCO2(g)]= 3.135E-06 -5.504

NOTES: - Water "molality" is mole fraction H2O in aqueous phase
 - "Descriptor" means:
 *dG/RT/ln10 for species with nonzero concs. (convergence criterion)
 *Saturation Index for minerals, SI=log10(IAP/Ksp)
 *log10(activity) for aqueous species with very small concentrations
 *log10(activity) for aqueous species Not Allowed to Form
 *NAF signifies that the species was Not Allowed to Form

Total G/RT= -2.05821101E+04

Total Diagonal Inversions 84
 Total Stoichiometric Reoptimizations 9

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ATTACHMENT 2

Molarity ap098_fmt_run012

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O WATER	8.12980E-01	7.32777E-01	0.9013	5.10331E+01	4.84005E+01	8.71945E+05	
CaSO4 Anhydrite	1.08767E+01	1.00000E+00	1.0000	9.99970E+00	9.48387E+00	1.29111E+06	
NaCl Halite	1.01559E+01	1.00000E+00	1.0000	9.33704E+00	8.85539E+00	5.17534E+05	
Mg(OH)2 Brucite	8.99681E+00	1.00000E+00	1.0000	8.27140E+00	7.84472E+00	4.57501E+05	
Cl-Cl-	6.22893E+00	8.06472E+00	1.2950	5.72669E+00	5.43128E+00	1.92555E+05	
Mg2Cl(OH)3.4H2O MgOxychloride	1.21677E+00	1.00000E+00	1.0000	1.11867E+00	1.06096E+00	2.19773E+05	
ThO2(am) Hydrus Thorium Oxide	1.08770E+00	1.00000E+00	1.0000	1.00000E+00	9.48415E-01	2.50417E+05	
Am(OH)3(s) Am(OH)3(s)	1.08770E+00	1.00000E+00	1.0000	1.00000E+00	9.48415E-01	2.78855E+05	
KNpO2CO3(s) KNpO2CO3(s)	1.08770E+00	1.00000E+00	1.0000	9.99999E-01	9.48414E-01	3.49163E+05	
CaCO3 Calcite	1.08728E+00	1.00000E+00	1.0000	9.99613E-01	9.48047E-01	9.48893E+04	
K+ K+	5.58961E-01	2.41936E-01	0.4328	5.13892E-01	4.87383E-01	1.90558E+04	
SO4= SO4=	2.08740E-01	4.44960E-03	0.0213	1.91909E-01	1.82010E-01	1.74834E+04	
MgB(OH)4+ MgB(OH)4+	7.36072E-02	1.40655E-01	1.9110	6.76723E-02	6.41814E-02	6.61994E+03	
Br- Br-	3.17313E-02	8.57994E-03	0.2704	2.91729E-02	2.76680E-02	2.21078E+03	
MgOx(aq) MgOx(aq)	2.58685E-02	3.27361E-02	1.2650	2.37827E-02	2.25559E-02	1.19873E+03	
Ac- Acetate-	3.10867E-03	1.72726E-03	0.5556	2.85802E-03	2.71059E-03	1.60044E+02	
MgCit- MgCit-	4.53252E-04	7.80549E-05	0.1722	4.16707E-04	3.95211E-04	8.43400E+01	
MgEDTA= MgEDTA=	4.58557E-06	5.96992E-07	0.1302	4.21584E-06	3.99837E-06	3.65128E+00	
Na+ Na+	4.96822E+00	4.61126E+00	0.9282	4.56763E+00	4.33201E+00	9.95919E+04	-3.80E-09
Mg++ Mg++	5.62017E-01	9.98313E-01	1.7760	5.16702E-01	4.90048E-01	1.19106E+04	-7.86E-09
B(OH)4- B(OH)4-	5.51524E-02	5.61813E-03	0.1019	5.07055E-02	4.80899E-02	3.79137E+03	-9.11E-08
B(OH)3(aq) B(OH)3(aq)	2.53793E-02	2.71440E-02	1.0700	2.33330E-02	2.21294E-02	1.36830E+03	-5.80E-08
Ca+++ Ca++	1.02664E-02	9.76394E-03	0.9511	9.43860E-03	8.95171E-03	3.58785E+02	-5.64E-09
B4O5(OH)4= B4O5(OH)4=	5.75024E-03	2.43095E-05	0.0042	5.28660E-03	5.01389E-03	9.58989E+02	1.67E-07
B3O3(OH)4- B3O3(OH)4-	3.30520E-03	5.41203E-04	0.1637	3.03870E-03	2.88195E-03	4.27847E+02	-1.75E-07
MgAc+ MgAc+	3.02471E-03	2.23728E-02	7.3970	2.78083E-03	2.63738E-03	2.19823E+02	-1.56E-08
CaB(OH)4+ CaB(OH)4+	2.11211E-03	2.45209E-03	1.1610	1.94181E-03	1.84164E-03	2.19006E+02	-5.98E-08
MgOH+ MgOH+	1.77392E-03	5.55943E-04	0.3134	1.63089E-03	1.54676E-03	6.39003E+01	1.52E-09
MgCO3(aq) MgCO3(aq)	3.40318E-04	3.40318E-04	1.0000	3.12879E-04	2.96739E-04	2.50193E+01	-6.43E-10
CaOx(aq) (Mg-analog)	2.53005E-04	3.20174E-04	1.2650	2.32606E-04	2.20607E-04	1.52042E+01	9.50E-10
Ox= Oxalate=	2.39096E-04	5.27999E-06	0.0221	2.19818E-04	2.08478E-04	6.01252E+00	1.71E-10
HCO3- HCO3-	5.04531E-05	1.79271E-05	0.3553	4.63851E-05	4.39924E-05	2.68429E+00	2.17E-09
CaAc+ (Mg-analog)	2.95830E-05	2.18816E-04	7.3970	2.71977E-05	2.57947E-05	2.55688E+00	-2.32E-08
CO3= CO3=	2.60940E-05	4.01949E-07	0.0154	2.39900E-05	2.27525E-05	1.36536E+00	4.48E-09
Citrate=- Citrate=-	9.74126E-06	3.92137E-10	0.0000	8.95583E-06	8.49384E-06	1.60618E+00	1.02E-09
OH- OH-	8.14131E-06	3.61595E-06	0.4441	7.48488E-06	7.09877E-06	1.20731E-01	2.73E-09
CaCO3(aq) CaCO3(aq)	5.55951E-06	5.55951E-06	1.0000	5.11125E-06	4.84759E-06	4.85191E-01	3.33E-10
CaCit- (Mg-analog)	4.43301E-06	7.63412E-07	0.1722	4.07558E-06	3.86534E-06	8.85858E-01	1.06E-09
NpO2Ox- NpO2Oxalate-	8.13552E-07	2.34930E-08	0.0289	7.47956E-07	7.09373E-07	2.11313E-01	1.79E-09
Am(OH)2+ Am(OH)2+	2.53918E-07	1.75244E-10	0.0007	2.33444E-07	2.21402E-07	6.13316E-02	5.56E-09
HAc(aq) Acetic Acid	2.01500E-07	2.01500E-07	1.0000	1.85253E-07	1.75696E-07	1.05509E-02	-1.16E-08
NpO2+ NpO2+	1.34592E-07	2.56029E-07	1.9020	1.23740E-07	1.17356E-07	3.15744E-02	-2.29E-09
NpO2CO3- NpO2CO3-	1.22337E-07	1.07011E-08	0.0875	1.12473E-07	1.06671E-07	3.51007E-02	5.17E-09

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ATTACHMENT 2

Molarity ap098_fmt_run012

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
AmEDTA- AmEDTA-	9.26150E-08	2.79284E-09	0.0302	8.51475E-08	8.07551E-08	9.14058E-02	4.11E-09
CaEDTA= (Mg-analog)	4.48489E-08	5.83884E-09	0.1302	4.12328E-08	3.91058E-08	3.63280E-02	1.07E-09
NpO2Ac(aq) NpO2Ac(aq)	3.81943E-08	1.04549E-08	0.2737	3.51147E-08	3.33033E-08	9.86085E-03	-7.27E-09
CO2(aq) CO2(aq)	3.14974E-08	1.08660E-07	3.4500	2.89577E-08	2.74640E-08	1.20868E-03	-4.58E-09
Th(OH)3(CO3)- Th(OH)3(CO3)-	1.34037E-08	3.62427E-09	0.2704	1.23230E-08	1.16873E-08	4.00955E-03	2.14E-10
NpO2OH(aq) NpO2OH(aq)	4.81688E-09	4.51642E-10	0.0938	4.42850E-09	4.20005E-09	1.20144E-03	5.74E-09
AmOH++ AmOH++	2.71323E-09	6.67753E-11	0.0246	2.49446E-09	2.36578E-09	6.15121E-04	-4.29E-09
NpO2(CO3)2-- NpO2(CO3)2--	1.49425E-09	1.15114E-13	0.0001	1.37377E-09	1.30290E-09	5.06913E-04	4.13E-09
HSO4- HSO4-	1.06268E-09	8.65080E-10	0.8141	9.76994E-10	9.26596E-10	8.99405E-05	-3.03E-09
Th(OH)4(aq) Th(OH)4(aq)	8.49114E-10	8.49114E-10	1.0000	7.80651E-10	7.40381E-10	2.22164E-04	-1.30E-09
HOx- Bioxalate-	6.97436E-10	1.96012E-10	0.2810	6.41202E-10	6.08125E-10	1.81513E-05	-2.09E-09
Am(OH)3(aq) Am(OH)3(aq)	6.94688E-10	6.30297E-12	0.0091	6.38676E-10	6.05729E-10	1.78098E-04	8.34E-09
AmAc++ AmAcetate++	5.59406E-10	6.38702E-12	0.0114	5.14301E-10	4.87771E-10	1.47328E-04	-4.07E-09
AmOx+ AmOxalate+	5.36269E-10	5.06481E-11	0.0944	4.93030E-10	4.67597E-10	1.27111E-04	-1.67E-08
H+ H+	4.60460E-10	2.04216E-09	4.4350	4.23333E-10	4.01495E-10	4.04667E-07	-5.88E-09
AmCO3+ AmCO3+	4.51352E-10	3.38847E-10	0.7507	4.14959E-10	3.93554E-10	1.19250E-04	-5.50E-09
HCitrate= HCitrate=	3.17410E-10	2.12199E-12	0.0067	2.91817E-10	2.76764E-10	5.26150E-05	-2.86E-09
AmCit(aq) AmCitrate(aq)	2.59295E-10	1.64885E-12	0.0064	2.38389E-10	2.26091E-10	9.76941E-05	7.84E-10
Am(CO3)2- Am(CO3)2-	1.68307E-10	1.08548E-11	0.0645	1.54736E-10	1.46754E-10	5.32744E-05	1.64E-09
AmSO4+ AmSO4+	1.14393E-10	5.27492E-11	0.4611	1.05169E-10	9.97441E-11	3.38190E-05	-6.74E-09
NpO2Cit= NpO2Citrate=	8.06230E-11	3.15258E-13	0.0039	7.41224E-11	7.02988E-11	3.22072E-05	-5.41E-09
EDTA== EDTA==	4.63900E-11	4.47396E-17	0.0000	4.26496E-11	4.04495E-11	3.59551E-05	6.50E-09
Am(CO3)3-- Am(CO3)3--	4.42527E-11	6.91717E-16	0.0000	4.06847E-11	3.85859E-11	1.63229E-05	9.28E-09
NpO2(CO3)3== NpO2(CO3)3==	1.87194E-11	3.56973E-21	0.0000	1.72101E-11	1.63223E-11	7.32994E-06	-1.11E-08
Am+++ Am+++	1.66564E-11	6.68916E-12	0.4016	1.53134E-11	1.45234E-11	3.52919E-06	-1.19E-08
Am(SO4)2- Am(SO4)2-	1.38315E-11	6.66715E-13	0.0482	1.27163E-11	1.20603E-11	5.24763E-06	8.81E-10
Am(CO3)4== Am(CO3)4==	1.34491E-11	1.73976E-24	0.0000	1.23647E-11	1.17268E-11	5.66449E-06	2.26E-08
NpO2(OH)2- NpO2(OH)2-	7.05331E-12	9.59175E-14	0.0136	6.48460E-12	6.15009E-12	1.86386E-06	9.34E-09
HEDTA= HEDTA=	4.18042E-12	3.40024E-15	0.0008	3.84336E-12	3.64510E-12	3.24376E-06	5.17E-09
AmCl++ AmCl++	1.83313E-12	9.35960E-11	51.0600	1.68533E-12	1.59839E-12	4.45076E-07	-8.80E-09
NpO2EDTA= NpO2EDTA=	2.30095E-13	3.92799E-15	0.0171	2.11543E-13	2.00630E-13	2.32317E-07	1.49E-09
AmCl2+ AmCl2+	9.88172E-14	7.91612E-11	801.1000	9.08496E-14	8.61631E-14	2.70471E-08	-4.72E-09
H2EDTA= H2EDTA=	5.21574E-15	5.25803E-17	0.0101	4.79520E-15	4.54784E-15	4.05168E-09	4.50E-10
H2Citrate= H2Citrate=	2.32399E-15	2.99647E-16	0.1289	2.13661E-15	2.02639E-15	3.87275E-10	-6.58E-09
Th(CO3)5=== Th(CO3)5===	4.69721E-16	1.35264E-29	0.0000	4.31848E-16	4.09571E-16	2.17926E-10	-3.38E-08
NpO2HEDTA= NpO2HEDTA=	4.54989E-16	8.23208E-17	0.1809	4.18304E-16	3.96725E-16	4.59782E-10	-4.78E-09
H2Ox(aq) OxalicAcid	9.90886E-18	9.90886E-18	1.0000	9.10991E-18	8.63997E-18	2.66593E-13	-1.25E-09
Th(SO4)3= Th(SO4)3=	9.18508E-18	2.33986E-19	0.0255	8.44450E-18	8.00889E-18	4.16631E-12	1.77E-11
ThEDTA(aq) ThEDTA(aq)	4.01319E-18	1.60170E-17	3.9910	3.68961E-18	3.49928E-18	3.92243E-12	-6.25E-09
Th(SO4)2(aq) Th(SO4)2(aq)	2.07146E-19	7.67867E-18	37.0700	1.90444E-19	1.80620E-19	7.66105E-14	-9.69E-09
NpO2H2EDTA= NpO2H2EDTA=	7.25011E-20	3.49921E-20	0.4826	6.66554E-20	6.32170E-20	7.33286E-14	-1.78E-08
ThCit+ ThCit+	3.32637E-20	6.69595E-19	20.1300	3.05817E-20	2.90041E-20	1.22147E-14	-4.19E-08
ThOx++ Th(C2O4)++	2.58076E-21	1.27601E-18	494.4000	2.37268E-21	2.25028E-21	5.87050E-16	-4.73E-08
ThAc2++ ThAcetate2++	1.75683E-21	5.13701E-19	292.4000	1.61518E-21	1.53186E-21	5.36343E-16	-4.95E-08
H3Citrate(aq) CitricAcid	1.08015E-21	1.08015E-21	1.0000	9.93062E-22	9.41835E-22	1.80949E-16	-1.07E-08

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Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H3EDTA- H3EDTA-	5.83392E-22	1.31314E-22	0.2251	5.36353E-22	5.08686E-22	4.53703E-16	-5.31E-09
ThAc+++ ThAc+++	4.10538E-22	3.94432E-20	96.0800	3.77436E-22	3.57966E-22	1.04198E-16	-4.32E-08
Th++++ Th++++	0.00000E+00	0.00000E+00	0.9093	0.00000E+00	0.00000E+00	0.00000E+00	-2.40E+01
AmOHC03(c) AmOHC03(c)	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-3.13E-01
NaAm(CO3)2.6H2O(c)	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-2.72E+00
Th(SO4)2.9H2O(s)	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-1.69E+01
Th(SO4)2.8H2O(s)	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-1.69E+01
Th(SO4)2.Na2SO4.6H2O(16C,s)	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-1.29E+01
Th(SO4)2.K2SO4.4H2O(16C,s)	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-1.48E+01
Th(SO4)2.2K2SO4.2H2O(16C,s)	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-1.49E+01
2[Th(SO4)2.7/2K2SO4(16C,s)]	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-3.32E+01
NpO2OH(aged) NpO2OH(aged)	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-2.55E+00
NpO2OH(amor) NpO2OH(amor)	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-3.25E+00
2[NaNpO2CO3.7/2H2O(s)]	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-3.41E+00
Na3NpO2(CO3)2(s) Na3NpO2(CO3)2(s)	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-3.21E+00
K3NpO2(CO3)2(s) K3NpO2(CO3)2(s)	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-5.30E+00
H2Ox.2H2O(s) H2C2O4.2H2O(s)	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-1.73E+01
NaHOx.H2O(s) NaHC2O4.H2O(s)	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-7.38E+00
Na2Ox(s) Na2C2O4(s)	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-1.54E+00
CO2("solid",DISABLED)	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-7.46E+01
NaK3(SO4)2 Aphthitalite/Glaserite	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-2.09E+00
CaCl2.6H2O Antarcticite	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-5.15E+00
CaCO3 Aragonite NAF	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-1.87E-01
K2SO4 Arcanite	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-1.81E+00
MgCl2.6H2O Bischofite	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-3.45E+00
Na2Mg(SO4)2.4H2O Bloedite	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-1.57E+00
Na6CO3(SO4)2 Burkeite	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-6.34E+00
CaCl2.4H2O CaCl2 Tetrahydrate	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-6.45E+00
Ca4Cl2(OH)6.13H2O CaOxychloride A	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-2.54E+01
Ca2Cl2(OH)2.H2O CaOxychloride B	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-1.18E+01
KMgCl3.6H2O Carnallite	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-3.04E+00
MgSO4.7H2O Epsomite	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-1.42E+00
CaNa2(CO3)2.5H2O Gaylussite NAF	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-4.73E+00
Na2Ca(SO4)2 Glauberite	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-1.42E-01
CaSO4.2H2O Gypsum	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-5.16E-02
MgSO4.6H2O Hexahydrate	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-1.53E+00
KMgClSO4.3H2O Kainite	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-2.27E+00
KHCO3 Kalicinite	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-5.64E+00
MgSO4.H2O Kieserite	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-2.36E+00
K2Mg(SO4)2.4H2O Leonite	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-2.50E+00
Na4Ca(SO4)3.2H2O Labile Salt	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-1.01E+00
MgCO3 Magnesite NAF	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	1.44E+00
KHSO4 Mercallite	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-1.03E+01
Na2SO4.10H2O Mirabilite	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-1.15E+00
K8H6(SO4)7 Misenite	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-6.27E+01

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Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
NaHCO ₃ Nahcolite	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-3.68E+00
Na ₂ CO ₃ .10H ₂ O Natron	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-5.59E+00
MgCO ₃ .3H ₂ O Nesquehonite NAF	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-1.63E+00
K ₂ Mg(SO ₄) ₂ .6H ₂ O Picromerite/Schoen	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-2.42E+00
Na ₂ Ca(CO ₃) ₂ .2H ₂ O Pirssonite NAF	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-4.50E+00
K ₂ MgCa ₂ (SO ₄) ₄ .2H ₂ O Polyhalite	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-1.19E+00
Ca(OH) ₂ Portlandite	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-7.70E+00
K ₂ CO ₃ .3/2H ₂ O Potassium Carbonate	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-1.09E+01
K ₈ H ₄ (CO ₃) ₆ .3H ₂ O K-Sequicarbonate	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-4.41E+01
KNaCO ₃ .6H ₂ O K-Na-Carbonate	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-7.04E+00
K ₂ NaH(CO ₃) ₂ .2H ₂ O Potassium Trona	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-1.32E+01
K ₃ H(SO ₄) ₂ Sesquipotassium Sulfate	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-1.17E+01
Na ₃ H(SO ₄) ₂ Sesquisodium Sulfate	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-1.06E+01
Na ₂ CO ₃ .7H ₂ O Na ₂ CO ₃ -Heptahydrate	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-5.55E+00
KCl Sylvite	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-6.10E-01
K ₂ Ca(SO ₄) ₂ .H ₂ O Syngenite	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-6.33E-01
Mg ₂ CaCl ₆ .12H ₂ O Tachyhydrite	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-1.56E+01
Na ₂ SO ₄ Thenardite	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-7.37E-01
Na ₂ CO ₃ .H ₂ O Thermonatrite	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-5.69E+00
Na ₃ H(CO ₃) ₂ .2H ₂ O Trona	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-8.38E+00
Na ₂ B ₄ O ₇ .10H ₂ O Borax	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-6.97E-01
B(OH) ₃ Boric Acid Solid	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-1.54E+00
KB ₅ O ₈ .4H ₂ O K-Pentaborate (30 C)	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-4.02E+00
K ₂ B ₄ O ₇ .4H ₂ O K-Tetraborate (30 C)	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-3.89E+00
NaBO ₂ .4H ₂ O Sodium Metaborate	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-2.19E+00
NaB ₅ O ₈ .5H ₂ O Sodium Pentaborate	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-4.10E+00
NaBO ₂ .NaCl.2H ₂ O Teepleite (20 C)	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-1.62E+00
CaMg(CO ₃) ₂ Dolomite NAF	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	2.28E+00
Mg ₅ (CO ₃) ₄ (OH) ₂ .4H ₂ O HydroMagne5424 NAF	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	8.68E-02
Mg ₄ (CO ₃) ₃ (OH) ₂ .3H ₂ O HydroMagne4323 NAF	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-2.78E-01
H+(solid) to.set.aH+ NAF	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-8.69E+00
OH-/H ₂ O(solid) to.set.aH+ NAF	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	8.69E+00
NaOH(aq) to.titrate.base.only	0.00000E+00	0.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-2.95E+02
HCl(aq) to.titrate.acid.only	0.00000E+00	0.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-2.48E+02
H ₄ EDTA(aq) H ₄ EDTA(aq)	0.00000E+00	0.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-2.81E+01

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ATTACHMENT 2

Molarity ap098_fmt_run018

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/Liter	Descriptor
H2O WATER	8.12976E-01	7.32772E-01	0.9013	5.10311E+01	4.84000E+01	8.71936E+05	
CaSO4 Anhydrite	1.08767E+01	1.00000E+00	1	9.99934E+00	9.48379E+00	1.29110E+06	
NaCl Halite	1.01563E+01	1.00000E+00	1	9.33702E+00	8.85562E+00	5.17547E+05	
Mg(OH)2 Brucite	8.99630E+00	1.00000E+00	1	8.27061E+00	7.84419E+00	4.57470E+05	
Cl- Cl-	6.22856E+00	8.06466E+00	1.295	5.72613E+00	5.43090E+00	1.92542E+05	
Mg2Cl(OH)3.4H2O MgOxychloride	1.21746E+00	1.00000E+00	1	1.11925E+00	1.06154E+00	2.19894E+05	
ThO2(am) Hydrus Thorium Oxide	1.08774E+00	1.00000E+00	1	1.00000E+00	9.48442E-01	2.50424E+05	
Am(OH)3(s) Am(OH)3(s)	1.08774E+00	1.00000E+00	1	1.00000E+00	9.48441E-01	2.78863E+05	
KNpO2CO3(s) KNpO2CO3(s)	1.08774E+00	1.00000E+00	1	9.99999E-01	9.48441E-01	3.49173E+05	
Mg5(CO3)4(OH)2.4H2O HydroMagne5424	1.08764E+00	1.00000E+00	1	9.99908E-01	9.48354E-01	4.43486E+05	
K+ K+	5.58983E-01	2.41930E-01	0.4328	5.13892E-01	4.87397E-01	1.90564E+04	
SO4= SO4=	2.09147E-01	4.45828E-03	2.13E-02	1.92276E-01	1.82363E-01	1.75173E+04	
MgB(OH)4+ MgB(OH)4+	7.36204E-02	1.40660E-01	1.911	6.76818E-02	6.41923E-02	6.62106E+03	
Br- Br-	3.17326E-02	8.57972E-03	0.2704	2.91729E-02	2.76688E-02	2.21084E+03	
MgOx(aq) MgOx(aq)	2.58700E-02	3.27376E-02	1.265	2.37832E-02	2.25570E-02	1.19879E+03	
Ac- Acetate-	3.10870E-03	1.72732E-03	0.5556	2.85793E-03	2.71058E-03	1.60044E+02	
MgCit- MgCit-	4.53282E-04	7.80384E-05	0.1722	4.16718E-04	3.95232E-04	8.43446E+01	
MgEDTA= MgEDTA=	4.58582E-06	5.97031E-07	0.1302	4.21590E-06	3.99854E-06	3.65144E+00	
Na+ Na+	4.96843E+00	4.61129E+00	0.9281	4.56766E+00	4.33215E+00	9.95952E+04	-1.43E-09
Mg++ Mg++	5.62129E-01	9.98382E-01	1.776	5.16785E-01	4.90140E-01	1.19129E+04	-1.07E-09
B(OH)4- B(OH)4-	5.51506E-02	5.61792E-03	0.1019	5.07019E-02	4.80878E-02	3.79120E+03	-3.47E-08
B(OH)3(aq) B(OH)3(aq)	2.53794E-02	2.71439E-02	1.07	2.33322E-02	2.21292E-02	1.36829E+03	-5.57E-08
Ca++ Ca++	1.02494E-02	9.74494E-03	0.9508	9.42263E-03	8.93682E-03	3.58188E+02	-2.93E-10
B4O5(OH)4= B4O5(OH)4=	5.75012E-03	2.43084E-05	4.23E-03	5.28629E-03	5.01374E-03	9.58958E+02	1.71E-07
B3O3(OH)4- B3O3(OH)4-	3.30528E-03	5.41191E-04	0.1637	3.03866E-03	2.88200E-03	4.27854E+02	-1.88E-07
MgAc+ MgAc+	3.02498E-03	2.23751E-02	7.397	2.78097E-03	2.63759E-03	2.19840E+02	-5.99E-09
CaB(OH)4+ CaB(OH)4+	2.10817E-03	2.44722E-03	1.161	1.93811E-03	1.83819E-03	2.18596E+02	-3.85E-08
MgOH+ MgOH+	1.77430E-03	5.55962E-04	0.3133	1.63117E-03	1.54707E-03	6.39132E+01	7.57E-10
MgCO3(aq) MgCO3(aq)	3.23737E-04	3.23737E-04	1	2.97623E-04	2.82278E-04	2.38000E+01	4.59E-10
CaOx(aq) (Mg-analog)	2.52510E-04	3.19543E-04	1.265	2.32142E-04	2.20173E-04	1.51743E+01	1.96E-10
Ox= Oxalate=	2.39059E-04	5.27986E-06	2.21E-02	2.19775E-04	2.08444E-04	6.01153E+00	2.39E-09
HCO3- HCO3-	4.79980E-05	1.70529E-05	0.3553	4.41262E-05	4.18511E-05	2.55364E+00	1.61E-09
CaAc+ (Mg-analog)	2.95260E-05	2.18398E-04	7.397	2.71443E-05	2.57448E-05	2.55193E+00	-7.40E-09
CO3= CO3=	2.48220E-05	3.82338E-07	1.54E-02	2.28198E-05	2.16432E-05	1.29879E+00	4.55E-09
Citrate=- Citrate=-	9.73857E-06	3.92027E-10	4.03E-05	8.95301E-06	8.49141E-06	1.60573E+00	4.97E-09
OH- OH-	8.14110E-06	3.61583E-06	0.4441	7.48440E-06	7.09852E-06	1.20727E-01	2.08E-09
CaCO3(aq) CaCO3(aq)	5.27798E-06	5.27798E-06	1	4.85223E-06	4.60206E-06	4.60616E-01	7.29E-10
CaCit- (Mg-analog)	4.42436E-06	7.61712E-07	0.1722	4.06747E-06	3.85776E-06	8.84121E-01	-2.98E-11
NpO2Ox- NpO2Oxalate-	8.55243E-07	2.46980E-08	2.89E-02	7.86255E-07	7.45717E-07	2.22139E-01	-8.15E-10
Am(OH)2+ Am(OH)2+	2.53799E-07	1.75250E-10	6.91E-04	2.33327E-07	2.21297E-07	6.13024E-02	-6.78E-11
HAc(aq) Acetic Acid	2.01512E-07	2.01512E-07	1	1.85257E-07	1.75706E-07	1.05515E-02	-4.13E-09
NpO2+ NpO2+	1.41523E-07	2.69168E-07	1.902	1.30107E-07	1.23399E-07	3.32002E-02	-7.39E-10
NpO2CO3- NpO2CO3-	1.22323E-07	1.07014E-08	8.75E-02	1.12456E-07	1.06658E-07	3.50963E-02	1.90E-09
AmEDTA- AmEDTA-	9.26408E-08	2.79312E-09	3.02E-02	8.51680E-08	8.07768E-08	9.14303E-02	-2.55E-09
CaEDTA= (Mg-analog)	4.47610E-08	5.82746E-09	0.1302	4.11503E-08	3.90287E-08	3.62564E-02	5.74E-10

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ATTACHMENT 2

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Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/Liter	Descriptor
NpO2Ac(aq) NpO2Ac(aq)	4.01527E-08	1.09918E-08	0.2737	3.69138E-08	3.50105E-08	1.03663E-02	-3.73E-09
CO2(aq) CO2(aq)	2.99576E-08	1.03365E-07	3.45	2.75411E-08	2.61211E-08	1.14958E-03	-1.09E-09
Th(OH)3(CO3)- Th(OH)3(CO3)-	1.27508E-08	3.44752E-09	0.2704	1.17223E-08	1.11179E-08	3.81422E-03	1.47E-09
NpO2OH(aq) NpO2OH(aq)	5.06319E-09	4.74803E-10	9.38E-02	4.65476E-09	4.41477E-09	1.26286E-03	7.57E-10
AmOH++ AmOH++	2.71415E-09	6.67799E-11	2.46E-02	2.49522E-09	2.36657E-09	6.15325E-04	-1.30E-09
NpO2(CO3)2-- NpO2(CO3)2--	1.42076E-09	1.09500E-13	7.71E-05	1.30615E-09	1.23881E-09	4.81978E-04	3.13E-09
HSO4- HSO4-	1.06478E-09	8.66791E-10	0.8141	9.78889E-10	9.28419E-10	9.01174E-05	-2.41E-09
Th(OH)4(aq) Th(OH)4(aq)	8.49103E-10	8.49103E-10	1	7.80610E-10	7.40363E-10	2.22159E-04	-1.92E-10
HOx- Bioxalate-	6.97384E-10	1.96013E-10	0.2811	6.41129E-10	6.08074E-10	1.81497E-05	-2.04E-10
Am(OH)3(aq) Am(OH)3(aq)	6.94652E-10	6.30297E-12	9.07E-03	6.38618E-10	6.05692E-10	1.78087E-04	1.09E-09
AmAc++ AmAcetate++	5.59815E-10	6.38791E-12	1.14E-02	5.14658E-10	4.88123E-10	1.47435E-04	-1.53E-09
AmOx+ AmOxalate+	5.35945E-10	5.06521E-11	9.45E-02	4.92713E-10	4.67310E-10	1.27033E-04	-6.62E-09
H+ H+	4.60477E-10	2.04222E-09	4.435	4.23333E-10	4.01506E-10	4.04678E-07	-1.43E-09
AmCO3+ AmCO3+	4.29385E-10	3.22348E-10	0.7507	3.94749E-10	3.74397E-10	1.13446E-04	-9.46E-10
HCitrate= HCitrate=	3.17357E-10	2.12145E-12	6.68E-03	2.91757E-10	2.76715E-10	5.26057E-05	8.88E-11
AmCit(aq) AmCitrate(aq)	2.59172E-10	1.64856E-12	6.36E-03	2.38266E-10	2.25981E-10	9.76464E-05	-2.09E-09
Am(CO3)2- Am(CO3)2-	1.52312E-10	9.82246E-12	6.45E-02	1.40025E-10	1.32806E-10	4.82110E-05	1.65E-09
AmSO4+ AmSO4+	1.14616E-10	5.28575E-11	0.4612	1.05370E-10	9.99374E-11	3.38845E-05	-2.28E-09
NpO2Cit= NpO2Citrate=	8.47292E-11	3.31343E-13	3.91E-03	7.78945E-11	7.38784E-11	3.38472E-05	-1.89E-09
EDTA== EDTA==	4.63790E-11	4.47394E-17	9.65E-07	4.26379E-11	4.04395E-11	3.59462E-05	1.21E-08
Am(CO3)3=- Am(CO3)3=-	3.80931E-11	5.95393E-16	1.56E-05	3.50203E-11	3.32147E-11	1.40508E-05	9.52E-09
NpO2(CO3)3=- NpO2(CO3)3=-	1.69191E-11	3.22998E-21	1.91E-10	1.55543E-11	1.47524E-11	6.62491E-06	-1.30E-09
Am+++ Am+++	1.66211E-11	6.68985E-12	0.4025	1.52804E-11	1.44926E-11	3.52169E-06	-1.95E-09
Am(SO4)2- Am(SO4)2-	1.38876E-11	6.69386E-13	4.82E-02	1.27674E-11	1.21091E-11	5.26887E-06	2.81E-10
Am(CO3)4=- Am(CO3)4=-	1.10105E-11	1.42443E-24	1.29E-13	1.01223E-11	9.60046E-12	4.63737E-06	2.89E-08
NpO2(OH)2- NpO2(OH)2-	7.41392E-12	1.00833E-13	1.36E-02	6.81588E-12	6.46446E-12	1.95913E-06	2.40E-09
HEDTA= HEDTA=	4.18055E-12	3.40032E-15	8.13E-04	3.84333E-12	3.64517E-12	3.24382E-06	5.45E-09
AmCl++ AmCl++	1.83511E-12	9.36050E-11	51.01	1.68708E-12	1.60010E-12	4.45552E-07	-1.93E-10
NpO2EDTA=-NpO2EDTA=-	2.41870E-13	4.12954E-15	1.71E-02	2.22359E-13	2.10895E-13	2.44203E-07	5.26E-09
AmCl2+ AmCl2+	9.88945E-14	7.91683E-11	800.5	9.09172E-14	8.62296E-14	2.70680E-08	1.76E-09
H2EDTA= H2EDTA=	5.21612E-15	5.25830E-17	1.01E-02	4.79536E-15	4.54812E-15	4.05194E-09	-8.61E-10
H2Citrate- H2Citrate-	2.32367E-15	2.99580E-16	0.1289	2.13623E-15	2.02609E-15	3.87218E-10	-2.73E-09
NpO2HEDTA= NpO2HEDTA=	4.78215E-16	8.65474E-17	0.181	4.39640E-16	4.16973E-16	4.83247E-10	-2.75E-09
Th(CO3)5=== Th(CO3)5===	3.66325E-16	1.05347E-29	2.88E-14	3.36776E-16	3.19412E-16	1.69954E-10	2.63E-08
H2Ox(aq) OxalicAcid	9.90916E-18	9.90916E-18	1	9.10984E-18	8.64015E-18	2.66599E-13	-4.46E-10
Th(SO4)3= Th(SO4)3=	9.23945E-18	2.35386E-19	2.55E-02	8.49415E-18	8.05621E-18	4.19093E-12	2.19E-09
ThEDTA(aq) ThEDTA(aq)	4.01400E-18	1.60190E-17	3.991	3.69021E-18	3.49995E-18	3.92319E-12	-4.82E-09
Th(SO4)2(aq) Th(SO4)2(aq)	2.08025E-19	7.70960E-18	37.06	1.91245E-19	1.81384E-19	7.69347E-14	-1.88E-09
NpO2H2EDTA- NpO2H2EDTA-	7.61829E-20	3.67897E-20	0.4829	7.00376E-20	6.64266E-20	7.70516E-14	-9.21E-09
ThCit+ ThCit+	3.32399E-20	6.69490E-20	20.14	3.05586E-20	2.89831E-20	1.22059E-14	-1.44E-08
ThOx++ Th(C2O4)++	2.58103E-21	1.27614E-18	494.4	2.37283E-21	2.25049E-21	5.87103E-16	-1.37E-08
ThAc2++ ThAcetate2++	1.75833E-21	5.13801E-19	292.2	1.61650E-21	1.53315E-21	5.36798E-16	-1.47E-08
H3Citrate(aq) CitricAcid	1.07994E-21	1.07994E-21	1	9.92827E-22	9.41639E-22	1.80911E-16	-4.34E-09
H3EDTA- H3EDTA-	5.83411E-22	1.31325E-22	0.2251	5.36350E-22	5.08697E-22	4.53713E-16	-4.34E-09
ThAc+++ ThAc+++	4.11306E-22	3.94495E-20	95.91	3.78128E-22	3.58632E-22	1.04391E-16	-1.05E-08

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ATTACHMENT 2

Molarity ap098_fmt_run018

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/Liter	Descriptor
Th++++ Th++++	0.00000E+00	0.00000E+00	0.9341	0.00000E+00	0.00000E+00	0.00000E+00	-2.40E+01
AmOHCO3(c) AmOHCO3(c)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-3.35E-01
NaAm(CO3)2.6H2O(c)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-2.76E+00
Th(SO4)2.9H2O(s)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.69E+01
Th(SO4)2.8H2O(s)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.69E+01
Th(SO4)2.Na2SO4.6H2O(16C,s)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.29E+01
Th(SO4)2.K2SO4.4H2O(16C,s)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.48E+01
Th(SO4)2.2K2SO4.2H2O(16C,s)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.49E+01
2Th(SO4)2.7/2K2SO4(16C,s)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-3.32E+01
NpO2OH(aged) NpO2OH(aged)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-2.53E+00
NpO2OH(amor) NpO2OH(amor)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-3.23E+00
2[NaNpO2CO3.7/2H2O(s)]	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-3.41E+00
Na3NpO2(CO3)2(s) Na3NpO2(CO3)2(s)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-3.23E+00
K3NpO2(CO3)2(s) K3NpO2(CO3)2(s)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-5.32E+00
H2Ox.2H2O(s) H2C2O4.2H2O(s)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.73E+01
NaHOx.H2O(s) NaHC2O4.H2O(s)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-7.38E+00
Na2Ox(s) Na2C2O4(s)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.54E+00
CO2("solid",DISABLED)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-7.46E+01
NaK3(SO4)2 Aphthalite/Glaserite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-2.08E+00
CaCl2.6H2O Antarcticite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-5.15E+00
CaCO3 Aragonite NAF	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-2.09E-01
K2SO4 Arcanite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.81E+00
MgCl2.6H2O Bischofite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-3.45E+00
Na2Mg(SO4)2.4H2O Bloedite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.57E+00
Na6CO3(SO4)2 Burkeite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-6.36E+00
CaCO3 Calcite NAF	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-2.26E-02
CaCl2.4H2O CaCl2 Tetrahydrite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-6.46E+00
Ca4Cl2(OH)6.13H2O CaOxychloride A	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-2.54E+01
Ca2Cl2(OH)2.H2O CaOxychloride B	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.18E+01
KMgCl3.6H2O Carnallite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-3.04E+00
MgSO4.7H2O Epsomite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.42E+00
CaNa2(CO3)2.5H2O Gaylussite NAF	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-4.77E+00
Na2Ca(SO4)2 Glauberite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.41E-01
CaSO4.2H2O Gypsum	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-5.16E-02
MgSO4.6H2O Hexahydrite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.53E+00
KMgClSO4.3H2O Kainite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-2.27E+00
KHCO3 Kalicinite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-5.67E+00
MgSO4.H2O Kieserite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-2.36E+00
K2Mg(SO4)2.4H2O Leonite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-2.50E+00
Na4Ca(SO4)3.2H2O Labile Salt	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.01E+00
MgCO3 Magnesite NAF	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	1.42E+00
KHSO4 Mercurite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.03E+01
Na2SO4.10H2O Mirabilite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.15E+00
K8H6(SO4)7 Misenite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-6.27E+01
NaHCO3 Nahcolite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-3.70E+00

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Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/Liter	Descriptor
Na2CO3.10H2O Natron	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-5.62E+00
MgCO3.3H2O Nesquehonite NAF	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.66E+00
K2Mg(SO4)2.6H2O Picromerite/Schoen	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-2.42E+00
Na2Ca(CO3)2.2H2O Pirssonite NAF	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-4.55E+00
K2MgCa2(SO4)4.2H2O Polyhalite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.19E+00
Ca(OH)2 Portlandite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-7.70E+00
K2CO3.3/2H2O Potassium Carbonate	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.09E+01
K8H4(CO3)6.3H2O K-Sequicarbonate	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-4.43E+01
KNaCO3.6H2O K-Na-Carbonate	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-7.06E+00
K2NaH(CO3)2.2H2O Potassium Trona	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.33E+01
K3H(SO4)2 Sesquipotassium Sulfate	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.17E+01
Na3H(SO4)2 Sesquisodium Sulfate	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.06E+01
Na2CO3.7H2O Na2CO3-Heptahydrate	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-5.57E+00
KCl Sylvite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-6.10E-01
K2Ca(SO4)2.H2O Syngenite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-6.32E-01
Mg2CaCl6.12H2O Tachyhydrite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.56E+01
Na2SO4 Thenardite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-7.36E-01
Na2CO3.H2O Thermonatrite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-5.71E+00
Na3H(CO3)2.2H2O Trona	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-8.42E+00
Na2B4O7.10H2O Borax	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-6.97E-01
B(OH)3 Borix Acid Solid	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.54E+00
KB5O8.4H2O K-Pentaborate (30 C)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-4.02E+00
K2B4O7.4H2O K-Tetraborate (30 C)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-3.89E+00
NaBO2.4H2O Sodium Metaborate	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-2.19E+00
NaB5O8.5H2O Sodium Pentaborate	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-4.10E+00
NaBO2.NaCl.2H2O Teepleite (20 C)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.62E+00
CaMg(CO3)2 Dolomite NAF	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	2.24E+00
Mg4(CO3)3(OH)2.3H2O HydroMagne4323 NAF	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-3.44E-01
H+(solid) to.set.aH+ NAF	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-8.69E+00
OH-/H2O(solid) to.set.aH+ NAF	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	8.69E+00
NaOH(aq) to.titrate.base.only	0.00000E+00	0.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-2.95E+02
HCl(aq) to.titrate.acid.only	0.00000E+00	0.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-2.48E+02
H4EDTA(aq) H4EDTA(aq)	0.00000E+00	0.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-2.81E+01

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Molarity ap098_fmt_run022

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/Liter	Descriptor
H2O WATER	8.15675E-01	7.47722E-01	0.9167	5.57240E+01	4.87923E+01	8.79004E+05	
CaSO4 Anhydrite	9.93453E+00	1.00000E+00	1	9.97307E+00	8.73249E+00	1.18882E+06	
Mg(OH)2 Brucite	9.81712E+00	1.00000E+00	1	9.85520E+00	8.62929E+00	5.03257E+05	
NaCl Halite	9.40465E+00	1.00000E+00	1	9.44114E+00	8.26673E+00	4.83130E+05	
Na+ Na+	6.02273E+00	5.82887E+00	0.9678	6.04609E+00	5.29400E+00	1.21708E+05	
CaCO3 Calcite	1.01406E+00	1.00000E+00	1	1.01800E+00	8.91364E-01	8.92159E+04	
ThO2(am) Hydrous Thorium Oxide	9.96136E-01	1.00000E+00	1	1.00000E+00	8.75607E-01	2.31193E+05	
Am(OH)3(s) Am(OH)3(s)	9.96135E-01	1.00000E+00	1	1.00000E+00	8.75607E-01	2.57448E+05	
KNpO2CO3(s) KNpO2CO3(s)	9.96111E-01	1.00000E+00	1	9.99976E-01	8.75586E-01	3.22351E+05	
SO4= SO4=	2.00245E-01	3.85784E-03	0.019266	2.01022E-01	1.76016E-01	1.69077E+04	
Mg++ Mg++	1.26674E-01	2.42161E-01	1.912	1.27165E-01	1.11347E-01	2.70629E+03	
K+ K+	1.09255E-01	5.22453E-02	0.4782	1.09678E-01	9.60351E-02	3.75481E+03	
B(OH)4- B(OH)4-	4.20899E-02	4.20581E-03	0.099925	4.22531E-02	3.69971E-02	2.91683E+03	
MgOx(aq) MgOx(aq)	2.26344E-02	2.83557E-02	1.253	2.27222E-02	1.98957E-02	1.05736E+03	
Br- Br-	1.23869E-02	3.46312E-03	0.2796	1.24350E-02	1.08882E-02	8.70008E+02	
Ac- Acetate-	3.99031E-03	3.01745E-03	0.7562	4.00579E-03	3.50750E-03	2.07097E+02	
MgCit- MgCit-	4.01358E-04	8.01307E-05	0.1996	4.02915E-04	3.52795E-04	7.52883E+01	
MgEDTA= MgEDTA=	4.07175E-06	1.05201E-06	0.2584	4.08755E-06	3.57908E-06	3.26839E+00	
Cl- Cl-	5.96192E+00	6.38005E+00	1.07	5.98504E+00	5.24055E+00	1.85793E+05	1.06E-09
MgB(OH)4+ MgB(OH)4+	1.34611E-02	2.55418E-02	1.897	1.35133E-02	1.18324E-02	1.22044E+03	-3.75E-09
B(OH)3(aq) B(OH)3(aq)	1.05362E-02	1.00081E-02	0.9499	1.05771E-02	9.26136E-03	5.72648E+02	6.68E-09
Ca++ Ca++	1.04548E-02	1.12616E-02	1.077	1.04954E-02	9.18981E-03	3.68328E+02	-3.96E-08
Na2Ca(SO4)2 Glauberite	9.00726E-03	1.00000E+00	1	9.04220E-03	7.91742E-03	2.20243E+03	-2.29E-08
CaB(OH)4+ CaB(OH)4+	1.79779E-03	2.11724E-03	1.178	1.80476E-03	1.58026E-03	1.87923E+02	-4.17E-08
MgAc+ MgAc+	1.62055E-03	9.48074E-03	5.85	1.62683E-03	1.42447E-03	1.18728E+02	7.58E-09
CaOx(aq) (Mg-analog)	1.05260E-03	1.31868E-03	1.253	1.05669E-03	9.25243E-04	6.37678E+01	-3.56E-08
MgOH+ MgOH+	7.64482E-04	2.73810E-04	0.3582	7.67447E-04	6.71982E-04	2.77611E+01	-4.37E-09
Ox= Oxalate=	6.13835E-04	1.88542E-05	0.030715	6.16216E-04	5.39563E-04	1.55610E+01	1.74E-08
B3O3(OH)4- B3O3(OH)4-	4.47392E-04	5.18404E-05	0.1159	4.49127E-04	3.93259E-04	5.83822E+01	9.17E-09
B4O5(OH)4= B4O5(OH)4=	4.29068E-04	1.67419E-06	0.0039019	4.30733E-04	3.77153E-04	7.21366E+01	2.16E-08
CaAc+ (Mg-analog)	7.53631E-05	4.40899E-04	5.85	7.56555E-05	6.62445E-05	6.56642E+00	-3.24E-08
MgCO3(aq) MgCO3(aq)	7.15726E-05	7.15726E-05	1	7.18503E-05	6.29126E-05	5.30442E+00	3.32E-08
NpO2Ox- NpO2Oxalate-	2.26486E-05	4.48068E-07	0.019783	2.27365E-05	1.99082E-05	5.93040E+00	-2.34E-08
HCO3- HCO3-	2.25305E-05	7.81124E-06	0.3467	2.26179E-05	1.98044E-05	1.20840E+00	4.17E-08
CaCit- (Mg-analog)	1.86650E-05	3.72646E-06	0.1996	1.87375E-05	1.64066E-05	3.76008E+00	-3.28E-08
CO3= CO3=	1.57891E-05	3.48493E-07	0.022072	1.58503E-05	1.38787E-05	8.32847E-01	4.19E-08
OH- OH-	1.40375E-05	7.34182E-06	0.523	1.40920E-05	1.23390E-05	2.09854E-01	3.40E-09
Citrate= Citrate=	1.12654E-05	1.65958E-09	0.00014732	1.13091E-05	9.90235E-06	1.87253E+00	7.87E-09
CaCO3(aq) CaCO3(aq)	5.55951E-06	5.55951E-06	1	5.58108E-06	4.88683E-06	4.89119E-01	3.09E-12
NpO2+ NpO2+	7.07352E-07	1.36747E-06	1.933	7.10096E-07	6.21765E-07	1.67284E-01	-3.63E-08
NpO2CO3- NpO2CO3-	4.56370E-07	4.95544E-08	0.1086	4.58140E-07	4.01151E-07	1.32001E-01	-7.06E-09
NpO2Ac(aq) NpO2Ac(aq)	3.37126E-07	9.75512E-08	0.2894	3.38433E-07	2.96335E-07	8.77424E-02	-4.69E-08
CaEDTA= (Mg-analog)	1.89355E-07	4.89236E-08	0.2584	1.90090E-07	1.66444E-07	1.54621E-01	-3.44E-08
HAc(aq) AceticAcid	1.76907E-07	1.76907E-07	1	1.77593E-07	1.55502E-07	9.33819E-03	-3.59E-09
Am(OH)2+ Am(OH)2+	1.02595E-07	8.63100E-11	0.00084127	1.02993E-07	9.01813E-08	2.49815E-02	-2.63E-08

Original Data
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Molarity ap098_fmt_run022

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/Liter	Descriptor
AmEDTA- AmEDTA-	9.68343E-08	2.42392E-09	0.025032	9.72100E-08	8.51178E-08	9.63438E-02	4.24E-09
NpO2OH(aq) NpO2OH(aq)	4.71966E-08	4.89784E-09	0.1038	4.73797E-08	4.14860E-08	1.18673E-02	-4.63E-08
CO2(aq) CO2(aq)	6.71361E-09	2.33184E-08	3.473	6.73965E-09	5.90129E-09	2.59714E-04	3.27E-08
Th(OH)3(CO3)- Th(OH)3(CO3)-	5.76364E-09	1.61139E-09	0.2796	5.78600E-09	5.06626E-09	1.73808E-03	4.11E-08
NpO2(CO3)2=- NpO2(CO3)2=-	2.56036E-09	4.62171E-13	0.00018051	2.57029E-09	2.25056E-09	8.75616E-04	2.56E-08
NpO2Cit= NpO2Citrate=	1.62788E-09	7.12617E-12	0.0043776	1.63420E-09	1.43092E-09	6.55570E-04	-2.40E-08
HOx- Bioxalate-	1.34888E-09	3.51759E-10	0.2608	1.35412E-09	1.18567E-09	3.53899E-05	1.48E-08
Th(OH)4(aq) Th(OH)4(aq)	8.84102E-10	8.84102E-10	1	8.87532E-10	7.77129E-10	2.33191E-04	1.64E-09
Am(OH)3(aq) Am(OH)3(aq)	7.95189E-10	6.30297E-12	0.0079264	7.98274E-10	6.98974E-10	2.05514E-04	-9.07E-09
AmOH++ AmOH++	6.48687E-10	1.61977E-11	0.02497	6.51204E-10	5.70199E-10	1.48256E-04	-2.43E-09
HSO4- HSO4-	6.36376E-10	3.76936E-10	0.5923	6.38845E-10	5.59377E-10	5.42962E-05	4.14E-08
HCitrate= HCitrate=	4.83192E-10	4.51327E-12	0.0093405	4.85067E-10	4.24728E-10	8.07441E-05	1.24E-08
AmOx+ AmOxalate+	3.21375E-10	2.16071E-11	0.067233	3.22622E-10	2.82490E-10	7.67921E-05	1.26E-09
H+ H+	2.31769E-10	1.02631E-09	4.428	2.32668E-10	2.03726E-10	2.05336E-07	1.29E-09
NpO2(OH)2- NpO2(OH)2-	1.32134E-10	2.11198E-12	0.015984	1.32647E-10	1.16147E-10	3.51996E-05	-4.21E-08
AmCit(aq) AmCitrate(aq)	1.05548E-10	8.33680E-13	0.0078986	1.05958E-10	9.27775E-11	4.00891E-05	-1.56E-08
AmAc++ AmAcetate++	8.55651E-11	1.33303E-12	0.015579	8.58971E-11	7.52121E-11	2.27174E-05	-1.20E-08
AmCO3+ AmCO3+	4.72195E-11	3.50981E-11	0.7433	4.74027E-11	4.15062E-11	1.25767E-05	3.21E-08
Am(CO3)2- Am(CO3)2-	1.77685E-11	9.74823E-13	0.054862	1.78375E-11	1.56186E-11	5.66984E-06	7.33E-08
AmSO4+ AmSO4+	1.27336E-11	5.46381E-12	0.4291	1.27830E-11	1.11929E-11	3.79503E-06	3.01E-08
EDTA== EDTA==	9.21112E-12	3.25018E-16	0.000035285	9.24685E-12	8.09661E-12	7.19698E-06	-9.14E-09
NpO2(CO3)3=- NpO2(CO3)3=-	4.49177E-12	1.24261E-20	2.7664E-09	4.50919E-12	3.94828E-12	1.77307E-06	4.27E-08
HEDTA=- HEDTA=-	2.68774E-12	1.24140E-14	0.0046188	2.69817E-12	2.36253E-12	2.10241E-06	1.80E-09
Am+++ Am+++	2.44867E-12	7.99150E-13	0.3264	2.45817E-12	2.15239E-12	5.23030E-07	-5.42E-08
Am(SO4)2- Am(SO4)2-	1.55447E-12	5.98748E-14	0.038518	1.56050E-12	1.36638E-12	5.94534E-07	7.39E-08
NpO2EDTA=- NpO2EDTA=-	-1.12E-12	1.52410E-13	0.1356	1.12850E-12	9.88125E-13	1.14418E-06	-3.56E-08
Am(CO3)3=- Am(CO3)3=-	1.03120E-12	5.38587E-17	0.000052229	1.03520E-12	9.06427E-13	3.83444E-07	1.04E-07
AmCl++ AmCl++	1.90901E-13	8.84605E-12	46.34	1.91642E-13	1.67803E-13	4.67252E-08	2.20E-08
AmCl2+ AmCl2+	7.25113E-15	5.91888E-12	816.3	7.27926E-15	6.37377E-15	2.00077E-09	1.83E-08
H2EDTA= H2EDTA=	6.80505E-15	9.64746E-17	0.014177	6.83145E-15	5.98166E-15	5.32908E-09	7.86E-09
NpO2HEDTA= NpO2HEDTA=	5.59755E-15	1.60525E-15	0.2868	5.61926E-15	4.92026E-15	5.70231E-09	-3.26E-08
H2Citrate- H2Citrate-	2.60985E-15	3.20292E-16	0.1227	2.61997E-15	2.29407E-15	4.38433E-10	1.09E-08
Am(CO3)4=- Am(CO3)4=-	2.23664E-15	1.17447E-25	5.251E-11	2.24531E-15	1.96601E-15	9.49657E-10	1.02E-07
H2Ox(aq) OxalicAcid	8.93662E-18	8.93662E-18	1	8.97129E-18	7.85533E-18	2.42382E-13	7.28E-09
ThEDTA(aq) ThEDTA(aq)	1.89533E-18	7.12870E-18	3.761	1.90268E-18	1.66600E-18	1.86746E-12	3.16E-09
NpO2H2EDTA- NpO2H2EDTA-	1.05668E-18	3.42917E-19	0.3245	1.06078E-18	9.28830E-19	1.07740E-12	-2.61E-08
Th(SO4)3= Th(SO4)3=	5.60534E-19	9.34270E-21	0.016667	5.62709E-19	4.92712E-19	2.56314E-13	1.09E-07
ThCit+ ThCit+	1.75195E-20	1.73614E-19	9.91	1.75875E-20	1.53997E-20	6.48541E-15	2.03E-08
Th(CO3)5=== Th(CO3)5===	1.14356E-20	4.05988E-31	3.5502E-11	1.14800E-20	1.00519E-20	5.34848E-15	2.29E-07
Th(SO4)2(aq) Th(SO4)2(aq)	1.11376E-20	3.53627E-19	31.75	1.11809E-20	9.79004E-21	4.15248E-15	8.07E-08
ThOx++ Th(C2O4)++	1.56831E-21	2.79153E-19	178	1.57439E-21	1.37855E-21	3.59633E-16	4.66E-08
H3EDTA- H3EDTA-	5.83347E-22	1.21085E-22	0.2076	5.85610E-22	5.12764E-22	4.57341E-16	7.07E-09
H3Citrate(aq) CitricAcid	5.80241E-22	5.80241E-22	1	5.82492E-22	5.10034E-22	9.79896E-17	4.95E-09
ThAc2++ ThAcetate2++	5.44279E-22	9.60484E-20	176.5	5.46391E-22	4.78424E-22	1.67509E-16	2.53E-08
ThAc+++ ThAc+++	0.00000E+00	0.00000E+00	48.92	0.00000E+00	0.00000E+00	0.00000E+00	-2.04E+01

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ATTACHMENT 2

Molarity ap098_fmt_run022

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/Liter	Descriptor
HCl(aq) to titrate.acid.only	0.00000E+00	0.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-2.48E+02
NaOH(aq) to titrate.base.only	0.00000E+00	0.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-2.95E+02
AmOHCO3(c) AmOHCO3(c)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-9.90E-01
NaAm(CO3)2.6H2O(c)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-3.61E+00
Th(SO4)2.9H2O(s)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.82E+01
Th(SO4)2.8H2O(s)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.82E+01
Th(SO4)2.Na2SO4.6H2O(16C,s)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.40E+01
Th(SO4)2.K2SO4.4H2O(16C,s)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.75E+01
Th(SO4)2.2K2SO4.2H2O(16C,s)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.90E+01
2[Th(SO4)2.7/2K2SO4(16C,s)]	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-4.56E+01
NpO2OH(aged) NpO2OH(aged)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.52E+00
NpO2OH(amor) NpO2OH(amor)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-2.22E+00
2[NaNpO2CO3.7/2H2O(s)]	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.82E+00
Na3NpO2(CO3)2(s) Na3NpO2(CO3)2(s)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-2.30E+00
K3NpO2(CO3)2(s) K3NpO2(CO3)2(s)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-6.69E+00
H2Ox.2H2O(s) H2C2O4.2H2O(s)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.73E+01
NaHOx.H2O(s) NaHC2O4.H2O(s)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-7.01E+00
Na2Ox(s) Na2C2O4(s)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-7.88E-01
CO2("solid",DISABLED)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-7.52E+01
NaK3(SO4)2 Aphthitalite/Glaserite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-4.10E+00
CaCl2.6H2O Antarcticite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-5.24E+00
CaCO3 Aragonite NAF	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.87E-01
K2SO4 Arcanite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-3.20E+00
MgCl2.6H2O Bischofite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-4.22E+00
Na2Mg(SO4)2.4H2O Bloedite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-2.07E+00
Na6CO3(SO4)2 Burkeite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-5.92E+00
CaCl2.4H2O CaCl2 Tetrahydrate	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-6.56E+00
Ca4Cl2(OH)6.13H2O CaOxychloride A	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-2.34E+01
Ca2Cl2(OH)2.H2O CaOxychloride B	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.12E+01
KMgCl3.6H2O Carnallite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-4.57E+00
MgSO4.7H2O Epsomite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-2.03E+00
CaNa2(CO3)2.5H2O Gaylussite NAF	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-4.54E+00
CaSO4.2H2O Gypsum	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-3.41E-02
MgSO4.6H2O Hexahydrate	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-2.15E+00
KMgClSO4.3H2O Kainite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-3.69E+00
KHCO3 Kalicinite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-6.67E+00
MgSO4.H2O Kieserite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-3.03E+00
K2Mg(SO4)2.4H2O Leonite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-4.53E+00
Na4Ca(SO4)3.2H2O Labile Salt	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-7.07E-01
MgCO3 Magnesite NAF	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	7.60E-01
Mg2Cl(OH)3.4H2O MgOxychloride	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-3.74E-01
KHSO4 Mercurite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.13E+01
Na2SO4.10H2O Mirabilite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-9.17E-01
K8H6(SO4)7 Misenite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-7.03E+01
NaHCO3 Nahcolite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-3.94E+00

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ATTACHMENT 2

Molarity ap098_fmt_run022

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/Liter	Descriptor
Na2CO3.10H2O Natron	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-5.36E+00
MgCO3.3H2O Nesquehonite NAF	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-2.29E+00
K2Mg(SO4)2.6H2O Picromerite/Schoen	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-4.44E+00
Na2Ca(CO3)2.2H2O Pirssonite NAF	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-4.34E+00
K2MgCa2(SO4)4.2H2O Polyhalite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-3.24E+00
Ca(OH)2 Portlandite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-7.03E+00
K2CO3.3/2H2O Potassium Carbonate	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.22E+01
K8H4(CO3)6.3H2O K-Sequicarbonate	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-5.10E+01
KNaCO3.6H2O K-Na-Carbonate	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-7.62E+00
K2NaH(CO3)2.2H2O Potassium Trona	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.49E+01
K3H(SO4)2 Sesquipotassium Sulfate	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.41E+01
Na3H(SO4)2 Sesquisodium Sulfate	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.07E+01
Na2CO3.7H2O Na2CO3-Heptahydrate	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-5.35E+00
KCl Sylvite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.38E+00
K2Ca(SO4)2.H2O Syngenite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-2.02E+00
Mg2CaCl6.12H2O Tachyhydrite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.73E+01
Na2SO4 Thenardite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-5.95E-01
Na2CO3.H2O Thermonatrite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-5.53E+00
Na3H(CO3)2.2H2O Trona	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-8.48E+00
Na2B4O7.10H2O Borax	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.59E+00
B(OH)3 Borix Acid Solid	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.97E+00
KB5O8.4H2O K-Pentaborate (30 C)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-6.58E+00
K2B4O7.4H2O K-Tetraborate (30 C)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-6.37E+00
NaBO2.4H2O Sodium Metaborate	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-2.19E+00
NaB5O8.5H2O Sodium Pentaborate	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-5.89E+00
NaBO2.NaCl.2H2O Teepleite (20 C)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.64E+00
CaMg(CO3)2 Dolomite NAF	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	1.60E+00
Mg5(CO3)4(OH)2.4H2O HydroMagne5424 NAF	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-2.59E+00
Mg4(CO3)3(OH)2.3H2O HydroMagne4323 NAF	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-2.28E+00
H+(solid) to.set.aH+ NAF	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-8.99E+00
OH-/H2O(solid) to.set.aH+ NAF	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	8.99E+00
H4EDTA(aq) H4EDTA(aq)	0.00000E+00	0.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-2.84E+01
Th++++ Th++++	0.00000E+00	0.00000E+00	0.5366	0.00000E+00	0.00000E+00	0.00000E+00	-2.52E+01

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Information Only

ATTACHMENT 2

Molarity ap098_fmt_run028

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/Liter	Descriptor
H2O WATER	8.15610E-01	7.48023E-01	0.9171	5.57064E+01	4.87988E+01	8.79121E+05	
CaSO4 Anhydrite	9.96388E+00	1.00000E+00	1	9.99937E+00	8.75946E+00	1.19249E+06	
Mg(OH)2 Brucite	9.81579E+00	1.00000E+00	1	9.85075E+00	8.62926E+00	5.03255E+05	
NaCl Halite	9.40421E+00	1.00000E+00	1	9.43770E+00	8.26743E+00	4.83172E+05	
Na+ Na+	6.04608E+00	5.86556E+00	0.9701	6.06761E+00	5.31524E+00	1.22196E+05	
Mg5(CO3)4(OH)2.4H2O HydroMagne5424	1.00083E+00	1.00000E+00	1	1.00439E+00	8.79846E-01	4.11449E+05	
ThO2(am) Hydrous Thorium Oxide	9.96451E-01	1.00000E+00	1	1.00000E+00	8.76001E-01	2.31297E+05	
Am(OH)3(s) Am(OH)3(s)	9.96451E-01	1.00000E+00	1	1.00000E+00	8.76001E-01	2.57563E+05	
KNpO2CO3(s) KNpO2CO3(s)	9.96446E-01	1.00000E+00	1	9.99994E-01	8.75996E-01	3.22502E+05	
SO4= SO4=	1.92124E-01	3.68404E-03	1.92E-02	1.92808E-01	1.68900E-01	1.62241E+04	
Mg++ Mg++	1.10758E-01	2.12856E-01	1.922	1.11152E-01	9.73696E-02	2.36657E+03	
K+ K+	1.09271E-01	5.25180E-02	0.4806	1.09660E-01	9.60622E-02	3.75587E+03	
B(OH)4- B(OH)4-	4.35256E-02	4.35008E-03	9.99E-02	4.36806E-02	3.82642E-02	3.01672E+03	
MgOx(aq) MgOx(aq)	2.24031E-02	2.80716E-02	1.253	2.24828E-02	1.96950E-02	1.04669E+03	
Br- Br-	1.23909E-02	3.47180E-03	0.2802	1.24350E-02	1.08931E-02	8.70400E+02	
Ac- Acetate-	4.12133E-03	3.14997E-03	0.7643	4.13601E-03	3.62315E-03	2.13925E+02	
MgCit- MgCit-	3.97229E-04	7.97748E-05	0.2008	3.98644E-04	3.49213E-04	7.45237E+01	
MgEDTA= MgEDTA=	4.04226E-06	1.07241E-06	0.2653	4.05666E-06	3.55364E-06	3.24516E+00	
Cl- Cl-	5.96723E+00	6.34014E+00	1.062	5.98848E+00	5.24592E+00	1.85983E+05	-7.36E-10
MgB(OH)4+ MgB(OH)4+	1.21800E-02	2.32209E-02	1.906	1.22233E-02	1.07077E-02	1.10443E+03	1.76E-09
Ca++ Ca++	1.08320E-02	1.17929E-02	1.089	1.08706E-02	9.52266E-03	3.81668E+02	-1.08E-09
B(OH)3(aq) B(OH)3(aq)	1.02774E-02	9.70483E-03	0.9443	1.03140E-02	9.03510E-03	5.58657E+02	-1.92E-09
CaB(OH)4+ CaB(OH)4+	1.93877E-03	2.29318E-03	1.183	1.94568E-03	1.70442E-03	2.02688E+02	-1.76E-09
MgAc+ MgAc+	1.48470E-03	8.69937E-03	5.859	1.48999E-03	1.30523E-03	1.08790E+02	-1.53E-09
CaOx(aq) (Mg-analog)	1.24121E-03	1.55526E-03	1.253	1.24563E-03	1.09117E-03	7.52034E+01	-8.97E-10
MgOH+ MgOH+	7.11798E-04	2.56708E-04	0.3606	7.14333E-04	6.25756E-04	2.58514E+01	9.89E-10
Ox= Oxalate=	6.81803E-04	2.12351E-05	3.11E-02	6.84231E-04	5.99387E-04	1.72863E+01	-2.37E-09
B3O3(OH)4- B3O3(OH)4-	4.39557E-04	5.03578E-05	0.1146	4.41122E-04	3.86424E-04	5.73674E+01	-2.50E-09
B4O5(OH)4= B4O5(OH)4=	4.31373E-04	1.68074E-06	3.90E-03	4.32909E-04	3.79229E-04	7.25337E+01	-5.05E-09
MgCO3(aq) MgCO3(aq)	3.17137E-04	3.17137E-04	1	3.18266E-04	2.78801E-04	2.35069E+01	1.78E-10
HCO3- HCO3-	1.06529E-04	3.69321E-05	0.3467	1.06909E-04	9.36522E-05	5.71439E+00	-1.90E-10
CaAc+ (Mg-analog)	8.22576E-05	4.81975E-04	5.859	8.25505E-05	7.23144E-05	7.16809E+00	-2.34E-09
CO3= CO3=	7.82755E-05	1.75676E-06	2.24E-02	7.85543E-05	6.88136E-05	4.12945E+00	-7.65E-10
CaCO3(aq) CaCO3(aq)	2.93478E-05	2.93478E-05	1	2.94524E-05	2.58003E-05	2.58233E+00	-6.70E-10
CaCit- (Mg-analog)	2.20079E-05	4.41980E-06	0.2008	2.20862E-05	1.93476E-05	4.43408E+00	-9.96E-10
OH- OH-	1.48628E-05	7.83093E-06	0.5269	1.49157E-05	1.30662E-05	2.22220E-01	-5.38E-10
Citrate= Citrate=	1.21894E-05	1.87969E-09	1.54E-04	1.22328E-05	1.07159E-05	2.02638E+00	-2.39E-09
NpO2Ox- NpO2Oxalate-	5.09495E-06	9.95885E-08	1.95E-02	5.11310E-06	4.47908E-06	1.33426E+00	-7.42E-10
NpO2CO3- NpO2CO3-	4.52521E-07	4.92971E-08	0.1089	4.54133E-07	3.97821E-07	1.30905E-01	6.42E-10
CaEDTA= (Mg-analog)	2.23955E-07	5.94154E-08	0.2653	2.24753E-07	1.96884E-07	1.82899E-01	-6.95E-10
HAc(aq) AceticAcid	1.73211E-07	1.73211E-07	1	1.73828E-07	1.52273E-07	9.14430E-03	5.65E-10
NpO2+ NpO2+	1.38778E-07	2.69860E-07	1.945	1.39272E-07	1.22003E-07	3.28245E-02	6.64E-11
Am(OH)2+ Am(OH)2+	9.68178E-08	8.09192E-11	8.36E-04	9.71626E-08	8.51146E-08	2.35780E-02	2.25E-09
AmEDTA- AmEDTA-	9.31020E-08	2.31659E-09	2.49E-02	9.34336E-08	8.18479E-08	9.26426E-02	2.29E-09
NpO2Ac(aq) NpO2Ac(aq)	6.95275E-08	2.00964E-08	0.289	6.97751E-08	6.11231E-08	1.80981E-02	1.57E-09

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ATTACHMENT 2

Molarity ap098_fmt_run028

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/Liter	Descriptor
CO2(aq) CO2(aq)	2.98386E-08	1.03365E-07	3.464	2.99448E-08	2.62317E-08	1.15445E-03	-4.99E-10
Th(OH)3(CO3)- Th(OH)3(CO3)-	2.72023E-08	7.62181E-09	0.2802	2.72991E-08	2.39141E-08	8.20418E-03	-5.68E-10
NpO2(CO3)2=- NpO2(CO3)2=-	1.25826E-08	2.31772E-12	1.84E-04	1.26275E-08	1.10617E-08	4.30371E-03	-1.66E-10
NpO2OH(aq) NpO2OH(aq)	9.95445E-09	1.03094E-09	0.1036	9.98990E-09	8.75117E-09	2.50331E-03	1.29E-09
HOx- Bioxalate-	1.42593E-09	3.71583E-10	0.2606	1.43101E-09	1.25356E-09	3.74163E-05	-1.87E-09
Th(OH)4(aq) Th(OH)4(aq)	8.84814E-10	8.84814E-10	1	8.87965E-10	7.77858E-10	2.33410E-04	-3.57E-10
Am(OH)3(aq) Am(OH)3(aq)	8.04366E-10	6.30297E-12	7.84E-03	8.07230E-10	7.07135E-10	2.07913E-04	2.14E-09
HSO4- HSO4-	5.76779E-10	3.37607E-10	0.5853	5.78833E-10	5.07058E-10	4.92178E-05	3.13E-10
AmOH++ AmOH++	5.65882E-10	1.42375E-11	2.52E-02	5.67897E-10	4.97478E-10	1.29348E-04	5.79E-10
HCitrate= HCitrate=	5.06620E-10	4.79449E-12	9.46E-03	5.08424E-10	4.45380E-10	8.46702E-05	-2.13E-09
Am(CO3)2- Am(CO3)2-	3.73861E-10	2.04143E-11	5.46E-02	3.75192E-10	3.28669E-10	1.19313E-04	2.81E-10
NpO2Cit= NpO2Citrate=	3.61777E-10	1.59280E-12	4.40E-03	3.63065E-10	3.18045E-10	1.45712E-04	-2.69E-09
AmOx+ AmOxalate+	3.01428E-10	2.00545E-11	6.65E-02	3.02502E-10	2.64992E-10	7.20353E-05	-2.97E-09
H+ H+	2.16767E-10	9.62591E-10	4.441	2.17538E-10	1.90564E-10	1.92069E-07	-6.80E-10
AmCO3+ AmCO3+	1.95503E-10	1.45805E-10	0.7458	1.96199E-10	1.71871E-10	5.20784E-05	-1.81E-10
NpO2(CO3)3=- NpO2(CO3)3=-	1.05595E-10	3.14131E-19	2.97E-09	1.05971E-10	9.28305E-11	4.16878E-05	-1.29E-09
Am(CO3)3=- Am(CO3)3=-	1.04453E-10	5.68570E-15	5.44E-05	1.04825E-10	9.18272E-11	3.88454E-05	8.03E-11
AmCit(aq) AmCitrate(aq)	9.89426E-11	7.78138E-13	7.86E-03	9.92949E-11	8.69825E-11	3.75851E-05	8.26E-10
AmAc++ AmAcetate++	7.25408E-11	1.14677E-12	1.58E-02	7.27991E-11	6.37721E-11	1.92620E-05	3.64E-09
NpO2(OH)2- NpO2(OH)2-	2.96765E-11	4.74164E-13	1.60E-02	2.97822E-11	2.60892E-11	7.90664E-06	1.17E-09
AmSO4+ AmSO4+	1.00272E-11	4.29978E-12	0.4288	1.00629E-11	8.81514E-12	2.98884E-06	3.43E-10
EDTA== EDTA==	9.42535E-12	3.76936E-16	4.00E-05	9.45892E-12	8.28602E-12	7.36535E-06	-1.68E-09
HEDTA=- HEDTA=-	2.74810E-12	1.35032E-14	4.91E-03	2.75789E-12	2.41591E-12	2.14991E-06	-2.53E-10
Am+++ Am+++	2.11708E-12	6.58566E-13	0.3111	2.12462E-12	1.86117E-12	4.52263E-07	-3.70E-10
Am(SO4)2- Am(SO4)2-	1.17596E-12	4.49960E-14	3.83E-02	1.18015E-12	1.03381E-12	4.49827E-07	1.46E-09
Am(CO3)4=- Am(CO3)4=-	9.75203E-13	6.25010E-23	6.41E-11	9.78676E-13	8.57321E-13	4.14118E-07	1.75E-10
NpO2EDTA=- NpO2EDTA=-	2.38462E-13	3.48814E-14	0.1463	2.39311E-13	2.09637E-13	2.42746E-07	-1.52E-09
AmCl++ AmCl++	1.52818E-13	7.24428E-12	47.4	1.53362E-13	1.34345E-13	3.74088E-08	-1.53E-08
H2EDTA= H2EDTA=	6.84860E-15	9.84245E-17	1.44E-02	6.87299E-15	6.02075E-15	5.36391E-09	2.65E-10
AmCl2+ AmCl2+	5.77023E-15	4.81682E-12	834.8	5.79078E-15	5.07273E-15	1.59236E-09	-3.35E-09
H2Citrate- H2Citrate-	2.60174E-15	3.19126E-16	0.1227	2.61101E-15	2.28725E-15	4.37129E-10	-1.86E-09
NpO2HEDTA= NpO2HEDTA=	1.18427E-15	3.44577E-16	0.291	1.18849E-15	1.04111E-15	1.20659E-09	-1.01E-09
Th(CO3)5=== Th(CO3)5===	2.12661E-17	1.02192E-27	4.81E-11	2.13418E-17	1.86955E-17	9.94756E-12	-1.44E-08
H2Ox(aq) OxalicAcid	8.85419E-18	8.85419E-18	1	8.88572E-18	7.78390E-18	2.40179E-13	-6.62E-10
ThEDTA(aq) ThEDTA(aq)	1.69762E-18	6.39265E-18	3.766	1.70367E-18	1.49242E-18	1.67289E-12	7.64E-10
Th(SO4)3= Th(SO4)3=	3.74092E-19	6.29103E-21	1.68E-02	3.75424E-19	3.28872E-19	1.71083E-13	1.17E-09
NpO2H2EDTA- NpO2H2EDTA-	2.14981E-19	6.90396E-20	0.3211	2.15746E-19	1.88994E-19	2.19224E-13	-2.97E-09
ThCit+ ThCit+	1.54954E-20	1.52049E-19	9.813	1.55505E-20	1.36223E-20	5.73687E-15	-7.76E-09
Th(SO4)2(aq) Th(SO4)2(aq)	7.82933E-21	2.49353E-19	31.85	7.85721E-21	6.88293E-21	2.91942E-15	-2.12E-10
ThOx++ Th(C2O4)++	1.36734E-21	2.43108E-19	177.8	1.37221E-21	1.20206E-21	3.13591E-16	-9.13E-09
H3EDTA- H3EDTA-	5.58798E-22	1.15863E-22	0.2073	5.60788E-22	4.91251E-22	4.38153E-16	4.01E-11
H3Citrate(aq) CitricAcid	5.42237E-22	5.42237E-22	1	5.44168E-22	4.76692E-22	9.15838E-17	-1.89E-09
ThAc2++ ThAcetate2++	4.52948E-22	8.09340E-20	178.7	4.54561E-22	3.98196E-22	1.39419E-16	-3.29E-09
ThAc+++ ThAc+++	6.77820E-23	3.40756E-21	50.27	6.80234E-23	5.95886E-23	1.73452E-17	-4.29E-09
HCl(aq) to.titrate.acid.only	0.00000E+00	0.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-2.48E+02

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ATTACHMENT 2

Molarity ap098_fmt_run028

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/Liter	Descriptor
NaOH(aq) to.titrate.base.only	0.00000E+00	0.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-2.95E+02
AmOHCO3(c) AmOHCO3(c)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-3.44E-01
NaAm(CO3)2.6H2O(c)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-2.29E+00
Th(SO4)2.9H2O(s)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.83E+01
Th(SO4)2.8H2O(s)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.83E+01
Th(SO4)2.Na2SO4.6H2O(16C,s)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.42E+01
Th(SO4)2.K2SO4.4H2O(16C,s)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.76E+01
Th(SO4)2.2K2SO4.2H2O(16C,s)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.92E+01
2Th(SO4)2.72K2SO4(16C,s)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-4.60E+01
NpO2OH(aged) NpO2OH(aged)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-2.19E+00
NpO2OH(amor) NpO2OH(amor)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-2.89E+00
2[NaNpO2CO3.72H2O(s)]	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.81E+00
Na3NpO2(CO3)2(s) Na3NpO2(CO3)2(s)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.59E+00
K3NpO2(CO3)2(s) K3NpO2(CO3)2(s)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-5.99E+00
H2Ox.2H2O(s) H2C2O4.2H2O(s)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.73E+01
NaHOx.H2O(s) NaHC2O4.H2O(s)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-6.99E+00
Na2Ox(s) Na2C2O4(s)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-7.31E-01
CO2("solid",DISABLED)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-7.46E+01
NaK3(SO4)2 Aphthitalite/Glaserite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-4.14E+00
CaCl2.6H2O Antarcticite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-5.22E+00
CaCO3 Aragonite NAF	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	5.36E-01
K2SO4 Arcanite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-3.22E+00
MgCl2.6H2O Bischofite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-4.28E+00
Na2Mg(SO4)2.4H2O Bloedite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-2.16E+00
Na6CO3(SO4)2 Burkeite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-5.24E+00
CaCO3 Calcite NAF	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	7.23E-01
CaCl2.4H2O CaCl2 Tetrahydrate	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-6.55E+00
Ca4Cl2(OH)6.13H2O CaOxychloride A	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-2.31E+01
Ca2Cl2(OH)2.H2O CaOxychloride B	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.11E+01
KMgCl3.6H2O Carnallite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-4.63E+00
MgSO4.7H2O Epsomite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-2.11E+00
CaNa2(CO3)2.5H2O Gaylussite NAF	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-3.11E+00
Na2Ca(SO4)2 Glauberite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.46E-02
CaSO4.2H2O Gypsum	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-3.37E-02
MgSO4.6H2O Hexahydrate	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-2.23E+00
KMgClSO4.3H2O Kainite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-3.77E+00
KHCO3 Kalicinite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-5.99E+00
MgSO4.H2O Kieserite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-3.11E+00
K2Mg(SO4)2.4H2O Leonite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-4.62E+00
Na4Ca(SO4)3.2H2O Labile Salt	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-7.36E-01
MgCO3 Magnesite NAF	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	1.41E+00
Mg2Cl(OH)3.4H2O MgOxychloride	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-4.04E-01
KHSO4 Mercallite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.13E+01
Na2SO4.10H2O Mirabilite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-9.30E-01
K8H6(SO4)7 Misenite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-7.06E+01

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Molarity ap098_fmt_run028

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/Liter	Descriptor
NaHCO3 Nahcolite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-3.26E+00
Na2CO3.10H2O Natron	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-4.65E+00
MgCO3.3H2O Nesquehonite NAF	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.64E+00
K2Mg(SO4)2.6H2O Picromerite/Schoen	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-4.53E+00
Na2Ca(CO3)2.2H2O Pirssonite NAF	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-2.91E+00
K2MgCa2(SO4)4.2H2O Polyhalite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-3.33E+00
Ca(OH)2 Portlandite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-6.95E+00
K2CO3.3/2H2O Potassium Carbonate	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.15E+01
K8H4(CO3)6.3H2O K-Sequicarbonate	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-4.69E+01
KNaCO3.6H2O K-Na-Carbonate	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-6.91E+00
K2NaH(CO3)2.2H2O Potassium Trona	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.35E+01
K3H(SO4)2 Sesquipotassium Sulfate	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.42E+01
Na3H(SO4)2 Sesquisodium Sulfate	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.08E+01
Na2CO3.7H2O Na2CO3-Heptahydrate	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-4.64E+00
KCl Sylvite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.38E+00
K2Ca(SO4)2.H2O Syngenite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-2.03E+00
Mg2CaCl6.12H2O Tachyhydrite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.74E+01
Na2SO4 Thenardite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-6.10E-01
Na2CO3.H2O Thermonatrite	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-4.83E+00
Na3H(CO3)2.2H2O Trona	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-7.09E+00
Na2B4O7.10H2O Borax	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.58E+00
B(OH)3 Borix Acid Solid	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.98E+00
KB5O8.4H2O K-Pentaborate (30 C)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-6.62E+00
K2B4O7.4H2O K-Tetraborate (30 C)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-6.36E+00
NaBO2.4H2O Sodium Metaborate	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-2.17E+00
NaB5O8.5H2O Sodium Pentaborate	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-5.92E+00
NaBO2.NaCl.2H2O Teepleite (20 C)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.62E+00
CaMg(CO3)2 Dolomite NAF	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	2.97E+00
Mg4(CO3)3(OH)2.3H2O HydroMagne4323 NAF	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-3.44E-01
H+(solid) to.set.aH+ NAF	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-9.02E+00
OH-/H2O(solid) to.set.aH+ NAF	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	9.02E+00
H4EDTA(aq) H4EDTA(aq)	0.00000E+00	0.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-2.85E+01
Th++++ Th++++	0.00000E+00	0.00000E+00	0.5481	0.00000E+00	0.00000E+00	0.00000E+00	-2.53E+01

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	A	B	C	D	E	F	G	H
1								
2	Aqueous Forms							
3	Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
4	Th(OH)3(CO3)- Th(OH)3(CO3)-	1.34037E-08	3.62427E-09	0.2704	1.23230E-08	1.16873E-08	4.00955E-03	2.14E-10
5	Th(OH)4(aq) Th(OH)4(aq)	8.49114E-10	8.49114E-10	1.0000	7.80651E-10	7.40381E-10	2.22164E-04	-1.30E-09
6	Th(CO3)5=== Th(CO3)5===	4.69721E-16	1.35264E-29	0.0000	4.31848E-16	4.09571E-16	2.17926E-10	-3.38E-08
7	Th(SO4)3= Th(SO4)3=	9.18508E-18	2.33986E-19	0.0255	8.44450E-18	8.00889E-18	4.16631E-12	1.77E-11
8	ThEDTA(aq) ThEDTA(aq)	4.01319E-18	1.60170E-17	3.9910	3.68961E-18	3.49928E-18	3.92243E-12	-6.25E-09
9	Th(SO4)2(aq) Th(SO4)2(aq)	2.07146E-19	7.67867E-18	37.0700	1.90444E-19	1.80620E-19	7.66105E-14	-9.69E-09
10	ThCit+ ThCit+	3.32637E-20	6.69595E-19	20.1300	3.05817E-20	2.90041E-20	1.22147E-14	-4.19E-08
11	ThOx++ Th(C2O4)++	2.58076E-21	1.27601E-18	494.4000	2.37268E-21	2.25028E-21	5.87050E-16	-4.73E-08
12	ThAc2++ ThAcetate2++	1.75683E-21	5.13701E-19	292.4000	1.61518E-21	1.53186E-21	5.36343E-16	-4.95E-08
13	ThAc+++ ThAc+++	4.10538E-22	3.94432E-20	96.0800	3.77436E-22	3.57966E-22	1.04198E-16	-4.32E-08
14	Th++++ Th++++	0.00000E+00	0.00000E+00	0.9093	0.00000E+00	0.00000E+00	0.00000E+00	-2.40E+01
15	Sum of Th Molarities					1.24277E-08		
16								
17								
18	Solid Forms							
19	Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
20	ThO2(am)_____Hydrous_Thorium_Oxide	1.08770E+00	1.00000E+00	1.0000	1.00000E+00	9.48415E-01	2.50417E+05	
21	2[Th(SO4)2.7/2K2SO4(16C,s)]	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-3.32E+01
22	Th(SO4)2.2K2SO4.2H2O(16C,s)_____	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-1.49E+01
23	Th(SO4)2.8H2O(s)	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-1.69E+01
24	Th(SO4)2.9H2O(s)	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-1.69E+01
25	Th(SO4)2.K2SO4.4H2O(16C,s)_____	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-1.48E+01
26	Th(SO4)2.Na2SO4.6H2O(16C,s)_____	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-1.29E+01

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	A	B	C	D	E	F	G	H
1								
2	Aqueous Forms							
3	Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
4	Th(OH)3(CO3)- Th(OH)3(CO3)-	0.0000000134037	0.00000000362427	0.2704	0.000000012323	0.0000000116873	0.00400955	0.000000000214
5	Th(OH)4(aq) Th(OH)4(aq)	0.000000000849114	0.000000000849114	1	0.000000000780651	0.000000000740381	0.000222164	-0.0000000013
6	Th(CO3)5=== Th(CO3)5===	4.69721E-16	1.35264E-29	0.000000000000028797	4.31848E-16	4.09571E-16	0.000000000217926	-0.0000000338
7	Th(SO4)3= Th(SO4)3=	9.18508E-18	2.33986E-19	0.025475	8.4445E-18	8.00889E-18	0.0000000000416631	0.000000000177
8	ThEDTA(aq) ThEDTA(aq)	4.01319E-18	1.6017E-17	3.991	3.68961E-18	3.49928E-18	0.0000000000392243	-0.00000000625
9	Th(SO4)2(aq) Th(SO4)2(aq)	2.07146E-19	7.67867E-18	37.07	1.90444E-19	1.8062E-19	0.000000000000766105	-0.00000000969
10	ThCit+ ThCit+	3.32637E-20	6.69595E-19	20.13	3.05817E-20	2.90041E-20	0.000000000000122147	-0.0000000419
11	ThOx++ Th(C2O4)++	2.58076E-21	1.27601E-18	494.4	2.37268E-21	2.25028E-21	5.8705E-16	-0.0000000473
12	ThAc2++ ThAcetate2++	1.75683E-21	5.13701E-19	292.4	1.61518E-21	1.53186E-21	5.36343E-16	-0.0000000495
13	ThAc+++ ThAc+++	4.10538E-22	3.94432E-20	96.08	3.77436E-22	3.57966E-22	1.04198E-16	-0.0000000432
14	Th++++ Th++++	0	0	0.9093	0	0	0	-24
15	Sum of Th Molarities =SUM(F4:F14)							
16								
17								
18	Solid Forms							
19	Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
20	ThO2(am)_____Hydrous_Thorium_Oxide	1.0877	1	1	1	0.948415	250417	
21	2[Th(SO4)2.7/2K2SO4(16C,s)]	0	1	1	0	0	0	-33.2
22	Th(SO4)2.2K2SO4.2H2O(16C,s)_____	0	1	1	0	0	0	-14.9
23	Th(SO4)2.8H2O(s)	0	1	1	0	0	0	-16.9
24	Th(SO4)2.9H2O(s)	0	1	1	0	0	0	-16.9
25	Th(SO4)2.K2SO4.4H2O(16C,s)_____	0	1	1	0	0	0	-14.8
26	Th(SO4)2.Na2SO4.6H2O(16C,s)_____	0	1	1	0	0	0	-12.9

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	A	B	C	D	E	F	G	H	
1	Aqueous Forms								
2	Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/Liter	Descriptor	
3	Th(OH)3(CO3)- Th(OH)3(CO3)-	1.27508E-08	3.44752E-09	0.2704	1.17223E-08	1.11179E-08	3.81422E-03	1.47E-09	
4	Th(OH)4(aq) Th(OH)4(aq)	8.49103E-10	8.49103E-10	1	7.80610E-10	7.40363E-10	2.22159E-04	-1.92E-10	
5	Th(CO3)5=== Th(CO3)5===	3.66325E-16	1.05347E-29	2.88E-14	3.36776E-16	3.19412E-16	1.69954E-10	2.63E-08	
6	Th(SO4)3= Th(SO4)3=	9.23945E-18	2.35386E-19	2.55E-02	8.49415E-18	8.05621E-18	4.19093E-12	2.19E-09	
7	ThEDTA(aq) ThEDTA(aq)	4.01400E-18	1.60190E-17	3.991	3.69021E-18	3.49995E-18	3.92319E-12	-4.82E-09	
8	Th(SO4)2(aq) Th(SO4)2(aq)	2.08025E-19	7.70960E-18	37.06	1.91245E-19	1.81384E-19	7.69347E-14	-1.88E-09	
9	ThCit+ ThCit+	3.32399E-20	6.69490E-19	20.14	3.05586E-20	2.89831E-20	1.22059E-14	-1.44E-08	
10	ThOx++ Th(C2O4)++	2.58103E-21	1.27614E-18	494.4	2.37283E-21	2.25049E-21	5.87103E-16	-1.37E-08	
11	ThAc2++ ThAcetate2++	1.75833E-21	5.13801E-19	292.2	1.61650E-21	1.53315E-21	5.36798E-16	-1.47E-08	
12	ThAc+++ ThAc+++	4.11306E-22	3.94495E-20	95.91	3.78128E-22	3.58632E-22	1.04391E-16	-1.05E-08	
13	Th++++ Th++++	0.00000E+00	0.00000E+00	0.9341	0.00000E+00	0.00000E+00	0.00000E+00	-2.40E+01	
14	Sum of Th Molarities						1.18583E-08		
15									
16									
17	Solid Forms								
18	Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/Liter	Descriptor	
19	ThO2(am)_____Hydrous_Thorium_Oxide	1.08774E+00	1.00000E+00	1	1.00000E+00	9.48442E-01	2.50424E+05		
20	2[Th(SO4)2.7/2K2SO4(16C,s)]_____	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-3.32E+01	
21	Th(SO4)2.2K2SO4.2H2O(16C,s)_____	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.49E+01	
22	Th(SO4)2.8H2O(s)_____	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.69E+01	
23	Th(SO4)2.9H2O(s)_____	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.69E+01	
24	Th(SO4)2.K2SO4.4H2O(16C,s)_____	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.48E+01	
25	Th(SO4)2.Na2SO4.6H2O(16C,s)_____	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.29E+01	

	A	B	C	D	E	F	G	H
1	Aqueous Forms							
2	Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/Liter	Descriptor
3	Th(OH)3(CO3)- Th(OH)3(CO3)-	0.0000000127508	0.00000000344752	0.2704	0.0000000117223	0.0000000111179	0.00381422	0.00000000147
4	Th(OH)4(aq) Th(OH)4(aq)	0.000000000849103	0.000000000849103	1	0.00000000078061	0.000000000740363	0.000222159	-0.000000000192
5	Th(CO3)5=== Th(CO3)5===	3.66325E-16	1.05347E-29	0.000000000000028758	3.36776E-16	3.19412E-16	0.000000000169954	0.00000000263
6	Th(SO4)3= Th(SO4)3=	9.23945E-18	2.35386E-19	0.025476	8.49415E-18	8.05621E-18	0.00000000000419093	0.00000000219
7	ThEDTA(aq) ThEDTA(aq)	4.014E-18	1.6019E-17	3.991	3.69021E-18	3.49995E-18	0.00000000000392319	-0.00000000482
8	Th(SO4)2(aq) Th(SO4)2(aq)	2.08025E-19	7.7096E-18	37.06	1.91245E-19	1.81384E-19	0.000000000000769347	-0.00000000188
9	ThCit+ ThCit+	3.32399E-20	6.6949E-19	20.14	3.05586E-20	2.89831E-20	0.0000000000000122059	-0.0000000144
10	ThOx++ Th(C2O4)++	2.58103E-21	1.27614E-18	494.4	2.37283E-21	2.25049E-21	5.87103E-16	-0.0000000137
11	ThAc2++ ThAcetate2++	1.75833E-21	5.13801E-19	292.2	1.6165E-21	1.53315E-21	5.36798E-16	-0.0000000147
12	ThAc+++ ThAc+++	4.11306E-22	3.94495E-20	95.91	3.78128E-22	3.58632E-22	1.04391E-16	-0.0000000105
13	Th++++ Th++++	0	0	0.9341	0	0	0	-24
14	Sum of Th Molarities =SUM(F3:F13)							
15								
16								
17	Solid Forms							
18	Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/Liter	Descriptor
19	ThO2(am) Hydrous Thorium Oxide	1.08774	1	1	1	0.948442	250424	
20	2[Th(SO4)2.7/2K2SO4(16C,s)]	0	1	1	0	0	0	-33.2
21	Th(SO4)2.2K2SO4.2H2O(16C,s)	0	1	1	0	0	0	-14.9
22	Th(SO4)2.8H2O(s)	0	1	1	0	0	0	-16.9
23	Th(SO4)2.9H2O(s)	0	1	1	0	0	0	-16.9
24	Th(SO4)2.K2SO4.4H2O(16C,s)	0	1	1	0	0	0	-14.8
25	Th(SO4)2.Na2SO4.6H2O(16C,s)	0	1	1	0	0	0	-12.9

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	A	B	C	D	E	F	G	H
1	Aqueous Forms							
2	Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/Liter	Descriptor
3	Th(OH)3(CO3)- Th(OH)3(CO3)-	5.76364E-09	1.61139E-09	0.2796	5.78600E-09	5.06626E-09	1.73808E-03	4.11E-08
4	Th(OH)4(aq) Th(OH)4(aq)	8.84102E-10	8.84102E-10	1	8.87532E-10	7.77129E-10	2.33191E-04	1.64E-09
5	ThEDTA(aq) ThEDTA(aq)	1.89533E-18	7.12870E-18	3.761	1.90268E-18	1.66600E-18	1.86746E-12	3.16E-09
6	Th(SO4)3= Th(SO4)3=	5.60534E-19	9.34270E-21	0.016667	5.62709E-19	4.92712E-19	2.56314E-13	1.09E-07
7	ThCit+ ThCit+	1.75195E-20	1.73614E-19	9.91	1.75875E-20	1.53997E-20	6.48541E-15	2.03E-08
8	Th(CO3)5=== Th(CO3)5===	1.14356E-20	4.05988E-31	3.5502E-11	1.14800E-20	1.00519E-20	5.34848E-15	2.29E-07
9	Th(SO4)2(aq) Th(SO4)2(aq)	1.11376E-20	3.53627E-19	31.75	1.11809E-20	9.79004E-21	4.15248E-15	8.07E-08
10	ThOx++ Th(C2O4)++	1.56831E-21	2.79153E-19	178	1.57439E-21	1.37855E-21	3.59633E-16	4.66E-08
11	ThAc2++ ThAcetate2++	5.44279E-22	9.60484E-20	176.5	5.46391E-22	4.78424E-22	1.67509E-16	2.53E-08
12	Th++++ Th++++	0.00000E+00	0.00000E+00	0.5366	0.00000E+00	0.00000E+00	0.00000E+00	-2.52E+01
13	ThAc+++ ThAc+++	0.00000E+00	0.00000E+00	48.92	0.00000E+00	0.00000E+00	0.00000E+00	-2.04E+01
14	Sum of Th Molarities					5.84339E-09		
15								
16								
17	Solid Forms							
18	Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/Liter	Descriptor
19	ThO2(am) Hydrus Thorium Oxide	9.96136E-01	1.00000E+00	1	1.00000E+00	8.75607E-01	2.31193E+05	
20	2[Th(SO4)2.7/2K2SO4(16C,s)]	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-4.56E+01
21	Th(SO4)2.2K2SO4.2H2O(16C,s)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.90E+01
22	Th(SO4)2.8H2O(s)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.82E+01
23	Th(SO4)2.9H2O(s)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.82E+01
24	Th(SO4)2.K2SO4.4H2O(16C,s)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.75E+01
25	Th(SO4)2.Na2SO4.6H2O(16C,s)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.40E+01

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	A	B	C	D	E	F	G	H
1	Aqueous Forms							
2	Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/Liter	Descriptor
3	Th(OH)3(CO3)- Th(OH)3(CO3)-	0.00000000576364	0.00000000161139	0.2796	0.000000005786	0.00000000506626	0.00173808	0.0000000411
4	Th(OH)4(aq) Th(OH)4(aq)	0.000000000884102	0.000000000884102	1	0.000000000887532	0.000000000777129	0.000233191	0.0000000164
5	ThEDTA(aq) ThEDTA(aq)	1.89533E-18	7.1287E-18	3.761	1.90268E-18	1.666E-18	0.0000000000186746	0.00000000316
6	Th(SO4)3= Th(SO4)3=	5.60534E-19	9.3427E-21	0.016667	5.62709E-19	4.92712E-19	0.00000000000256314	0.000000109
7	ThCit+ ThCit+	1.75195E-20	1.73614E-19	9.91	1.75875E-20	1.53997E-20	6.48541E-15	0.0000000203
8	Th(CO3)5=== Th(CO3)5===	1.14356E-20	4.05988E-31	0.000000000035502	1.148E-20	1.00519E-20	5.34848E-15	0.000000229
9	Th(SO4)2(aq) Th(SO4)2(aq)	1.11376E-20	3.53627E-19	31.75	1.11809E-20	9.79004E-21	4.15248E-15	0.0000000807
10	ThOx++ Th(C2O4)++	1.56831E-21	2.79153E-19	178	1.57439E-21	1.37855E-21	3.59633E-16	0.0000000466
11	ThAc2++ ThAcetate2++	5.44279E-22	9.60484E-20	176.5	5.46391E-22	4.78424E-22	1.67509E-16	0.0000000253
12	Th++++ Th++++	0	0	0.5366	0	0	0	-25.2
13	ThAc+++ ThAc+++	0	0	48.92	0	0	0	-20.4
14	Sum of Th Molarities =SUM(F3:F13)							
15								
16								
17	Solid Forms							
18	Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/Liter	Descriptor
19	ThO2(am) Hydrus Thorium Oxide	0.996136	1	1	1	0.875607	231193	
20	2[Th(SO4)2.7/2K2SO4(16C,s)]	0	1	1	0	0	0	-45.6
21	Th(SO4)2.2K2SO4.2H2O(16C,s)	0	1	1	0	0	0	-19
22	Th(SO4)2.8H2O(s)	0	1	1	0	0	0	-18.2
23	Th(SO4)2.9H2O(s)	0	1	1	0	0	0	-18.2
24	Th(SO4)2.K2SO4.4H2O(16C,s)	0	1	1	0	0	0	-17.5
25	Th(SO4)2.Na2SO4.6H2O(16C,s)	0	1	1	0	0	0	-14

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	A	B	C	D	E	F	G	H	
1	Aqueous Forms								
2	Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/Liter	Descriptor	
3	Th++++ Th++++	0.00000E+00	0.00000E+00	0.5481	0.00000E+00	0.00000E+00	0.00000E+00	-2.53E+01	
4	ThAc+++ ThAc+++	6.77820E-23	3.40756E-21	50.27	6.80234E-23	5.95886E-23	1.73452E-17	-4.29E-09	
5	ThAc2++ ThAcetate2++	4.52948E-22	8.09340E-20	178.7	4.54561E-22	3.98196E-22	1.39419E-16	-3.29E-09	
6	ThOx++ Th(C2O4)++	1.36734E-21	2.43108E-19	177.8	1.37221E-21	1.20206E-21	3.13591E-16	-9.13E-09	
7	Th(SO4)2(aq) Th(SO4)2(aq)	7.82933E-21	2.49353E-19	31.85	7.85721E-21	6.88293E-21	2.91942E-15	-2.12E-10	
8	ThCit+ ThCit+	1.54954E-20	1.52049E-19	9.813	1.55505E-20	1.36223E-20	5.73687E-15	-7.76E-09	
9	Th(SO4)3= Th(SO4)3=	3.74092E-19	6.29103E-21	1.68E-02	3.75424E-19	3.28872E-19	1.71083E-13	1.17E-09	
10	ThEDTA(aq) ThEDTA(aq)	1.69762E-18	6.39265E-18	3.766	1.70367E-18	1.49242E-18	1.67289E-12	7.64E-10	
11	Th(CO3)5=== Th(CO3)5===	2.12661E-17	1.02192E-27	4.81E-11	2.13418E-17	1.86955E-17	9.94756E-12	-1.44E-08	
12	Th(OH)4(aq) Th(OH)4(aq)	8.84814E-10	8.84814E-10	1	8.87965E-10	7.77858E-10	2.33410E-04	-3.57E-10	
13	Th(OH)3(CO3)- Th(OH)3(CO3)-	2.72023E-08	7.62181E-09	0.2802	2.72991E-08	2.39141E-08	8.20418E-03	-5.68E-10	
14	Sum of Th Molarities						2.46920E-08		
15									
16									
17	Solid Forms								
18	Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/Liter	Descriptor	
19	2[Th(SO4)2.7/2K2SO4(16C,s)]	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-4.60E+01	
20	Th(SO4)2.2K2SO4.2H2O(16C,s)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.92E+01	
21	Th(SO4)2.8H2O(s)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.83E+01	
22	Th(SO4)2.9H2O(s)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.83E+01	
23	Th(SO4)2.K2SO4.4H2O(16C,s)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.76E+01	
24	Th(SO4)2.Na2SO4.6H2O(16C,s)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.42E+01	
25	ThO2(am) Hydrus Thorium Oxide	9.96451E-01	1.00000E+00	1	1.00000E+00	8.76001E-01	2.31297E+05		

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	A	B	C	D	E	F	G	H
1	Aqueous Forms							
2	Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/Liter	Descriptor
3	Th++++ Th++++	0	0	0.5481	0	0	0	-25.3
4	ThAc+++ ThAc+++	6.7782E-23	3.40756E-21	50.27	6.80234E-23	5.95886E-23	1.73452E-17	-0.00000000429
5	ThAc2++ ThAcetate2++	4.52948E-22	8.0934E-20	178.7	4.54561E-22	3.98196E-22	1.39419E-16	-0.00000000329
6	ThOx++ Th(C2O4)++	1.36734E-21	2.43108E-19	177.8	1.37221E-21	1.20206E-21	3.13591E-16	-0.00000000913
7	Th(SO4)2(aq) Th(SO4)2(aq)	7.82933E-21	2.49353E-19	31.85	7.85721E-21	6.88293E-21	2.91942E-15	-0.00000000212
8	ThCit+ ThCit+	1.54954E-20	1.52049E-19	9.813	1.55505E-20	1.36223E-20	5.73687E-15	-0.00000000776
9	Th(SO4)3= Th(SO4)3=	3.74092E-19	6.29103E-21	0.016817	3.75424E-19	3.28872E-19	0.00000000000171083	0.0000000117
10	ThEDTA(aq) ThEDTA(aq)	1.69762E-18	6.39265E-18	3.766	1.70367E-18	1.49242E-18	0.0000000000167289	0.00000000764
11	Th(CO3)5=== Th(CO3)5===	2.12661E-17	1.02192E-27	0.00000000048054	2.13418E-17	1.86955E-17	0.0000000000994756	-0.000000144
12	Th(OH)4(aq) Th(OH)4(aq)	0.000000000884814	0.000000000884814	1	0.00000000887965	0.00000000777858	0.00023341	-0.00000000357
13	Th(OH)3(CO3)- Th(OH)3(CO3)-	0.0000000272023	0.00000000762181	0.2802	0.0000000272991	0.0000000239141	0.00820418	-0.00000000568
14	Sum of Th Molarities =SUM(F3:F13)							
15								
16								
17	Solid Forms							
18	Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/Liter	Descriptor
19	2[Th(SO4)2.7/2K2SO4(16C,s)]	0	1	1	0	0	0	-46
20	Th(SO4)2.2K2SO4.2H2O(16C,s)	0	1	1	0	0	0	-19.2
21	Th(SO4)2.8H2O(s)	0	1	1	0	0	0	-18.3
22	Th(SO4)2.9H2O(s)	0	1	1	0	0	0	-18.3
23	Th(SO4)2.K2SO4.4H2O(16C,s)	0	1	1	0	0	0	-17.6
24	Th(SO4)2.Na2SO4.6H2O(16C,s)	0	1	1	0	0	0	-14.2
25	ThO2(am) Hydrus Thorium Oxide	0.996451	1	1	1	0.876001	231297	

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	A	B	C	D	E	F	G	H
1								
2	Aqueous Forms							
3	Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
4	NpO2Ox- NpO2Oxalate-	8.13552E-07	2.34930E-08	0.0289	7.47956E-07	7.09373E-07	2.11313E-01	1.79E-09
5	NpO2+ NpO2+	1.34592E-07	2.56029E-07	1.9020	1.23740E-07	1.17356E-07	3.15744E-02	-2.29E-09
6	NpO2CO3- NpO2CO3-	1.22337E-07	1.07011E-08	0.0875	1.12473E-07	1.06671E-07	3.51007E-02	5.17E-09
7	NpO2Ac(aq) NpO2Ac(aq)	3.81943E-08	1.04549E-08	0.2737	3.51147E-08	3.33033E-08	9.86085E-03	-7.27E-09
8	NpO2OH(aq) NpO2OH(aq)	4.81688E-09	4.51642E-10	0.0938	4.42850E-09	4.20005E-09	1.20144E-03	5.74E-09
9	NpO2(CO3)2=- NpO2(CO3)2=-	1.49425E-09	1.15114E-13	0.0001	1.37377E-09	1.30290E-09	5.06913E-04	4.13E-09
10	NpO2Cit= NpO2Citrate=	8.06230E-11	3.15258E-13	0.0039	7.41224E-11	7.02988E-11	3.22072E-05	-5.41E-09
11	NpO2(CO3)3=- NpO2(CO3)3=-	1.87194E-11	3.56973E-21	0.0000	1.72101E-11	1.63223E-11	7.32994E-06	-1.11E-08
12	NpO2(OH)2- NpO2(OH)2-	7.05331E-12	9.59175E-14	0.0136	6.48460E-12	6.15009E-12	1.86386E-06	9.34E-09
13	NpO2EDTA=- NpO2EDTA=-	2.30095E-13	3.92799E-15	0.0171	2.11543E-13	2.00630E-13	2.32317E-07	1.49E-09
14	NpO2HEDTA= NpO2HEDTA=	4.54989E-16	8.23208E-17	0.1809	4.18304E-16	3.96725E-16	4.59782E-10	-4.78E-09
15	NpO2H2EDTA- NpO2H2EDTA-	7.25011E-20	3.49921E-20	0.4826	6.66554E-20	6.32170E-20	7.33286E-14	-1.78E-08
16	Sum of Np Molarities					9.72299E-07		
17								
18								
19	Solid Forms							
20	Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
21	KNpO2CO3(s) KNpO2CO3(s)	1.08770E+00	1.00000E+00	1.0000	9.99999E-01	9.48414E-01	3.49163E+05	
22	2[NaNpO2CO3.7/2H2O(s)]	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-3.41E+00
23	K3NpO2(CO3)2(s) K3NpO2(CO3)2(s)	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-5.30E+00
24	Na3NpO2(CO3)2(s) Na3NpO2(CO3)2(s)	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-3.21E+00
25	NpO2OH(aged) NpO2OH(aged)	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-2.55E+00
26	NpO2OH(amor) NpO2OH(amor)	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-3.25E+00

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	A	B	C	D	E	F	G	H
1								
2	Aqueous Forms							
3	Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
4	NpO2Ox- NpO2Oxalate-	0.000000813552	0.000000023493	0.028877	0.000000747956	0.000000709373	0.211313	0.00000000179
5	NpO2+ NpO2+	0.000000134592	0.000000256029	1.902	0.00000012374	0.000000117356	0.0315744	-0.00000000229
6	NpO2CO3- NpO2CO3-	0.000000122337	0.0000000107011	0.087473	0.000000112473	0.000000106671	0.0351007	0.00000000517
7	NpO2Ac(aq) NpO2Ac(aq)	0.0000000381943	0.0000000104549	0.2737	0.0000000351147	0.0000000333033	0.00986085	-0.00000000727
8	NpO2OH(aq) NpO2OH(aq)	0.00000000481688	0.00000000451642	0.093762	0.0000000044285	0.00000000420005	0.00120144	0.00000000574
9	NpO2(CO3)2= NpO2(CO3)2=-	0.00000000149425	0.00000000000115114	0.000077038	0.00000000137377	0.0000000013029	0.000506913	0.00000000413
10	NpO2Cit= NpO2Citrate=	0.000000000080623	0.00000000000315258	0.0039103	0.0000000000741224	0.0000000000702988	0.0000322072	-0.00000000541
11	NpO2(CO3)3=- NpO2(CO3)3=-	0.0000000000187194	3.56973E-21	0.0000000001907	0.0000000000172101	0.0000000000163223	0.00000732994	-0.0000000111
12	NpO2(OH)2- NpO2(OH)2-	0.00000000000705331	0.000000000000959175	0.013599	0.0000000000064846	0.00000000000615009	0.00000186386	0.00000000934
13	NpO2EDTA= NpO2EDTA=-	0.00000000000230095	3.92799E-15	0.017071	0.00000000000211543	0.0000000000020063	0.000000232317	0.00000000149
14	NpO2HEDTA= NpO2HEDTA=	4.54989E-16	8.23208E-17	0.1809	4.18304E-16	3.96725E-16	0.000000000459782	-0.00000000478
15	NpO2H2EDTA- NpO2H2EDTA-	7.25011E-20	3.49921E-20	0.4826	6.66554E-20	6.3217E-20	0.000000000000733286	-0.0000000178
16	Sum of Np Molarities =SUM(F4:F15)							
17								
18								
19	Solid Forms							
20	Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
21	KNpO2CO3(s) KNpO2CO3(s)	1.0877	1	1	0.999999	0.948414	349163	
22	2[NaNpO2CO3.7/2H2O(s)]	0	1	1	0	0	0	-3.41
23	K3NpO2(CO3)2(s) K3NpO2(CO3)2(s)	0	1	1	0	0	0	-5.3
24	Na3NpO2(CO3)2(s) Na3NpO2(CO3)2(s)	0	1	1	0	0	0	-3.21
25	NpO2OH(aged) NpO2OH(aged)	0	1	1	0	0	0	-2.55
26	NpO2OH(amor) NpO2OH(amor)	0	1	1	0	0	0	-3.25

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	A	B	C	D	E	F	G	H
1	Aqueous Forms							
2	Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/Liter	Descriptor
3	NpO2Ox- NpO2Oxalate-	8.55243E-07	2.46980E-08	2.89E-02	7.86255E-07	7.45717E-07	2.22139E-01	-8.15E-10
4	NpO2+ NpO2+	1.41523E-07	2.69168E-07	1.902	1.30107E-07	1.23399E-07	3.32002E-02	-7.39E-10
5	NpO2CO3- NpO2CO3-	1.22323E-07	1.07014E-08	8.75E-02	1.12456E-07	1.06658E-07	3.50963E-02	1.90E-09
6	NpO2Ac(aq) NpO2Ac(aq)	4.01527E-08	1.09918E-08	0.2737	3.69138E-08	3.50105E-08	1.03663E-02	-3.73E-09
7	NpO2OH(aq) NpO2OH(aq)	5.06319E-09	4.74803E-10	9.38E-02	4.65476E-09	4.41477E-09	1.26286E-03	7.57E-10
8	NpO2(CO3)2=- NpO2(CO3)2=-	1.42076E-09	1.09500E-13	7.71E-05	1.30615E-09	1.23881E-09	4.81978E-04	3.13E-09
9	NpO2Cit= NpO2Citrate=	8.47292E-11	3.31343E-13	3.91E-03	7.78945E-11	7.38784E-11	3.38472E-05	-1.89E-09
10	NpO2(CO3)3=- NpO2(CO3)3=-	1.69191E-11	3.22998E-21	1.91E-10	1.55543E-11	1.47524E-11	6.62491E-06	-1.30E-09
11	NpO2(OH)2- NpO2(OH)2-	7.41392E-12	1.00833E-13	1.36E-02	6.81588E-12	6.46446E-12	1.95913E-06	2.40E-09
12	NpO2EDTA=-NpO2EDTA=-	2.41870E-13	4.12954E-15	1.71E-02	2.22359E-13	2.10895E-13	2.44203E-07	5.26E-09
13	NpO2HEDTA= NpO2HEDTA=	4.78215E-16	8.65474E-17	0.181	4.39640E-16	4.16973E-16	4.83247E-10	-2.75E-09
14	NpO2H2EDTA- NpO2H2EDTA-	7.61829E-20	3.67897E-20	0.4829	7.00376E-20	6.64266E-20	7.70516E-14	-9.21E-09
15	Sum of Np Molarities					1.01653E-06		
16								
17								
18	Solid Forms							
19	Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/Liter	Descriptor
20	KNpO2CO3(s) KNpO2CO3(s)	1.08774E+00	1.00000E+00	1	9.99999E-01	9.48441E-01	3.49173E+05	
21	2[NaNpO2CO3.7/2H2O(s)]	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-3.41E+00
22	K3NpO2(CO3)2(s) K3NpO2(CO3)2(s)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-5.32E+00
23	Na3NpO2(CO3)2(s) Na3NpO2(CO3)2(s)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-3.23E+00
24	NpO2OH(aged) NpO2OH(aged)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-2.53E+00
25	NpO2OH(amor) NpO2OH(amor)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-3.23E+00

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A	B	C	D	E	F	G	H	
1	Aqueous Forms							
2	Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/Liter	Descriptor
3	NpO2Ox- NpO2Oxalate-	0.000000855243	0.000000024698	0.028878	0.000000786255	0.000000745717	0.222139	-0.000000000815
4	NpO2+ NpO2+	0.000000141523	0.000000269168	1.902	0.000000130107	0.000000123399	0.0332002	-0.000000000739
5	NpO2CO3- NpO2CO3-	0.000000122323	0.0000000107014	0.087485	0.000000112456	0.000000106658	0.0350963	0.00000000019
6	NpO2Ac(aq) NpO2Ac(aq)	0.0000000401527	0.0000000109918	0.2737	0.0000000369138	0.0000000350105	0.0103663	-0.000000000373
7	NpO2OH(aq) NpO2OH(aq)	0.0000000506319	0.000000000474803	0.093775	0.00000000465476	0.00000000441477	0.00126286	0.000000000757
8	NpO2(CO3)2-- NpO2(CO3)2--	0.00000000142076	0.0000000000001095	0.000077072	0.00000000130615	0.00000000123881	0.000481978	0.000000000313
9	NpO2Cit= NpO2Citrate=	0.000000000847292	0.0000000000000331343	0.0039106	0.0000000000778945	0.0000000000738784	0.0000338472	-0.00000000189
10	NpO2(CO3)3=== NpO2(CO3)3===	0.0000000000169191	3.22998E-21	0.00000000019091	0.0000000000155543	0.0000000000147524	0.00000662491	-0.0000000013
11	NpO2(OH)2- NpO2(OH)2-	0.00000000000741392	0.000000000000100833	0.0136	0.00000000000681588	0.00000000000646446	0.00000195913	0.00000000024
12	NpO2EDTA= NpO2EDTA=	0.00000000000024187	4.12954E-15	0.017073	0.000000000000222359	0.000000000000210895	0.000000244203	0.00000000526
13	NpO2HEDTA= NpO2HEDTA=	4.78215E-16	8.65474E-17	0.181	4.3964E-16	4.16973E-16	0.000000000483247	-0.00000000275
14	NpO2H2EDTA- NpO2H2EDTA-	7.61829E-20	3.67897E-20	0.4829	7.00376E-20	6.64266E-20	0.0000000000000770516	-0.000000000921
15	Sum of Np Molarities =SUM(F3:F14)							
16								
17								
18	Solid Forms							
19	Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/Liter	Descriptor
20	KNpO2CO3(s) KNpO2CO3(s)	1.08774	1	1	0.999999	0.948441	349173	
21	2[NaNpO2CO3.7/2H2O(s)]	0	1	1	0	0	0	-3.41
22	K3NpO2(CO3)2(s) K3NpO2(CO3)2(s)	0	1	1	0	0	0	-5.32
23	Na3NpO2(CO3)2(s) Na3NpO2(CO3)2(s)	0	1	1	0	0	0	-3.23
24	NpO2OH(aged) NpO2OH(aged)	0	1	1	0	0	0	-2.53
25	NpO2OH(amor) NpO2OH(amor)	0	1	1	0	0	0	-3.23

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	A	B	C	D	E	F	G	H
1	Aqueous Forms							
2	Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/Liter	Descriptor
3	NpO2Ox- NpO2Oxalate-	2.26486E-05	4.48068E-07	0.019783	2.27365E-05	1.99082E-05	5.93040E+00	-2.34E-08
4	NpO2+ NpO2+	7.07352E-07	1.36747E-06	1.933	7.10096E-07	6.21765E-07	1.67284E-01	-3.63E-08
5	NpO2CO3- NpO2CO3-	4.56370E-07	4.95544E-08	0.1086	4.58140E-07	4.01151E-07	1.32001E-01	-7.06E-09
6	NpO2Ac(aq) NpO2Ac(aq)	3.37126E-07	9.75512E-08	0.2894	3.38433E-07	2.96335E-07	8.77424E-02	-4.69E-08
7	NpO2OH(aq) NpO2OH(aq)	4.71966E-08	4.89784E-09	0.1038	4.73797E-08	4.14860E-08	1.18673E-02	-4.63E-08
8	NpO2(CO3)2-- NpO2(CO3)2--	2.56036E-09	4.62171E-13	0.00018051	2.57029E-09	2.25056E-09	8.75616E-04	2.56E-08
9	NpO2Cit= NpO2Citrate=	1.62788E-09	7.12617E-12	0.0043776	1.63420E-09	1.43092E-09	6.55570E-04	-2.40E-08
10	NpO2(OH)2- NpO2(OH)2-	1.32134E-10	2.11198E-12	0.015984	1.32647E-10	1.16147E-10	3.51996E-05	-4.21E-08
11	NpO2(CO3)3=== NpO2(CO3)3===	4.49177E-12	1.24261E-20	2.7664E-09	4.50919E-12	3.94828E-12	1.77307E-06	4.27E-08
12	NpO2HEDTA= NpO2HEDTA=	5.59755E-15	1.60525E-15	0.2868	5.61926E-15	4.92026E-15	5.70231E-09	-3.26E-08
13	NpO2H2EDTA- NpO2H2EDTA-	1.05668E-18	3.42917E-19	0.3245	1.06078E-18	9.28830E-19	1.07740E-12	-2.61E-08
14	NpO2EDTA=- NpO2EDTA=-	-1.12E-12	1.52410E-13	0.1356	1.12850E-12	9.88125E-13	1.14418E-06	-3.56E-08
15	Sum of Np Molarities					2.127274E-05		
16								
17								
18	Solid Forms							
19	Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/Liter	Descriptor
20	KNpO2CO3(s) KNpO2CO3(s)	9.96111E-01	1.00000E+00	1	9.99976E-01	8.75586E-01	3.22351E+05	
21	2[NaNpO2CO3.7/2H2O(s)]	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.82E+00
22	K3NpO2(CO3)2(s) K3NpO2(CO3)2(s)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-6.69E+00
23	Na3NpO2(CO3)2(s) Na3NpO2(CO3)2(s)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-2.30E+00
24	NpO2OH(aged) NpO2OH(aged)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.52E+00
25	NpO2OH(amor) NpO2OH(amor)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-2.22E+00

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	A	B	C	D	E	F	G	H
1	Aqueous Forms							
2	Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/Liter	Descriptor
3	NpO2Ox- NpO2Oxalate-	0.0000226486	0.000000448068	0.019783	0.0000227365	0.0000199082	5.9304	-0.0000000234
4	NpO2+ NpO2+	0.000000707352	0.00000136747	1.933	0.000000710096	0.00000621765	0.167284	-0.0000000363
5	NpO2CO3- NpO2CO3-	0.00000045637	0.0000000495544	0.1086	0.00000045814	0.000000401151	0.132001	-0.00000000706
6	NpO2Ac(aq) NpO2Ac(aq)	0.000000337126	0.0000000975512	0.2894	0.000000338433	0.000000296335	0.0877424	-0.0000000469
7	NpO2OH(aq) NpO2OH(aq)	0.0000000471966	0.00000000489784	0.1038	0.0000000473797	0.000000041486	0.0118673	-0.0000000463
8	NpO2(CO3)2-- NpO2(CO3)2--	0.00000000256036	0.00000000000462171	0.00018051	0.00000000257029	0.00000000225056	0.000875616	0.00000000256
9	NpO2Cit= NpO2Citrate=	0.00000000162788	0.00000000000712617	0.0043776	0.0000000016342	0.00000000143092	0.00065557	-0.0000000024
10	NpO2(OH)2- NpO2(OH)2-	0.000000000132134	0.00000000000211198	0.015984	0.000000000132647	0.000000000116147	0.0000351996	-0.0000000421
11	NpO2(CO3)3== NpO2(CO3)3==	0.00000000000449177	1.24261E-20	0.0000000027664	0.00000000000450919	0.00000000000394828	0.00000177307	0.0000000427
12	NpO2HEDTA= NpO2HEDTA=	5.59755E-15	1.60525E-15	0.2868	5.61926E-15	4.92026E-15	0.00000000570231	-0.0000000326
13	NpO2H2EDTA- NpO2H2EDTA-	1.05668E-18	3.42917E-19	0.3245	1.06078E-18	9.2883E-19	0.0000000000010774	-0.0000000261
14	NpO2EDTA-- NpO2EDTA--	-0.00000000000112414	0.00000000000015241	0.1356	0.0000000000011285	0.000000000000988125	0.00000114418	-0.0000000356
15	Sum of Np Molarities =SUM(F3:F14)							
16								
17								
18	Solid Forms							
19	Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/Liter	Descriptor
20	KNpO2CO3(s) KNpO2CO3(s)	0.996111	1	1	0.999976	0.875586	322351	
21	2[NaNpO2CO3.7/2H2O(s)]	0	1	1	0	0	0	-1.82
22	K3NpO2(CO3)2(s) K3NpO2(CO3)2(s)	0	1	1	0	0	0	-6.69
23	Na3NpO2(CO3)2(s) Na3NpO2(CO3)2(s)	0	1	1	0	0	0	-2.3
24	NpO2OH(aged) NpO2OH(aged)	0	1	1	0	0	0	-1.52
25	NpO2OH(amor) NpO2OH(amor)	0	1	1	0	0	0	-2.22

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	A	B	C	D	E	F	G	H
1	Aqueous Forms							
2	Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/Liter	Descriptor
3	NpO2H2EDTA- NpO2H2EDTA-	2.14981E-19	6.90396E-20	0.3211	2.15746E-19	1.88994E-19	2.19224E-13	-2.97E-09
4	NpO2HEDTA= NpO2HEDTA=	1.18427E-15	3.44577E-16	0.291	1.18849E-15	1.04111E-15	1.20659E-09	-1.01E-09
5	NpO2EDTA=- NpO2EDTA=-	2.38462E-13	3.48814E-14	0.1463	2.39311E-13	2.09637E-13	2.42746E-07	-1.52E-09
6	NpO2(OH)2- NpO2(OH)2-	2.96765E-11	4.74164E-13	1.60E-02	2.97822E-11	2.60892E-11	7.90664E-06	1.17E-09
7	NpO2(CO3)3=- NpO2(CO3)3=-	1.05595E-10	3.14131E-19	2.97E-09	1.05971E-10	9.28305E-11	4.16878E-05	-1.29E-09
8	NpO2Cit= NpO2Citrate=	3.61777E-10	1.59280E-12	4.40E-03	3.63065E-10	3.18045E-10	1.45712E-04	-2.69E-09
9	NpO2OH(aq) NpO2OH(aq)	9.95445E-09	1.03094E-09	0.1036	9.98990E-09	8.75117E-09	2.50331E-03	1.29E-09
10	NpO2(CO3)2=- NpO2(CO3)2=-	1.25826E-08	2.31772E-12	1.84E-04	1.26275E-08	1.10617E-08	4.30371E-03	-1.66E-10
11	NpO2Ac(aq) NpO2Ac(aq)	6.95275E-08	2.00964E-08	0.289	6.97751E-08	6.11231E-08	1.80981E-02	1.57E-09
12	NpO2+ NpO2+	1.38778E-07	2.69860E-07	1.945	1.39272E-07	1.22003E-07	3.28245E-02	6.64E-11
13	NpO2CO3- NpO2CO3-	4.52521E-07	4.92971E-08	0.1089	4.54133E-07	3.97821E-07	1.30905E-01	6.42E-10
14	NpO2Ox- NpO2Oxalate-	5.09495E-06	9.95885E-08	1.95E-02	5.11310E-06	4.47908E-06	1.33426E+00	-7.42E-10
15	Sum of Np Molarities					5.08028E-06		
16								
17								
18	Solid Forms							
19	Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/Liter	Descriptor
20	2[NaNpO2CO3.7/2H2O(s)]	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.81E+00
21	K3NpO2(CO3)2(s) K3NpO2(CO3)2(s)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-5.99E+00
22	KNpO2CO3(s) KNpO2CO3(s)	9.96446E-01	1.00000E+00	1	9.99994E-01	8.75996E-01	3.22502E+05	
23	Na3NpO2(CO3)2(s) Na3NpO2(CO3)2(s)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-1.59E+00
24	NaOH(aq) to.titrate.base.only	0.00000E+00	0.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-2.95E+02
25	NpO2OH(aged) NpO2OH(aged)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-2.19E+00
26	NpO2OH(amor) NpO2OH(amor)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-2.89E+00

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	A	B	C	D	E	F	G	H
1	Aqueous Forms							
2	Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/Liter	Descriptor
3	NpO2H2EDTA- NpO2H2EDTA-	2.14981E-19	6.90396E-20	0.3211	2.15746E-19	1.88994E-19	0.00000000000219224	-0.00000000297
4	NpO2HEDTA= NpO2HEDTA=	1.18427E-15	3.44577E-16	0.291	1.18849E-15	1.04111E-15	0.0000000120659	-0.0000000101
5	NpO2EDTA=- NpO2EDTA=-	0.00000000000238462	0.000000000000348814	0.1463	0.00000000000239311	0.00000000000209637	0.000000242746	-0.0000000152
6	NpO2(OH)2- NpO2(OH)2-	0.0000000000296765	0.000000000000474164	0.015978	0.0000000000297822	0.0000000000260892	0.00000790664	0.0000000117
7	NpO2(CO3)3=- NpO2(CO3)3=-	0.00000000105595	3.14131E-19	0.0000000029749	0.00000000105971	0.000000000928305	0.0000416878	-0.0000000129
8	NpO2Cit= NpO2Citrate=	0.000000000361777	0.000000000015928	0.0044027	0.000000000363065	0.000000000318045	0.000145712	-0.0000000269
9	NpO2OH(aq) NpO2OH(aq)	0.0000000995445	0.0000000103094	0.1036	0.000000099899	0.0000000875117	0.00250331	0.0000000129
10	NpO2(CO3)2= NpO2(CO3)2=-	0.000000125826	0.0000000000231772	0.0001842	0.000000126275	0.000000110617	0.00430371	-0.00000000166
11	NpO2Ac(aq) NpO2Ac(aq)	0.0000000695275	0.0000000200964	0.289	0.0000000697751	0.0000000611231	0.0180981	0.0000000157
12	NpO2+ NpO2+	0.00000138778	0.00000026986	1.945	0.00000139272	0.00000122003	0.0328245	0.000000000664
13	NpO2CO3- NpO2CO3-	0.000000452521	0.0000000492971	0.1089	0.000000454133	0.000000397821	0.130905	0.000000000642
14	NpO2Ox- NpO2Oxalate-	0.00000509495	0.0000000995885	0.019546	0.0000051131	0.00000447908	1.33426	-0.00000000742
15	Sum of Np Molarities =SUM(F3:F14)							
16								
17								
18	Solid Forms							
19	Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/Liter	Descriptor
20	2[NaNpO2CO3.7/2H2O(s)]	0	1	1	0	0	0	-1.81
21	K3NpO2(CO3)2(s) K3NpO2(CO3)2(s)	0	1	1	0	0	0	-5.99
22	KNpO2CO3(s) KNpO2CO3(s)	0.996446	1	1	0.999994	0.875996	322502	
23	Na3NpO2(CO3)2(s) Na3NpO2(CO3)2(s)	0	1	1	0	0	0	-1.59
24	NaOH(aq) to.titrate.base.only	0	0	1	0	0	0	-2.95
25	NpO2OH(aged) NpO2OH(aged)	0	1	1	0	0	0	-2.19
26	NpO2OH(amor) NpO2OH(amor)	0	1	1	0	0	0	-2.89

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	A	B	C	D	E	F	G	H
1								
2	Aqueous Forms							
3	Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
4	Am(OH)2+ Am(OH)2+	2.53918E-07	1.75244E-10	0.0007	2.33444E-07	2.21402E-07	6.13316E-02	5.56E-09
5	AmEDTA- AmEDTA-	9.26150E-08	2.79284E-09	0.0302	8.51475E-08	8.07551E-08	9.14058E-02	4.11E-09
6	AmOH++ AmOH++	2.71323E-09	6.67753E-11	0.0246	2.49446E-09	2.36578E-09	6.15121E-04	-4.29E-09
7	Am(OH)3(aq) Am(OH)3(aq)	6.94688E-10	6.30297E-12	0.0091	6.38676E-10	6.05729E-10	1.78098E-04	8.34E-09
8	AmAc++ AmAcetate++	5.59406E-10	6.38702E-12	0.0114	5.14301E-10	4.87771E-10	1.47328E-04	-4.07E-09
9	AmOx+ AmOxalate+	5.36269E-10	5.06481E-11	0.0944	4.93030E-10	4.67597E-10	1.27111E-04	-1.67E-08
10	AmCO3+ AmCO3+	4.51352E-10	3.38847E-10	0.7507	4.14959E-10	3.93554E-10	1.19250E-04	-5.50E-09
11	AmCit(aq) AmCitrate(aq)	2.59295E-10	1.64885E-12	0.0064	2.38389E-10	2.26091E-10	9.76941E-05	7.84E-10
12	Am(CO3)2- Am(CO3)2-	1.68307E-10	1.08548E-11	0.0645	1.54736E-10	1.46754E-10	5.32744E-05	1.64E-09
13	AmSO4+ AmSO4+	1.14393E-10	5.27492E-11	0.4611	1.05169E-10	9.97441E-11	3.38190E-05	-6.74E-09
14	Am(CO3)3-- Am(CO3)3--	4.42527E-11	6.91717E-16	0.0000	4.06847E-11	3.85859E-11	1.63229E-05	9.28E-09
15	Am+++ Am+++	1.66564E-11	6.68916E-12	0.4016	1.53134E-11	1.45234E-11	3.52919E-06	-1.19E-08
16	Am(SO4)2- Am(SO4)2-	1.38315E-11	6.66715E-13	0.0482	1.27163E-11	1.20603E-11	5.24763E-06	8.81E-10
17	Am(CO3)4=== Am(CO3)4===	1.34491E-11	1.73976E-24	0.0000	1.23647E-11	1.17268E-11	5.66449E-06	2.26E-08
18	AmCl++ AmCl++	1.83313E-12	9.35960E-11	51.0600	1.68533E-12	1.59839E-12	4.45076E-07	-8.80E-09
19	AmCl2+ AmCl2+	9.88172E-14	7.91612E-11	801.1000	9.08496E-14	8.61631E-14	2.70471E-08	-4.72E-09
20	Sum of Am Molarities					3.07029E-07		
21								
22								
23	Solid Forms							
24	Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
25	Am(OH)3(s) Am(OH)3(s)	1.08770E+00	1.00000E+00	1.0000	1.00000E+00	9.48415E-01	2.78855E+05	
26	AmOHCO3(c) AmOHCO3(c)	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-3.13E-01
27	NaAm(CO3)2.6H2O(c)	0.00000E+00	1.00000E+00	1.0000	0.00000E+00	0.00000E+00	0.00000E+00	-2.72E+00

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	A	B	C	D	E	F	G	H
1								
2	Aqueous Forms							
3	Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
4	Am(OH)2+ Am(OH)2+	0.000000253918	0.00000000175244	0.00069016	0.000000233444	0.000000221402	0.0613316	0.00000000556
5	AmEDTA- AmEDTA-	0.000000092615	0.00000000279284	0.030155	0.0000000851475	0.0000000807551	0.0914058	0.00000000411
6	AmOH++ AmOH++	0.00000000271323	0.0000000000667753	0.024611	0.00000000249446	0.00000000236578	0.000615121	-0.00000000429
7	Am(OH)3(aq) Am(OH)3(aq)	0.00000000694688	0.0000000000630297	0.0090731	0.00000000638676	0.00000000605729	0.000178098	0.00000000834
8	AmAc++ AmAcetate++	0.00000000559406	0.0000000000638702	0.011418	0.00000000514301	0.00000000487771	0.000147328	-0.00000000407
9	AmOx+ AmOxalate+	0.00000000536269	0.000000000506481	0.094445	0.0000000049303	0.00000000467597	0.000127111	-0.0000000167
10	AmCO3+ AmCO3+	0.00000000451352	0.000000000338847	0.7507	0.00000000414959	0.00000000393554	0.00011925	-0.0000000055
11	AmCit(aq) AmCitrate(aq)	0.00000000259295	0.0000000000164885	0.006359	0.00000000238389	0.00000000226091	0.0000976941	0.000000000784
12	Am(CO3)2- Am(CO3)2-	0.00000000168307	0.000000000108548	0.064494	0.00000000154736	0.00000000146754	0.0000532744	0.00000000164
13	AmSO4+ AmSO4+	0.00000000114393	0.000000000527492	0.4611	0.00000000105169	0.000000000997441	0.000033819	-0.00000000674
14	Am(CO3)3-- Am(CO3)3--	0.000000000442527	6.91717E-16	0.000015631	0.000000000406847	0.000000000385859	0.0000163229	0.00000000928
15	Am+++ Am+++	0.000000000166564	0.0000000000668916	0.4016	0.000000000153134	0.000000000145234	0.00000352919	-0.0000000119
16	Am(SO4)2- Am(SO4)2-	0.000000000138315	0.0000000000666715	0.048203	0.000000000127163	0.000000000120603	0.00000524763	0.000000000881
17	Am(CO3)4=== Am(CO3)4===	0.000000000134491	1.73976E-24	0.0000000000012936	0.000000000123647	0.000000000117268	0.00000566449	0.00000000226
18	AmCl++ AmCl++	0.0000000000183313	0.000000000093596	51.06	0.0000000000168533	0.0000000000159839	0.000000445076	-0.0000000088
19	AmCl2+ AmCl2+	0.00000000000988172	0.0000000000791612	801.1	0.00000000000908496	0.000000000000861631	0.0000000270471	-0.00000000472
20	Sum of Am Molarities =SUM(F4:F19)							
21								
22								
23	Solid Forms							
24	Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
25	Am(OH)3(s) Am(OH)3(s)	1.0877	1	1	1	0.948415	278855	
26	AmOHCO3(c) AmOHCO3(c)	0	1	1	0	0	0	-0.313
27	NaAm(CO3)2.6H2O(c)	0	1	1	0	0	0	-2.72

	A	B	C	D	E	F	G	H
1	Aqueous Forms							
2	Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/Liter	Descriptor
3	Am(OH) ₂ + Am(OH) ₂ +	2.53799E-07	1.75250E-10	6.91E-04	2.33327E-07	2.21297E-07	6.13024E-02	-6.78E-11
4	AmEDTA- AmEDTA-	9.26408E-08	2.79312E-09	3.02E-02	8.51680E-08	8.07768E-08	9.14303E-02	-2.55E-09
5	AmOH++ AmOH++	2.71415E-09	6.67799E-11	2.46E-02	2.49522E-09	2.36657E-09	6.15325E-04	-1.30E-09
6	Am(OH) ₃ (aq) Am(OH) ₃ (aq)	6.94652E-10	6.30297E-12	9.07E-03	6.38618E-10	6.05692E-10	1.78087E-04	1.09E-09
7	AmAc++ AmAcetate++	5.59815E-10	6.38791E-12	1.14E-02	5.14658E-10	4.88123E-10	1.47435E-04	-1.53E-09
8	AmOx+ AmOxalate+	5.35945E-10	5.06521E-11	9.45E-02	4.92713E-10	4.67310E-10	1.27033E-04	-6.62E-09
9	AmCO ₃ + AmCO ₃ +	4.29385E-10	3.22348E-10	0.7507	3.94749E-10	3.74397E-10	1.13446E-04	-9.46E-10
10	AmCit(aq) AmCitrate(aq)	2.59172E-10	1.64856E-12	6.36E-03	2.38266E-10	2.25981E-10	9.76464E-05	-2.09E-09
11	Am(CO ₃) ₂ - Am(CO ₃) ₂ -	1.52312E-10	9.82246E-12	6.45E-02	1.40025E-10	1.32806E-10	4.82110E-05	1.65E-09
12	AmSO ₄ + AmSO ₄ +	1.14616E-10	5.28575E-11	0.4612	1.05370E-10	9.99374E-11	3.38845E-05	-2.28E-09
13	Am(CO ₃) ₃ =- Am(CO ₃) ₃ =-	3.80931E-11	5.95393E-16	1.56E-05	3.50203E-11	3.32147E-11	1.40508E-05	9.52E-09
14	Am+++ Am+++	1.66211E-11	6.68985E-12	0.4025	1.52804E-11	1.44926E-11	3.52169E-06	-1.95E-09
15	Am(SO ₄) ₂ - Am(SO ₄) ₂ -	1.38876E-11	6.69386E-13	4.82E-02	1.27674E-11	1.21091E-11	5.26887E-06	2.81E-10
16	Am(CO ₃) ₄ === Am(CO ₃) ₄ ===	1.10105E-11	1.42443E-24	1.29E-13	1.01223E-11	9.60046E-12	4.63737E-06	2.89E-08
17	AmCl++ AmCl++	1.83511E-12	9.36050E-11	51.01	1.68708E-12	1.60010E-12	4.45552E-07	-1.93E-10
18	AmCl ₂ + AmCl ₂ +	9.88945E-14	7.91683E-11	800.5	9.09172E-14	8.62296E-14	2.70680E-08	1.76E-09
19	Sum of Am Molarities					3.06906E-07		
20								
21								
22	Solid Forms							
23	Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/Liter	Descriptor
24	Am(OH) ₃ (s) Am(OH) ₃ (s)	1.08774E+00	1.00000E+00	1	1.00000E+00	9.48441E-01	2.78863E+05	
25	AmOHCO ₃ (c) AmOHCO ₃ (c)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-3.35E-01
26	NaAm(CO ₃) ₂ .6H ₂ O(c)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-2.76E+00

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	A	B	C	D	E	F	G	H
1	Aqueous Forms							
2	Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/Liter	Descriptor
3	Am(OH)2+ Am(OH)2+	0.000000253799	0.0000000017525	0.0006905	0.000000233327	0.000000221297	0.0613024	-0.000000000678
4	AmEDTA- AmEDTA-	0.0000000926408	0.00000000279312	0.03015	0.000000085168	0.0000000807768	0.0914303	-0.00000000255
5	AmOH++ AmOH++	0.00000000271415	0.000000000667799	0.024604	0.00000000249522	0.00000000236657	0.000615325	-0.0000000013
6	Am(OH)3(aq) Am(OH)3(aq)	0.00000000694652	0.0000000000630297	0.0090736	0.00000000638618	0.00000000605692	0.000178087	-0.00000000109
7	AmAc++ AmAcetate++	0.00000000559815	0.0000000000638791	0.011411	0.00000000514658	0.00000000488123	0.000147435	-0.00000000153
8	AmOx+ AmOxalate+	0.00000000535945	0.000000000506521	0.09451	0.00000000492713	0.0000000046731	0.000127033	-0.00000000662
9	AmCO3+ AmCO3+	0.00000000429385	0.000000000322348	0.7507	0.00000000394749	0.00000000374397	0.000113446	-0.000000000946
10	AmCit(aq) AmCitrate(aq)	0.00000000259172	0.0000000000164856	0.0063609	0.00000000238266	0.00000000225981	0.0000976464	-0.00000000209
11	Am(CO3)2- Am(CO3)2-	0.00000000152312	0.0000000000982246	0.064489	0.00000000140025	0.00000000132806	0.000048211	0.00000000165
12	AmSO4+ AmSO4+	0.00000000114616	0.000000000528575	0.4612	0.0000000010537	0.000000000999374	0.0000338845	-0.00000000228
13	Am(CO3)3=- Am(CO3)3=-	0.000000000380931	5.95393E-16	0.00001563	0.000000000350203	0.000000000332147	0.0000140508	0.000000000952
14	Am+++ Am+++	0.000000000166211	0.0000000000668985	0.4025	0.000000000152804	0.000000000144926	0.00000352169	-0.00000000195
15	Am(SO4)2- Am(SO4)2-	0.000000000138876	0.00000000000669386	0.0482	0.000000000127674	0.000000000121091	0.00000526887	0.000000000281
16	Am(CO3)4=- Am(CO3)4=-	0.000000000110105	1.42443E-24	0.0000000000012937	0.000000000101223	0.0000000000960046	0.00000463737	0.00000000289
17	AmCl++ AmCl++	0.0000000000183511	0.000000000093605	51.01	0.0000000000168708	0.000000000016001	0.000000445552	-0.000000000193
18	AmCl2+ AmCl2+	0.00000000000988945	0.0000000000791683	800.5	0.00000000000909172	0.000000000000862296	0.000000027068	0.000000000176
19	Sum of Am Molarities =SUM(F3:F18)							
20								
21								
22	Solid Forms							
23	Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/Liter	Descriptor
24	Am(OH)3(s) Am(OH)3(s)	1.08774	1	1	1	0.948441	278863	
25	AmOHCO3(c) AmOHCO3(c)	0	1	1	0	0	0	-0.335
26	NaAm(CO3)2.6H2O(c)	0	1	1	0	0	0	-2.76

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	A	B	C	D	E	F	G	H	
1	Aqueous Forms								
2	Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/Liter	Descriptor	
3	Am(OH) ₂ + Am(OH) ₂ +	1.02595E-07	8.63100E-11	0.00084127	1.02993E-07	9.01813E-08	2.49815E-02	-2.63E-08	
4	AmEDTA- AmEDTA-	9.68343E-08	2.42392E-09	0.025032	9.72100E-08	8.51178E-08	9.63438E-02	4.24E-09	
5	Am(OH) ₃ (aq) Am(OH) ₃ (aq)	7.95189E-10	6.30297E-12	0.0079264	7.98274E-10	6.98974E-10	2.05514E-04	-9.07E-09	
6	AmOH++ AmOH++	6.48687E-10	1.61977E-11	0.02497	6.51204E-10	5.70199E-10	1.48256E-04	-2.43E-09	
7	AmOx+ AmOxalate+	3.21375E-10	2.16071E-11	0.067233	3.22622E-10	2.82490E-10	7.67921E-05	1.26E-09	
8	AmCit(aq) AmCitrate(aq)	1.05548E-10	8.33680E-13	0.0078986	1.05958E-10	9.27775E-11	4.00891E-05	-1.56E-08	
9	AmAc++ AmAcetate++	8.55651E-11	1.33303E-12	0.015579	8.58971E-11	7.52121E-11	2.27174E-05	-1.20E-08	
10	AmCO ₃ + AmCO ₃ +	4.72195E-11	3.50981E-11	0.7433	4.74027E-11	4.15062E-11	1.25767E-05	3.21E-08	
11	Am(CO ₃) ₂ - Am(CO ₃) ₂ -	1.77685E-11	9.74823E-13	0.054862	1.78375E-11	1.56186E-11	5.66984E-06	7.33E-08	
12	AmSO ₄ + AmSO ₄ +	1.27336E-11	5.46381E-12	0.4291	1.27830E-11	1.11929E-11	3.79503E-06	3.01E-08	
13	Am+++ Am+++	2.44867E-12	7.99150E-13	0.3264	2.45817E-12	2.15239E-12	5.23030E-07	-5.42E-08	
14	Am(SO ₄) ₂ - Am(SO ₄) ₂ -	1.55447E-12	5.98748E-14	0.038518	1.56050E-12	1.36638E-12	5.94534E-07	7.39E-08	
15	Am(CO ₃) ₃ =- Am(CO ₃) ₃ =-	1.03120E-12	5.38587E-17	0.000052229	1.03520E-12	9.06427E-13	3.83444E-07	1.04E-07	
16	AmCl++ AmCl++	1.90901E-13	8.84605E-12	46.34	1.91642E-13	1.67803E-13	4.67252E-08	2.20E-08	
17	AmCl ₂ + AmCl ₂ +	7.25113E-15	5.91888E-12	816.3	7.27926E-15	6.37377E-15	2.00077E-09	1.83E-08	
18	Am(CO ₃) ₄ == Am(CO ₃) ₄ ==	2.23664E-15	1.17447E-25	5.251E-11	2.24531E-15	1.96601E-15	9.49657E-10	1.02E-07	
19	Sum of Am Molarities						1.77092E-07		
20									
21									
22	Solid Forms								
23	Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/Liter	Descriptor	
24	Am(OH) ₃ (s) Am(OH) ₃ (s)	9.96135E-01	1.00000E+00	1	1.00000E+00	8.75607E-01	2.57448E+05		
25	AmOHCO ₃ (c) AmOHCO ₃ (c)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-9.90E-01	
26	NaAm(CO ₃) ₂ .6H ₂ O(c)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-3.61E+00	

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	A	B	C	D	E	F	G	H
1	Aqueous Forms							
2	Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/Liter	Descriptor
3	Am(OH)2+ Am(OH)2+	0.000000102595	0.00000000008631	0.00084127	0.000000102993	0.0000000901813	0.0249815	-0.0000000263
4	AmEDTA- AmEDTA-	0.0000000968343	0.00000000242392	0.025032	0.00000009721	0.0000000851178	0.0963438	0.00000000424
5	Am(OH)3(aq) Am(OH)3(aq)	0.000000000795189	0.0000000000630297	0.0079264	0.000000000798274	0.00000000698974	0.000205514	-0.00000000907
6	AmOH++ AmOH++	0.000000000648687	0.0000000000161977	0.02497	0.000000000651204	0.000000000570199	0.000148256	-0.00000000243
7	AmOx+ AmOxalate+	0.000000000321375	0.0000000000216071	0.067233	0.000000000322622	0.00000000028249	0.0000767921	0.00000000126
8	AmCit(aq) AmCitrate(aq)	0.000000000105548	0.0000000000083368	0.0078986	0.000000000105958	0.0000000000927775	0.0000400891	-0.0000000156
9	AmAc++ AmAcetate++	0.0000000000855651	0.0000000000133303	0.015579	0.0000000000858971	0.0000000000752121	0.0000227174	-0.0000000012
10	AmCO3+ AmCO3+	0.0000000000472195	0.0000000000350981	0.7433	0.0000000000474027	0.0000000000415062	0.0000125767	0.00000000321
11	Am(CO3)2- Am(CO3)2-	0.0000000000177685	0.00000000000974823	0.054862	0.0000000000178375	0.0000000000156186	0.00000566984	0.00000000733
12	AmSO4+ AmSO4+	0.0000000000127336	0.00000000000546381	0.4291	0.000000000012783	0.0000000000111929	0.00000379503	0.00000000301
13	Am+++ Am+++	0.00000000000244867	0.00000000000079915	0.3264	0.00000000000245817	0.00000000000215239	0.00000052303	-0.0000000542
14	Am(SO4)2- Am(SO4)2-	0.00000000000155447	0.0000000000000598748	0.038518	0.0000000000015605	0.00000000000136638	0.000000594534	0.00000000739
15	Am(CO3)3-- Am(CO3)3--	0.0000000000010312	5.38587E-17	0.000052229	0.0000000000010352	0.000000000000906427	0.000000383444	0.000000104
16	AmCl++ AmCl++	0.000000000000190901	0.00000000000884605	46.34	0.000000000000191642	0.000000000000167803	0.0000000467252	0.0000000022
17	AmCl2+ AmCl2+	7.25113E-15	0.00000000000591888	816.3	7.27926E-15	6.37377E-15	0.00000000200077	0.00000000183
18	Am(CO3)4== Am(CO3)4==	2.23664E-15	1.17447E-25	0.000000000005251	2.24531E-15	1.96601E-15	0.000000000949657	0.000000102
19	Sum of Am Molarities =SUM(F3:F18)							
20								
21								
22	Solid Forms							
23	Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/Liter	Descriptor
24	Am(OH)3(s) Am(OH)3(s)	0.996135	1	1	1	0.875607	257448	
25	AmOHCO3(c) AmOHCO3(c)	0	1	1	0	0	0	-0.99
26	NaAm(CO3)2.6H2O(c)	0	1	1	0	0	0	-3.61

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	A	B	C	D	E	F	G	H	
1	Aqueous Forms								
2	Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/Liter	Descriptor	
3	AmCl2+ AmCl2+	5.77023E-15	4.81682E-12	834.8	5.79078E-15	5.07273E-15	1.59236E-09	-3.35E-09	
4	AmCl++ AmCl++	1.52818E-13	7.24428E-12	47.4	1.53362E-13	1.34345E-13	3.74088E-08	-1.53E-08	
5	Am(CO3)4=- Am(CO3)4=-	9.75203E-13	6.25010E-23	6.41E-11	9.78676E-13	8.57321E-13	4.14118E-07	1.75E-10	
6	Am(SO4)2- Am(SO4)2-	1.17596E-12	4.49960E-14	3.83E-02	1.18015E-12	1.03381E-12	4.49827E-07	1.46E-09	
7	Am+++ Am+++	2.11708E-12	6.58566E-13	0.3111	2.12462E-12	1.86117E-12	4.52263E-07	-3.70E-10	
8	AmSO4+ AmSO4+	1.00272E-11	4.29978E-12	0.4288	1.00629E-11	8.81514E-12	2.98884E-06	3.43E-10	
9	AmAc++ AmAcetate++	7.25408E-11	1.14677E-12	1.58E-02	7.27991E-11	6.37721E-11	1.92620E-05	3.64E-09	
10	AmCit(aq) AmCitrate(aq)	9.89426E-11	7.78138E-13	7.86E-03	9.92949E-11	8.69825E-11	3.75851E-05	8.26E-10	
11	Am(CO3)3=- Am(CO3)3=-	1.04453E-10	5.68570E-15	5.44E-05	1.04825E-10	9.18272E-11	3.88454E-05	8.03E-11	
12	AmCO3+ AmCO3+	1.95503E-10	1.45805E-10	0.7458	1.96199E-10	1.71871E-10	5.20784E-05	-1.81E-10	
13	AmOx+ AmOxalate+	3.01428E-10	2.00545E-11	6.65E-02	3.02502E-10	2.64992E-10	7.20353E-05	-2.97E-09	
14	Am(CO3)2- Am(CO3)2-	3.73861E-10	2.04143E-11	5.46E-02	3.75192E-10	3.28669E-10	1.19313E-04	2.81E-10	
15	AmOH++ AmOH++	5.65882E-10	1.42375E-11	2.52E-02	5.67897E-10	4.97478E-10	1.29348E-04	5.79E-10	
16	Am(OH)3(aq) Am(OH)3(aq)	8.04366E-10	6.30297E-12	7.84E-03	8.07230E-10	7.07135E-10	2.07913E-04	2.14E-09	
17	AmEDTA- AmEDTA-	9.31020E-08	2.31659E-09	2.49E-02	9.34336E-08	8.18479E-08	9.26426E-02	2.29E-09	
18	Am(OH)2+ Am(OH)2+	9.68178E-08	8.09192E-11	8.36E-04	9.71626E-08	8.51146E-08	2.35780E-02	2.25E-09	
19	Sum of Am Molarities						1.69188E-07		
20									
21									
22	Solid Forms								
23	Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/Liter	Descriptor	
24	AmOHCO3(c) AmOHCO3(c)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-3.44E-01	
25	NaAm(CO3)2.6H2O(c)	0.00000E+00	1.00000E+00	1	0.00000E+00	0.00000E+00	0.00000E+00	-2.29E+00	
26	Am(OH)3(s) Am(OH)3(s)	9.96451E-01	1.00000E+00	1	1.00000E+00	8.76001E-01	2.57563E+05		

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	A	B	C	D	E	F	G	H
1	Aqueous Forms							
2	Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/Liter	Descriptor
3	AmCl2+ AmCl2+	5.77023E-15	0.0000000000481682	834.8	5.79078E-15	5.07273E-15	0.0000000159236	-0.00000000335
4	AmCl++ AmCl++	0.00000000000152818	0.0000000000724428	47.4	0.0000000000153362	0.0000000000134345	0.0000000374088	-0.0000000153
5	Am(CO3)4== Am(CO3)4==	0.00000000000975203	6.2501E-23	0.0000000006409	0.0000000000978676	0.00000000000857321	0.000000414118	-0.00000000175
6	Am(SO4)2- Am(SO4)2-	0.0000000000117596	0.0000000000044996	0.038263	0.0000000000118015	0.0000000000103381	0.000000449827	0.00000000146
7	Am+++ Am+++	0.0000000000211708	0.00000000000658566	0.3111	0.0000000000212462	0.0000000000186117	0.000000452263	-0.00000000037
8	AmSO4+ AmSO4+	0.000000000100272	0.0000000000429978	0.4288	0.000000000100629	0.0000000000881514	0.0000298884	0.000000000343
9	AmAc++ AmAcetate++	0.000000000725408	0.0000000000114677	0.015809	0.000000000727991	0.0000000000637721	0.000019262	0.000000000364
10	AmCit(aq) AmCitrate(aq)	0.000000000989426	0.00000000000778138	0.0078645	0.000000000992949	0.0000000000869825	0.0000375851	0.000000000826
11	Am(CO3)3- Am(CO3)3-	0.000000000104453	0.00000000000056857	0.000054433	0.000000000104825	0.0000000000918272	0.0000388454	0.0000000000803
12	AmCO3+ AmCO3+	0.000000000195503	0.000000000145805	0.7458	0.000000000196199	0.000000000171871	0.0000520784	-0.000000000181
13	AmOx+ AmOxalate+	0.000000000301428	0.000000000200545	0.066532	0.000000000302502	0.000000000264992	0.0000720353	-0.000000000297
14	Am(CO3)2- Am(CO3)2-	0.000000000373861	0.000000000204143	0.054604	0.000000000375192	0.000000000328669	0.000119313	0.000000000281
15	AmOH++ AmOH++	0.000000000565882	0.000000000142375	0.02516	0.000000000567897	0.000000000497478	0.000129348	0.0000000000579
16	Am(OH)3(aq) Am(OH)3(aq)	0.000000000804366	0.0000000000630297	0.007836	0.00000000080723	0.000000000707135	0.000207913	0.000000000214
17	AmEDTA- AmEDTA-	0.000000093102	0.0000000231659	0.024882	0.0000000934336	0.0000000818479	0.0926426	0.000000000229
18	Am(OH)2+ Am(OH)2+	0.000000968178	0.0000000000809192	0.00083579	0.0000000971626	0.0000000851146	0.023578	0.000000000225
19	Sum of Am Molarities =SUM(F3:F18)							
20								
21								
22	Solid Forms							
23	Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/Liter	Descriptor
24	AmOHCO3(c) AmOHCO3(c)	0	1	1	0	0	0	-0.344
25	NaAm(CO3)2.6H2O(c)	0	1	1	0	0	0	-2.29
26	Am(OH)3(s) Am(OH)3(s)	0.996451	1	1	1	0.876001	257563	

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