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MODELING MONOMETHYLMERCURY AND TRIBUTYLTIN SPECIATION WITH EPA's GEOCHEMICAL SPECIATION MODEL MINTEQA2

by

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FOREWORD

The Ecosystems Assessment Branch of the Ecosystems Research Division, National Exposure Research Laboratory, Office of Research and Development, U.S. Environmental Protection Agency conducts research that is designed to meet the agency's needs in areas related to assessing the ecological health of diverse biological communities. As part of this mission, a significant amount of research is devoted to improving tools to assess low level, ecological exposures to toxicants of national concern.

The United States Environmental Protection Agency's Science Advisory Board is currently exploring the use of the Free Ion Activity and Biotic Ligand Models as means of reducing the uncertainty in EPA's ability to assess the bioavailability and toxicity of ionic toxicants present in aquatic media. Achieving this objective requires a thorough understanding of the chemical speciation of these ionic toxicants in our nation's waterbodies. MINTEQA2 is a geochemical speciation model that has received widespread support from the U.S. EPA Center for Exposure Assessment Modeling and is perhaps one of the most widespread geochemical speciation models available to the technical research community. This report constitutes part of an ongoing series of upgrades to MINTEQA2 by developing a modeling capability for describing the aquatic speciation of two species of widespread interest: monomethylmercury and tributyltin.

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ABSTRACT

Monomethylmercury (MMHg) is the compound responsible for the majority of fish consumption advisories in forty eight states in the United States of America. These widespread low level (but toxicologically significant) ecological exposures to MMHg result from microbial methylation of atmospherically deposited inorganic mercury in our national waterbodies. Tributyltin (TBT) is an industrially synthesized antifoulant compound that was historically added to paints applied to the hulls of ships, boats and other watercraft. There is an extensive technical literature on the adverse effects associated with low level ecological exposures to this compound. Although the use of TBT has been restricted in recent years, there exists a significant reservoir of TBT in the sediments underlying our nation's boatyards and marinas.

Although there is extensive ongoing research devoted to the behavior of MMHg and TBT in the environment, there does not currently exist a widely available chemical speciation modeling capability for these two toxicants in aquatic media. This report addresses this limitation by initiating a modeling capability for these two species using EPA's geochemical speciation model MINTEQA2. Alterations to the MINTEQA2 components database (COMP.DBS) are documented and a template input file is provided (and documented) that will permit researchers to simulate the aqueous chemical speciation of MMHg and TBT.

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CHAPTER 1

INTRODUCTION

Monomethylmercury [CH_3Hg^+] and tributyltin [$(C_4H_9)_3Sn^+$] are two organometallic compounds of widespread concern to EPA. Monomethylmercury (MMHg) is the mercury species responsible for approximately 80 percent of fish consumption advisories in forty eight states in North America; however, it represents only a relatively small percentage of the total global mercury inventory. Although most anthropogenic mercury is emitted to the atmosphere, this atmospheric inorganic mercury is deposited to aquatic and terrestrial surfaces and ultimately serves as a substrate for biological methylation to the far more toxic and bioaccumulative monomethyl species.

Tributyltin (TBT) is primarily an industrially synthesized antifoulant compound historically added to the paints applied to the hulls of marine and freshwater transport vehicles. Because TBT is extremely ecotoxic, major efforts have been made to find more ecofriendly alternatives. Nevertheless, residual unacceptable concentrations of TBT have been found in the sediments underlying many boatyards and marinas.

The EPA Science Advisory Board is currently exploring the Free Ion Activity (FIA) paradigm for potential use as a more accurate predictor of ionic toxicant bioavailability in natural waters. An implicit requirement of the FIA model is a fundamental understanding of the aqueous speciation behavior of those ionic species of interest. For example, both MMHg and TBT can exist as a suite of species in natural waters: CH_3Hg^+, CH_3HgOH, CH_3HgCl, CH_3HgS^-, CH_3HgSR, $(C_4H_9)_3Sn^+$, $(C_4H_9)_3SnOH$, $(C_4H_9)_3SnCl$, and $(C_4H_9)_3SnBr$.

Given the complexity of the various, simultaneous (and competing) equilibrium reactions governing the speciation of ionic species in aquatic systems, EPA has developed and distributed the geochemical speciation model MINTEQA2 (Brown and Allison, 1987, Allison et al., 1991; Hydrogeologic, 1999a, 1999b). The present work is designed to at least partially address a limitation found in earlier versions of MINTEQA2 by initiating a capability for modeling the aqueous speciation behavior of MMHg and TBT in environmental aquatic systems.

Generally speaking, geochemical speciation models require both an innate database of reaction constants that enable one to model complex competitive geochemical speciation simulations and user input containing the total analytical concentrations of the reacting species of interest. It is the purpose of this document to develop a “first cut” modeling capability for both MMHg and TBT in EPA’s geochemical speciation model MINTEQA2 by extending the existing reaction constant database. There is extensive ongoing research concerning the environmental speciation behavior of both MMHg and TBT and it is anticipated that future upgrades in this area will be necessary as more data becomes available.

CHAPTER 2

ALTERATIONS TO MINTEQA2

I. COMP.DBS

MINTEQA2 conceptually divides chemical species into two categories: components (individual ionic species) and products (all species that can be derived from the components entered into a given simulation). Because there are no components for either MMHg of TBT in earlier versions of MINTEQ, a new component database was developed that includes these two components. In addition, recent research findings (Haitzer et al., 2002) suggest that environmental aquatic mercury species may interact with reduced sulfur in natural organic carbon (e.g., RS- and RSS- binding sites). Hence an overall reduced sulfur component of RS- also was added to the component database.

The new component database is given in APPENDIX A. Specific additions to COMP.DBS include components 362 (MMHg), 733 (RS-) and 792 (TBT). The "+1" and "-1" to the right of the names of the components represents the net charge of each component. The two consecutive terms "0.0" to the right of the net charge designate Debye-Huckel A and B parameters for these species. These numbers are set to zero because values for MMHg, TBT and RS- could not be found in the technical literature. Consequently, all activity coefficient calculations with these species are performed using the default Davies extension in MINTEQA2. The final entry for components 362, 733 and 792 include the gram formula weights for these compounds (because the "R" in "RS-" does not exist as a unique compound, a molecular weight for "RS-" cannot be determined and hence this value is set to 0 in the revised version of COMP.DBS) . Users seeking to model MMHg and TBT speciation will have to use this file to replace the earlier versions of COMP.DBS distributed with previous installations of MINTEQA2.

II. MMHg&TBT.INP

Additional chemical reactions can be implemented in MINTEQA2 via two procedures: 1) permanently altering the thermodynamic database and 2) generating input files with appended reactions. Because of the general uncertainty concerning the environmental speciation of MMHg and TBT, the second option has been exercised in this effort. APPENDIX B depicts the sample template input file MMHg&TBT.INP that contains chemical reactions (and formation constants) for MMHg and TBT with various environmental ligands. The aquatic concentration data in this input file are generally those used in previous simulations by Loux (1998). It is anticipated that the user will access this template with PRODEF, alter the values as per the user's requirements and save it under a different name for future runs with MINRUN.BAT. Note that the revised (newer) version of COMP.DBS also must be present in the same directory in order to alter the file MMHg&TBT.INP with PRODEF.

The bottom half of APPENDIX B contains the actual reactions for MMHg, RS- and TBT. The thermodynamic reaction constants listed in the template input file were obtained from Erni (1981) and Dyrssen and Wedborg (1991) for MMHg and from Arnold et al. (1997) for TBT. The individual entries in the reaction constant section of this input file are described in Allison et al. (1991) and Hydrogeologic and Allison Geosciences (1999a). Because neither enthalpies of reactions nor Debye-Huckel "A" and "B" parameters could be found in the technical literature for these species, values of zero for each of these terms is entered into the designated position in the input file. The net effect is that as with the components, the default Davies activity coefficient algorithm will be used for estimating activity coefficients for these species and no temperature corrections will be made to the reaction constants in MINTEQA2 simulations. The reader also should note that in order to formulate some of these reactions into expressions compatible with MINTEQA2, an ionization constant for water of 10^{-14} was assumed and the second ionization (acidity) constant for HS^- was ascribed a value of $10^{-17.3}$. Lastly, the MINTEQA2 ionization constant ($10^{6.194}$) for the reaction $Hg(OH)_2 + 2H^+ <==> Hg^{2+} + 2H_2O$ also was utilized in order to simulate the reactions between Hg^{2+} and RS^-.

III. MMHg&TBT.OUT

APPENDIX III contains a copy of the file MMHg&TBT.OUT. This file represents the output generated in a MINTEQA2 simulation of MMHg&TBT.INP and is included for the purpose of illustrating what can be expected from MINTEQA2 simulations with MMHg&TBT.INP.

IV. FUTURE EXTENSIONS TO THE MMHg AND TBT REACTION DATABASE

The user will likely desire to extend the list of reactions given in the input file MMHg&TBT.INP. Those seeking to estimate reaction constants unavailable in the technical research literature are referred to Dzombak (1986), Loux et al. (1989) and Loux (1998) for sample exercises of this nature.

Note:

The author would appreciate constructive feedback from users of these files.

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APPENDIX A

REVISED VERSION OF COM.DBS IN MINTEQA2 (VERSION 4.0)

```
COMP v4.00 09/30/1999
001 E-1          -1.0   0.0  0.0      0.0000
002 H2O           0.0   0.0  0.0     18.0153
020 Ag+1          1.0   0.0  0.0    107.8682
030 Al+3          3.0   9.0  0.0     26.9815
060 H3AsO3        0.0   0.0  0.0    125.9436
061 H3AsO4        0.0   0.0  0.0    141.9430
090 H3BO3         0.0   0.0  0.0     61.833
100 Ba+2          2.0   5.0  0.0    137.33
110 Be+2          2.0   0.0  0.0     9.0122
130 Br-1         -1.0   4.0  0.0     79.904
140 CO3-2        -2.0   5.4  0.0     60.0094
143 CN-          -1.0   0.0  0.0     26.0177
144 DOM1         -2.8   0.0  0.0     0.000
145 DOM2         -2.8   0.0  0.0     0.000
146 DOM3         -2.8   0.0  0.0     0.000
150 Ca+2          2.0   6.0  .165    40.078
160 Cd+2          2.0   0.0  0.0    112.41
180 Cl-1         -1.0   3.0  .015    35.453
200 Co+2          2.0   0.0  0.0     58.9332
201 Co+3          3.0   0.0  0.0     58.9332
210 Cr+2          2.0   0.0  0.0     51.9961
211 Cr(OH)2+      1.0   0.0  0.0     86.0108
212 CrO4-2       -2.0   4.0  0.0    115.9937
230 Cu+1          1.0   2.5  0.0     63.546
231 Cu+2          2.0   6.0  0.0     63.546
270 F-1          -1.0   3.5  0.0     18.9984
280 Fe+2          2.0   6.0  0.0     55.847
281 Fe+3          3.0   9.0  0.0     55.847
330 H+1           1.0   9.0  0.0     1.0079
360 Hg2+2         2.0   4.0  0.0    401.18
361 Hg(OH)2       0.0   0.0  0.0    234.60
362 Hg(CH3)+      1.0   0.0  0.0    215.6247
380 I-1          -1.0   0.0  0.0    126.9045
410 K+1           1.0   3.0  .015    39.0983
440 Li+1          1.0   6.0  0.0      6.941
460 Mg+2          2.0   6.5  .20     24.305
470 Mn+2          2.0   6.0  0.0     54.9380
```

471	Mn+3	3.0	9.0	0.0	54.9380
480	MoO4-2	-2.0	0.0	0.0	159.9376
490	NH4+1	1.0	2.5	0.0	18.0385
491	NO2-1	-1.0	0.0	0.0	46.0055
492	NO3-1	-1.0	3.0	0.0	62.0049
500	Na+1	1.0	4.0	.075	22.9898
540	Ni+2	2.0	0.0	0.0	58.6900
580	PO4-3	-3.0	5.0	0.0	94.9714
600	Pb+2	2.0	0.0	0.0	207.2
730	HS-1	-1.0	3.5	0.0	33.073
731	S	0.0	0.0	0.0	32.066
732	SO4-2	-2.0	4.0	-.04	96.063
733	RS-	-1.0	0.0	0.0	0.000
740	Sb(OH)3	0.0	0.0	0.0	172.77
741	Sb(OH)6-	-1.0	0.0	0.0	223.79
760	HSe-1	-1.0	0.0	0.0	79.96
761	HSeO3-1	-1.0	0.0	0.0	127.96
762	SeO4-2	-2.0	4.0	0.0	142.95
770	H4SiO4	0.0	0.0	0.0	96.1149
790	Sn(OH)2	0.0	0.0	0.0	152.7246
791	Sn(OH)6-	-2.0	0.0	0.0	220.7538
792	Sn3But+	1.0	0.0	0.0	290.0553
800	Sr+2	2.0	5.0	0.0	87.62
811	ADS1TYP1	0.0	0.0	0.0	0.0000
812	ADS1TYP2	0.0	0.0	0.0	0.0000
813	ADS1PSIo	0.0	0.0	0.0	0.0000
814	ADS1PSIb	0.0	0.0	0.0	0.0000
815	ADS1PSId	0.0	0.0	0.0	0.0000
821	ADS2TYP1	0.0	0.0	0.0	0.0000
822	ADS2TYP2	0.0	0.0	0.0	0.0000
823	ADS2PSIo	0.0	0.0	0.0	0.0000
824	ADS2PSIb	0.0	0.0	0.0	0.0000
825	ADS2PSId	0.0	0.0	0.0	0.0000
831	ADS3TYP1	0.0	0.0	0.0	0.0000
832	ADS3TYP2	0.0	0.0	0.0	0.0000
833	ADS3PSIo	0.0	0.0	0.0	0.0000
834	ADS3PSIb	0.0	0.0	0.0	0.0000
835	ADS3PSId	0.0	0.0	0.0	0.0000
841	ADS4TYP1	0.0	0.0	0.0	0.0000
842	ADS4TYP2	0.0	0.0	0.0	0.0000
843	ADS4PSIo	0.0	0.0	0.0	0.0000
844	ADS4PSIb	0.0	0.0	0.0	0.0000
845	ADS4PSId	0.0	0.0	0.0	0.0000

851	ADS5TYP1	0.0	0.0	0.0	0.0000
852	ADS5TYP2	0.0	0.0	0.0	0.0000
853	ADS5PSIo	0.0	0.0	0.0	0.0000
854	ADS5PSIb	0.0	0.0	0.0	0.0000
855	ADS5PSId	0.0	0.0	0.0	0.0000
870	Tl+1	1.0	0.0	0.0	204.383
871	Tl(OH)3	0.0	0.0	0.0	255.405
890	U+3	3.0	0.0	0.0	238.0289
891	U+4	4.0	0.0	0.0	238.0289
892	UO2+1	1.0	0.0	0.0	270.0277
893	UO2+2	2.0	0.0	0.0	270.0277
900	V+2	2.0	0.0	0.0	50.9425
901	V+3	3.0	0.0	0.0	50.9425
902	VO+2	2.0	0.0	0.0	66.9419
903	VO2+1	1.0	0.0	0.0	82.9413
917	Benzoate	-1.0	0.0	0.0	121.116
918	PhAcO	-1.0	0.0	0.0	135.142
920	iPhthal	-2.0	0.0	0.0	164.117
950	Zn+2	2.0	6.0	0.0	65.39
955	DiEtAm	0.0	0.0	0.0	73.138
956	BuAm	0.0	0.0	0.0	73.138
958	MeAm	0.0	0.0	0.0	31.057
959	DiMeAm	0.0	0.0	0.0	45.084
961	HexylAm	0.0	0.0	0.0	101.192
963	EtDiAm	0.0	0.0	0.0	60.099
964	PrAm	0.0	0.0	0.0	59.111
965	iPrAm	0.0	0.0	0.0	59.111
966	TriMeAm	0.0	0.0	0.0	59.111
967	Citrate	-3.0	0.0	0.0	189.102
968	NTA	-3.0	0.0	0.0	188.117
969	EDTA	-4.0	0.0	0.0	288.214
971	Propion	-1.0	0.0	0.0	73.072
972	Butyr	-1.0	0.0	0.0	87.098
973	iButyr	-1.0	0.0	0.0	87.098
980	2Picol	0.0	0.0	0.0	93.128
981	3Picol	0.0	0.0	0.0	93.128
982	4Picol	0.0	0.0	0.0	93.128
983	Formate	-1.0	0.0	0.0	45.018
984	iValerat	-1.0	0.0	0.0	101.125
985	Valerate	-1.0	0.0	0.0	101.125
992	Acetate	-1.0	0.0	0.0	59.045
993	Tartrat	-2.0	0.0	0.0	148.072
994	Glycine	-1.0	0.0	0.0	74.059

995 Salicyl	-2.0	0.0	0.0	136.107
996 Glutam	-2.0	0.0	0.0	145.115
997 Phthal	-2.0	0.0	0.0	164.117

APPENDIX B

MMHg&TBT.INP; MINTEQA2 input file for modeling monomethylmercury and tributyltin speciation in environmental systems. Simulated data for Kissimmee River as described in Loux (1998).

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Refs. Dyrssen & Wedborg '91, WASP, 56:507; Erni in Stumm & Morgan,
'81, Aq. Chem. and Arnold et al., '97, Env.Sci.Tech., 31:2596-2602
25.00 MOLAL  0.000  0.00000E+00
0 0 1 0 1 0 0 0 1 1 0 0 0
0   0   0
   330  0.000E+00   -7.00 y              /H+1
   362  1.000E-12   -6.00 y              /Hg(CH3)+
   180  7.616E-04   -6.00 y              /Cl-1
   140  0.000E+00   -7.00 y              /CO3-2
   732  1.790E-04   -7.00                /SO4-2
   730  1.000E-09   -7.00                /HS-1
   792  1.000E-12   -7.00                /Sn3But+
   130  1.000E-06   -7.00                /Br-1
   500  6.980E-04   -3.16                /Na+1
   492  3.568E-06   -5.45 y              /NO3-1
   490  7.137E-06   -5.15 y              /NH4+1
   491  1.070E-06   -5.97 y              /NO2-1
   410  6.138E-05   -4.21 y              /K+1
   460  1.748E-04   -3.76 y              /Mg+2
   150  4.000E-04   -3.40 y              /Ca+2
   281  3.760E-06   -5.42 y              /Fe+3
   270  1.053E-05   -4.98 y              /F-1
   770  9.240E-05   -4.03 y              /H4SiO4
   580  4.035E-06   -5.39 y              /PO4-3
   733  5.000E-08   -7.30 y              /RS-
   361  1.000E-11  -11.00 y              /Hg(OH)2

  3   2
3301403    21.5847    -4.0600              /CO2 (g)
   330     7.0000     0.0000              /H+1

  2  13
3623300 Hg(CH3)OH       0.0000   -4.6300   0.000   0.000 0.00 0.00 0.00 307.0126
 0.00 2  -1.000 330   1.000 362   0.000   0   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
3621800 Hg(CH3)Cl       0.0000    5.2500   0.000   0.000 0.00 0.00 0.00 325.4580
```

0.00 2 1.000 180 1.000 362 0.000 0 0.000 0 0.000 0 0.000 0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
0 0.000 0 0.000 0 0.000 0
3621400 Hg(CH3)C03- 0.0000 6.1000 0.000 0.000-1.00 0.00 0.00 350.0145
0.00 2 1.000 140 1.000 362 0.000 0 0.000 0 0.000 0 0.000 0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
0 0.000 0 0.000 0 0.000 0
3627320 Hg(CH3)SO4- 0.0000 0.9400 0.000 0.000-1.00 0.00 0.00 386.0689
0.00 2 1.000 732 1.000 362 0.000 0 0.000 0 0.000 0 0.000 0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
0 0.000 0 0.000 0 0.000 0
3627300 Hg(CH3)S- 0.0000 3.7200 0.000 0.000-1.00 0.00 0.00 247.6907
0.00 3 -1.000 330 1.000 362 1.000 730 0.000 0 0.000 0 0.000 0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
0 0.000 0 0.000 0 0.000 0
3627301 (Hg(CH3))2S 0.0000 20.0600 0.000 0.000 0.00 0.00 0.00 463.3154
0.00 3 1.000 730 2.000 362 -1.000 330 0.000 0 0.000 0 0.000 0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
0 0.000 0 0.000 0 0.000 0
7920020 Sn3ButOH 0.0000 -6.2500 0.000 0.000 0.00 0.00 0.00 307.0122
0.00 3 1.000 2 1.000 792 -1.000 330 0.000 0 0.000 0 0.000 0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
0 0.000 0 0.000 0 0.000 0
7921800 Sn3ButCl 0.0000 0.6000 0.000 0.000 0.00 0.00 0.00 325.5083
0.00 2 1.000 180 1.000 792 0.000 0 0.000 0 0.000 0 0.000 0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
0 0.000 0 0.000 0 0.000 0
7921300 Sn3ButBr 0.0000 0.4300 0.000 0.000 0.00 0.00 0.00 369.9593
0.00 2 1.000 130 1.000 792 0.000 0 0.000 0 0.000 0 0.000 0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
0 0.000 0 0.000 0 0.000 0
3307330 RSH 0.0000 9.3400 0.000 0.000 0.00 0.00 0.00 0.0000
0.00 2 1.000 330 1.000 733 0.000 0 0.000 0 0.000 0 0.000 0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
0 0.000 0 0.000 0 0.000 0
3627330 CH3HgSR 0.0000 16.1200 0.000 0.000 0.00 0.00 0.00 0.0000
0.00 2 1.000 362 1.000 733 0.000 0 0.000 0 0.000 0 0.000 0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
0 0.000 0 0.000 0 0.000 0
3617330 HgSR+ 0.0000 28.2940 0.000 0.000 1.00 0.00 0.00 0.0000
0.00 4 1.000 361 1.000 733 2.000 330 -2.000 2 0.000 0 0.000 0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
0 0.000 0 0.000 0 0.000 0

3617331 Hg(SR)2 0.0000 47.7940 0.000 0.000 0.00 0.00 0.00 0.0000
0.00 4 2.000 733 1.000 361 2.000 330 -2.000 2 0.000 0 0.000 0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
0 0.000 0 0.000 0 0.000 0

APPENDIX C

MMHg&TBT.OUT; MINTEQA2 output file generated from a simulation with MMHg&TBT.INP.

PART 1 of OUTPUT FILE

MINTEQA2 v4.02 DATE OF CALCULATIONS: 28-OCT-2004 TIME: 4: 3:59

Refs. Dyrssen & Wedborg '91, WASP, 56:507; Erni in Stumm & Morgan, '81, Aq. Chem. and Arnold et al., '97, Env.Sci.Tech., 31:2596-2602
Component file (COMP.DBS): comp.dbs COMP v4.00 09/30/1999
Thermodynamic file (THERMO.UNF): thermo.unf THERMO V4.00 09/30/1999
Gaussian DOM file (GAUSSIAN.DBS): gaussian.dbsGAUSSIAN V4.00 09/30/1999
Solids file (TYPE6.UNF): type6.unf TYPE6 V4.00 09/30/1999

Temperature (Celsius): 25.00
Units of concentration: MOLAL
Ionic strength to be computed.
If specified, carbonate concentration represents total inorganic carbon.
Do not automatically terminate if charge imbalance exceeds 30%
Precipitation is allowed only for those solids specified as ALLOWED in the input file (if any).
Maximum iterations: 200
The method used to compute activity coefficients is: Davies equation
Intermediate output file

330	0.000E+00	-7.00 y
362	1.000E-12	-6.00 y
180	7.616E-04	-6.00 y
140	0.000E+00	-7.00 y
732	1.790E-04	-7.00
730	1.000E-09	-7.00
792	1.000E-12	-7.00
130	1.000E-06	-7.00
500	6.980E-04	-3.16
492	3.568E-06	-5.45 y
490	7.137E-06	-5.15 y
491	1.070E-06	-5.97 y
410	6.138E-05	-4.21 y

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   460  1.748E-04    -3.76 y
   150  4.000E-04    -3.40 y
   281  3.760E-06    -5.42 y
   270  1.053E-05    -4.98 y
   770  9.240E-05    -4.03 y
   580  4.035E-06    -5.39 y
   733  5.000E-08    -7.30 y
   361  1.000E-11   -11.00 y

 H2O has been inserted as a COMPONENT
  3   2
3301403    21.5847    -4.0600
   330     7.0000     0.0000
  2  13
3623300 Hg(CH3)OH       0.0000   -4.6300   0.000   0.000 0.00 0.00 0.00 307.0126
0.00 2  -1.000 330   1.000 362   0.000   0   0.000   0   0.000   0   0.000   0
 0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0
3621800 Hg(CH3)Cl       0.0000    5.2500   0.000   0.000 0.00 0.00 0.00 325.4580
0.00 2   1.000 180   1.000 362   0.000   0   0.000   0   0.000   0   0.000   0
 0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0
3621400 Hg(CH3)C03-     0.0000    6.1000   0.000   0.000-1.00 0.00 0.00 350.0145
0.00 2   1.000 140   1.000 362   0.000   0   0.000   0   0.000   0   0.000   0
 0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0
3627320 Hg(CH3)SO4-     0.0000    0.9400   0.000   0.000-1.00 0.00 0.00 386.0689
0.00 2   1.000 732   1.000 362   0.000   0   0.000   0   0.000   0   0.000   0
 0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0
3627300 Hg(CH3)S-       0.0000    3.7200   0.000   0.000-1.00 0.00 0.00 247.6907
0.00 3  -1.000 330   1.000 362   1.000 730   0.000   0   0.000   0   0.000   0
 0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0
3627301 (Hg(CH3))2S     0.0000   20.0600   0.000   0.000 0.00 0.00 0.00 463.3154
0.00 3   1.000 730   2.000 362  -1.000 330   0.000   0   0.000   0   0.000   0
 0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0
7920020 Sn3ButOH        0.0000   -6.2500   0.000   0.000 0.00 0.00 0.00 307.0122
0.00 3   1.000   2   1.000 792  -1.000 330   0.000   0   0.000   0   0.000   0
 0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0
7921800 Sn3ButCl        0.0000    0.6000   0.000   0.000 0.00 0.00 0.00 325.5083
```

0.00 2 1.000 180 1.000 792 0.000 0 0.000 0 0.000 0 0.000 0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
0.000 0 0.000 0 0.000 0
7921300 Sn3ButBr 0.0000 0.4300 0.000 0.000 0.00 0.00 0.00 369.9593
0.00 2 1.000 130 1.000 792 0.000 0 0.000 0 0.000 0 0.000 0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
0.000 0 0.000 0 0.000 0
3307330 RSH 0.0000 9.3400 0.000 0.000 0.00 0.00 0.00 0.0000
0.00 2 1.000 330 1.000 733 0.000 0 0.000 0 0.000 0 0.000 0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
0.000 0 0.000 0 0.000 0
3627330 CH3HgSR 0.0000 16.1200 0.000 0.000 0.00 0.00 0.00 0.0000
0.00 2 1.000 362 1.000 733 0.000 0 0.000 0 0.000 0 0.000 0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
0.000 0 0.000 0 0.000 0
3617330 HgSR+ 0.0000 28.2940 0.000 0.000 1.00 0.00 0.00 0.0000
0.00 4 1.000 361 1.000 733 2.000 330 -2.000 2 0.000 0 0.000 0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
0.000 0 0.000 0 0.000 0
3617331 Hg(SR)2 0.0000 47.7940 0.000 0.000 0.00 0.00 0.00 0.0000
0.00 4 2.000 733 1.000 361 2.000 330 -2.000 2 0.000 0 0.000 0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
0.000 0 0.000 0 0.000 0

INPUT DATA BEFORE TYPE MODIFICATIONS

ID	Name	ACTIVITY GUESS	log GUESS	ANAL TOTAL
330	H+1	1.000E-07	-7.000	0.000E+00
362	Hg(CH3)+	1.000E-06	-6.000	1.000E-12
180	Cl-1	1.000E-06	-6.000	7.616E-04
140	CO3-2	1.000E-07	-7.000	0.000E+00
732	SO4-2	1.000E-07	-7.000	1.790E-04
730	HS-1	1.000E-07	-7.000	1.000E-09
792	Sn3But+	1.000E-07	-7.000	1.000E-12
130	Br-1	1.000E-07	-7.000	1.000E-06
500	Na+1	6.918E-04	-3.160	6.980E-04
492	NO3-1	3.548E-06	-5.450	3.568E-06
490	NH4+1	7.079E-06	-5.150	7.137E-06
491	NO2-1	1.072E-06	-5.970	1.070E-06
410	K+1	6.166E-05	-4.210	6.138E-05
460	Mg+2	1.738E-04	-3.760	1.748E-04
150	Ca+2	3.981E-04	-3.400	4.000E-04
281	Fe+3	3.802E-06	-5.420	3.760E-06

270	F-1	1.047E-05	-4.980	1.053E-05
770	H4SiO4	9.333E-05	-4.030	9.240E-05
580	PO4-3	4.074E-06	-5.390	4.035E-06
733	RS-	5.012E-08	-7.300	5.000E-08
361	Hg(OH)2	1.000E-11	-11.000	1.000E-11
2	H2O	1.000E+00	0.000	0.000E+00

Charge Balance: UNSPECIATED

Sum of CATIONS= 1.927E-03 Sum of ANIONS = 1.148E-03

PERCENT DIFFERENCE = 2.535E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

IMPROVED ACTIVITY GUESSES PRIOR TO FIRST ITERATION:		
CO3-2	Log activity guess:	-7.58
SO4-2	Log activity guess:	-3.75
HS-1	Log activity guess:	-9.27
Fe+3	Log activity guess:	-14.88
H4SiO4	Log activity guess:	-4.03
PO4-3	Log activity guess:	-11.18
Hg(OH)2	Log activity guess:	-11.00

PART 2 of OUTPUT FILE

MINTEQA2 v4.02 DATE OF CALCULATIONS: 28-OCT-2004 TIME: 4: 4: 0

CONSTRAINTS ON COMPONENT ACTIVITIES

As specified, this chemical system is OPEN with respect to the following components:

H2O H+1 CO3-2

Activities of the following components are constrained
by the species shown:

COMPONENT	SPECIES	TYPE
H+1	H+1	3
CO3-2	CO2 (g)	3
H2O	H2O	3

PART 3 of OUTPUT FILE

MINTEQA2 v4.02 DATE OF CALCULATIONS: 28-OCT-2004 TIME: 4: 4: 0

PARAMETERS OF THE COMPONENT MOST OUT OF BALANCE:

ITER	NAME	TOTAL mol/L	DIFF FXN	LOG ACTVTY	RESIDUAL
0	PO4-3	4.035E-06	5.203E-07	-11.18037	5.199E-07
1	PO4-3	4.035E-06	4.404E-07	-11.23147	4.400E-07
2	PO4-3	4.035E-06	1.386E-08	-11.26807	1.346E-08
3	Ca+2	4.000E-04	4.263E-08	-3.50040	2.630E-09
4	HS-1	1.000E-09	3.281E-05	-13.54370	3.281E-05
5	HS-1	1.000E-09	7.469E-07	-13.18608	7.469E-07
6	HS-1	1.000E-09	3.539E-08	-12.50700	3.539E-08
7	HS-1	1.000E-09	3.926E-08	-11.16767	3.926E-08
8	HS-1	1.000E-09	1.866E-07	-10.28749	1.866E-07
9	HS-1	1.000E-09	3.333E-07	-9.66148	3.333E-07
10	HS-1	1.000E-09	3.642E-08	-9.63932	3.641E-08
11	HS-1	1.000E-09	3.202E-09	-9.63587	3.202E-09
12	HS-1	1.000E-09	-5.197E-10	-9.60680	5.196E-10
13	HS-1	1.000E-09	-7.324E-12	-9.28849	7.224E-12

ID No	Name	Total Conc(M)	Conc (M)	log Activity	Diff fxn
733	RS-	5.000E-08	2.398E-10	-9.64307	4.216E-15
362	Hg(CH3)+	1.000E-12	3.516E-19	-18.47676	-3.900E-20
180	Cl-1	7.616E-04	7.616E-04	-3.14111	2.181E-14
361	Hg(OH)2	1.000E-11	3.061E-26	-25.51396	5.822E-16

732	SO4-2	1.790E-04	1.654E-04	-3.87293	1.895E-14
730	HS-1	1.000E-09	5.466E-10	-9.28521	-3.052E-15
792	Sn3But+	1.000E-12	1.579E-13	-12.82459	4.011E-24
130	Br-1	1.000E-06	1.000E-06	-6.02284	2.864E-17
500	Na+1	6.980E-04	6.975E-04	-3.17932	1.999E-14
492	NO3-1	3.568E-06	3.564E-06	-5.47085	1.022E-16
490	NH4+1	7.137E-06	7.088E-06	-5.17228	2.033E-16
491	NO2-1	1.070E-06	1.070E-06	-5.99346	3.065E-17
410	K+1	6.138E-05	6.132E-05	-4.23522	1.758E-15
460	Mg+2	1.748E-04	1.710E-04	-3.85827	1.960E-14
150	Ca+2	4.000E-04	3.899E-04	-3.50045	4.467E-14
281	Fe+3	3.760E-06	2.038E-15	-14.89642	9.747E-17
270	F-1	1.053E-05	1.033E-05	-5.00881	3.015E-16
770	H4SiO4	9.240E-05	9.229E-05	-4.03464	-5.234E-17
580	PO4-3	4.035E-06	8.632E-12	-11.26943	2.421E-16
2	H2O	0.000E+00	-7.940E-05	-0.00002	0.000E+00
140	CO3-2	0.000E+00	3.211E-08	-7.58472	0.000E+00
330	H+1	0.000E+00	1.054E-07	-7.00000	0.000E+00

Type I - COMPONENTS AS SPECIES IN SOLUTION

ID No	Name	Conc (M)	log Act	Charge	Act Coef	New logK
330	H+1	1.054E-07	-7.00000	1.00	0.94877	0.023
362	Hg(CH3)+	3.516E-19	-18.47676	1.00	0.94877	0.023
180	Cl-1	7.616E-04	-3.14111	-1.00	0.94877	0.023
140	CO3-2	3.211E-08	-7.58472	-2.00	0.81030	0.091
732	SO4-2	1.654E-04	-3.87293	-2.00	0.81030	0.091
730	HS-1	5.466E-10	-9.28521	-1.00	0.94877	0.023
792	Sn3But+	1.579E-13	-12.82459	1.00	0.94877	0.023
130	Br-1	1.000E-06	-6.02284	-1.00	0.94877	0.023
500	Na+1	6.975E-04	-3.17932	1.00	0.94877	0.023
492	NO3-1	3.564E-06	-5.47085	-1.00	0.94877	0.023
490	NH4+1	7.088E-06	-5.17228	1.00	0.94877	0.023
491	NO2-1	1.070E-06	-5.99346	-1.00	0.94877	0.023
410	K+1	6.132E-05	-4.23522	1.00	0.94877	0.023
460	Mg+2	1.710E-04	-3.85827	2.00	0.81030	0.091
150	Ca+2	3.899E-04	-3.50045	2.00	0.81030	0.091
281	Fe+3	2.038E-15	-14.89642	3.00	0.62295	0.206
270	F-1	1.033E-05	-5.00881	-1.00	0.94877	0.023
770	H4SiO4	9.229E-05	-4.03464	0.00	1.00052	0.000
580	PO4-3	8.632E-12	-11.26943	-3.00	0.62295	0.206

733	RS-	2.398E-10	-9.64307	-1.00	0.94877	0.023
361	Hg(OH)2	3.061E-26	-25.51396	0.00	1.00052	0.000

Type II - OTHER SPECIES IN SOLUTION OR ADSORBED

ID No	Name	Conc (M)	log Act	Charge	Act Coef	New logK
361 7331	Hg(SR)2	9.856E-12	-11.00607	0.00	1.00052	47.794
330 7700	H3SiO4-	1.146E-07	-6.96365	-1.00	0.94877	-9.906
330 7301	S-2	3.207E-20	-19.58521	-2.00	0.81030	-17.209
361 3300	Hg+2	5.908E-34	-33.31993	2.00	0.81030	6.285
330 0020	OH-	1.061E-07	-6.99702	-1.00	0.94877	-13.974
361 3302	HgOH+	2.023E-30	-29.71695	1.00	0.94877	2.820
361 3303	Hg(OH)3-1	4.091E-34	-33.41098	-1.00	0.94877	-14.874
281 3300	FeOH+2	1.018E-10	-10.08344	2.00	0.81030	-2.096
281 3301	Fe(OH)2+	3.407E-06	-5.49046	1.00	0.94877	-4.571
281 3302	Fe(OH)3 (aq)	3.494E-07	-6.45648	0.00	1.00052	-12.560
281 3303	Fe(OH)4-	3.454E-09	-8.48450	-1.00	0.94877	-21.565
281 3304	Fe2(OH)2+4	5.230E-19	-18.64688	4.00	0.43110	-2.489
281 3305	Fe3(OH)4+5	3.923E-23	-22.97734	5.00	0.26855	-5.717
460 3300	MgOH+	2.399E-09	-8.64278	1.00	0.94877	-11.762
150 3300	CaOH+	6.689E-10	-9.19746	1.00	0.94877	-12.674
330 2700	HF (aq)	1.449E-09	-8.83881	0.00	1.00052	3.170
330 2701	HF2-	5.691E-14	-13.26762	-1.00	0.94877	3.773
330 2702	H2F2 (aq)	5.625E-18	-17.24962	0.00	1.00052	6.768
770 2700	SiF6-2	1.527E-32	-31.90744	-2.00	0.81030	30.271
361 2701	HgF+	1.833E-37	-36.75974	1.00	0.94877	7.786
281 2700	FeF+2	1.683E-14	-13.86524	2.00	0.81030	6.131
281 2701	FeF2+	3.770E-15	-14.44655	1.00	0.94877	10.490
281 2702	FeF3 (aq)	4.942E-17	-16.30586	0.00	1.00052	13.617
460 2700	MgF+	1.606E-07	-6.81708	1.00	0.94877	2.073
150 2700	CaF+	3.561E-08	-7.47126	1.00	0.94877	1.061
500 2700	NaF (aq)	4.089E-09	-8.38813	0.00	1.00052	-0.200
361 1800	HgCl+	7.274E-30	-29.16104	1.00	0.94877	13.517
361 1801	HgCl2 (aq)	2.498E-26	-25.60215	0.00	1.00052	20.194
361 1802	HgCl3-1	1.904E-28	-27.74326	-1.00	0.94877	21.217
361 1803	HgCl4-2	6.412E-31	-30.28438	-2.00	0.81030	21.885
361 1805	HgClOH (aq)	6.148E-26	-25.21106	0.00	1.00052	10.444
281 1800	FeCl+2	3.418E-17	-16.55754	2.00	0.81030	1.571
281 1801	FeCl2+	9.423E-20	-19.04865	1.00	0.94877	2.153
281 1802	FeCl3 (aq)	6.457E-24	-23.18976	0.00	1.00052	1.130
361 1301	HgBr+	1.946E-30	-29.73377	1.00	0.94877	15.826

361	1302	HgBr2 (aq)	5.160E-28	-27.28711	0.00	1.00052	24.272
361	1303	HgBr3-1	1.390E-31	-30.87995	-1.00	0.94877	26.725
361	1304	HgBr4-2	2.625E-36	-35.67228	-2.00	0.81030	28.024
361	1305	HgBrCl (aq)	3.184E-27	-26.49678	0.00	1.00052	22.181
361	3301	HgBrOH (aq)	7.870E-27	-26.10379	0.00	1.00052	12.433
330	7300	H2S (aq)	4.532E-10	-9.34353	0.00	1.00052	6.941
361	7300	HgS2-2	2.636E-15	-14.67034	-2.00	0.81030	29.505
361	7301	Hg(HS)2 (aq)	2.700E-14	-13.56834	0.00	1.00052	44.516
361	7302	HgHS2-1	1.149E-13	-12.96234	-1.00	0.94877	38.145
330	7320	HSO4-	1.370E-09	-8.88598	-1.00	0.94877	2.010
490	7320	NH4SO4-	1.018E-08	-8.01521	-1.00	0.94877	1.053
361	7320	HgSO4 (aq)	1.678E-35	-34.77485	0.00	1.00052	8.612
281	7320	FeSO4+	2.011E-15	-14.71935	1.00	0.94877	4.073
281	7321	Fe(SO4)2-	5.762E-18	-17.26228	-1.00	0.94877	5.403
460	7320	MgSO4 (aq)	3.377E-06	-5.47119	0.00	1.00052	2.260
150	7320	CaSO4 (aq)	9.692E-06	-5.01337	0.00	1.00052	2.360
500	7320	NaSO4-	5.019E-07	-6.32224	-1.00	0.94877	0.753
410	7320	KSO4-	5.773E-08	-7.26142	-1.00	0.94877	0.870
330	4900	NH3 (aq)	3.831E-08	-7.41650	0.00	1.00052	-9.244
361	4900	HgNH3+2	1.429E-32	-31.93621	2.00	0.81030	5.841
361	4901	Hg(NH3)2+2	5.481E-31	-30.35250	2.00	0.81030	5.597
361	4902	Hg(NH3)3+2	8.367E-38	-37.16878	2.00	0.81030	-3.047
361	4903	Hg(NH3)4+2	2.549E-44	-43.68507	2.00	0.81030	-11.391
150	4901	CaNH3+2	1.882E-11	-10.81673	2.00	0.81030	-9.053
150	4902	Ca(NH3)2+2	2.873E-19	-18.63301	2.00	0.81030	-18.697
361	4920	HgNO3+	6.300E-40	-39.22348	1.00	0.94877	5.784
361	4921	Hg(NO3)2 (aq)	8.397E-46	-45.07562	0.00	1.00052	5.380
281	4921	FeNO3+2	5.298E-20	-19.36727	2.00	0.81030	1.091
150	4921	CaNO3+	3.561E-09	-8.47129	1.00	0.94877	0.523
330	5800	HPO4-2	1.574E-06	-5.89443	-2.00	0.81030	12.466
330	5801	H2PO4-	2.120E-06	-5.69643	-1.00	0.94877	19.596
330	5802	H3PO4	2.827E-11	-10.54843	0.00	1.00052	21.721
281	5801	FeH2PO4+2	5.984E-17	-16.31436	2.00	0.81030	23.943
281	5800	FeHPO4+	1.409E-11	-10.87386	1.00	0.94877	22.315
460	5800	MgPO4-	3.541E-11	-10.47370	-1.00	0.94877	4.677
460	5801	MgH2PO4+	1.417E-08	-7.87160	1.00	0.94877	21.279
460	5802	MgHPO4 (aq)	1.114E-07	-6.95270	0.00	1.00052	15.175
150	5800	CaHPO4 (aq)	1.840E-07	-6.73488	0.00	1.00052	15.035
150	5801	CaPO4-	5.164E-09	-8.30988	-1.00	0.94877	6.483
150	5802	CaH2PO4+	1.500E-08	-7.84688	1.00	0.94877	20.946
500	5800	NaHPO4-	1.045E-08	-8.00375	-1.00	0.94877	13.468
410	5800	KHPO4-	5.932E-10	-9.24966	-1.00	0.94877	13.278
330	1400	HCO3-	5.858E-05	-4.25507	-1.00	0.94877	10.352

330 1401	H2CO3 (aq)	1.248E-05	-4.90372	0.00	1.00052	16.681
361 1401	HgCO3 (aq)	1.490E-29	-28.82665	0.00	1.00052	18.272
361 1402	Hg(CO3)2-2	1.514E-33	-32.91136	-2.00	0.81030	21.863
361 1403	HgHCO3+	2.925E-32	-31.55665	1.00	0.94877	22.565
460 1400	MgCO3 (aq)	3.439E-09	-8.46332	0.00	1.00052	2.979
460 1401	MgHCO3+	9.441E-08	-7.04780	1.00	0.94877	11.418
150 1400	CaHCO3+	1.917E-07	-6.74012	1.00	0.94877	11.368
150 1401	CaCO3 (aq)	1.167E-08	-7.93265	0.00	1.00052	3.152
500 1400	NaCO3-	3.379E-10	-9.49404	-1.00	0.94877	1.293
500 1401	NaHCO3 (aq)	2.064E-08	-7.68504	0.00	1.00052	10.079
330 7701	H2SiO4-2	2.750E-12	-11.65198	-2.00	0.81030	-21.526
362 3300	Hg(CH3)OH	7.817E-17	-16.10676	0.00	1.00052	-4.630
362 1800	Hg(CH3)Cl	4.285E-17	-16.36787	0.00	1.00052	5.250
362 1400	Hg(CH3)C03-	1.152E-20	-19.96148	-1.00	0.94877	6.123
362 7320	Hg(CH3)SO4-	4.104E-22	-21.40968	-1.00	0.94877	0.963
362 7300	Hg(CH3)S-	9.569E-18	-17.04197	-1.00	0.94877	3.743
362 7301	(Hg(CH3))2S	6.623E-20	-19.17872	0.00	1.00052	20.060
792 0020	Sn3ButOH	8.417E-13	-12.07461	0.00	1.00052	-6.250
792 1800	Sn3ButCl	4.306E-16	-15.36570	0.00	1.00052	0.600
792 1300	Sn3ButBr	3.822E-19	-18.41743	0.00	1.00052	0.430
330 7330	RSH	4.974E-08	-7.30307	0.00	1.00052	9.340
362 7330	CH3HgSR	9.999E-13	-11.99983	0.00	1.00052	16.120
361 7330	HgSR+	1.445E-21	-20.86300	1.00	0.94877	28.317

Type III - SPECIES WITH FIXED ACTIVITY

ID No	Name	Conc (M)	New logK	Enthalpy
2	H2O	-7.940E-05	0.000	0.000
3301403	CO2 (g)	-7.141E-05	21.585	-4.060
330	H+1	6.079E-05	7.000	0.000

Type VI - EXCLUDED SPECIES (not included in mole balance)

ID No	Name	Conc (M)	New logK	Enthalpy
361 2700	HgF2 (g)	0.000E+00	-12.565	165.186
361 1300	HgBr2 (g)	6.737E-34	18.388	-54.494
330 7302	H2S (g)	5.306E-09	8.010	0.000

PERCENTAGE DISTRIBUTION OF COMPONENTS AMONG
TYPE I and TYPE II (dissolved and adsorbed) species

RS-
99.5 Percent bound in species #3307330 RSH

Hg(CH3)+
100.0 Percent bound in species #3627330 CH3HgSR

Cl-1
100.0 Percent bound in species # 180 Cl-1

Hg(OH)2
98.6 Percent bound in species #3617331 Hg(SR)2

1.1 Percent bound in species #3617302 HgHS2-1

SO4-2
92.4 Percent bound in species # 732 SO4-2

1.9 Percent bound in species #4607320 MgSO4 (aq)

5.4 Percent bound in species #1507320 CaSO4 (aq)

HS-1
54.7 Percent bound in species # 730 HS-1

45.3 Percent bound in species #3307300 H2S (aq)

Sn3But+

15.8 Percent bound in species # 792 Sn3But+

84.2 Percent bound in species #7920020 Sn3ButOH

Br-1

100.0 Percent bound in species # 130 Br-1

Na+1

99.9 Percent bound in species # 500 Na+1

NO3-1

99.9 Percent bound in species # 492 NO3-1

NH4+1

99.3 Percent bound in species # 490 NH4+1

NO2-1

100.0 Percent bound in species # 491 NO2-1

K+1

99.9 Percent bound in species # 410 K+1

Mg+2

97.8 Percent bound in species # 460 Mg+2

1.9 Percent bound in species #4607320 MgSO4 (aq)

Ca+2

97.5 Percent bound in species # 150 Ca+2

2.4 Percent bound in species #1507320 CaSO4 (aq)

Fe+3

90.6 Percent bound in species #2813301 Fe(OH)2+

9.3 Percent bound in species #2813302 Fe(OH)3 (aq)

F-1

98.1 Percent bound in species # 270 F-1

1.5 Percent bound in species #4602700 MgF+

H4SiO4

99.9 Percent bound in species # 770 H4SiO4

PO4-3

39.0 Percent bound in species #3305800 HPO4-2

52.5 Percent bound in species #3305801 H2PO4-

2.8 Percent bound in species #4605802 MgHPO4 (aq)

4.6 Percent bound in species #1505800 CaHPO4 (aq)

H2O

1.3 Percent bound in species #3300020 OH-

85.3 Percent bound in species #2813301 Fe(OH)2+

13.1 Percent bound in species #2813302 Fe(OH)3 (aq)

CO3-2

82.0 Percent bound in species #3301400 HCO3-

17.5 Percent bound in species #3301401 H2CO3 (aq)

H+1

1.9 Percent bound in species #3305800 HPO4-2

5.2 Percent bound in species #3305801 H2PO4-

71.4 Percent bound in species #3301400 HCO3-

30.4 Percent bound in species #3301401 H2CO3 (aq)

PART 5 of OUTPUT FILE

MINTEQA2 v4.02 DATE OF CALCULATIONS: 28-OCT-2004 TIME: 4: 4: 0

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	Name	DISSOLVED		SORBED		PRECIPITATED	
		mol/L	percent	mol/L	percent	mol/L	percent
733	RS-	5.000E-08	100.0	0.000E+00	0.0	0.000E+00	0.0
362	Hg(CH3)+	1.000E-12	100.0	0.000E+00	0.0	0.000E+00	0.0
180	Cl-1	7.616E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
361	Hg(OH)2	1.000E-11	100.0	0.000E+00	0.0	0.000E+00	0.0
732	SO4-2	1.790E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
730	HS-1	1.000E-09	100.0	0.000E+00	0.0	0.000E+00	0.0
792	Sn3But+	1.000E-12	100.0	0.000E+00	0.0	0.000E+00	0.0
130	Br-1	1.000E-06	100.0	0.000E+00	0.0	0.000E+00	0.0
500	Na+1	6.980E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
492	NO3-1	3.568E-06	100.0	0.000E+00	0.0	0.000E+00	0.0
490	NH4+1	7.137E-06	100.0	0.000E+00	0.0	0.000E+00	0.0
491	NO2-1	1.070E-06	100.0	0.000E+00	0.0	0.000E+00	0.0
410	K+1	6.138E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
460	Mg+2	1.748E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
150	Ca+2	4.000E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
281	Fe+3	3.760E-06	100.0	0.000E+00	0.0	0.000E+00	0.0
270	F-1	1.053E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
770	H4SiO4	9.240E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
580	PO4-3	4.035E-06	100.0	0.000E+00	0.0	0.000E+00	0.0
2	H2O	7.985E-06	100.0	0.000E+00	0.0	0.000E+00	0.0
140	CO3-2	7.141E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
330	H+1	8.204E-05	100.0	0.000E+00	0.0	0.000E+00	0.0

Charge Balance: SPECIATED

Sum of CATIONS = 1.892E-03 Sum of ANIONS 1.173E-03

PERCENT DIFFERENCE = 2.345E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

EQUILIBRIUM IONIC STRENGTH (m) = 2.260E-03

EQUILIBRIUM pH = 7.000

DATE ID NUMBER: 20041028
TIME ID NUMBER: 4040022

PART 6 of OUTPUT FILE

MINTEQA2 v4.02 DATE OF CALCULATIONS: 28-OCT-2004 TIME: 4: 4: 0

Saturation indices and stoichiometry of all minerals

ID No	Name	SI	Composition by stoich. of components
1036100	CINNABAR	3.895	[1.000]361 [-2.000] 2 [1.000]330 [1.000]730
1036101	METACINNABAR	3.295	[1.000]361 [-2.000] 2 [1.000]330 [1.000]730
2077000	CHALCEDONY	-0.485	[1.000]770 [-2.000] 2
2077001	CRISTOBALITE	-0.685	[1.000]770 [-2.000] 2
2077002	QUARTZ	-0.035	[1.000]770 [-2.000] 2
2077003	SiO2 (am,gel)	-1.325	[1.000]770 [-2.000] 2
2077004	SiO2 (am,ppt)	-1.295	[1.000]770 [-2.000] 2
2036100	MONTROYDITE	-21.874	[1.000]361 [-1.000] 2 [0.000]330
2036101	Hg(OH)2	-22.018	[1.000]361
2028100	FERRIHYDRITE	2.913	[1.000]281 [3.000] 2 [-3.000]330
2028102	GOETHITE	5.613	[1.000]281 [2.000] 2 [-3.000]330
2046000	BRUCITE	-6.702	[1.000]460 [2.000] 2 [-2.000]330
2046001	PERICLASE	-11.442	[-2.000]330 [1.000]460 [1.000] 2
2046002	Mg(OH)2 (active)	-8.652	[1.000]460 [2.000] 2 [-2.000]330
2015000	LIME	-22.200	[-2.000]330 [1.000]150 [1.000] 2
2015001	PORTLANDITE	-12.304	[1.000]150 [2.000] 2 [-2.000]330
3028100	HEMATITE	13.625	[2.000]281 [3.000] 2 [-6.000]330
3028101	MAGHEMITE	5.821	[-6.000]330 [2.000]281 [3.000] 2
3028102	LEPIDOCROCITE	4.733	[-3.000]330 [1.000]281 [2.000] 2
3046001	MAGNESIOFERRITE	5.489	[-8.000]330 [1.000]460 [2.000]281 [4.000] 2
3050000	NATRON	-12.633	[2.000]500 [1.000]140 [10.000] 2
4246001	MgF2	-5.746	[1.000]460 [2.000]270
4215000	FLUORITE	-2.569	[1.000]150 [2.000]270

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4136100 HgCl2                   -24.534 [  1.000]361 [  2.000]180 [  2.000]330
                                        [ -2.000]  2
4128100 Fe(OH)2.7Cl.3           6.101 [ -2.700]330 [  1.000]281 [  2.700]  2
                                        [  0.300]180
4150000 HALITE                  -7.923 [  1.000]500 [  1.000]180
4036100 HgBr2                   -26.286 [  1.000]361 [  2.000]130 [  2.000]330
                                        [ -2.000]  2
5036101 Hg3O2CO3                -68.445 [  3.000]361 [ -4.000]  2 [  2.000]330
                                        [  1.000]140
5046000 ARTINITE                -10.901 [ -2.000]330 [  2.000]460 [  1.000]140
                                        [  5.000]  2
5046001 HYDROMAGNESITE          -26.864 [  5.000]460 [  4.000]140 [ -2.000]330
                                        [  6.000]  2
5046002 MAGNESITE               -3.983 [  1.000]460 [  1.000]140
5046003 NESQUEHONITE            -6.773 [  1.000]460 [  1.000]140 [  3.000]  2
5015000 ARAGONITE               -2.749 [  1.000]150 [  1.000]140
5015001 CALCITE                 -2.610 [  1.000]150 [  1.000]140
5015002 DOLOMITE (ordered)      -5.438 [  1.000]150 [  1.000]460 [  2.000]140
5015004 DOLOMITE (disordered)   -5.988 [  1.000]150 [  1.000]460 [  2.000]140
5015003 HUNTITE                 -15.446 [  3.000]460 [  1.000]150 [  4.000]140
5050001 THERMONATRITE           -14.580 [  2.000]500 [  1.000]140 [  1.000]  2
6036100 HgSO4                   -33.968 [  1.000]361 [  1.000]732 [  2.000]330
                                        [ -2.000]  2
6028100 Fe2(SO4)3               -37.677 [  2.000]281 [  3.000]732
6028101 H-JAROSITE              -5.335 [ -5.000]330 [  3.000]281 [  2.000]732
                                        [  7.000]  2
6050000 Na-JAROSITE             -2.415 [ -6.000]330 [  1.000]500 [  3.000]281
                                        [  2.000]732 [  6.000]  2
6041002 K-JAROSITE              0.130 [ -6.000]330 [  1.000]410 [  3.000]281
                                        [  2.000]732 [  6.000]  2
6046000 EPSOMITE                -5.605 [  1.000]460 [  1.000]732 [  7.000]  2
6015000 ANHYDRITE               -3.013 [  1.000]150 [  1.000]732
6015001 GYPSUM                  -2.763 [  1.000]150 [  1.000]732 [  2.000]  2
6050001 MIRABILITE              -9.118 [  2.000]500 [  1.000]732 [ 10.000]  2
6050002 THENARDITE              -10.553 [  2.000]500 [  1.000]732
7028100 STRENGITE               0.234 [  1.000]281 [  1.000]580 [  2.000]  2
7046002 Mg3(PO4)2               -10.834 [  3.000]460 [  2.000]580
7046001 MgHPO4:3H2O             -3.953 [  1.000]460 [  1.000]330 [  1.000]580
                                        [  3.000]  2
7015002 FCO3APATITE             4.473 [  9.316]150 [  0.360]500 [  0.144]460
                                        [  4.800]580 [  1.200]140 [  2.480]270
7015003 HYDROXYLAPATITE         0.022 [  5.000]150 [  3.000]580 [  1.000]  2
                                        [ -1.000]330
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7015004 CaHPO4:2H2O -2.775 [1.000]150 [1.000]330 [1.000]580
[2.000] 2
7015005 CaHPO4 -2.495 [1.000]150 [1.000]330 [1.000]580
7015006 Ca3(PO4)2 (beta) -4.120 [3.000]150 [2.000]580
7015007 Ca4H(PO4)3:3H2O -7.730 [4.000]150 [1.000]330 [3.000]580
[3.000] 2
8646000 CHRYSOTILE -9.844 [3.000]460 [2.000]770 [1.000] 2
[-6.000]330
8646003 SEPIOLITE -7.580 [2.000]460 [3.000]770 [-4.000]330
[-0.500] 2
8646004 SEPIOLITE (A) -10.600 [-0.500] 2 [2.000]460 [3.000]770
[-4.000]330