

US EPA ARCHIVE DOCUMENT

**Diffuse-Layer Sorption Reactions  
for use in MINTEQA2 for  
HWIR Metals and Metalloids**

prepared for

U.S. Environmental Protection Agency  
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## SUMMARY

This report outlines the development of the database of diffuse-layer sorption reactions for hydrous ferric oxide (HFO) to be used in equilibrium speciation calculations for the Hazardous Waste Identification Rule (HWIR). The sorption of contaminant metals and metalloids is important in that it retards contaminant transport in the subsurface. In HWIR, the results of the speciation modeling are used to compute the contaminant sorption distribution coefficient,  $K_d$ , a transport model parameter that must be included to account for this retardation. The contaminant metals and metalloids of interest in HWIR are: arsenic (As), antimony (Sb), barium (Ba), beryllium (Be), cadmium (Cd), chromium (Cr), cobalt (Co), copper (Cu), lead (Pb), mercury (Hg), molybdenum (Mo), nickel (Ni), selenium (Se), silver (Ag), thallium (Tl), tin (Sn), vanadium (V), and zinc (Zn). Although not a metal, cyanide (CN) is also of interest as a transportable contaminant. A consistent set of sorption reactions are presented for all HWIR contaminants of interest. The corresponding MINTEQA2 database is also presented.

## 1.0 BACKGROUND

The U.S. Environmental Protection Agency has used the MINTEQA2/PRODEFA2 equilibrium speciation model (Allison *et al.*, 1991) to evaluate metal speciation and to estimate metal sorption for previous modeling in the Hazardous Waste Identification Rule (US EPA, 1996). In particular, the model has been used to estimate  $K_d$  as a function of metal concentration for a number of metal contaminants. Public and EPA peer reviews of the HWIR methodology have resulted in numerous comments, some of which pertain to the role of the MINTEQA2/PRODEFA2 model (hereafter referred to simply as "MINTEQA2"). Two specific areas of weakness in the application of the model in HWIR were identified:

- 1) The general thermodynamic database used by MINTEQA2 needs to be updated. This database contains thermodynamic data for dissolved (aqueous) phase and solid phase reactions and reactions used to represent oxidation-reduction and gas phase species at constant partial pressure. The database was originally compiled more than ten years ago and has been supplemented over the years with data that may not always have been consistent with earlier entries. The database requires a thorough review of all entries impacting the HWIR calculations. Also, certain metals of interest in HWIR are not currently represented in the general thermodynamic database.
- 2) The specialized thermodynamic database of reactions between metals and the hydrous ferric oxide (HFO) sorbent used in the diffuse-layer model (DLM) needs to be supplemented with reactions for those metals that form oxoanions in aqueous solution (e.g., arsenic, chromium (VI), and selenium). These metals have been included in the HWIR methodology, but have not been included in previous MINTEQA2 modeling. Hydrous ferric oxide reactions for cationic metals also need to be reviewed and updated if necessary. In addition, the database needs to be supplemented with reactions for new HWIR species not included in the original HWIR modeling and not currently represented in the MINTEQA2 HFO database.

The first of these concerns has been addressed in a separate task (Task 2) under this same work assignment. Concern (2) is the focus of this study. The objective has been to provide the MINTEQA2 model with the latest available data for all HWIR contaminant metals pertinent to diffuse-layer model sorption reactions on hydrous ferric oxide.

## 2.0 DATA SOURCES AND METHODOLOGY

The previous database used in earlier HWIR modeling was developed from data presented in a Ph.D dissertation by David Dzombak (1986). It included species representing sorption reactions for the cations: hydrogen (protons), barium, cadmium, copper, lead, nickel, and zinc; and the anions: arsenite and arsenate. The arsenic reactions have not previously been used in HWIR modeling. Reactions for chromium(III) and mercury(II), although not included in the previous MINTEQA2 (version 3.11) database, are given in the

Dzombak dissertation and have been used in HWIR modeling. The objective of this task was to provide HFO diffuse-layer model reactions to represent sorbed species for all HWIR metals, metalloids, and cyanide. Reactions for those metals that were previously represented have been checked for completeness and accuracy. Reactions to represent HWIR sorbed metal species not in the previous database have been added. The HWIR metals not represented in the version 3.11 database include: chromium, mercury, silver, vanadium, selenium, thallium, antimony, molybdenum, tin, and cobalt. If experimentally derived sorption reactions with equilibrium constants were not found, estimates using linear free energy relationships relating the magnitude of sorption constants to hydrolysis or acidity constants have been employed.

The primary source of data for updating the diffuse-layer sorption database was a compilation of reactions representing a unified and consistent database for HFO by Dzombak and Morel (1990). This work presents many of the same reactions given in the compilation of Dzombak (1986) with some revised constants. It also presents data not included in the earlier compilation.

## 2.1 HFO SORPTION REACTIONS

The diffuse-layer sorption reactions for the contaminant metals of interest were obtained from Dzombak and Morel (1990). The presentation follows theirs in presenting the results for metals grouped according to similar surface reactions. The log equilibrium constants are referenced by a subscript 1 or 2 ( $\log K_1^{intr}$ ,  $\log K_2^{intr}$ ) to indicate the specific sorption reaction. The “*intr*” superscript indicates that these are the values of the intrinsic constants (exclusive of electrostatic effects). For certain transition and post-transition cations, Dzombak and Morel derived constants for both low-affinity (weak) and high-affinity (strong) sites. These are identified with a superscript in the site names as in:  $\text{Fe}^w\text{OH}^0$  and  $\text{Fe}^s\text{OH}^0$  for the (neutral) weak and strong sites, respectively. The superscript “*n*” appearing in the reactions below refers to charge on the metal M.

### 2.1.1 HFO Surface Reactions for Cations

The HFO surface reactions for cations as given by (Dzombak and Morel, 1990) differ somewhat among the various groups of metals. In particular, the alkaline earth metals (with the exception of beryllium) behave similarly and the transition and post-transition metals behave similarly. They present data for a single trivalent cation,  $\text{Cr}^{3+}$ , with a surface reaction that differs from the other two groups. Beryllium, although it belongs the alkaline earths, behaves somewhat anomalously for its group. The hydroxide of beryllium is amphoteric, whereas the hydroxides of calcium, strontium, and barium are strong bases. Its behavior as regards surface reactions is more similar to the transition metals; it will be listed with those metals for the purposes of defining its HFO reactions. Also, note that although magnesium, calcium, and manganese are not contaminant metals in HWIR, their relevant surface constants are provided below because their concentration levels in natural systems can result in effective competition for trace metal sorption sites.

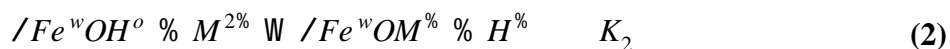
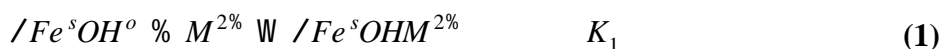
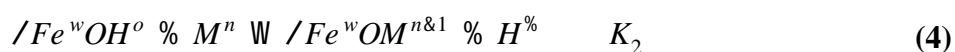
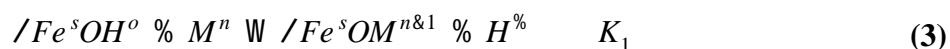
Reactions for Ba, Mg, and CaReactions for Divalent Be, Cd, Co, Cu, Hg, Ni, Pb, Mn, Sn, Zn, and Monovalent AgReaction for the Trivalent Cr**2.1.2 Intrinsic Constants for Cations**

Table 2.1 presents values for the intrinsic constants as given by Dzombak and Morel (1990). They used linear free energy relationships (LFER) between the cations and their first hydrolysis constants to extrapolate some values for metals whose intrinsic constants were not derivable from experimental data. The use of LFER is predicated on the assumption that the relative affinity among various cations for the hydroxyl sites on HFO reflect their relative affinities for OH<sup>-</sup> complexation in solution. Values estimated from LFER (as opposed to those derived from experimental results) are indicated in Table 2.1 with an asterisk. A dash entry means no constant could be determined.

**Table 2.1 Intrinsic Sorption Constants for some Cations on HFO.**

Metal	$\log K_1^{intr}$	$\log K_2^{intr}$
Ba <sup>2+</sup>	5.46	-7.2*
Ca <sup>2+</sup>	4.97	-5.85
Mg <sup>2+</sup>	—	-4.6*
Tl <sup>+</sup>	-3.5*	-6.9*
Ag <sup>+</sup>	-1.72	-5.3*
Mn <sup>2+</sup>	-0.4*	-3.5*
Co <sup>2+</sup>	-4.6	-3.01
Ni <sup>2+</sup>	0.37	-2.5*
Cd <sup>2+</sup>	0.47	-2.90
Zn <sup>2+</sup>	0.99	-1.99
Cu <sup>2+</sup>	2.89	0.6*
Pb <sup>2+</sup>	4.65	0.3*
Be <sup>2+</sup>	5.7*	3.3*
Hg <sup>2+</sup>	7.76	6.45
Sn <sup>2+</sup>	8.0*	5.9*
Cr <sup>3+</sup>	2.06	--

The constants shown in Table 2.1 are given by Dzombak and Morel (1990) with the exception of the values for Tl<sup>+</sup>. In most natural freshwater systems, the +1 oxidation state of thallium is expected to dominate (World Health Organization, 1996). Using the LFER expressions from Dzombak and Morel (determined by regression of the first hydrolysis constant with experimentally derived  $\log K_1^{intr}$  and  $\log K_2^{intr}$ , respectively) gives:

$$\log K_{1,Tl}^{intr} = 1.166 \log K_{TlOH} + 4.374 \quad (6)$$



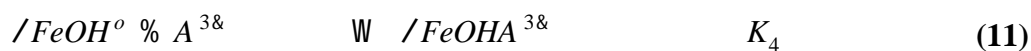
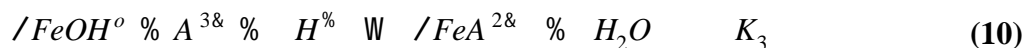
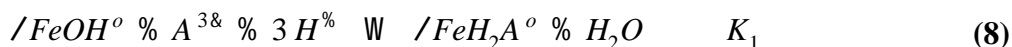
$$\log K_{2,Tl}^{intr} = 1.299 \log K_{TlOH} + 7.893 \quad (7)$$

The National Institute of Standards and Technology database *Critical Stability Constants of Metal Complexes, Version 4.0* gives a value of 0.79 for the first hydrolysis constant for  $Tl^+$  and the resulting estimates of  $\log K_1^{intr}$  and  $\log K_2^{intr}$  are -3.5 and -6.9, respectively. These values correspond to surface reactions (3) and (4) above, respectively.

### 2.1.3 HFO Surface Reactions for Anions

The HFO surface reactions for anions as given by (Dzombak and Morel, 1990) are also grouped by similar behavior. In particular, certain trivalent (deprotonated) anions behave similarly, the fully protonated (neutral) species of arsenite and borate behave similarly, and the divalent (deprotonated) anions behave similarly. The pertinent surface reactions are somewhat different for these groups, so they are presented separately below. Antimony (as  $SbO(OH)_4^-$ ) and cyanide are grouped with the divalent anions for the purposes of describing their surface reactions. Also, note that although the anionic species of sulfate, phosphate, and borate are not contaminant species in HWIR, their concentration levels relative to trace metals in natural water can be such as to influence competition for sorption sites, so their constants are included below. The generic anion is represented by "A" with the charge indicated in the reaction. Where appropriate, "n" represents the unsigned charge of the anion.

#### Reactions for phosphate, arsenate, and vanadate



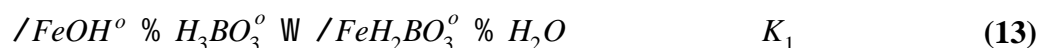
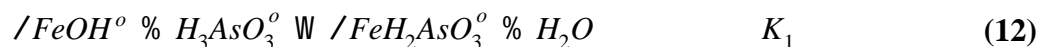
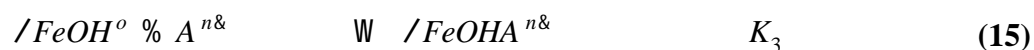
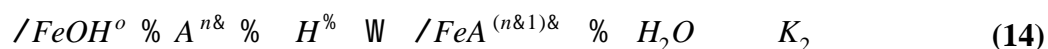
Reactions for arsenite and borateReactions for sulfate, selenate, selenite, chromate, molybdate, antimonate, and cyanide**2.1.4 Intrinsic Constants for Anions**

Table 2.2 presents values for the intrinsic constants as given by Dzombak and Morel (1990). They used linear free energy relationships (LFER) between the anions and their acidity constants ( $pK_a$ 's) to extrapolate some values for metals whose intrinsic constants were not derivable from experimental data. The use of LFER is predicated on the assumption that the relative site affinity among various anions reflects their relative affinities for protonation in solution. Values estimated from LFER (as opposed to those derived from experimental results) are indicated in Table 2.2 with an asterisk. The number of surface species needed to represent sorption on the HFO surface depends on the number of deprotonation reactions the anion undergoes within the range of relevant pH. Phosphate undergoes three deprotonations, so four surface reactions are required. An entry box crossed out in the table means that the surface constant is not applicable for that anion. A dash entry means that the constant is relevant, but its value could not be determined.

**Table 2.2 Intrinsic Sorption Constants for some Anions on HFO.**

Metal	$\log K_1^{intr}$	$\log K_2^{intr}$	$\log K_3^{intr}$	$\log K_4^{intr}$
H <sub>3</sub> AsO <sub>3</sub> <sup>0</sup>	5.41			
H <sub>3</sub> BO <sub>3</sub> <sup>0</sup>	0.62			
PO <sub>4</sub> <sup>3-</sup>	31.29	25.39	17.72	--
AsO <sub>4</sub> <sup>3-</sup>	29.31	23.51	--	10.58
VO <sub>4</sub> <sup>3-</sup>	--	—	—	13.57
SO <sub>4</sub> <sup>2-</sup>		7.78	0.79	
SeO <sub>4</sub> <sup>2-</sup>		7.73	0.80	
SeO <sub>3</sub> <sup>2-</sup>		12.69	5.17	
CrO <sub>4</sub> <sup>2-</sup>		10.85	3.9*	
MoO <sub>4</sub> <sup>2-</sup>		9.5*	2.4*	
SbO(OH) <sub>4</sub> <sup>-</sup>		8.4*	1.3*	
CN <sup>-</sup>		13.0*	5.7*	

The data in Table 5.2 represent a reasonably complete compilation for modeling the HWIR anions. The presence of only one constant for vanadate is the most detrimental omission. Dzombak and Morel (1990) note that this one constant is sufficient to describe the existing experimental data for vanadate sorption on HFO, but that this data corresponds to high pH and low sorption density only. Constants for other reactions are likely to be needed to describe vanadate sorption across the entire pH range of interest in HWIR. However, omission of the other constants will result in less sorption in the model, implying an environmentally conservative outcome. A LFER could, in principle, be used to estimate the missing constants, but the database of trivalent anions whose sorption constants are known is too small to develop a statistically sound relationship.

### 3.0 REVISED DATABASE FOR DIFFUSE-LAYER SORPTION ON HFO

The HFO diffuse-layer database is stored in the file FEO-DLM.DBS on the MINTEQA2 distribution diskettes. This file is not a part of the general thermodynamic database and is not directly used by MINTEQA2. Rather, the user invokes an option in PRODEFA2 to append the reactions in this file to the MINTEQA2 input file to be treated as added reactions for a particular model run. A revised FEO-

DLM.DBS file containing reactions that may be useful in the HWIR modeling is reproduced in Appendix A. This database has the reactions listed in Tables 2.1 and 2.2 with their associated constants and electrostatic terms. Reactions for protonation and deprotonation, as given in Dzombak and Morel (1990) are necessary to describe the complete set of surface species and to account for competition for binding sites.

#### 4.0 REFERENCES

- Allison, J.D., D.S. Brown, and K.J. Novo-Gradac (1991) *MINTEQA2/PRODEFA2, A Geochemical Assessment Model for Environmental Systems: Version 3.0 User's Manual*. United States Environmental Protection Agency, Office of Research and Development, Washington, DC, EPA/600/3-91/021, 106p.
- Dzombak, D.A., 1986. Toward a Uniform Model for the Sorption of Inorganic Ions on Hydrous Oxides, Ph.D. Dissertation, Massachusetts Institute of Technology, Cambridge, MA.
- Dzombak, D.A. and F.M.M. Morel, 1990. Surface Complexation Modeling: Hydrous Ferric Oxide, John Wiley and Sons, New York.
- US EPA (1996) EPA's composite model for leachate migration with transformation products (EPACMTP): Background document for metals. United States Environmental Protection Agency unpublished report, Office of Solid Waste, Washington, DC, 77p.
- World Health Organization, 1996. Thallium: Environmental Health Criteria 182, World Health Organization, Geneva.

**APPENDIX A**

**LISTING OF THE HFO DATABASE  
FOR MINTEQA2**

The following reactions presented for use in MINTEQA2. The HFO sorption reactions are as described by Dzombak and Morel (1990). In this compilation, the high affinity site is represented by MINTEQA2 component 811 and the low affinity site by component 812. Although there is no site affinity distinction for anions or for protons, separate reactions using components 811 and 812 are present (but using the same log *K* value for both sites) to correctly represent competition among all components.

```

2 78
8113302 =FeOH2+      0.0000  7.2900  0.000  0.000  1.00  0.00  0.00  0.0000
0.00 3  1.000 811  1.000 330  1.000 813  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
8113301 =FeO-        0.0000 -8.9300  0.000  0.000 -1.00  0.00  0.00  0.0000
0.00 3  1.000 811 -1.000 330 -1.000 813  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
8123302 =FeOH2+      0.0000  7.2900  0.000  0.000  1.00  0.00  0.00  0.0000
0.00 3  1.000 812  1.000 330  1.000 813  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
8123301 =FeO-        0.0000 -8.9300  0.000  0.000 -1.00  0.00  0.00  0.0000
0.00 3  1.000 812 -1.000 330 -1.000 813  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
8111000 =FeOHBa+2    0.0000  5.4600  0.000  0.000  2.00  0.00  0.00  0.0000
0.00 3  1.000 811  1.000 100  2.000 813  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
8121000 =FeOBa+      0.0000 -7.2000  0.000  0.000  1.00  0.00  0.00  0.0000
0.00 4  1.000 812  1.000 100 -1.000 330  1.000 813  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
8111500 =FeOHCa+2    0.0000  4.9700  0.000  0.000  2.00  0.00  0.00  0.0000
0.00 3  1.000 811  1.000 150  2.000 813  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
8121500 =FeOCa+      0.0000 -5.8500  0.000  0.000  1.00  0.00  0.00  0.0000
0.00 4  1.000 812  1.000 150 -1.000 330  1.000 813  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
8124600 =FeOMg+      0.0000 -4.6000  0.000  0.000  1.00  0.00  0.00  0.0000
0.00 4  1.000 812  1.000 460 -1.000 330  1.000 813  0.000  0  0.000  0
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0 0.000 0  0.000  0  0.000  0
8118700 =FeOTl       0.0000 -3.5000  0.000  0.000  0.00  0.00  0.00  0.0000
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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
8128700 =FeOTl       0.0000 -6.9000  0.000  0.000  0.00  0.00  0.00  0.0000
0.00 3  1.000 812  1.000 870 -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
8110200 =FeOAg       0.0000 -1.7200  0.000  0.000  0.00  0.00  0.00  0.0000

```

0.00 3 1.000 811 1.000 020 -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

8120200 =FeOAg 0.0000 -5.3000 0.000 0.000 0.00 0.00 0.00 0.0000  
 0.00 3 1.000 812 1.000 020 -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  
 8115400 =FeONi+ 0.0000 0.3700 0.000 0.000 1.00 0.00 0.00 0.0000  
 0.00 4 1.000 811 1.000 540 -1.000 330 1.000 813 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  
 8125400 =FeONi+ 0.0000 -2.5000 0.000 0.000 1.00 0.00 0.00 0.0000  
 0.00 4 1.000 812 1.000 540 -1.000 330 1.000 813 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  
 8112000 =FeOCO+ 0.0000 -0.4600 0.000 0.000 1.00 0.00 0.00 0.0000  
 0.00 4 1.000 811 1.000 200 -1.000 330 1.000 813 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  
 8122000 =FeOCO+ 0.0000 -3.0100 0.000 0.000 1.00 0.00 0.00 0.0000  
 0.00 4 1.000 812 1.000 200 -1.000 330 1.000 813 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  
 8111600 =FeOCD+ 0.0000 0.4700 0.000 0.000 1.00 0.00 0.00 0.0000  
 0.00 4 1.000 811 1.000 160 -1.000 330 1.000 813 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  
 8121600 =FeOCD+ 0.0000 -2.9000 0.000 0.000 1.00 0.00 0.00 0.0000  
 0.00 4 1.000 812 1.000 160 -1.000 330 1.000 813 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  
 8119500 =FeOZn+ 0.0000 0.9900 0.000 0.000 1.00 0.00 0.00 0.0000  
 0.00 4 1.000 811 1.000 950 -1.000 330 1.000 813 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  
 8129500 =FeOZn+ 0.0000 -1.9900 0.000 0.000 1.00 0.00 0.00 0.0000  
 0.00 4 1.000 812 1.000 950 -1.000 330 1.000 813 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  
 8112310 =FeOCu+ 0.0000 2.8900 0.000 0.000 1.00 0.00 0.00 0.0000  
 0.00 4 1.000 811 1.000 231 -1.000 330 1.000 813 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  
 8123100 =FeOCu+ 0.0000 0.6000 0.000 0.000 1.00 0.00 0.00 0.0000  
 0.00 4 1.000 812 1.000 231 -1.000 330 1.000 813 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  
 8116000 =FeOPb+ 0.0000 4.6500 0.000 0.000 1.00 0.00 0.00 0.0000  
 0.00 4 1.000 811 1.000 600 -1.000 330 1.000 813 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  
 8126000 =FeOPb+ 0.0000 0.3000 0.000 0.000 1.00 0.00 0.00 0.0000

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0.00 4 1.000 812 1.000 600 -1.000 330 1.000 813 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
8111100 =FeOBe+ 0.0000 5.7000 0.000 0.000 1.00 0.00 0.00 0.0000
0.00 4 1.000 811 1.000 110 -1.000 330 1.000 813 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
8121100 =FeOBe+ 0.0000 3.3000 0.000 0.000 1.00 0.00 0.00 0.0000
0.00 4 1.000 812 1.000 110 -1.000 330 1.000 813 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
8113610 =FeOHg+ 0.0000 13.9500 0.000 0.000 1.00 0.00 0.00 0.0000
0.00 5 1.000 811 1.000 361 -2.000 2 1.000 330 1.000 813 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
8123610 =FeOHg+ 0.0000 12.6400 0.000 0.000 1.00 0.00 0.00 0.0000
0.00 5 1.000 812 1.000 361 -2.000 2 1.000 330 1.000 813 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
8117900 =FeOSn+ 0.0000 15.1000 0.000 0.000 1.00 0.00 0.00 0.0000
0.00 5 1.000 811 1.000 790 -2.000 2 1.000 330 1.000 813 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
8127900 =FeOSn+ 0.0000 13.0000 0.000 0.000 1.00 0.00 0.00 0.0000
0.00 5 1.000 812 1.000 790 -2.000 2 1.000 330 1.000 813 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
8112110 =FeOCrOH+ 0.0000 11.6300 0.000 0.000 1.00 0.00 0.00 0.0000
0.00 4 1.000 811 1.000 211 -1.000 002 1.000 813 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
8110600 =FeH2AsO3 0.0000 5.4100 0.000 0.000 0.00 0.00 0.00 0.0000
0.00 3 1.000 811 1.000 60 -1.000 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 0.000 0 0.000 0 0.000 0
8120600 =FeH2AsO3 0.0000 5.4100 0.000 0.000 0.00 0.00 0.00 0.0000
0.00 3 1.000 812 1.000 60 -1.000 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 0.000 0 0.000 0 0.000 0
8110900 =FeH2BO3 0.0000 0.6200 0.000 0.000 0.00 0.00 0.00 0.0000
0.00 3 1.000 811 1.000 90 -1.000 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 0.000 0 0.000 0 0.000 0
8120900 =FeH2BO3 0.0000 0.6200 0.000 0.000 0.00 0.00 0.00 0.0000
0.00 3 1.000 812 1.000 90 -1.000 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 0.000 0 0.000 0 0.000 0
8115800 =FeH2PO4 0.0000 31.2900 0.000 0.000 0.00 0.00 0.00 0.0000
0.00 4 1.000 811 1.000 580 3.000 330 -1.000 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
8125800 =FeH2PO4 0.0000 31.2900 0.000 0.000 0.00 0.00 0.00 0.0000
0.00 4 1.000 812 1.000 580 3.000 330 -1.000 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

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8115801 =FeHPO4-      0.0000  25.3900  0.000  0.000-1.00 0.00 0.00  0.0000
  0.00 5  1.000 811  1.000 580  2.000 330  -1.000  2  -1.000 813  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
8125801 =FeHPO4-      0.0000  25.3900  0.000  0.000-1.00 0.00 0.00  0.0000
  0.00 5  1.000 812  1.000 580  2.000 330  -1.000  2  -1.000 813  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
8115802 =FePO4-2      0.0000  17.7200  0.000  0.000-2.00 0.00 0.00  0.0000
  0.00 5  1.000 811  1.000 580  1.000 330  -1.000  2  -2.000 813  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
8125802 =FePO4-2      0.0000  17.7200  0.000  0.000-2.00 0.00 0.00  0.0000
  0.00 5  1.000 812  1.000 580  1.000 330  -1.000  2  -2.000 813  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
8110610 =FeH2AsO4     0.0000  8.6100  0.000  0.000 0.00 0.00 0.00  0.0000
  0.00 3  1.000 811  1.000  61  -1.000  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 0.000  0  0.000  0  0.000  0
8120610 =FeH2AsO4     0.0000  8.6100  0.000  0.000 0.00 0.00 0.00  0.0000
  0.00 3  1.000 812  1.000  61  -1.000  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 0.000  0  0.000  0  0.000  0
8110611 =FeHAsO4-     0.0000  2.8100  0.000  0.000-1.00 0.00 0.00  0.0000
  0.00 5  1.000 811  1.000  61  -1.000  2  -1.000 330  -1.000 813  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
8120611 =FeHAsO4-     0.0000  2.8100  0.000  0.000-1.00 0.00 0.00  0.0000
  0.00 5  1.000 812  1.000  61  -1.000  2  -1.000 330  -1.000 813  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
8110613 =FeOHAsO4-3   0.0000 -10.1200  0.000  0.000-3.00 0.00 0.00  0.0000
  0.00 4  1.000 811  1.000  61  -3.000 330  -3.000 813  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
8120613 =FeOHAsO4-3   0.0000 -10.1200  0.000  0.000-3.00 0.00 0.00  0.0000
  0.00 4  1.000 812  1.000  61  -3.000 330  -3.000 813  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
8119031 =FeOHVO4-3    0.0000 -16.6300  0.000  0.000-3.00 0.00 0.00  0.0000
  0.00 5  1.000 811  1.000 903  2.000 002  -4.000 330  -3.000 813  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
8129031 =FeOHVO4-3    0.0000 -16.6300  0.000  0.000-3.00 0.00 0.00  0.0000
  0.00 5  1.000 812  1.000 903  2.000 002  -4.000 330  -3.000 813  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
8117320 =FeSO4-       0.0000  7.7800  0.000  0.000-1.00 0.00 0.00  0.0000
  0.00 5  1.000 811  1.000 732  1.000 330  -1.000 002  -1.000 813  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
8127320 =FeSO4-       0.0000  7.7800  0.000  0.000-1.00 0.00 0.00  0.0000
  0.00 5  1.000 812  1.000 732  1.000 330  -1.000 002  -1.000 813  0.000  0
  0.000  0  0.000  0  0.000  0  0.000  0  0.000  0  0.000  0

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0 0.000 0 0.000 0 0.000 0
8117321 =FeHSO4-2 0.0000 0.7900 0.000 0.000-2.00 0.00 0.00 0.0000
0.00 3 1.000 811 1.000 732 -2.000 813 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
8127321 =FeHSO4-2 0.0000 0.7900 0.000 0.000-2.00 0.00 0.00 0.0000
0.00 3 1.000 812 1.000 732 -2.000 813 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
8117610 =FeSeO3- 0.0000 4.2900 0.000 0.000-1.00 0.00 0.00 0.0000
0.00 4 1.000 811 1.000 761 -1.000 2 -1.000 813 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
8127610 =FeSeO3- 0.0000 4.2900 0.000 0.000-1.00 0.00 0.00 0.0000
0.00 4 1.000 812 1.000 761 -1.000 2 -1.000 813 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
8117611 =FeOHSeO3-2 0.0000 -3.2300 0.000 0.000-2.00 0.00 0.00 0.0000
0.00 4 1.000 811 1.000 761 -1.000 330 -2.000 813 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
8127611 =FeOHSeO3-2 0.0000 -3.2300 0.000 0.000-2.00 0.00 0.00 0.0000
0.00 4 1.000 812 1.000 761 -1.000 330 -2.000 813 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
8117620 =FeSeO4- 0.0000 7.7300 0.000 0.000-1.00 0.00 0.00 0.0000
0.00 5 1.000 811 1.000 762 1.000 330 -1.000 002 -1.000 813 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
8127620 =FeSeO4- 0.0000 7.7300 0.000 0.000-1.00 0.00 0.00 0.0000
0.00 5 1.000 812 1.000 762 1.000 330 -1.000 002 -1.000 813 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
8117621 =FeOHSeO4-2 0.0000 0.8000 0.000 0.000-2.00 0.00 0.00 0.0000
0.00 3 1.000 811 1.000 762 -2.000 813 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
8127621 =FeOHSeO4-2 0.0000 0.8000 0.000 0.000-2.00 0.00 0.00 0.0000
0.00 3 1.000 812 1.000 762 -2.000 813 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
8112120 =FeCrO4- 0.0000 10.8500 0.000 0.000-1.00 0.00 0.00 0.0000
0.00 5 1.000 811 1.000 212 1.000 330 -1.000 002 -1.000 813 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
8122120 =FeCrO4- 0.0000 10.8500 0.000 0.000-1.00 0.00 0.00 0.0000
0.00 5 1.000 812 1.000 212 1.000 330 -1.000 002 -1.000 813 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
8112121 =FeOHCrO4-2 0.0000 3.9000 0.000 0.000-2.00 0.00 0.00 0.0000
0.00 3 1.000 811 1.000 212 -2.000 813 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
8122121 =FeOHCrO4-2 0.0000 3.9000 0.000 0.000-2.00 0.00 0.00 0.0000
0.00 3 1.000 812 1.000 212 -2.000 813 0.000 0 0.000 0 0.000 0

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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
8114800 =FeMoO4- 0.0000 9.5000 0.000 0.000-1.00 0.00 0.00 0.0000
0.00 5 1.000 811 1.000 480 1.000 330 -1.000 002 -1.000 813 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
8124800 =FeMoO4- 0.0000 9.5000 0.000 0.000-1.00 0.00 0.00 0.0000
0.00 5 1.000 812 1.000 480 1.000 330 -1.000 002 -1.000 813 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
8114801 =FeOHMoO4-2 0.0000 2.4000 0.000 0.000-2.00 0.00 0.00 0.0000
0.00 3 1.000 811 1.000 480 -2.000 813 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
8124801 =FeOHMoO4-2 0.0000 2.4000 0.000 0.000-2.00 0.00 0.00 0.0000
0.00 3 1.000 812 1.000 480 -2.000 813 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
8117410 =FeSbO(OH)4 0.0000 8.4000 0.000 0.000 0.00 0.00 0.00 0.0000
0.00 4 1.000 811 1.000 741 1.000 330 -2.000 002 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
8127410 =FeSbO(OH)4 0.0000 8.4000 0.000 0.000 0.00 0.00 0.00 0.0000
0.00 4 1.000 812 1.000 741 1.000 330 -2.000 002 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
8117411 =FeOHSbO(OH)4 0.0000 1.3000 0.000 0.000-1.00 0.00 0.00 0.0000
0.00 4 1.000 811 1.000 741 -1.000 002 -1.000 813 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
8127411 =FeOHSbO(OH)4 0.0000 1.3000 0.000 0.000-1.00 0.00 0.00 0.0000
0.00 4 1.000 812 1.000 741 -1.000 002 -1.000 813 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
8111430 =FeCN 0.0000 13.0000 0.000 0.000 0.00 0.00 0.00 0.0000
0.00 4 1.000 811 1.000 143 1.000 330 -1.000 002 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
8121430 =FeCN 0.0000 13.0000 0.000 0.000 0.00 0.00 0.00 0.0000
0.00 4 1.000 812 1.000 143 1.000 330 -1.000 002 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
8111431 =FeOHCN- 0.0000 5.7000 0.000 0.000-1.00 0.00 0.00 0.0000
0.00 3 1.000 811 1.000 143 -1.000 813 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
8121431 =FeOHCN- 0.0000 5.7000 0.000 0.000-1.00 0.00 0.00 0.0000
0.00 3 1.000 812 1.000 143 -1.000 813 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

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