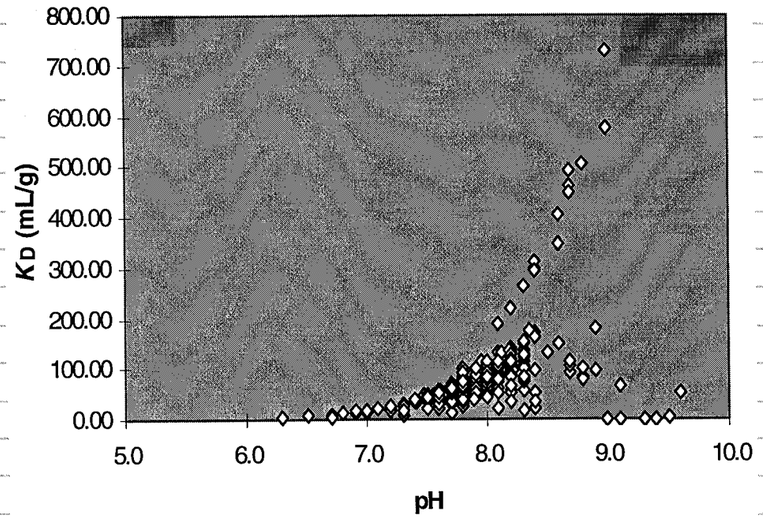
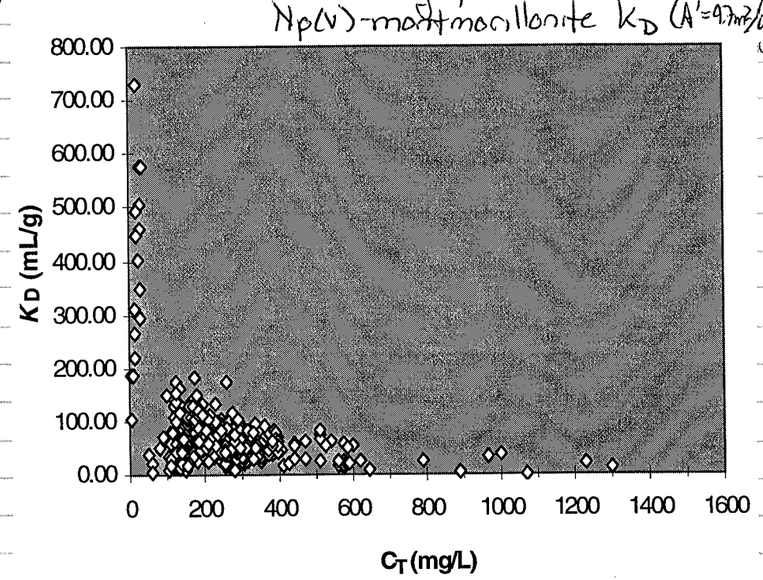
6/4/98 DRL



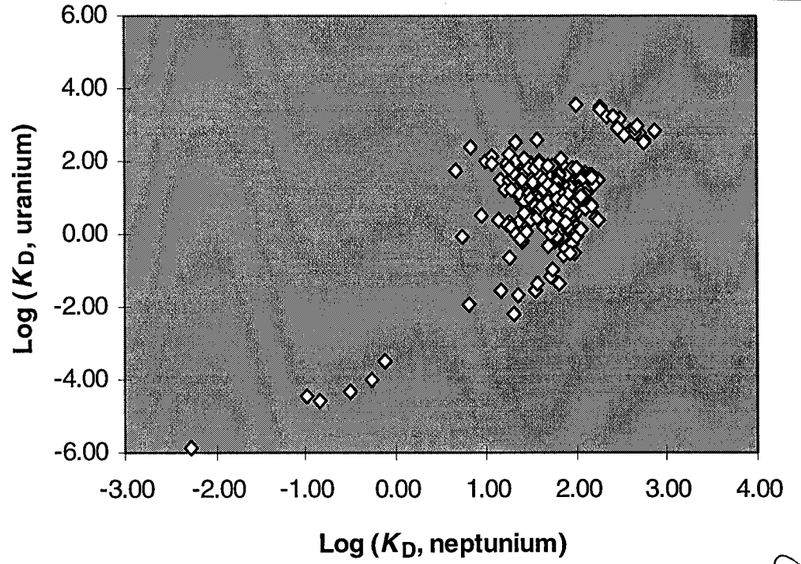

DRLumm

Correct graphs for
Np(V)-montmorillonite $K_D$ ($A' = 97 m^2/g$)






6/4/98 DRL

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The recalculated log $K_D$ for Np(V)-montmorillonite also has a slightly greater correlation to U(VI) of 0.6 (see previous log $K_D$ [Np(V)]-log $K_D$ [U(VI)] plot) as opposed to the value of 0.5 originally used in the report:

| | |
|---|---|
| Covariance | 0.250482 |
| Correlation | 0.609696 |

Change pages (4-5 through 4-9 & 4-11) sent to distribution list on 4/29/98 deliverable

6/5/98 (DR)

**Developing sorption coefficient statistics for input into TPA.**

As described previously, one goal of this work has been to develop information that can be used to incorporate, at least indirectly, the effects of chemistry on radionuclide sorption coefficients. Based on the method outlined in Pabalan et al. (1998), Bertetti et al. (1998), and Turner (1998), we have used the Diffuse-Layer Model (DLM) to model sorption for the range in water chemistries represented by the data of Perfect et al. (1995).

Assumptions include:

- Sorption behavior as a function of pH and carbonate concentration is similar for aluminosilicate minerals when expressed in terms of $K_D$/A', where A' is the effective surface area (BET surface area in the case of nonporous minerals, 10 % of BET in the case of sheet minerals such as montmorillonite, gibbsite, and kaolinite). Also implicit in this assumption is that aluminosilicate minerals will dominate sorption in the tuff units at YM.
- The effect outlined above has been demonstrated for U(VI) and Np(V) (Pabalan et al., 1998 and Bertetti et al., 1998). It is assumed that it is also true for other actinides such as Am(III), Pu(V), and Th(IV).
- The mean pore size in the matrix at YM is 0.1 μm (Travis and Nuttall, 1987), which is assumed to be true for all hydrostratigraphic units used in TPA.
- The water chemistries of Perfect et al. (1995) as screened and culled in Turner (1998) represent the likely range in water chemistry at YM.
- As appropriate, mean values from tpa.inp for solubility limits, density, and porosity are used in DLM simulations.

The steps involved in this modeling exercise are:

1. Identify sorption experiments that can be used to calibrate the DLM parameters.

   We used the following sorption experiments for Am(III), Th(IV), and Pu(V) sorption on γ-alumina (Righetto et al., 1988; 1991); Np(V) and U(VI) sorption on montmorillonite (Turner et al., 1998a; Pabalan and Turner, 1997). DLM parameters were determined assuming A' = 10 % of BET measured area for both γ-alumina (BET=130 $m^2/g$; A'=13.0 $m^2/g$) and montmorillonite (BET=97 $m^2/g$; A'=9.7 $m^2/g$).

2. Determine the DLM parameters for these experiments.

   The DLM parameters in Turner et al. (1998a) and Pabalan and Turner (1997) were used for Np(V)- and U(VI)-montmorillonite. The computer code FITEQL, Version 2.0 was used to determine DLM parameters for Am(III)-, Pu(V)-, and Th(IV)- γ-alumina. Turner (1995) used FITEQL with the BET surface area for γ-alumina (130 $m^2/g$), to determine that the surface species >AlOAm$^{+2}$, >AlOPuO2$^{o}$, and >AlOTh$^{+3}$ were adequate to fit the data. We reinterpreted the data using A' = 13.0 $m^2/g$ and the updated CNWRA radionuclide database [updated Am(III) data to the NEA database and PuO2+ data to the EQ3/6 database (data0.com.r2, 02aug95)] to derive new binding constants:



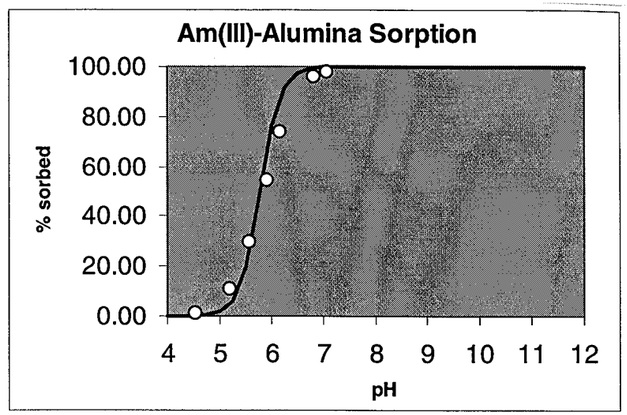
6/5/98 (DR)

| Radionuclide-Mineral | Surface Complex | Binding constant | Reference |
|---|---|---|---|
| Np(V)-montmorillonite | >AlO$^-$ | -9.73 | Turner et al. (1998a) |
| | >AlOH$_2^+$ | 8.33 | Turner et al. (1998a) |
| | >SiO$^-$ | -7.20 | Turner et al. (1998a) |
| | >AlO-NpO$_2$(OH)$^-$ | -13.79 | Turner et al. (1998a) |
| | >SiOH-NpO$_2^+$ | 4.05 | Turner et al. (1998a) |
| U(VI)-montmorillonite | >AlO$^-$ | -9.73 | Pabalan and Turner (1997) |
| | >AlOH$_2^+$ | 8.33 | Pabalan and Turner (1997) |
| | >SiO$^-$ | -7.20 | Pabalan and Turner (1997) |
| | >AlO-UO$_2^+$ | 2.70 | Pabalan and Turner (1997) |
| | >SiO-UO$_2^+$ | 2.60 | Pabalan and Turner (1997) |
| | >AlO-(UO$_2$)$_3$(OH)$_5^o$ | -14.95 | Pabalan and Turner (1997) |
| | >SiO-(UO$_2$)$_3$(OH)$_5^o$ | -15.29 | Pabalan and Turner (1997) |
| Am(III)-γ alumina | >AlO$^-$ | -9.73 | Turner and Sassman (1996) |
| | >AlOH$_2^+$ | 8.33 | Turner and Sassman (1996) |
| | >AlO-Am$^{2+}$ | 4.66 | This study [modified Turner(1995)] |
| Pu(V)-γ alumina | >AlO$^-$ | -9.73 | Turner and Sassman (1996) |
| | >AlOH$_2^+$ | 8.33 | Turner and Sassman (1996) |
| | >AlO-PuO$_2^o$ | -2.18 | This study [modified Turner(1995)] |
| Th(IV)-γ alumina | >AlO$^-$ | -9.73 | Turner and Sassman (1996) |
| | >AlOH$_2^+$ | 8.33 | Turner and Sassman (1996) |
| | >AlO-Th$^{3+}$ | 15.3 | This study [modified Turner(1995)] |

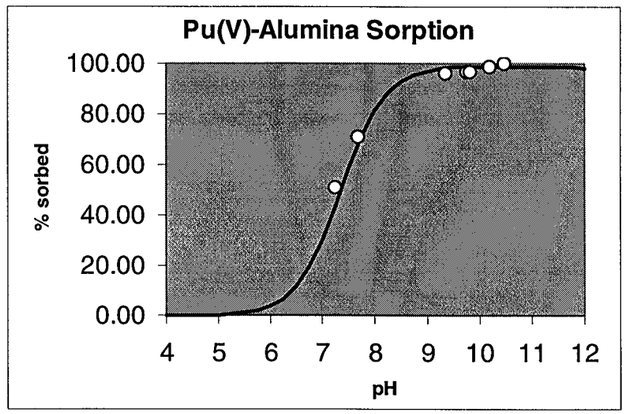
The models for U(VI) and Np(V)-montmorillonite have been demonstrated in Pabalan and Turner (1997) and Turner et al. (1998a), respectively. The DLM for Am(III)-, Pu(V)-, and Th(IV)- γ-alumina are shown here.

DLM: Model Calibration for Am(III), Pu(V), Th(IV) & alumina

Righetto et al. (1988)
$Am(III)_{total}$ = 5E-11 M
M/V = 0.01 g/L (γ alumina)
BET = 130 $m^2/g$
A' = 13.0 $m^2/g$
$T_{XOH}$ = 4.990E-07 M




Righetto et al. (1991)
$Pu(V)_{total}$ = 2e-10 M
M/V = 0.20 g/L (γ alumina)
BET = 130 $m^2/g$
A' = 13.0 $m^2/g$
$T_{XOH}$ = 9.972E-06 M




Righetto et al. (1988)
$Th(IV)_{total}$ = 1e-11 M
M/V = 0.01 g/L (γ alumina)
BET = 130 $m^2/g$
A' = 13.0 $m^2/g$
$T_{XOH}$ = 4.990E-07 M

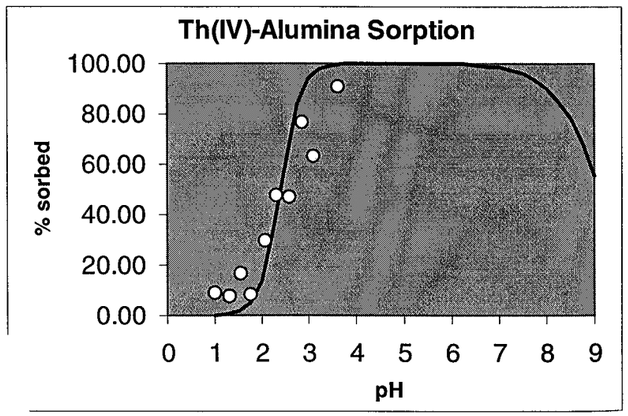



Figure 5.



DLM: Model Calibration for Np(V)-montmorillonite.



Information potentially subject to copyright protection was redacted from this location. The redacted material (two graphs) is from the following reference:

Turner, D.R., R.T. Pabalan, and F.P. Bertetti. "Neptunium(V) Sorption on Montmorillonite: An experimental and Surface Complexation Modeling Study. Clays and Clay Materials. 1998

6/5/98 DRJ

DLM: Model Calibration for U(VI).



Information potentially subject to copyright protection was redacted from this location. The redacted material (graphs) is from the following reference:

Pabalan, R.T. and D.R. Turner. "Uranium(6+) Sorption on Montmorillonite: Experimental and Surface Complexation Modeling Study. Aqueous Geochemistry. Vol. 2. pp. 203-226. 1997.

*Figure 4.*



With the DLM parameters presented in the previous table, MINTEQA2 input files were prepared for the 460 analyses in the culled Perfect et al. (1995) database. The mean solubility limit from TPA 3.1.4 is used for the radionuclide concentrations of Am(III), Pu(V), and Th(IV). Radionuclide concentrations for Np(V) and U(VI) were set at 1E-6 M. Work presented in Turner (1995) and Turner et al. (1998) suggest sorption expressed in terms of $K_D$ and $K_A$, are relatively insenstive to radionuclide concentration:

6/5/98 DRJ

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## Am(III)-γ alumina

```
MANSE SPRING NESESW 3-21S-54E NYE ;SampID=492-SPRING   ;ArcID=492
UTM=4000644.3 North; 599584.8 East; Date=10/28/64
23.90 MG/L    0.000  0.00000E-01
0 0 1 0 3 0 0 0 1 1 0 0 0
4   1   7
1.000E+00   13.00 0.000 0.000 81
    330  0.000E-01   -7.30 y                    /H+1
    040  1.200E-01   -6.30 y                    /Am+3
    150  0.500E+02   -2.90 y                    /Ca+2
    460  0.220E+02   -3.04 y                    /Mg+2
    500  0.470E+01   -3.69 y                    /Na+1
    410  0.900E+00   -4.64 y                    /K+1
    180  0.310E+01   -4.06 y                    /Cl-1
    732  0.270E+02   -3.55 y                    /SO4-2
    140  0.240E+03   -2.41 y                    /CO3-2
    492  0.800E+00   -4.89 y                    /NO3-1
    770  0.813E+01   -3.87 y                    /H4SiO4
    281  0.200E-01   -6.45 y                    /Fe+3
    813  0.000E-01    0.00 y                    /ADS1PSIo
    811  4.986E-05   -4.30 y                    /ADS1TYP1

  3   1
    330      7.3000      0.0000                 /H+1
  6   1
    813      0.0000      0.0000                 /ADS1PSIo

  2   3
8113300 >AlO-            0.0000   -9.0500   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 >AlOH2+          0.0000    6.8500   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
8110400 >AlOAm+2         0.0000    4.6600   0.000   0.000 2.00 0.00 0.00   0.0000
 0.00 4   1.000 811   1.000 040  -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
```

## Pu(V)-γ alumina

```
MANSE SPRING NESESW 3-21S-54E NYE ;SampID=492-SPRING   ;ArcID=492
UTM=4000644.3 North; 599584.8 East; Date=10/28/64
23.90 MG/L    0.000  0.00000E-01
0 0 1 0 3 0 0 0 1 1 0 0 0
4   1   7
1.000E+00   13.00 0.000 0.000 81
    330  0.000E-01   -7.30 y                    /H+1
    642  1.200E-01   -6.36 y                    /PuO2+1
    150  0.500E+02   -2.90 y                    /Ca+2
    460  0.220E+02   -3.04 y                    /Mg+2
    500  0.470E+01   -3.69 y                    /Na+1
    410  0.900E+00   -4.64 y                    /K+1
    180  0.310E+01   -4.06 y                    /Cl-1
    732  0.270E+02   -3.55 y                    /SO4-2
    140  0.240E+03   -2.41 y                    /CO3-2
    492  0.800E+00   -4.89 y                    /NO3-1
    770  0.813E+01   -3.87 y                    /H4SiO4
    281  0.200E-01   -6.45 y                    /Fe+3
    813  0.000E-01    0.00 y                    /ADS1PSIo
    811  4.986E-05   -4.30 y                    /ADS1TYP1

  3   1
    330      7.3000      0.0000                 /H+1
  6   1
    813      0.0000      0.0000                 /ADS1PSIo

  2   3
8113300 >AlO-            0.0000   -9.0500   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 >AlOH2+          0.0000    6.8500   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
8116420 >AlOPuO2         0.0000   -2.1800   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 3   1.000 811   1.000 642  -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
```

6/5/98
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## Th(IV)-γ alumina

```
MANSE SPRING NESESW 3-21S-54E NYE ;SampID=492-SPRING    ;ArcID=492
UTM=4000644.3 North; 599584.8 East; Date=10/28/64
23.90 MG/L    0.000  0.00000E-01
0 0 1 0 3 0 0 0 1 1 0 0 0
4   1   7
1.000E+00    13.00 0.000 0.000 81
     330  0.000E-01    -7.30 y                    /H+1
     866  2.300E-01    -6.01 y                    /Th+4
     150  0.500E+02    -2.90 y                    /Ca+2
     460  0.220E+02    -3.04 y                    /Mg+2
     500  0.470E+01    -3.69 y                    /Na+1
     410  0.900E+00    -4.64 y                    /K+1
     180  0.310E+01    -4.06 y                    /Cl-1
     732  0.270E+02    -3.55 y                    /SO4-2
     140  0.240E+03    -2.41 y                    /CO3-2
     492  0.800E+00    -4.89 y                    /NO3-1
     770  0.813E+01    -3.87 y                    /H4SiO4
     281  0.200E-01    -6.45 y                    /Fe+3
     813  1.000E-07    -7.00 y                    /ADS1PSIo
     811  4.986E-05    -4.30 y                    /ADS1TYP1

  3   1
     330      7.3000      0.0000                  /H+1
  6   1
     813      0.0000      0.0000                  /ADS1PSIo

  2   3
8113300 >AlO-              0.0000    -9.0500    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 >AlOH2+            0.0000     6.8500    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
8118660 >AlOTh+3           0.0000    15.3000    0.000    0.000 3.00 0.00 0.00    0.0000
 0.00 4    1.000 811    1.000 866   -1.000 330    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
```

Running these MINTEQA2 models allows generation of sorption coefficients for the observed ranges in water chemistry for the five radionuclide-mineral systems considered here. Normalized to effective surface area $K_A$, of the minerals used in the calibration experiments, and assuming that the pH- and $PCO_2$-dependent sorption behavior is similar for aluminosilicates, these sorption coefficient distributions can be recast in terms of $K_D$ for each of the hydrostratigraphic units used in TPA.

The log $K_A$, distributions and descriptive statistics calculated using Microsoft Excel 97 are given here:

**Descriptive Statistics**

| log $K_A$, (mL/m$^2$) | *Am(III)* | *Np(V)* | *Pu(V)* | *Th(IV)* | *U(VI)* |
|---|---|---|---|---|---|
| Mean | 6.54859 | 0.742079 | 2.706992 | 4.248341 | -0.03166 |
| Standard Error | 0.034889 | 0.019686 | 0.01421 | 0.027168 | 0.045466 |
| Median | 6.539491 | 0.773163 | 2.714884 | 4.329547 | 0.001593 |
| Mode | 6.337242 | 0.737717 | 2.650028 | 4.438974 | -0.15772 |
| Standard Deviation | 0.748294 | 0.422223 | 0.304776 | 0.582685 | 0.975139 |
| Sample Variance | 0.559944 | 0.178273 | 0.092889 | 0.339521 | 0.950896 |
| Kurtosis | 1.924308 | 26.57647 | 5.055398 | 34.22761 | 12.92837 |
| Skewness | 0.118437 | -3.55611 | -0.14772 | -4.41437 | -2.3184 |
| Range | 5.958202 | 5.140419 | 2.97415 | 7.714598 | 9.407036 |
| Minimum | 3.16042 | -3.26427 | 0.906492 | -1.77969 | -6.83733 |
| Maximum | 9.118622 | 1.876154 | 3.880642 | 5.934907 | 2.569708 |
| Sum | 3012.351 | 341.3565 | 1245.216 | 1954.237 | -14.5616 |
| Count | 460 | 460 | 460 | 460 | 460 |
| Confidence Level(95.0%) | 0.068563 | 0.038686 | 0.027925 | 0.053389 | 0.089347 |

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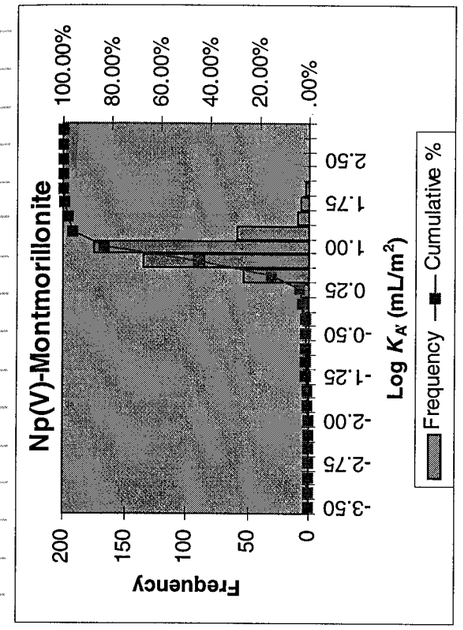


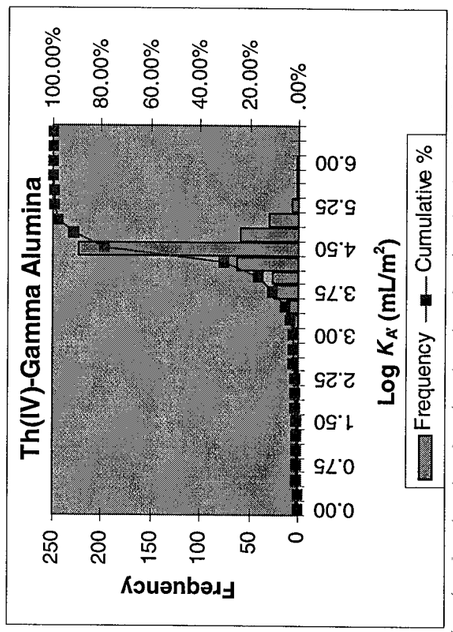


6/5/98
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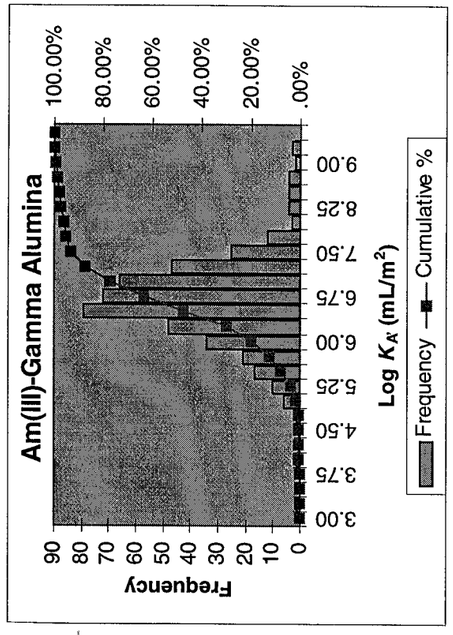


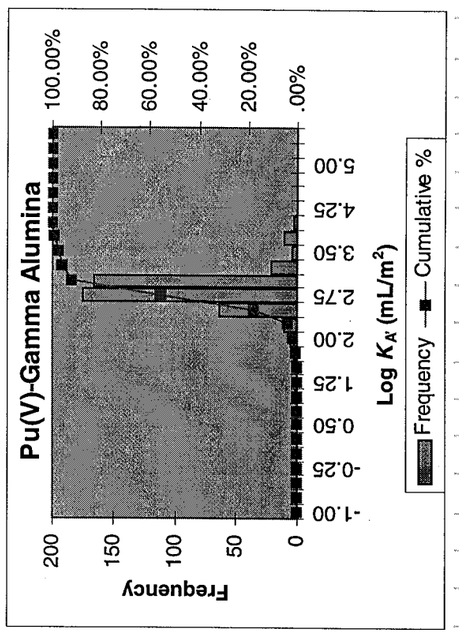

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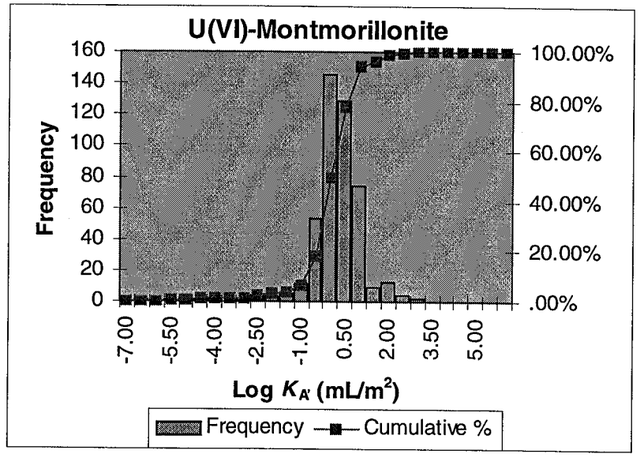


The distributions for each radionuclide appear to be log normal, although the kurtosis of the distributions varies. The final step in using this information in TPA is to apply this distribution to each hydrostratigraphic unit and transform the $K_A$ into $K_D$ (in mL/g). Assuming that aluminosilicates will dominate sorption in these units, it follows that the chemical dependent sorption behavior, and therefore these distributions, should hold for each unit. The key parameter for each transform to $K_A$ will therefore be the surface area.

Arthur (1996) presents a relationship among porosity, dry density, and pore radius such that:

DRJ mm

$$\text{Specific Surface Area} = \frac{3\phi_r}{\rho_r \mathrm{r}}$$

where $\phi_r$ is porosity of the rock, $\rho_r$ is density of the rock in g/m$^3$, and r is the radius of the pore in meters. For the YM region, parameter values were taken from the input file for TPA 3.1.4. The value for the pore radius was set at 0.05 μm based on work by Travis and Nuttall (1987) that suggests that more than 50 percent (median value) of the pores are less than 0.1 μm in diameter. Parameter values and calculated surface area is presented here. It is interesting to note that the calculated surface areas agree very well with measured surface areas (2.6 to 10 m$^2$/g) reported for total surface areas of tuff samples in Triay et al. (1996):

| Unit | $\phi_r$ (m$^3$/m$^3$) | $\rho_r$ (g/m$^3$) | r (m) | Surface area (m$^2$/g) |
|---|---|---|---|---|
| TSw | 0.12 | 2.46E+3 | 5.0E-08 | 2.9 |
| CHnv | 0.33 | 2.26E+3 | 5.0E-08 | 8.8 |
| CHnz | 0.32 | 2.40E+3 | 5.0E-08 | 8.0 |
| PPw | 0.28 | 2.54E+3 | 5.0E-08 | 6.6 |
| UCF | 0.28 | 2.42E+3 | 5.0E-08 | 6.9 |
| BFw | 0.12 | 2.57E+3 | 5.0E-08 | 2.8 |
| UFZ | 0.12 | 2.63E+3 | 5.0E-08 | 2.7 |



6/5/98 DRJ

By using the relationship $K_A$*(A')= $K_D$, sorption coefficients are determined for each radionuclide (5 total) for each of seven hydrostratigraphic units (in m$^3$/g = 1000 mL/g):

| Log KD(m3/kg) | Am(III)-TSw | Am(III)-CHnv | Am(III)-CHnz | Am(III)-PPw | Am(III)-UCF | Am(III)-BFw | Am(III)-UFZ |
|---|---|---|---|---|---|---|---|
| Mean | 4.0109879 | 4.4930726 | 4.4516799 | 4.3681338 | 4.387439 | 3.9957479 | 3.9799537 |
| Standard Error | 0.0348894 | 0.0348894 | 0.0348894 | 0.0348894 | 0.0348894 | 0.0348894 | 0.0348894 |
| Median | 4.0018887 | 4.4839733 | 4.4425807 | 4.3590346 | 4.3783398 | 3.9866487 | 3.9708544 |
| Mode | 3.7996402 | 4.2817248 | 4.2403322 | 4.1567861 | 4.1760913 | 3.7844002 | 3.7686059 |
| Standard Deviation | 0.7482941 | 0.7482941 | 0.7482941 | 0.7482941 | 0.7482941 | 0.7482941 | 0.7482941 |
| Sample Variance | 0.559944 | 0.559944 | 0.559944 | 0.559944 | 0.559944 | 0.559944 | 0.559944 |
| Kurtosis | 1.9243078 | 1.9243078 | 1.9243078 | 1.9243078 | 1.9243078 | 1.9243078 | 1.9243078 |
| Skewness | 0.1184368 | 0.1184368 | 0.1184368 | 0.1184368 | 0.1184368 | 0.1184368 | 0.1184368 |
| Range | 5.9582018 | 5.9582018 | 5.9582018 | 5.9582018 | 5.9582018 | 5.9582018 | 5.9582018 |
| Minimum | 0.6228182 | 1.1049028 | 1.0635102 | 0.9799641 | 0.9992693 | 0.6075782 | 0.5917839 |
| Maximum | 6.5810199 | 7.0631046 | 7.0217119 | 6.9381659 | 6.957471 | 6.56578 | 6.5499857 |
| Sum | 1845.0544 | 2066.8134 | 2047.7727 | 2009.3416 | 2018.2219 | 1838.044 | 1830.7787 |
| Count | 460 | 460 | 460 | 460 | 460 | 460 | 460 |
| Confidence Level(95.0%) | 0.0685627 | 0.0685627 | 0.0685627 | 0.0685627 | 0.0685627 | 0.0685627 | 0.0685627 |

| Log KD(m3/kg) | Np(V)-TSw | Np(V)-CHnv | Np(V)-CHnz | Np(V)-PPw | Np(V)-UCF | Np(V)-BFw | Np(V)-UFZ |
|---|---|---|---|---|---|---|---|
| Mean | -1.7955226 | -1.313438 | -1.3548307 | -1.4383767 | -1.4190716 | -1.8107626 | -1.8265569 |
| Standard Error | 0.0196863 | 0.0196863 | 0.0196863 | 0.0196863 | 0.0196863 | 0.0196863 | 0.0196863 |
| Median | -1.7644388 | -1.2823542 | -1.3237468 | -1.4072929 | -1.3879877 | -1.7796788 | -1.7954731 |
| Mode | -1.7998849 | -1.3178002 | -1.3591929 | -1.442739 | -1.4234338 | -1.8151249 | -1.8309191 |
| Standard Deviation | 0.4222233 | 0.4222233 | 0.4222233 | 0.4222233 | 0.4222233 | 0.4222233 | 0.4222233 |
| Sample Variance | 0.1782725 | 0.1782725 | 0.1782725 | 0.1782725 | 0.1782725 | 0.1782725 | 0.1782725 |
| Kurtosis | 26.576465 | 26.576465 | 26.576465 | 26.576465 | 26.576465 | 26.576465 | 26.576465 |
| Skewness | -3.5561097 | -3.5561097 | -3.5561097 | -3.5561097 | -3.5561097 | -3.5561097 | -3.5561097 |
| Range | 5.1404194 | 5.1404194 | 5.1404194 | 5.1404194 | 5.1404194 | 5.1404194 | 5.1404194 |
| Minimum | -5.8018677 | -5.319783 | -5.3611757 | -5.4447217 | -5.4254166 | -5.8171076 | -5.8329019 |
| Maximum | -0.6614482 | -0.1793635 | -0.2207562 | -0.3043023 | -0.2849971 | -0.6766882 | -0.6924825 |
| Sum | -825.94042 | -604.18147 | -623.2221 | -661.65329 | -652.77291 | -832.9508 | -840.21616 |
| Count | 460 | 460 | 460 | 460 | 460 | 460 | 460 |
| Confidence Level(95.0%) | 0.0386864 | 0.0386864 | 0.0386864 | 0.0386864 | 0.0386864 | 0.0386864 | 0.0386864 |

DRJ mm

| Log KD(m3/kg) | Pu(V)-TSw | Pu(V)-CHnv | Pu(V)-CHnz | Pu(V)-PPw | Pu(V)-UCF | Pu(V)-BFw | Pu(V)-UFZ |
|---|---|---|---|---|---|---|---|
| Mean | 0.1693902 | 0.6514749 | 0.6100822 | 0.5265361 | 0.5458413 | 0.1541502 | 0.138356 |
| Standard Error | 0.0142103 | 0.0142103 | 0.0142103 | 0.0142103 | 0.0142103 | 0.0142103 | 0.0142103 |
| Median | 0.1772819 | 0.6593666 | 0.6179739 | 0.5344279 | 0.553733 | 0.162042 | 0.1462477 |
| Mode | 0.1124258 | 0.5945105 | 0.5531178 | 0.4695718 | 0.4888769 | 0.0971859 | 0.0813916 |
| Standard Deviation | 0.3047764 | 0.3047764 | 0.3047764 | 0.3047764 | 0.3047764 | 0.3047764 | 0.3047764 |
| Sample Variance | 0.0928886 | 0.0928886 | 0.0928886 | 0.0928886 | 0.0928886 | 0.0928886 | 0.0928886 |
| Kurtosis | 5.0553979 | 5.0553979 | 5.0553979 | 5.0553979 | 5.0553979 | 5.0553979 | 5.0553979 |
| Skewness | -0.1477231 | -0.1477231 | -0.1477231 | -0.1477231 | -0.1477231 | -0.1477231 | -0.1477231 |
| Range | 2.9741497 | 2.9741497 | 2.9741497 | 2.9741497 | 2.9741497 | 2.9741497 | 2.9741497 |
| Minimum | -1.6311101 | -1.1490254 | -1.1904181 | -1.2739641 | -1.254659 | -1.64635 | -1.6621443 |
| Maximum | 1.3430397 | 1.8251244 | 1.7837317 | 1.7001856 | 1.7194908 | 1.3277997 | 1.3120054 |
| Sum | 77.919493 | 299.67844 | 280.63781 | 242.20662 | 251.087 | 70.909108 | 63.643745 |
| Count | 460 | 460 | 460 | 460 | 460 | 460 | 460 |
| Confidence Level(95.0%) | 0.0279252 | 0.0279252 | 0.0279252 | 0.0279252 | 0.0279252 | 0.0279252 | 0.0279252 |

| Log KD(m3/kg) | Th(IV)-TSw | Th(IV)-CHnv | Th(IV)-CHnz | Th(IV)-PPw | Th(IV)-UCF | Th(IV)-BFw | Th(IV)-UFZ |
|---|---|---|---|---|---|---|---|
| Mean | 1.7107391 | 2.1928238 | 2.1514311 | 2.067885 | 2.0871902 | 1.6954991 | 1.6797049 |
| Standard Error | 0.0271678 | 0.0271678 | 0.0271678 | 0.0271678 | 0.0271678 | 0.0271678 | 0.0271678 |
| Median | 1.7919453 | 2.27403 | 2.2326373 | 2.1490913 | 2.1683964 | 1.7767054 | 1.7609111 |
| Mode | 1.9013719 | 2.3834566 | 2.3420639 | 2.2585178 | 2.277823 | 1.8861319 | 1.8703377 |
| Standard Deviation | 0.5826846 | 0.5826846 | 0.5826846 | 0.5826846 | 0.5826846 | 0.5826846 | 0.5826846 |
| Sample Variance | 0.3395214 | 0.3395214 | 0.3395214 | 0.3395214 | 0.3395214 | 0.3395214 | 0.3395214 |
| Kurtosis | 34.22761 | 34.22761 | 34.22761 | 34.22761 | 34.22761 | 34.22761 | 34.22761 |
| Skewness | -4.4143746 | -4.4143746 | -4.4143746 | -4.4143746 | -4.4143746 | -4.4143746 | -4.4143746 |
| Range | 7.7145982 | 7.7145982 | 7.7145982 | 7.7145982 | 7.7145982 | 7.7145982 | 7.7145982 |
| Minimum | -4.3172929 | -3.8352082 | -3.8766009 | -3.9601469 | -3.9408418 | -4.3325328 | -4.3483271 |
| Maximum | 3.3973053 | 3.87939 | 3.8379973 | 3.7544512 | 3.7737564 | 3.3820653 | 3.3662711 |
| Sum | 786.93998 | 1008.6989 | 989.6583 | 951.22712 | 960.10749 | 779.9296 | 772.66424 |
| Count | 460 | 460 | 460 | 460 | 460 | 460 | 460 |
| Confidence Level(95.0%) | 0.0533887 | 0.0533887 | 0.0533887 | 0.0533887 | 0.0533887 | 0.0533887 | 0.0533887 |

6/5/98 DRJ

| Log KD(m3/kg) | U(VI)-TSw | U(VI)-CHnv | U(VI)-CHnz | U(VI)-PPw | U(VI)-UCF | U(VI)-BFw | U(VI)-UFZ |
|---|---|---|---|---|---|---|---|
| Mean | -2.5692576 | -2.0871729 | -2.1285656 | -2.2121116 | -2.1928065 | -2.5844975 | -2.6002918 |
| Standard Error | 0.0454661 | 0.0454661 | 0.0454661 | 0.0454661 | 0.0454661 | 0.0454661 | 0.0454661 |
| Median | -2.5360089 | -2.0539242 | -2.0953169 | -2.178863 | -2.1595578 | -2.5512489 | -2.5670431 |
| Mode | -2.6953176 | -2.213233 | -2.2546257 | -2.3381717 | -2.3188666 | -2.7105576 | -2.7263519 |
| Standard Deviation | 0.9751387 | 0.9751387 | 0.9751387 | 0.9751387 | 0.9751387 | 0.9751387 | 0.9751387 |
| Sample Variance | 0.9508956 | 0.9508956 | 0.9508956 | 0.9508956 | 0.9508956 | 0.9508956 | 0.9508956 |
| Kurtosis | 12.928374 | 12.928374 | 12.928374 | 12.928374 | 12.928374 | 12.928374 | 12.928374 |
| Skewness | -2.3183959 | -2.3183959 | -2.3183959 | -2.3183959 | -2.3183959 | -2.3183959 | -2.3183959 |
| Range | 9.407036 | 9.407036 | 9.407036 | 9.407036 | 9.407036 | 9.407036 | 9.407036 |
| Minimum | -9.3749296 | -8.8928449 | -8.9342376 | -9.0177836 | -8.9984785 | -9.3901696 | -9.4059638 |
| Maximum | 0.0321064 | 0.5141911 | 0.4727984 | 0.3892523 | 0.4085575 | 0.0168664 | 0.0010721 |
| Sum | -1181.8585 | -960.09953 | -979.14017 | -1017.5714 | -1008.691 | -1188.8689 | -1196.1342 |
| Count | 460 | 460 | 460 | 460 | 460 | 460 | 460 |
| Confidence Level(95.0%) | 0.0893474 | 0.0893474 | 0.0893474 | 0.0893474 | 0.0893474 | 0.0893474 | 0.0893474 |

It is important to note that for a given radionuclide, the method used here results in the same distribution for each hydrostratigraphic unit, since $K_D$ is determined by multiplying $K_A$ by a unit-specific constant (A'). It is also possible to use this information to develop correlation coefficients between each of the radionuclides. Using the data analysis tools in Microsoft Excel 97, the following correlation coefficients are developed for $K_A$ (and therefore $K_D$):

| $K_A$ ($mL/m^2$) | Am(III) | Np(V) | Pu(V) | Th(IV) | U(VI) |
|---|---|---|---|---|---|
| Am(III) | 1 | | | | |
| Np(V) | 0.9056426 | 1 | | | |
| Pu(V) | 0.9025125 | 0.9628663 | 1 | | |
| Th(IV) | -0.0349612 | -0.0448095 | -0.0682032 | 1 | |
| U(VI) | 0.3419898 | 0.4073383 | 0.4786748 | -0.0173596 | 1 |

For log $K_A$ (and log $K_D$), the correlation coefficients are different:

| log $K_A$ ($mL/m^2$) | Am(III) | Np(V) | Pu(V) | Th(IV) | U(VI) |
|---|---|---|---|---|---|
| Am(III) | 1 | | | | |
| Np(V) | 0.8373419 | 1 | | | |
| Pu(V) | 0.9640062 | 0.8813727 | 1 | | |
| Th(IV) | 0.1119944 | 0.2598956 | 0.1087378 | 1 | |
| U(VI) | 0.3455182 | 0.6096958 | 0.4893751 | 0.1648243 | 1 |

These $K_D$ distributions and correlation coefficients were passed to the PA element for incorporation in TPA 3.1.4.



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6/5/98 DRJ

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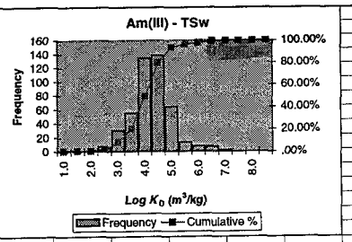
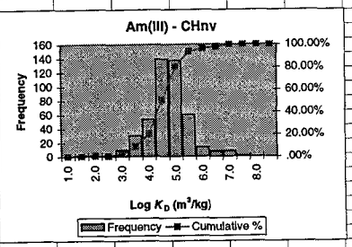
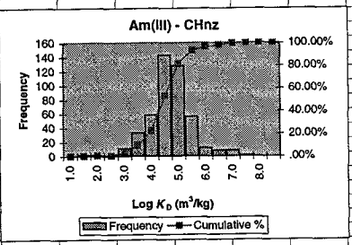
| TSw | Frequency | Cumulative % |
|---|---|---|
| 1.0 | 1 | .22% |
| 1.5 | 1 | .43% |
| 2.0 | 0 | .43% |
| 2.5 | 7 | 1.96% |
| 3.0 | 30 | 8.48% |
| 3.5 | 55 | 20.43% |
| 4.0 | 134 | 49.57% |
| 4.5 | 138 | 79.57% |
| 5.0 | 64 | 93.48% |
| 5.5 | 13 | 96.30% |
| 6.0 | 8 | 98.04% |
| 6.5 | 7 | 99.57% |
| 7.0 | 2 | 100.00% |
| 7.5 | 0 | 100.00% |
| 8.0 | 0 | 100.00% |
| More | 0 | 100.00% |



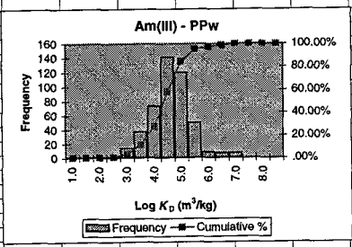

| CHnv | Frequency | Cumulative % |
|---|---|---|
| 1.0 | 0 | .00% |
| 1.5 | 1 | .22% |
| 2.0 | 1 | .43% |
| 2.5 | 0 | .43% |
| 3.0 | 9 | 2.39% |
| 3.5 | 30 | 8.91% |
| 4.0 | 53 | 20.43% |
| 4.5 | 139 | 50.65% |
| 5.0 | 137 | 80.43% |
| 5.5 | 60 | 93.48% |
| 6.0 | 13 | 96.30% |
| 6.5 | 8 | 98.04% |
| 7.0 | 8 | 99.78% |
| 7.5 | 1 | 100.00% |
| 8.0 | 0 | 100.00% |
| More | 0 | 100.00% |



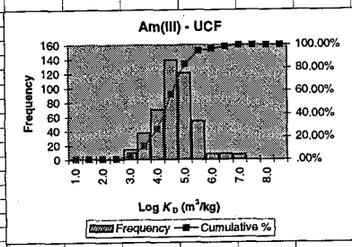

| Bin | Frequency | Cumulative % |
|---|---|---|
| 1.0 | 0 | .00% |
| 1.5 | 1 | .22% |
| 2.0 | 1 | .43% |
| 2.5 | 0 | .43% |
| 3.0 | 11 | 2.83% |
| 3.5 | 33 | 10.00% |
| 4.0 | 58 | 22.61% |
| 4.5 | 143 | 53.70% |
| 5.0 | 128 | 81.52% |
| 5.5 | 56 | 93.70% |
| 6.0 | 12 | 96.30% |
| 6.5 | 8 | 98.04% |
| 7.0 | 8 | 99.78% |
| 7.5 | 1 | 100.00% |
| 8.0 | 0 | 100.00% |
| More | 0 | 100.00% |



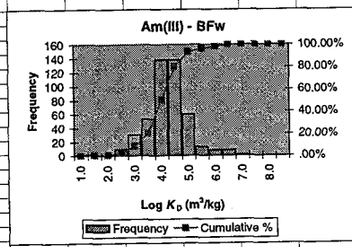

| Bin | Frequency | Cumulative % |
|---|---|---|
| 1.0 | 1 | .22% |
| 1.5 | 0 | .22% |
| 2.0 | 1 | .43% |
| 2.5 | 1 | .65% |
| 3.0 | 14 | 3.70% |
| 3.5 | 37 | 11.74% |
| 4.0 | 73 | 27.61% |
| 4.5 | 141 | 58.26% |
| 5.0 | 120 | 84.35% |
| 5.5 | 50 | 95.22% |
| 6.0 | 8 | 96.96% |
| 6.5 | 7 | 98.48% |
| 7.0 | 7 | 100.00% |
| 7.5 | 0 | 100.00% |
| 8.0 | 0 | 100.00% |
| More | 0 | 100.00% |



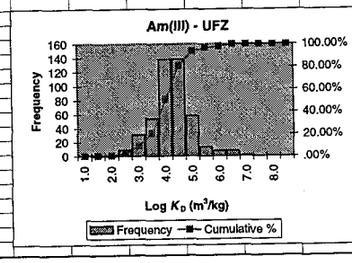

| Bin | Frequency | Cumulative % |
|---|---|---|
| 1.0 | 1 | .22% |
| 1.5 | 0 | .22% |
| 2.0 | 1 | .43% |
| 2.5 | 0 | .43% |
| 3.0 | 14 | 3.48% |
| 3.5 | 37 | 11.52% |
| 4.0 | 70 | 26.74% |
| 4.5 | 139 | 56.96% |
| 5.0 | 121 | 83.26% |
| 5.5 | 54 | 95.00% |
| 6.0 | 8 | 96.74% |
| 6.5 | 8 | 98.48% |
| 7.0 | 7 | 100.00% |
| 7.5 | 0 | 100.00% |
| 8.0 | 0 | 100.00% |
| More | 0 | 100.00% |




| Bin | Frequency | Cumulative % |
|---|---|---|
| 1.0 | 1 | .22% |
| 1.5 | 1 | .43% |
| 2.0 | 0 | .43% |
| 2.5 | 9 | 2.39% |
| 3.0 | 30 | 8.91% |
| 3.5 | 53 | 20.43% |
| 4.0 | 138 | 50.43% |
| 4.5 | 138 | 80.43% |
| 5.0 | 60 | 93.48% |
| 5.5 | 13 | 96.30% |
| 6.0 | 8 | 98.04% |
| 6.5 | 8 | 99.78% |
| 7.0 | 1 | 100.00% |
| 7.5 | 0 | 100.00% |
| 8.0 | 0 | 100.00% |
| More | 0 | 100.00% |




| Bin | Frequency | Cumulative % |
|---|---|---|
| 1.0 | 1 | .22% |
| 1.5 | 1 | .43% |
| 2.0 | 0 | .43% |
| 2.5 | 9 | 2.39% |
| 3.0 | 31 | 9.13% |
| 3.5 | 54 | 20.87% |
| 4.0 | 138 | 50.87% |
| 4.5 | 138 | 80.87% |
| 5.0 | 58 | 93.48% |
| 5.5 | 13 | 96.30% |
| 6.0 | 8 | 98.04% |
| 6.5 | 8 | 99.78% |
| 7.0 | 1 | 100.00% |
| 7.5 | 0 | 100.00% |
| 8.0 | 0 | 100.00% |
| More | 0 | 100.00% |

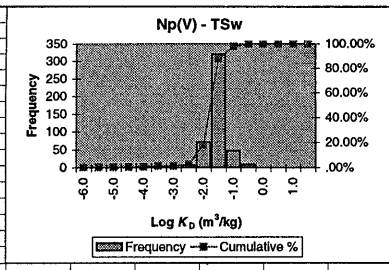



| Log KD(m3/kg) | Am(III)-TSw | Am(III)-CHnv | Am(III)-CHnz | Am(III)-PPw | Am(III)-UCF | Am(III)-BFw | Am(III)-UFZ |
|---|---|---|---|---|---|---|---|
| | | | | | | | |
| Mean | 4.01098789 | 4.49307256 | 4.45167988 | 4.36813383 | 4.38743898 | 3.99574792 | 3.97995365 |
| Standard Error | 0.03488939 | 0.03488939 | 0.03488939 | 0.03488939 | 0.03488939 | 0.03488939 | 0.03488939 |
| Median | 4.00188867 | 4.48397334 | 4.44258066 | 4.35903461 | 4.37833976 | 3.9866487 | 3.97065443 |
| Mode | 3.79964017 | 4.28172484 | 4.24033216 | 4.1567961 | 4.17609126 | 3.7844002 | 3.76860593 |
| Standard Deviation | 0.74829408 | 0.74829408 | 0.74829408 | 0.74829408 | 0.74829408 | 0.74829408 | 0.74829408 |
| Sample Variance | 0.55994403 | 0.55994403 | 0.55994403 | 0.55994403 | 0.55994403 | 0.55994403 | 0.55994403 |
| Kurtosis | 1.92430783 | 1.92430783 | 1.92430783 | 1.92430783 | 1.92430783 | 1.92430783 | 1.92430783 |
| Skewness | 0.11843681 | 0.11843681 | 0.11843681 | 0.11843681 | 0.11843681 | 0.11843681 | 0.11843681 |
| Range | 5.95820176 | 5.95820176 | 5.95820176 | 5.95820176 | 5.95820176 | 5.95820176 | 5.95820176 |
| Minimum | 0.62281817 | 1.10490284 | 1.06351016 | 0.9789641 | 0.99920926 | 0.6075782 | 0.59178393 |
| Maximum | 6.58101993 | 7.0631046 | 7.02171192 | 6.93816587 | 6.95747102 | 6.56577996 | 6.5499857 |
| Sum | 1845.05443 | 2066.81338 | 2047.77274 | 2009.34156 | 2018.22193 | 1838.04404 | 1830.77868 |
| Count | 460 | 460 | 460 | 460 | 460 | 460 | 460 |
| Confidence Level(95.0%) | 0.06856272 | 0.06856272 | 0.06856272 | 0.06856272 | 0.06856272 | 0.06856272 | 0.06856272 |

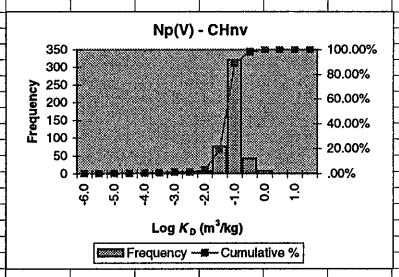
Calculated $K_D$ (in $m^3$/kg) based on DLM.

1/2 1/8/04 DBD

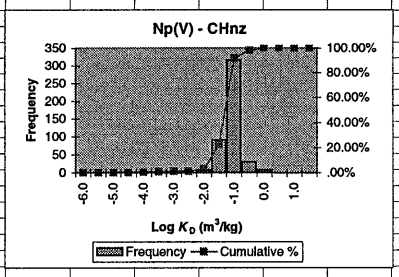
| Bin | Frequency | Cumulative % |
|---|---|---|
| -6.0 | 0 | .00% |
| -5.5 | 1 | .22% |
| -5.0 | 0 | .22% |
| -4.5 | 1 | .43% |
| -4.0 | 2 | .87% |
| -3.5 | 2 | 1.30% |
| -3.0 | 0 | 1.30% |
| -2.5 | 7 | 2.83% |
| -2.0 | 71 | 18.26% |
| -1.5 | 320 | 87.83% |
| -1.0 | 47 | 98.04% |
| -0.5 | 9 | 100.00% |
| 0.0 | 0 | 100.00% |
| 0.5 | 0 | 100.00% |
| 1.0 | 0 | 100.00% |
| More | 0 | 100.00% |



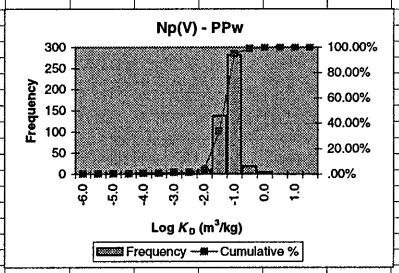

| Bin | Frequency | Cumulative % |
|---|---|---|
| -6.0 | 0 | .00% |
| -5.5 | 0 | .00% |
| -5.0 | 1 | .22% |
| -4.5 | 0 | .22% |
| -4.0 | 1 | .43% |
| -3.5 | 2 | .87% |
| -3.0 | 2 | 1.30% |
| -2.5 | 0 | 1.30% |
| -2.0 | 7 | 2.83% |
| -1.5 | 76 | 19.35% |
| -1.0 | 321 | 89.13% |
| -0.5 | 42 | 98.26% |
| 0.0 | 8 | 100.00% |
| 0.5 | 0 | 100.00% |
| 1.0 | 0 | 100.00% |
| More | 0 | 100.00% |



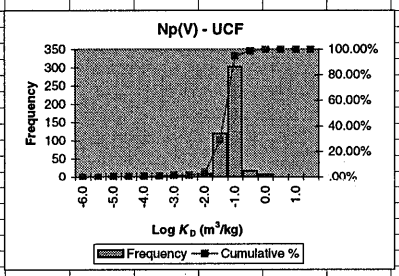

| Bin | Frequency | Cumulative % |
|---|---|---|
| -6.0 | 0 | .00% |
| -5.5 | 0 | .00% |
| -5.0 | 1 | .22% |
| -4.5 | 0 | .22% |
| -4.0 | 1 | .43% |
| -3.5 | 2 | .87% |
| -3.0 | 2 | 1.30% |
| -2.5 | 0 | 1.30% |
| -2.0 | 8 | 3.04% |
| -1.5 | 91 | 22.83% |
| -1.0 | 317 | 91.74% |
| -0.5 | 30 | 98.26% |
| 0.0 | 8 | 100.00% |
| 0.5 | 0 | 100.00% |
| 1.0 | 0 | 100.00% |
| More | 0 | 100.00% |



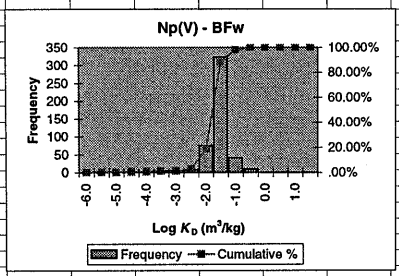

| Bin | Frequency | Cumulative % |
|---|---|---|
| -6.0 | 0 | .00% |
| -5.5 | 0 | .00% |
| -5.0 | 1 | .22% |
| -4.5 | 0 | .22% |
| -4.0 | 2 | .65% |
| -3.5 | 1 | .87% |
| -3.0 | 2 | 1.30% |
| -2.5 | 1 | 1.52% |
| -2.0 | 10 | 3.70% |
| -1.5 | 138 | 33.70% |
| -1.0 | 282 | 95.00% |
| -0.5 | 18 | 98.91% |
| 0.0 | 5 | 100.00% |
| 0.5 | 0 | 100.00% |
| 1.0 | 0 | 100.00% |
| More | 0 | 100.00% |



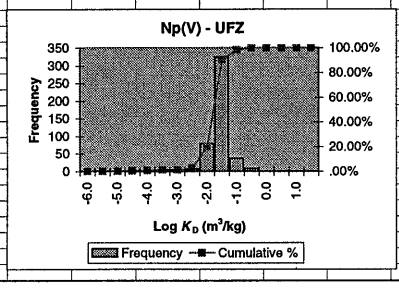

| Bin | Frequency | Cumulative % |
|---|---|---|
| -6.0 | 0 | .00% |
| -5.5 | 0 | .00% |
| -5.0 | 1 | .22% |
| -4.5 | 0 | .22% |
| -4.0 | 1 | .43% |
| -3.5 | 2 | .87% |
| -3.0 | 2 | 1.30% |
| -2.5 | 0 | 1.30% |
| -2.0 | 9 | 3.26% |
| -1.5 | 119 | 29.13% |
| -1.0 | 302 | 94.78% |
| -0.5 | 17 | 98.48% |
| 0.0 | 7 | 100.00% |
| 0.5 | 0 | 100.00% |
| 1.0 | 0 | 100.00% |
| More | 0 | 100.00% |




| Bin | Frequency | Cumulative % |
|---|---|---|
| -6.0 | 0 | .00% |
| -5.5 | 1 | .22% |
| -5.0 | 0 | .22% |
| -4.5 | 1 | .43% |
| -4.0 | 2 | .87% |
| -3.5 | 2 | 1.30% |
| -3.0 | 0 | 1.30% |
| -2.5 | 7 | 2.83% |
| -2.0 | 74 | 18.91% |
| -1.5 | 323 | 89.13% |
| -1.0 | 41 | 98.04% |
| -0.5 | 9 | 100.00% |
| 0.0 | 0 | 100.00% |
| 0.5 | 0 | 100.00% |
| 1.0 | 0 | 100.00% |
| More | 0 | 100.00% |




| Bin | Frequency | Cumulative % |
|---|---|---|
| -6.0 | 0 | .00% |
| -5.5 | 1 | .22% |
| -5.0 | 0 | .22% |
| -4.5 | 1 | .43% |
| -4.0 | 2 | .87% |
| -3.5 | 2 | 1.30% |
| -3.0 | 0 | 1.30% |
| -2.5 | 7 | 2.83% |
| -2.0 | 79 | 20.00% |
| -1.5 | 323 | 90.22% |
| -1.0 | 37 | 98.26% |
| -0.5 | 8 | 100.00% |
| 0.0 | 0 | 100.00% |
| 0.5 | 0 | 100.00% |
| 1.0 | 0 | 100.00% |
| More | 0 | 100.00% |




| Log KD(m3/kg) | Np(V)-TSw | Np(V)-CHnv | Np(V)-CHnz | Np(V)-PPw | Np(V)-UCF | Np(V)-BFw | Np(V)-UFZ |
|---|---|---|---|---|---|---|---|
| Mean | -1.7955226 | -1.313438 | -1.3548307 | -1.4383767 | -1.4190716 | -1.8107626 | -1.8265569 |
| Standard Error | 0.01968626 | 0.01968626 | 0.01968626 | 0.01968626 | 0.01968626 | 0.01968626 | 0.01968626 |
| Median | -1.7644388 | -1.2823542 | -1.3237468 | -1.4072929 | -1.3879877 | -1.7796788 | -1.7954731 |
| Mode | -1.7998849 | -1.3178002 | -1.3591929 | -1.442739 | -1.4234338 | -1.8151249 | -1.8309191 |
| Standard Deviation | 0.42222331 | 0.42222331 | 0.42222331 | 0.42222331 | 0.42222331 | 0.42222331 | 0.42222331 |
| Sample Variance | 0.17827252 | 0.17827252 | 0.17827252 | 0.17827252 | 0.17827252 | 0.17827252 | 0.17827252 |
| Kurtosis | 26.5764652 | 26.5764652 | 26.5764652 | 26.5764652 | 26.5764652 | 26.5764652 | 26.5764652 |
| Skewness | -3.5561097 | -3.5561097 | -3.5561097 | -3.5561097 | -3.5561097 | -3.5561097 | -3.5561097 |
| Range | 5.14041944 | 5.14041944 | 5.14041944 | 5.14041944 | 5.14041944 | 5.14041944 | 5.14041944 |
| Minimum | -5.8018677 | -5.319783 | -5.3611757 | -5.4447217 | -5.4254166 | -5.8171076 | -5.8329019 |
| Maximum | -0.6614482 | -0.1793635 | -0.2207562 | -0.3043023 | -0.2849971 | -0.6766882 | -0.6924825 |
| Sum | -825.94042 | -604.18147 | -623.2221 | -661.65329 | -652.77291 | -832.9508 | -840.21616 |
| Count | 460 | 460 | 460 | 460 | 460 | 460 | 460 |
| Confidence Level(95.0%) | 0.03868637 | 0.03868637 | 0.03868637 | 0.03868637 | 0.03868637 | 0.03868637 | 0.03868637 |

6/18/98 JRL 73

74
Lab Log
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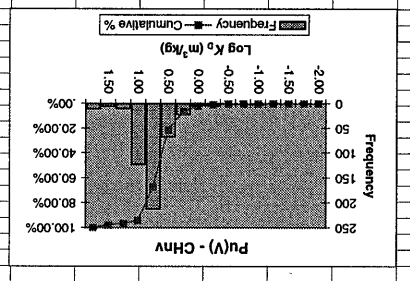
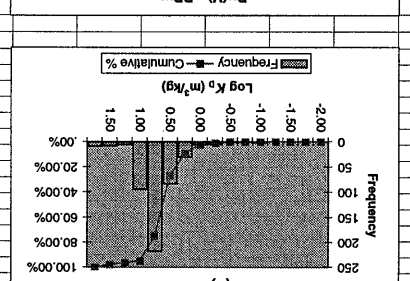
| Log KD(m3/kg) | Pu(V)-TSw | Pu(V)-CHnv | Pu(V)-CHnz | Pu(V)-PPw | Pu(V)-UCF | Pu(V)-BFw | Pu(V)-UFZ |
|---|---|---|---|---|---|---|---|
| Mean | 0.1693902 | 0.6514748 | 0.6100821 | 0.5265361 | 0.5456412 | 0.1541502 | 0.1383597 |
| Standard Error | 0.0142102 | 0.0142102 | 0.0142102 | 0.0142102 | 0.0142102 | 0.0142102 | 0.0142102 |
| Median | 0.1772819 | 0.6583666 | 0.6179739 | 0.5344278 | 0.5373043 | 0.1620419 | 0.1462477 |
| Mode | 0.1124266 | 0.5945152 | 0.5531176 | 0.4695717 | 0.4888769 | 0.0971658 | 0.0813916 |
| Standard Deviation | 0.3047759 | 0.3047759 | 0.3047759 | 0.3047759 | 0.3047759 | 0.3047759 | 0.3047759 |
| Sample Variance | 0.0928866 | 0.0928866 | 0.0928866 | 0.0928866 | 0.0928866 | 0.0928866 | 0.0928866 |
| Kurtosis | 5.0553979 | 5.0553979 | 5.0553979 | 5.0553979 | 5.0553979 | 5.0553979 | 5.0553979 |
| Skewness | -0.147723 | -0.147723 | -0.147723 | -0.147723 | -0.147723 | -0.147723 | -0.147723 |
| Range | 2.9741497 | 2.9741497 | 2.9741497 | 2.9741497 | 2.9741497 | 2.9741497 | 2.9741497 |
| Minimum | -1.631111 | -1.149025 | -1.190416 | -1.273964 | -1.25466 | -1.64635 | -1.662144 |
| Maximum | 1.3430398 | 1.8251243 | 1.7837316 | 1.7001856 | 1.7194907 | 1.3277997 | 1.3120064 |
| Sum | 77.91948 | 299.5764 | 280.6378 | 242.2066 | 251.0868 | 70.80901 | 63.64374 |
| Count | 460 | 460 | 460 | 460 | 460 | 460 | 460 |
| Confidence Level(95.0%) | 0.0279252 | 0.0279252 | 0.0279252 | 0.0279252 | 0.0279252 | 0.0279252 | 0.0279252 |



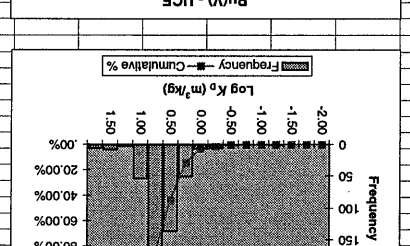

| Bin | Frequency | Cumulative % |
|---|---|---|
| -2.00 | 0 | .00% |
| -1.75 | 0 | .00% |
| -1.50 | 0 | .00% |
| -1.25 | 1 | .22% |
| -1.00 | 0 | .22% |
| -0.75 | 0 | .22% |
| -0.50 | 1 | .43% |
| -0.25 | 6 | 1.74% |
| 0.00 | 7 | 3.26% |
| 0.25 | 44 | 12.83% |
| 0.50 | 129 | 40.87% |
| 0.75 | 190 | 82.17% |
| 1.00 | 64 | 96.09% |
| 1.25 | 3 | 96.74% |
| 1.50 | 9 | 98.70% |
| More | 6 | 100.00% |



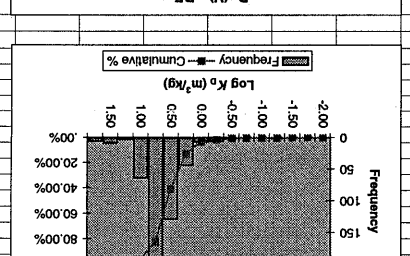

| Bin | Frequency | Cumulative % |
|---|---|---|
| -2.00 | 0 | .00% |
| -1.75 | 0 | .00% |
| -1.50 | 0 | .00% |
| -1.25 | 0 | .00% |
| -1.00 | 1 | .22% |
| -0.75 | 0 | .22% |
| -0.50 | 0 | .22% |
| -0.25 | 4 | 1.09% |
| 0.00 | 4 | 1.96% |
| 0.25 | 22 | 6.74% |
| 0.50 | 67 | 21.30% |
| 0.75 | 212 | 67.39% |
| 1.00 | 123 | 94.13% |
| 1.25 | 10 | 96.30% |
| 1.50 | 6 | 97.61% |
| More | 11 | 100.00% |



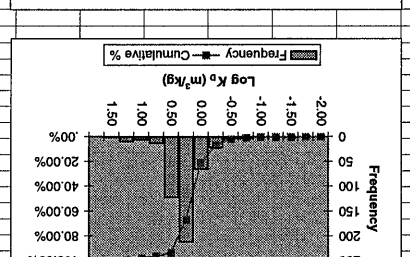

| Bin | Frequency | Cumulative % |
|---|---|---|
| -2.00 | 0 | .00% |
| -1.75 | 0 | .00% |
| -1.50 | 0 | .00% |
| -1.25 | 0 | .00% |
| -1.00 | 1 | .22% |
| -0.75 | 0 | .22% |
| -0.50 | 0 | .22% |
| -0.25 | 5 | 1.30% |
| 0.00 | 6 | 2.61% |
| 0.25 | 30 | 9.13% |
| 0.50 | 83 | 27.17% |
| 0.75 | 218 | 74.57% |
| 1.00 | 94 | 95.00% |
| 1.25 | 6 | 96.30% |
| 1.50 | 8 | 98.04% |
| More | 9 | 100.00% |



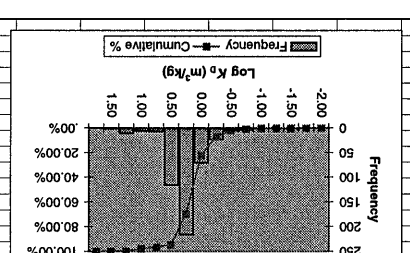

| Bin | Frequency | Cumulative % |
|---|---|---|
| -2.00 | 0 | .00% |
| -1.75 | 0 | .00% |
| -1.50 | 0 | .00% |
| -1.25 | 1 | .22% |
| -1.00 | 0 | .22% |
| -0.75 | 0 | .22% |
| -0.50 | 1 | .43% |
| -0.25 | 6 | 1.74% |
| 0.00 | 7 | 3.26% |
| 0.25 | 51 | 14.35% |
| 0.50 | 136 | 43.91% |
| 0.75 | 187 | 84.57% |
| 1.00 | 54 | 96.96% |
| 1.25 | 3 | 98.70% |
| 1.50 | 8 | 100.00% |
| More | 6 | 100.00% |




| Bin | Frequency | Cumulative % |
|---|---|---|
| -2.00 | 0 | .00% |
| -1.75 | 0 | .00% |
| -1.50 | 0 | .00% |
| -1.25 | 1 | .22% |
| -1.00 | 0 | .22% |
| -0.75 | 0 | .22% |
| -0.50 | 1 | .43% |
| -0.25 | 6 | 1.74% |
| 0.00 | 7 | 3.26% |
| 0.25 | 44 | 12.83% |
| 0.50 | 129 | 40.87% |
| 0.75 | 190 | 82.17% |
| 1.00 | 64 | 96.09% |
| 1.25 | 3 | 96.74% |
| 1.50 | 9 | 98.70% |
| More | 6 | 100.00% |

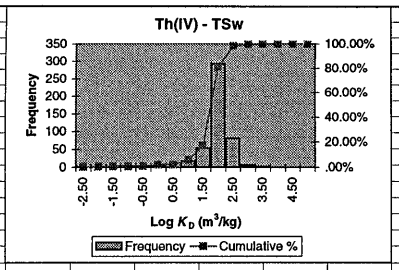



| Bin | Frequency | Cumulative % |
|---|---|---|
| -2.00 | 0 | .00% |
| -1.75 | 0 | .00% |
| -1.50 | 1 | .22% |
| -1.25 | 0 | .22% |
| -1.00 | 0 | .22% |
| -0.75 | 4 | 1.09% |
| -0.50 | 4 | 1.96% |
| -0.25 | 22 | 6.74% |
| 0.00 | 65 | 20.87% |
| 0.25 | 212 | 66.96% |
| 0.50 | 122 | 93.48% |
| 0.75 | 13 | 96.30% |
| 1.00 | 6 | 97.61% |
| 1.25 | 10 | 99.78% |
| 1.50 | 1 | 100.00% |
| More | 0 | 100.00% |

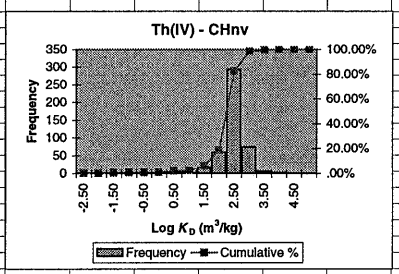



| Bin | Frequency | Cumulative % |
|---|---|---|
| -2.00 | 0 | .00% |
| -1.75 | 0 | .00% |
| -1.50 | 1 | .22% |
| -1.25 | 0 | .22% |
| -1.00 | 0 | .22% |
| -0.75 | 4 | 1.09% |
| -0.50 | 5 | 2.17% |
| -0.25 | 23 | 7.17% |
| 0.00 | 71 | 22.61% |
| 0.25 | 216 | 69.57% |
| 0.50 | 118 | 94.78% |
| 0.75 | 7 | 96.30% |
| 1.00 | 6 | 97.61% |
| 1.25 | 10 | 99.78% |
| 1.50 | 1 | 100.00% |
| More | 0 | 100.00% |

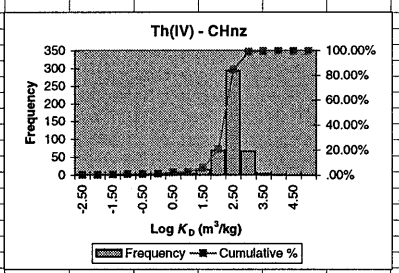
| Bin | Frequency | Cumulative % |
|---|---|---|
| -2.50 | 1 | .22% |
| -2.00 | 1 | .43% |
| -1.50 | 2 | .87% |
| -1.00 | 0 | .87% |
| -0.50 | 1 | 1.09% |
| 0.00 | 4 | 1.96% |
| 0.50 | 0 | 1.96% |
| 1.00 | 17 | 5.65% |
| 1.50 | 53 | 17.17% |
| 2.00 | 293 | 80.87% |
| 2.50 | 80 | 98.26% |
| 3.00 | 6 | 99.57% |
| 3.50 | 2 | 100.00% |
| 4.00 | 0 | 100.00% |
| 4.50 | 0 | 100.00% |
| More | 0 | 100.00% |



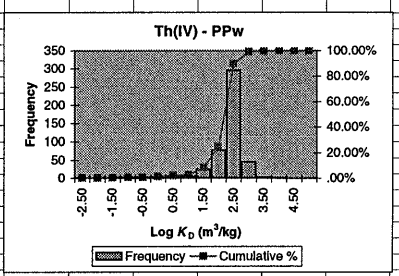

| Bin | Frequency | Cumulative % |
|---|---|---|
| -2.50 | 1 | .22% |
| -2.00 | 0 | .22% |
| -1.50 | 1 | .43% |
| -1.00 | 2 | .87% |
| -0.50 | 0 | .87% |
| 0.00 | 1 | 1.09% |
| 0.50 | 4 | 1.96% |
| 1.00 | 2 | 2.39% |
| 1.50 | 16 | 5.87% |
| 2.00 | 59 | 18.70% |
| 2.50 | 293 | 82.39% |
| 3.00 | 74 | 98.48% |
| 3.50 | 5 | 99.57% |
| 4.00 | 2 | 100.00% |
| 4.50 | 0 | 100.00% |
| More | 0 | 100.00% |



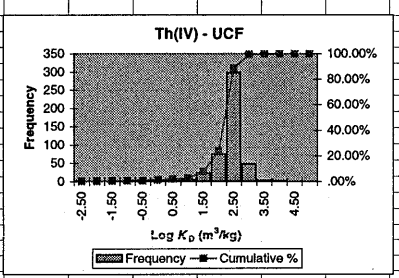

| Bin | Frequency | Cumulative % |
|---|---|---|
| -2.50 | 1 | .22% |
| -2.00 | 0 | .22% |
| -1.50 | 1 | .43% |
| -1.00 | 2 | .87% |
| -0.50 | 0 | .87% |
| 0.00 | 1 | 1.09% |
| 0.50 | 4 | 1.96% |
| 1.00 | 3 | 2.61% |
| 1.50 | 15 | 5.87% |
| 2.00 | 68 | 20.65% |
| 2.50 | 294 | 84.57% |
| 3.00 | 66 | 98.91% |
| 3.50 | 4 | 99.78% |
| 4.00 | 1 | 100.00% |
| 4.50 | 0 | 100.00% |
| More | 0 | 100.00% |



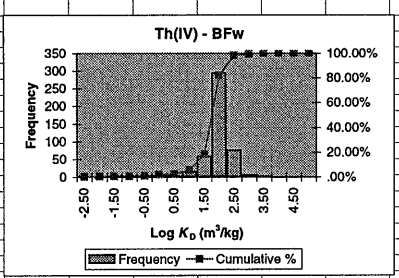

| Bin | Frequency | Cumulative % |
|---|---|---|
| -2.50 | 1 | .22% |
| -2.00 | 0 | .22% |
| -1.50 | 1 | .43% |
| -1.00 | 2 | .87% |
| -0.50 | 0 | .87% |
| 0.00 | 2 | 1.30% |
| 0.50 | 3 | 1.96% |
| 1.00 | 4 | 2.83% |
| 1.50 | 25 | 8.26% |
| 2.00 | 77 | 25.00% |
| 2.50 | 296 | 89.35% |
| 3.00 | 45 | 99.13% |
| 3.50 | 3 | 99.78% |
| 4.00 | 1 | 100.00% |
| 4.50 | 0 | 100.00% |
| More | 0 | 100.00% |



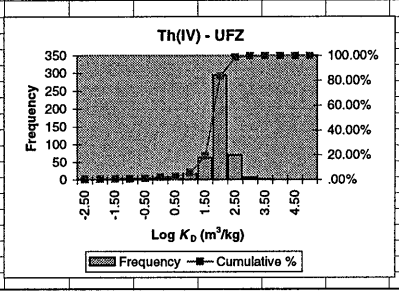

| Bin | Frequency | Cumulative % |
|---|---|---|
| -2.50 | 1 | .22% |
| -2.00 | 0 | .22% |
| -1.50 | 1 | .43% |
| -1.00 | 2 | .87% |
| -0.50 | 0 | .87% |
| 0.00 | 2 | 1.30% |
| 0.50 | 3 | 1.96% |
| 1.00 | 4 | 2.83% |
| 1.50 | 23 | 7.83% |
| 2.00 | 74 | 23.91% |
| 2.50 | 298 | 88.70% |
| 3.00 | 48 | 99.13% |
| 3.50 | 3 | 99.78% |
| 4.00 | 1 | 100.00% |
| 4.50 | 0 | 100.00% |
| More | 0 | 100.00% |




| Bin | Frequency | Cumulative % |
|---|---|---|
| -2.50 | 1 | .22% |
| -2.00 | 1 | .43% |
| -1.50 | 2 | .87% |
| -1.00 | 0 | .87% |
| -0.50 | 1 | 1.09% |
| 0.00 | 4 | 1.96% |
| 0.50 | 2 | 2.39% |
| 1.00 | 15 | 5.65% |
| 1.50 | 58 | 18.26% |
| 2.00 | 294 | 82.17% |
| 2.50 | 75 | 98.48% |
| 3.00 | 5 | 99.57% |
| 3.50 | 2 | 100.00% |
| 4.00 | 0 | 100.00% |
| 4.50 | 0 | 100.00% |
| More | 0 | 100.00% |



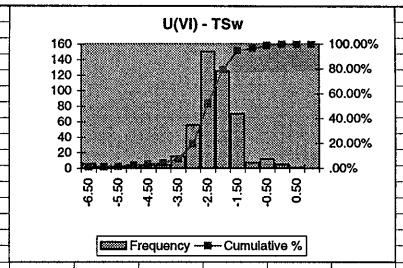

| Bin | Frequency | Cumulative % |
|---|---|---|
| -2.50 | 1 | .22% |
| -2.00 | 1 | .43% |
| -1.50 | 2 | .87% |
| -1.00 | 0 | .87% |
| -0.50 | 1 | 1.09% |
| 0.00 | 4 | 1.96% |
| 0.50 | 2 | 2.39% |
| 1.00 | 16 | 5.87% |
| 1.50 | 62 | 19.35% |
| 2.00 | 294 | 83.26% |
| 2.50 | 70 | 98.48% |
| 3.00 | 6 | 99.78% |
| 3.50 | 1 | 100.00% |
| 4.00 | 0 | 100.00% |
| 4.50 | 0 | 100.00% |
| More | 0 | 100.00% |



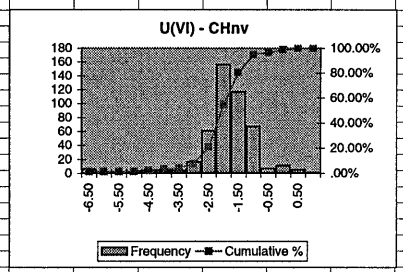

| Log KD(m3/kg) | Th(IV)-TSw | Th(IV)-CHnv | Th(IV)-CHnz | Th(IV)-PPw | Th(IV)-UCF | Th(IV)-BFw | Th(iV)-UFZ |
|---|---|---|---|---|---|---|---|
| | | | | | | | |
| Mean | 1.7107391 | 2.19282377 | 2.15143109 | 2.06788504 | 2.08719019 | 1.69549913 | 1.67970486 |
| Standard Error | 0.02716781 | 0.02716781 | 0.02716781 | 0.02716781 | 0.02716781 | 0.02716781 | 0.02716781 |
| Median | 1.79194534 | 2.27403002 | 2.23263733 | 2.14909128 | 2.16839644 | 1.77670538 | 1.76091111 |
| Mode | 1.90137189 | 2.38345657 | 2.34206388 | 2.25851783 | 2.27782298 | 1.88613193 | 1.87033766 |
| Standard Deviation | 0.58268461 | 0.58268461 | 0.58268461 | 0.58268461 | 0.58268461 | 0.58268461 | 0.58268461 |
| Sample Variance | 0.33952136 | 0.33952136 | 0.33952136 | 0.33952136 | 0.33952136 | 0.33952136 | 0.33952136 |
| Kurtosis | 34.2276103 | 34.2276103 | 34.2276103 | 34.2276103 | 34.2276103 | 34.2276103 | 34.2276103 |
| Skewness | -4.4143746 | -4.4143746 | -4.4143746 | -4.4143746 | -4.4143746 | -4.4143746 | -4.4143746 |
| Range | 7.71459817 | 7.71459817 | 7.71459817 | 7.71459817 | 7.71459817 | 7.71459817 | 7.71459817 |
| Minimum | -4.3172929 | -3.8352082 | -3.8766009 | -3.9601469 | -3.9408418 | -4.3325328 | -4.3483271 |
| Maximum | 3.3973053 | 3.87938897 | 3.83799729 | 3.75445123 | 3.77375639 | 3.38206533 | 3.36627106 |
| Sum | 786.939985 | 1008.69894 | 989.6583 | 951.227116 | 960.107488 | 779.9296 | 772.664237 |
| Count | 460 | 460 | 460 | 460 | 460 | 460 | 460 |
| Confidence Level(95.0%) | 0.05338869 | 0.05338869 | 0.05338869 | 0.05338869 | 0.05338869 | 0.05338869 | 0.05338869 |

64/98 75

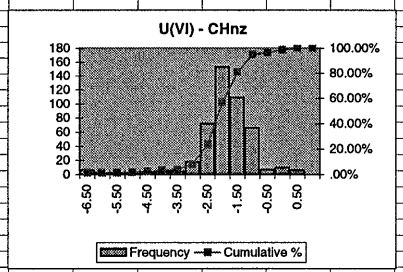
| Bin | Frequency | Cumulative % |
|---|---|---|
| -6.50 | 6 | 1.30% |
| -6.00 | 0 | 1.30% |
| -5.50 | 1 | 1.52% |
| -5.00 | 4 | 2.39% |
| -4.50 | 4 | 3.26% |
| -4.00 | 4 | 4.13% |
| -3.50 | 15 | 7.39% |
| -3.00 | 56 | 19.57% |
| -2.50 | 150 | 52.17% |
| -2.00 | 125 | 79.35% |
| -1.50 | 70 | 94.57% |
| -1.00 | 7 | 96.09% |
| -0.50 | 12 | 98.70% |
| 0.00 | 5 | 99.78% |
| 0.50 | 1 | 100.00% |
| More | 0 | 100.00% |



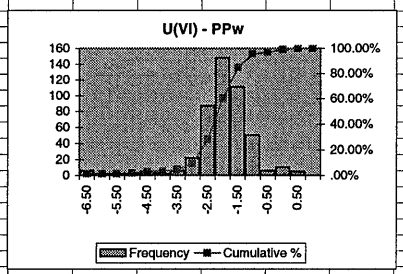

| Bin | Frequency | Cumulative % |
|---|---|---|
| -6.50 | 6 | 1.30% |
| -6.00 | 0 | 1.30% |
| -5.50 | 0 | 1.30% |
| -5.00 | 1 | 1.52% |
| -4.50 | 4 | 2.39% |
| -4.00 | 4 | 3.26% |
| -3.50 | 4 | 4.13% |
| -3.00 | 16 | 7.61% |
| -2.50 | 61 | 20.87% |
| -2.00 | 156 | 54.78% |
| -1.50 | 117 | 80.22% |
| -1.00 | 67 | 94.78% |
| -0.50 | 7 | 96.30% |
| 0.00 | 11 | 98.70% |
| 0.50 | 5 | 99.78% |
| More | 1 | 100.00% |



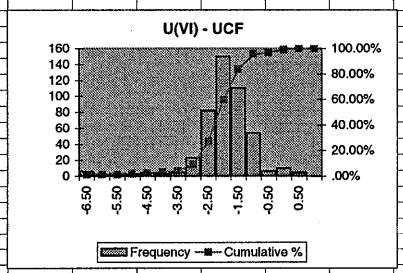

| Bin | Frequency | Cumulative % |
|---|---|---|
| -6.50 | 6 | 1.30% |
| -6.00 | 0 | 1.30% |
| -5.50 | 0 | 1.30% |
| -5.00 | 2 | 1.74% |
| -4.50 | 3 | 2.39% |
| -4.00 | 4 | 3.26% |
| -3.50 | 4 | 4.13% |
| -3.00 | 18 | 8.04% |
| -2.50 | 72 | 23.70% |
| -2.00 | 153 | 56.96% |
| -1.50 | 109 | 80.65% |
| -1.00 | 66 | 95.00% |
| -0.50 | 7 | 96.52% |
| 0.00 | 10 | 98.70% |
| 0.50 | 6 | 100.00% |
| More | 0 | 100.00% |



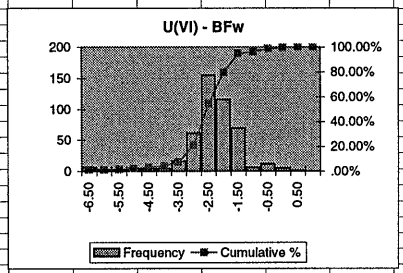

| Bin | Frequency | Cumulative % |
|---|---|---|
| -6.50 | 6 | 1.30% |
| -6.00 | 0 | 1.30% |
| -5.50 | 0 | 1.30% |
| -5.00 | 2 | 1.74% |
| -4.50 | 5 | 2.83% |
| -4.00 | 2 | 3.26% |
| -3.50 | 6 | 4.57% |
| -3.00 | 22 | 9.35% |
| -2.50 | 87 | 28.26% |
| -2.00 | 148 | 60.43% |
| -1.50 | 111 | 84.57% |
| -1.00 | 50 | 95.43% |
| -0.50 | 6 | 96.74% |
| 0.00 | 10 | 98.91% |
| 0.50 | 5 | 100.00% |
| More | 0 | 100.00% |



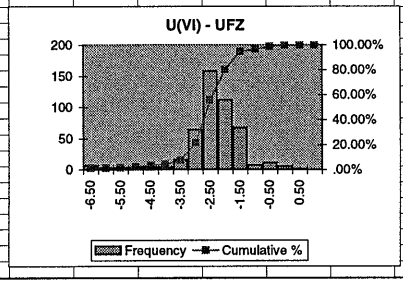

| Bin | Frequency | Cumulative % |
|---|---|---|
| -6.50 | 6 | 1.30% |
| -6.00 | 0 | 1.30% |
| -5.50 | 0 | 1.30% |
| -5.00 | 2 | 1.74% |
| -4.50 | 4 | 2.61% |
| -4.00 | 3 | 3.26% |
| -3.50 | 5 | 4.35% |
| -3.00 | 23 | 9.35% |
| -2.50 | 82 | 27.17% |
| -2.00 | 150 | 59.78% |
| -1.50 | 110 | 83.70% |
| -1.00 | 54 | 95.43% |
| -0.50 | 6 | 96.74% |
| 0.00 | 10 | 98.91% |
| 0.50 | 5 | 100.00% |
| More | 0 | 100.00% |




| Bin | Frequency | Cumulative % |
|---|---|---|
| -6.50 | 6 | 1.30% |
| -6.00 | 0 | 1.30% |
| -5.50 | 1 | 1.52% |
| -5.00 | 4 | 2.39% |
| -4.50 | 4 | 3.26% |
| -4.00 | 4 | 4.13% |
| -3.50 | 16 | 7.61% |
| -3.00 | 61 | 20.87% |
| -2.50 | 155 | 54.57% |
| -2.00 | 116 | 79.78% |
| -1.50 | 69 | 94.78% |
| -1.00 | 6 | 96.09% |
| -0.50 | 12 | 98.70% |
| 0.00 | 5 | 99.78% |
| 0.50 | 1 | 100.00% |
| More | 0 | 100.00% |




| Bin | Frequency | Cumulative % |
|---|---|---|
| -6.50 | 6 | 1.30% |
| -6.00 | 0 | 1.30% |
| -5.50 | 1 | 1.52% |
| -5.00 | 4 | 2.39% |
| -4.50 | 4 | 3.26% |
| -4.00 | 4 | 4.13% |
| -3.50 | 16 | 7.61% |
| -3.00 | 64 | 21.52% |
| -2.50 | 158 | 55.87% |
| -2.00 | 112 | 80.22% |
| -1.50 | 67 | 94.78% |
| -1.00 | 7 | 96.30% |
| -0.50 | 11 | 98.70% |
| 0.00 | 5 | 99.78% |
| 0.50 | 1 | 100.00% |
| More | 0 | 100.00% |

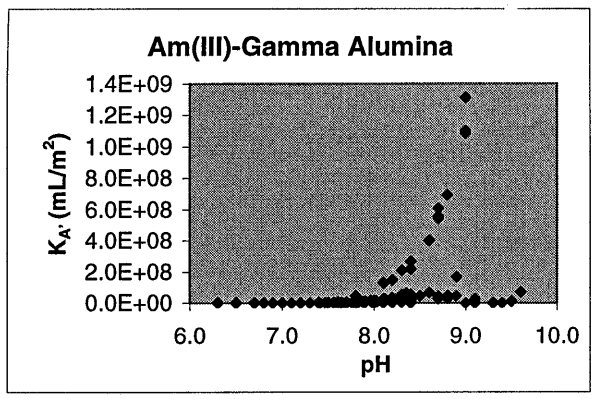


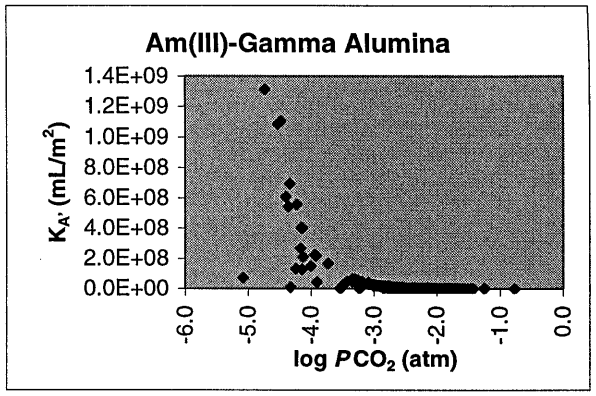

| Log KD(m3/kg) | U(VI)-TSw | U(VI)-CHnv | U(VI)-CHnz | U(VI)-PPw | U(VI)-UCF | U(VI)-BFw | U(VI)-UFZ |
|---|---|---|---|---|---|---|---|
| Mean | -2.5692576 | -2.0871729 | -2.1285656 | -2.2121116 | -2.1928065 | -2.5844975 | -2.6002918 |
| Standard Error | 0.04546608 | 0.04546608 | 0.04546608 | 0.04546608 | 0.04546608 | 0.04546608 | 0.04546608 |
| Median | -2.5360089 | -2.0539242 | -2.0953169 | -2.178863 | -2.1595578 | -2.5512489 | -2.5670431 |
| Mode | -2.6953176 | -2.213233 | -2.2546257 | -2.3381717 | -2.3188666 | -2.7105576 | -2.7263519 |
| Standard Deviation | 0.97513874 | 0.97513874 | 0.97513874 | 0.97513874 | 0.97513874 | 0.97513874 | 0.97513874 |
| Sample Variance | 0.95089556 | 0.95089556 | 0.95089556 | 0.95089556 | 0.95089556 | 0.95089556 | 0.95089556 |
| Kurtosis | 12.928374 | 12.928374 | 12.928374 | 12.928374 | 12.928374 | 12.928374 | 12.928374 |
| Skewness | -2.3183959 | -2.3183959 | -2.3183959 | -2.3183959 | -2.3183959 | -2.3183959 | -2.3183959 |
| Range | 9.40703597 | 9.40703597 | 9.40703597 | 9.40703597 | 9.40703597 | 9.40703597 | 9.40703597 |
| Minimum | -9.3749296 | -8.8928449 | -8.9342376 | -9.0177836 | -8.9984785 | -9.3901696 | -9.4059638 |
| Maximum | 0.03210638 | 0.51419106 | 0.47279837 | 0.38925232 | 0.40855747 | 0.01686641 | 0.00107215 |
| Sum | -1181.8585 | -960.09953 | -979.14017 | -1017.5714 | -1008.691 | -1188.8689 | -1196.1342 |
| Count | 460 | 460 | 460 | 460 | 460 | 460 | 460 |
| Confidence Level(95.0%) | 0.08934745 | 0.08934745 | 0.08934745 | 0.08934745 | 0.08934745 | 0.08934745 | 0.08934745 |

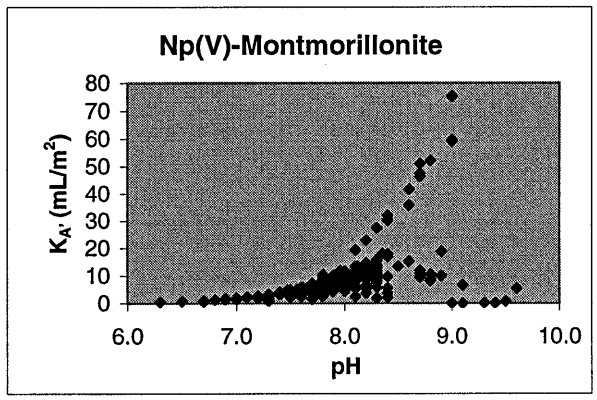
X-axis = Log $K_D$ ($m^3/kg$)

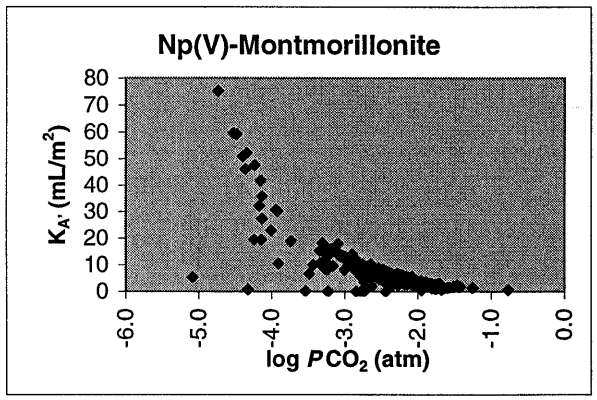
Left y-axis = Frequency

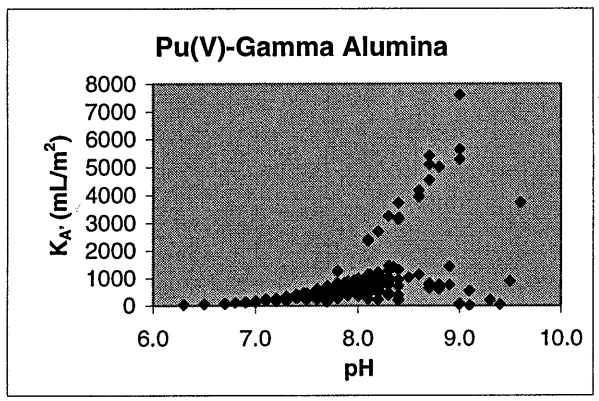
Right y-axis = Cumulative %

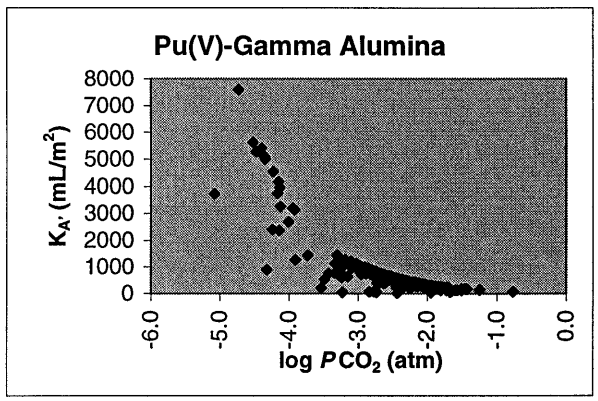

Am(III)-Gamma Alumina
1.4E+09
1.2E+09
1.0E+09
8.0E+08
6.0E+08
4.0E+08
2.0E+08
0.0E+00
$K_{A'}$ (mL/m$^2$)
6.0
7.0
8.0
9.0
10.0
pH

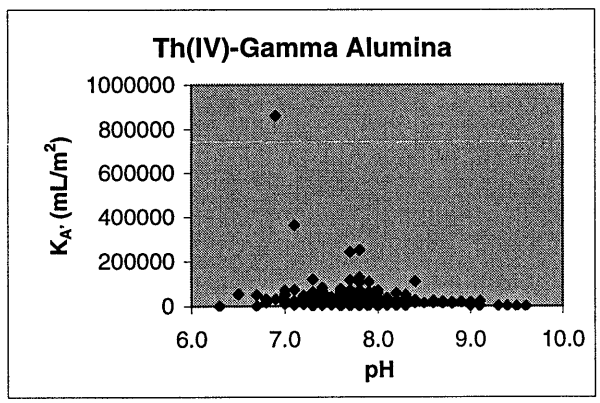

Am(III)-Gamma Alumina
1.4E+09
1.2E+09
1.0E+09
8.0E+08
6.0E+08
4.0E+08
2.0E+08
0.0E+00
$K_{A'}$ (mL/m$^2$)
-6.0
-5.0
-4.0
-3.0
-2.0
-1.0
0.0
log $PCO_2$ (atm)

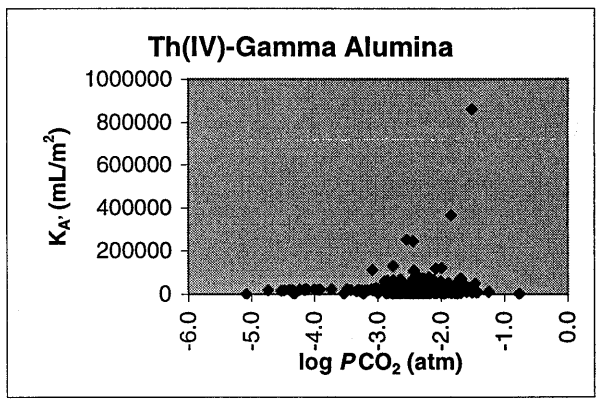

Np(V)-Montmorillonite
80
70
60
50
40
30
20
10
0
$K_{A'}$ (mL/m$^2$)
6.0
7.0
8.0
9.0
10.0
pH

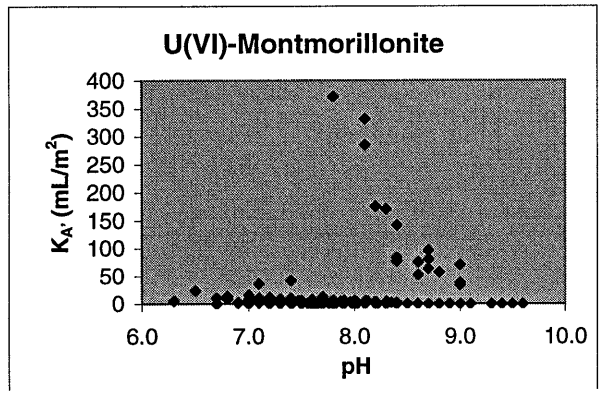

Np(V)-Montmorillonite
80
70
60
50
40
30
20
10
0
$K_{A'}$ (mL/m$^2$)
-6.0
-5.0
-4.0
-3.0
-2.0
-1.0
0.0
log $PCO_2$ (atm)

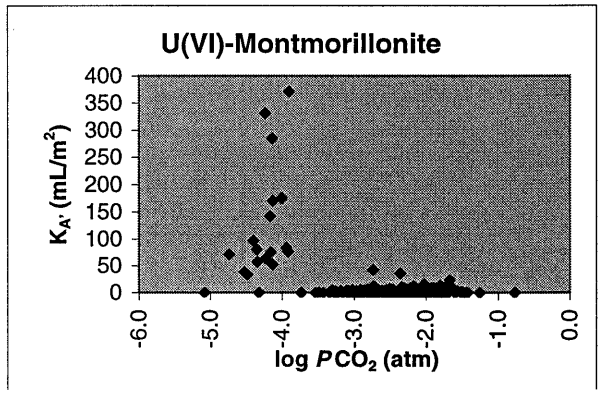

Pu(V)-Gamma Alumina
8000
7000
6000
5000
4000
3000
2000
1000
0
$K_{A'}$ (mL/m$^2$)
6.0
7.0
8.0
9.0
10.0
pH


Pu(V)-Gamma Alumina
8000
7000
6000
5000
4000
3000
2000
1000
0
$K_{A'}$ (mL/m$^2$)
-6.0
-5.0
-4.0
-3.0
-2.0
-1.0
0.0
log $PCO_2$ (atm)


Th(IV)-Gamma Alumina
1000000
800000
600000
400000
200000
0
$K_{A'}$ (mL/m$^2$)
6.0
7.0
8.0
9.0
10.0
pH


Th(IV)-Gamma Alumina
1000000
800000
600000
400000
200000
0
$K_{A'}$ (mL/m$^2$)
-6.0
-5.0
-4.0
-3.0
-2.0
-1.0
0.0
log $PCO_2$ (atm)

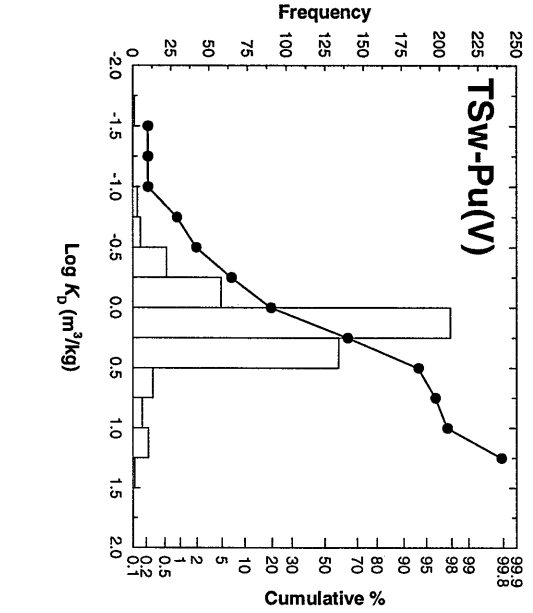

U(VI)-Montmorillonite
400
350
300
250
200
150
100
50
0
$K_{A'}$ (mL/m$^2$)
6.0
7.0
8.0
9.0
10.0
pH

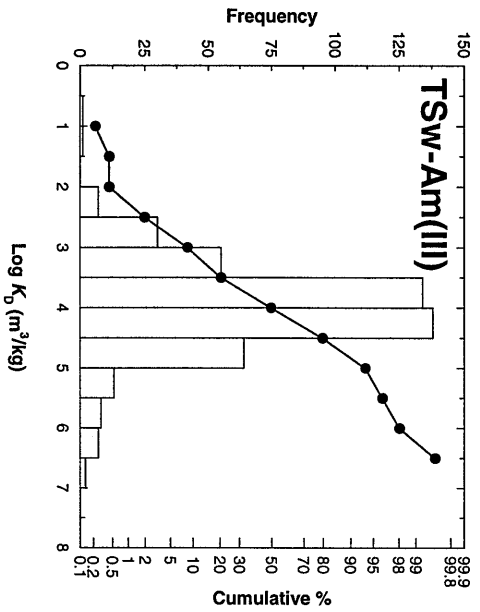

U(VI)-Montmorillonite
400
350
300
250
200
150
100
50
0
$K_{A'}$ (mL/m$^2$)
-6.0
-5.0
-4.0
-3.0
-2.0
-1.0
0.0
log $PCO_2$ (atm)

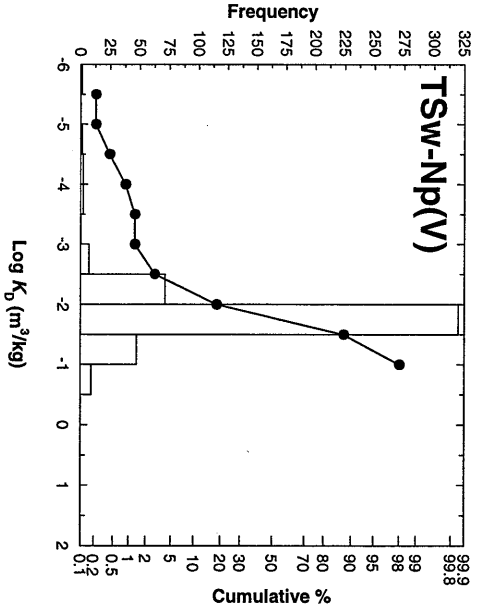
78

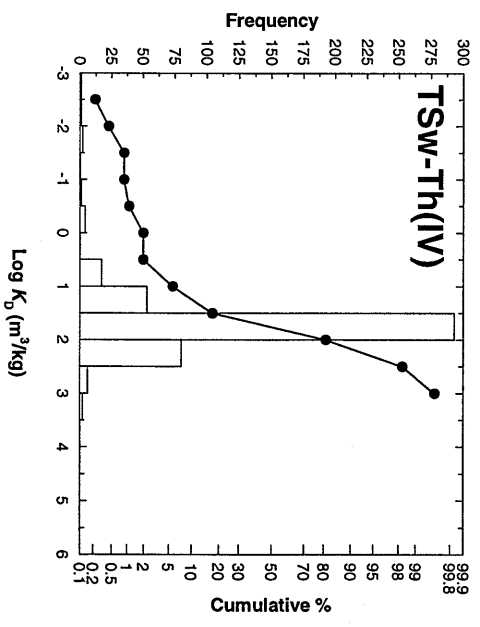
6/15/98

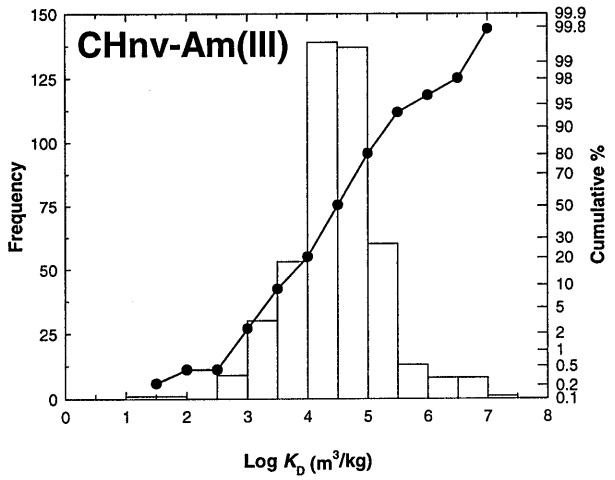
Alternative representation - The following graphs present the same data shown in pp. 72-77, with a probability axis for cumulative % to evaluate distribution.

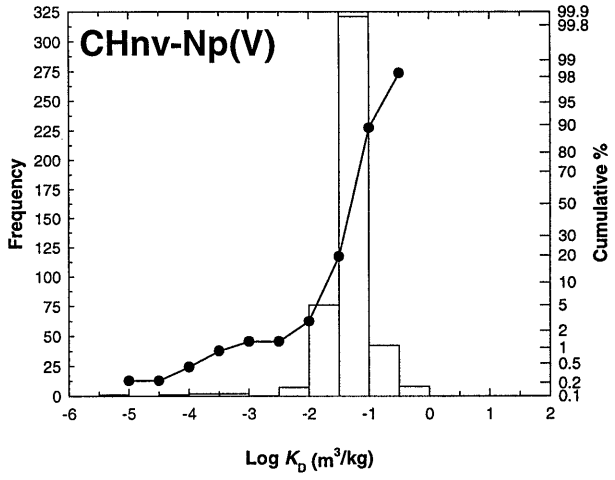


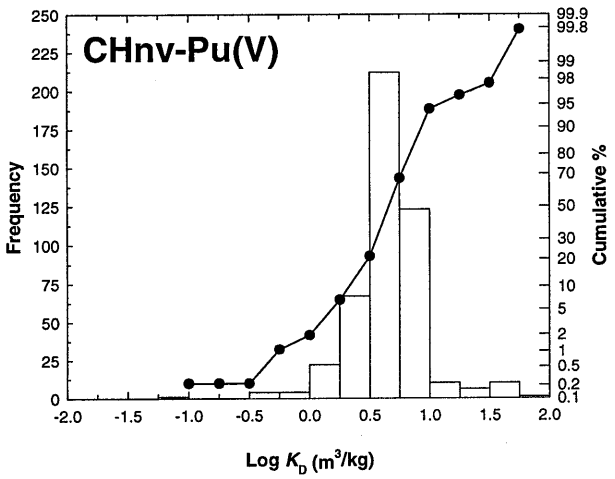



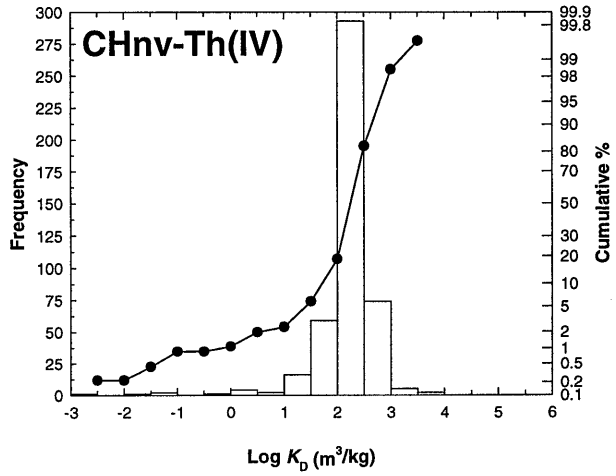



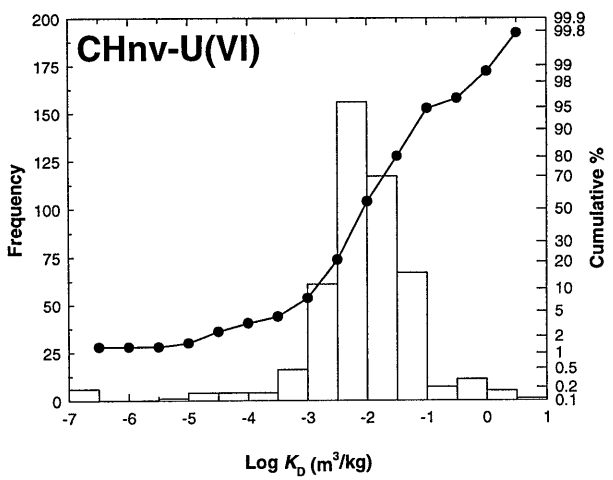



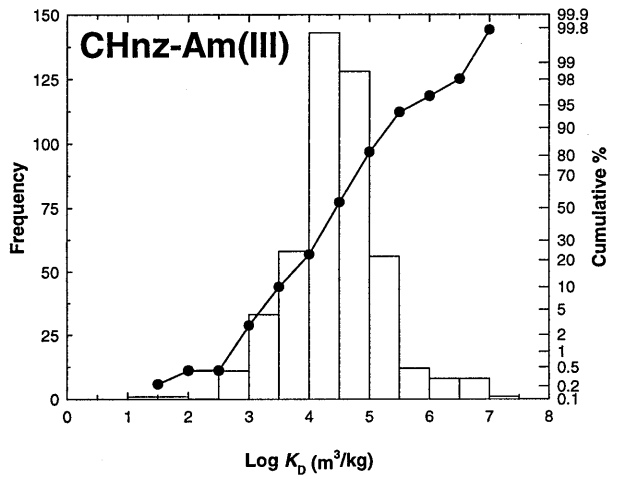

CHnv-Am(III)
Frequency
Cumulative %
Log $K_D$ (m³/kg)

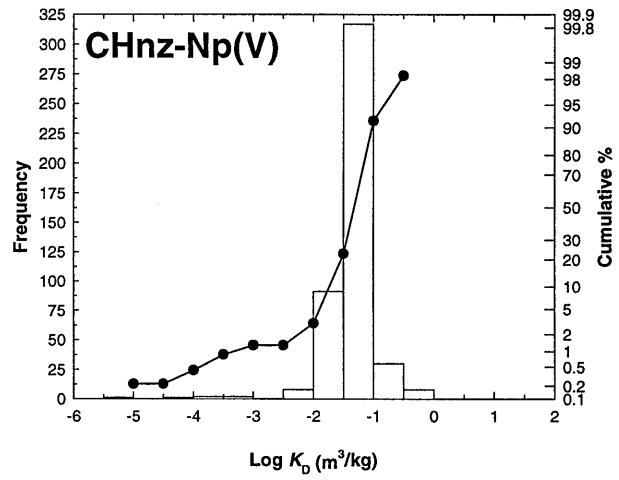

CHnv-Np(V)
Frequency
Cumulative %
Log $K_D$ (m³/kg)

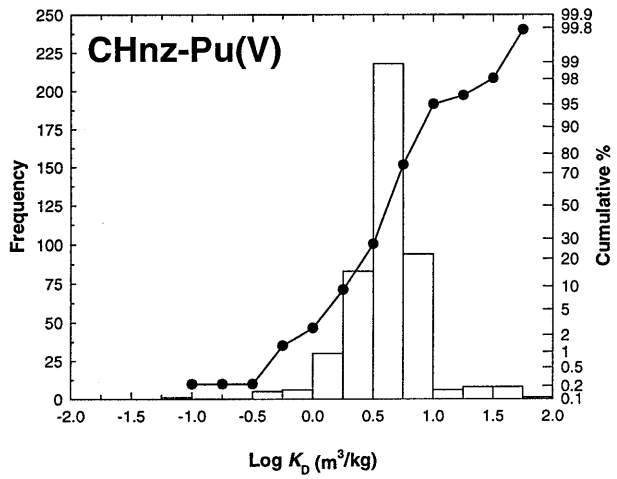

CHnv-Pu(V)
Frequency
Cumulative %
Log $K_D$ (m³/kg)

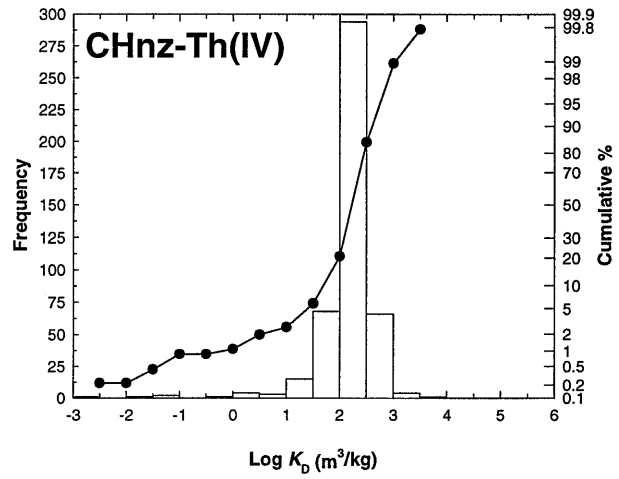

CHnv-Th(IV)
Frequency
Cumulative %
Log $K_D$ (m³/kg)

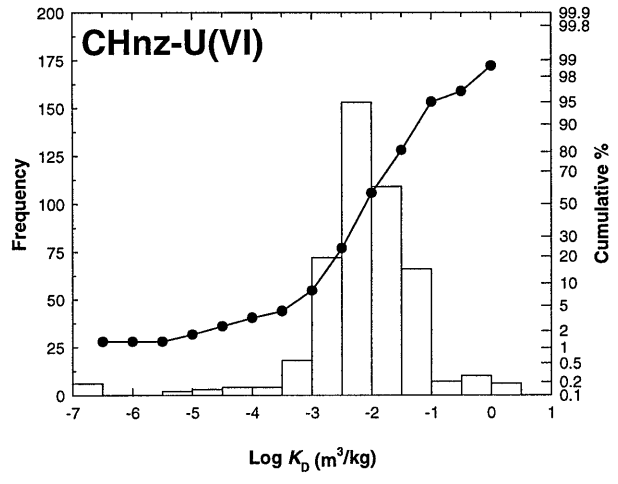

CHnv-U(VI)
Frequency
Cumulative %
Log $K_D$ (m³/kg)

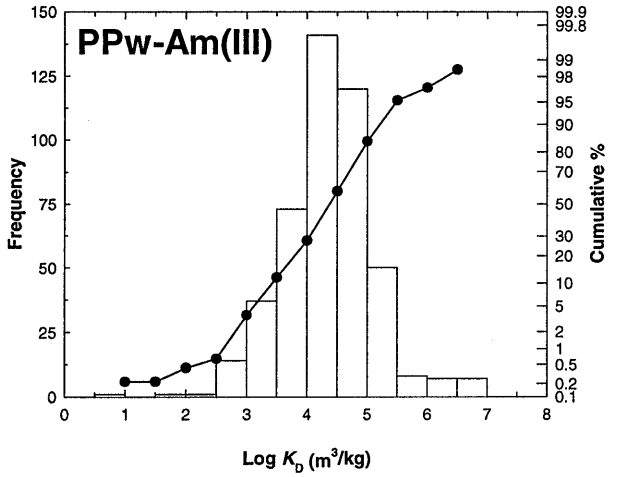

CHnz-Am(III)
Frequency
Cumulative %
Log $K_D$ (m$^3$/kg)

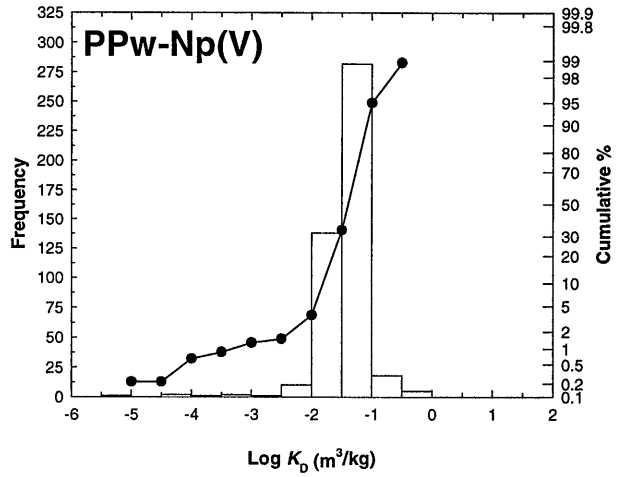

CHnz-Np(V)
Frequency
Cumulative %
Log $K_D$ (m$^3$/kg)

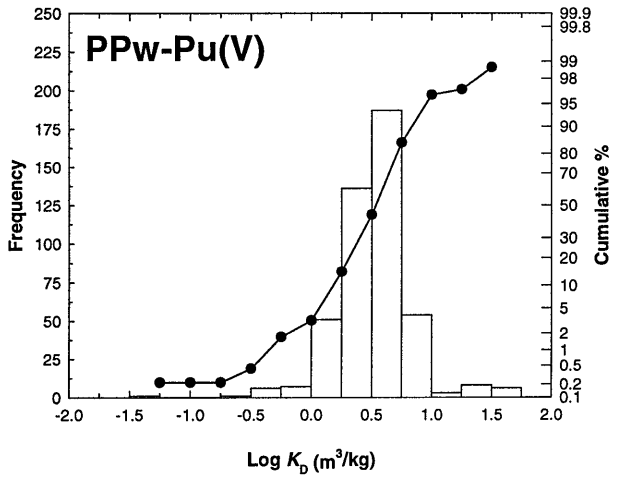

CHnz-Pu(V)
Frequency
Cumulative %
Log $K_D$ (m$^3$/kg)

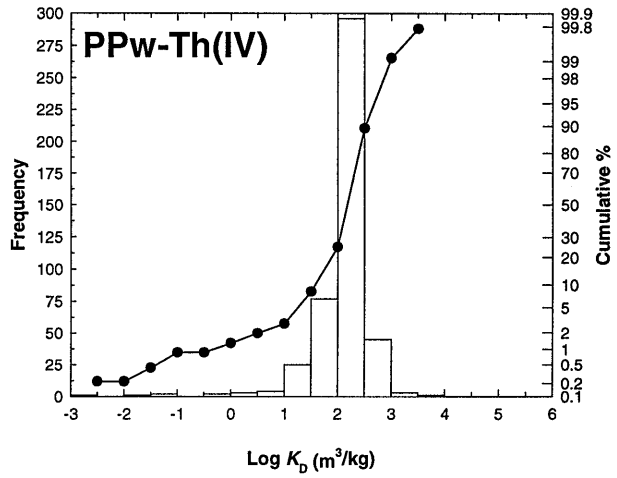

CHnz-Th(IV)
Frequency
Cumulative %
Log $K_D$ (m$^3$/kg)

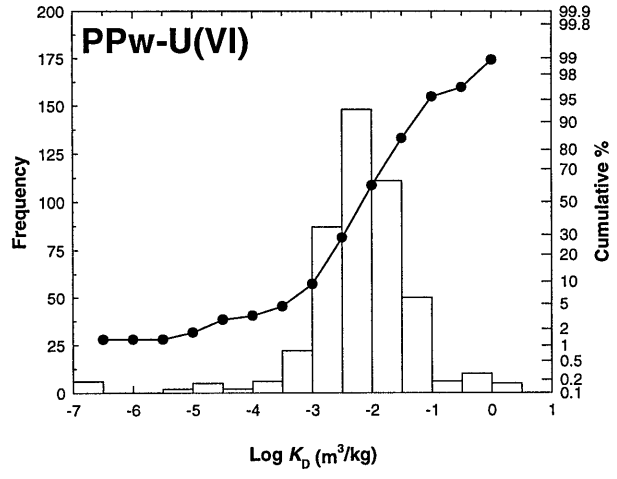

CHnz-U(VI)
Frequency
Cumulative %
Log $K_D$ (m$^3$/kg)

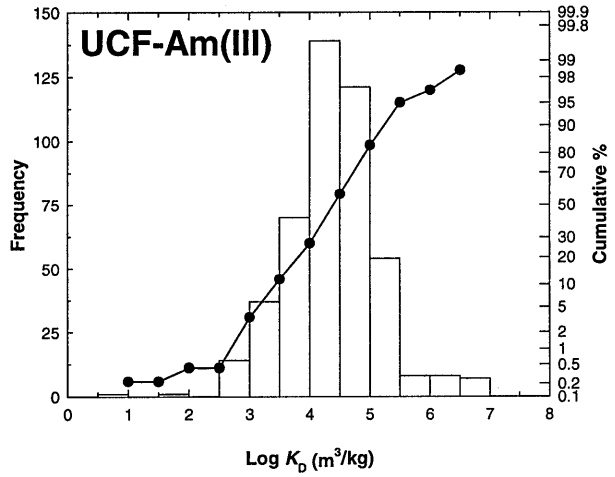

PPw-Am(III)
Frequency
Cumulative %
Log $K_D$ ($m^3$/kg)

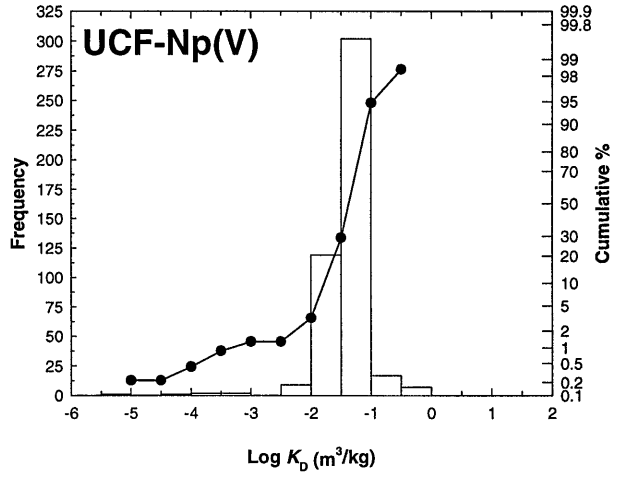

PPw-Np(V)
Frequency
Cumulative %
Log $K_D$ ($m^3$/kg)

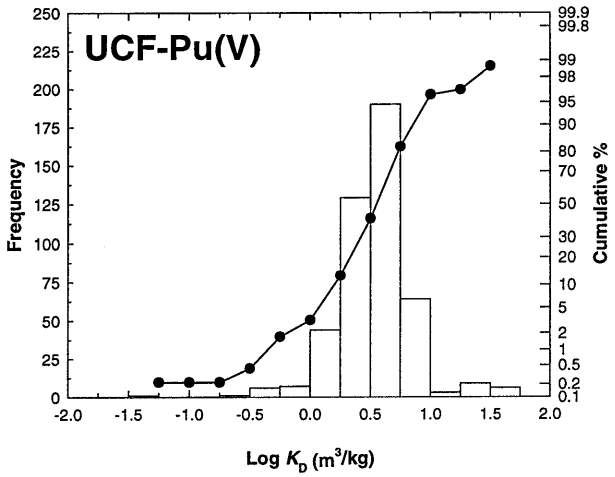

PPw-Pu(V)
Frequency
Cumulative %
Log $K_D$ ($m^3$/kg)

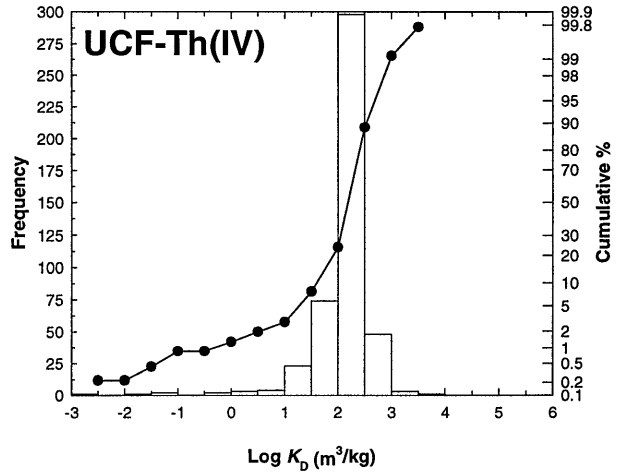

PPw-Th(IV)
Frequency
Cumulative %
Log $K_D$ ($m^3$/kg)

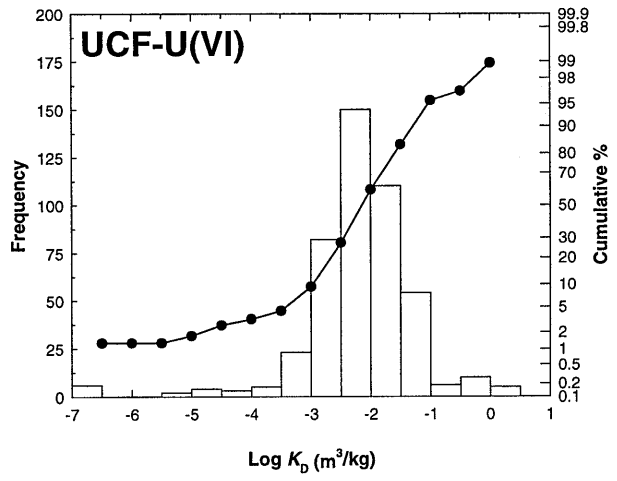

PPw-U(VI)
Frequency
Cumulative %
Log $K_D$ ($m^3$/kg)

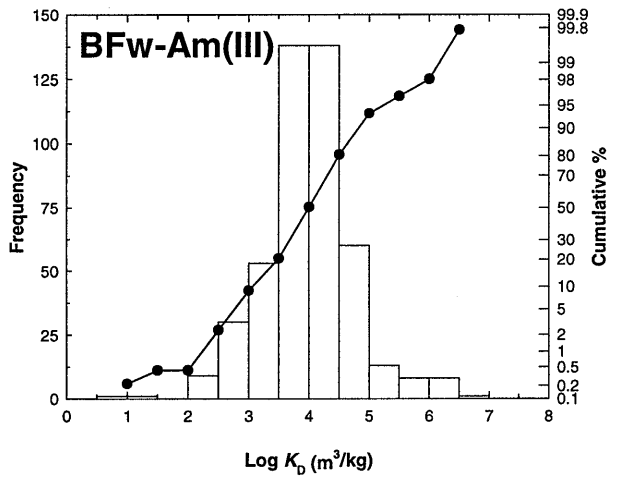

UCF-Am(III)
Frequency
Cumulative %
Log $K_D$ ($m^3$/kg)

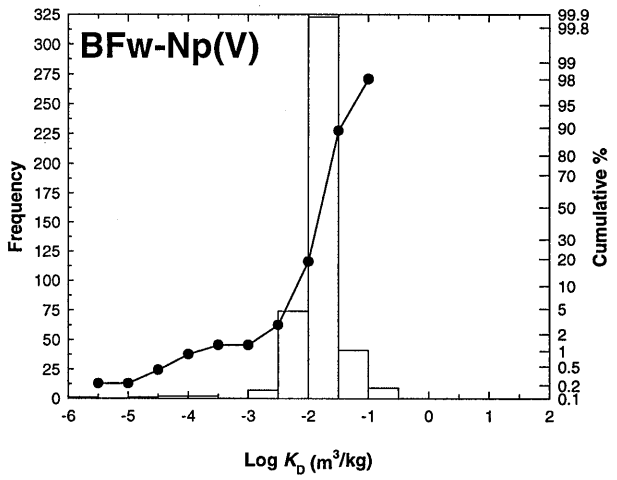

UCF-Np(V)
Frequency
Cumulative %
Log $K_D$ ($m^3$/kg)

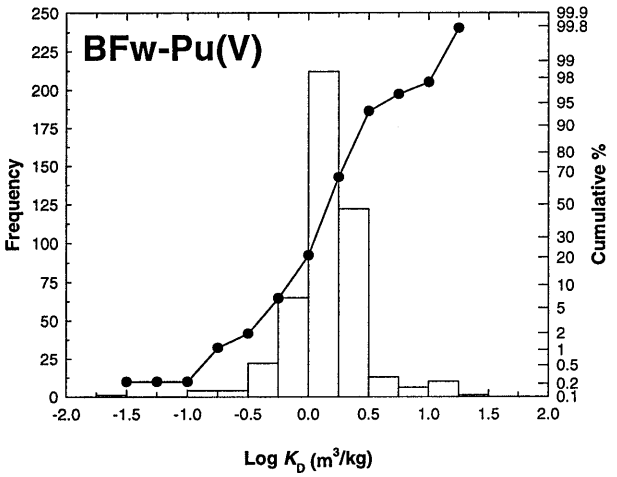

UCF-Pu(V)
Frequency
Cumulative %
Log $K_D$ ($m^3$/kg)

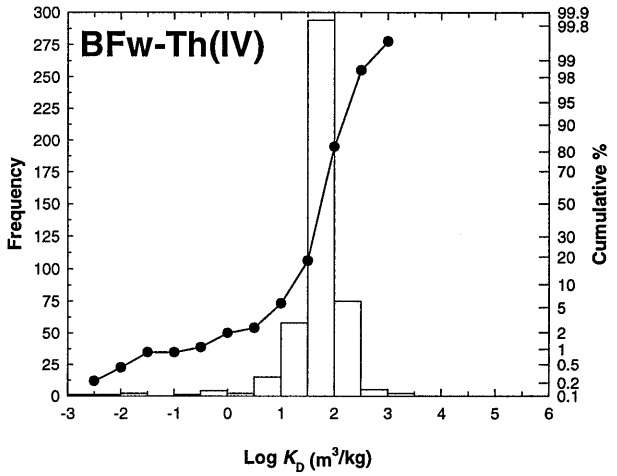

UCF-Th(IV)
Frequency
Cumulative %
Log $K_D$ ($m^3$/kg)

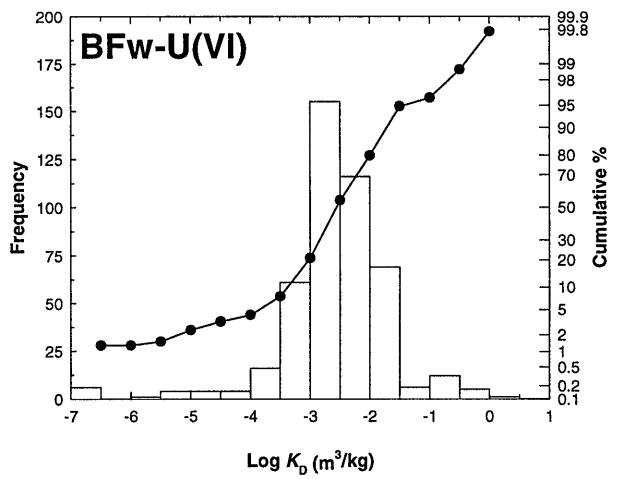

UCF-U(VI)
Frequency
Cumulative %
Log $K_D$ ($m^3$/kg)

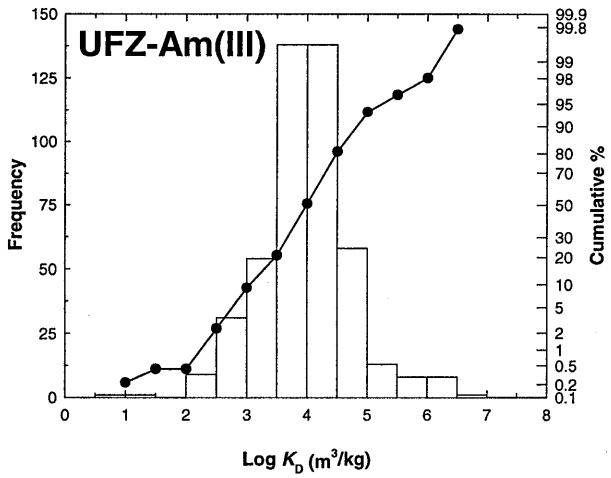

BFw-Am(III)
Frequency
Cumulative %
Log $K_D$ ($m^3$/kg)

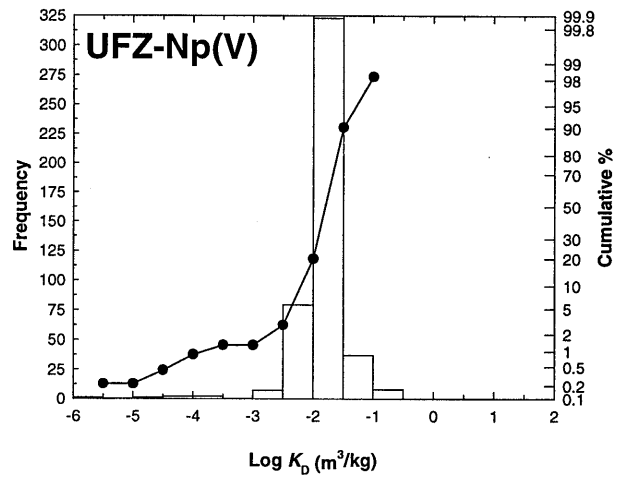

BFw-Np(V)
Frequency
Cumulative %
Log $K_D$ ($m^3$/kg)

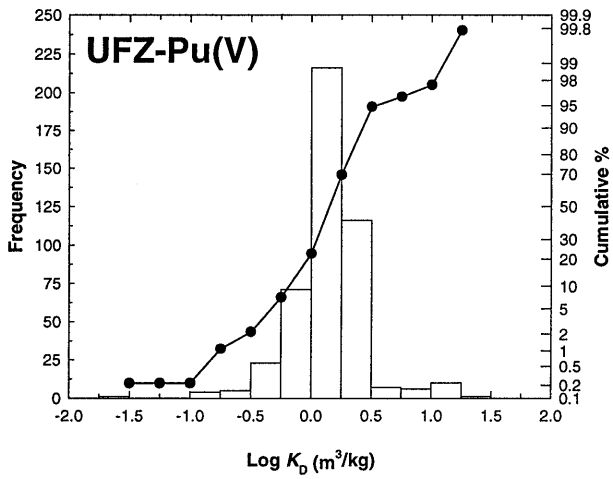

BFw-Pu(V)
Frequency
Cumulative %
Log $K_D$ ($m^3$/kg)

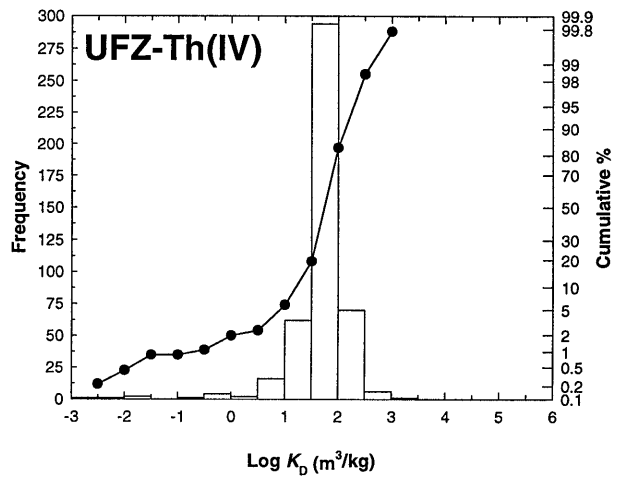

BFw-Th(IV)
Frequency
Cumulative %
Log $K_D$ ($m^3$/kg)

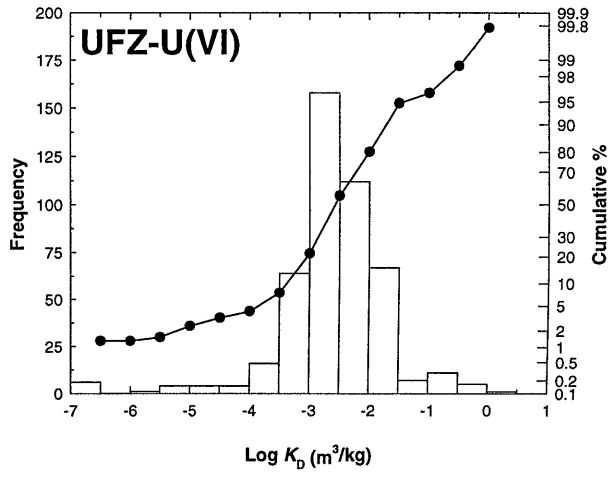

BFw-U(VI)
Frequency
Cumulative %
Log $K_D$ ($m^3$/kg)


UFZ-Am(III)
Frequency
Cumulative %
Log $K_D$ ($m^3$/kg)


UFZ-Np(V)
Frequency
Cumulative %
Log $K_D$ ($m^3$/kg)


UFZ-Pu(V)
Frequency
Cumulative %
Log $K_D$ ($m^3$/kg)


UFZ-Th(IV)
Frequency
Cumulative %
Log $K_D$ ($m^3$/kg)


UFZ-U(VI)
Frequency
Cumulative %
Log $K_D$ ($m^3$/kg)

**Developing sorption coefficient statistics for input into TPA.**

As noted earlier, the shape of the distributions for a given radionuclide are the same for each hydrostratigraphic unit. This is because the distributions are based on a $K_{A'}$ calculated using the DLM and the water chemistries of Perfect et al. (1995), screened according to criteria outlined in Turner (1998). Each radionuclide distribution is converted to $K_D$ by multiplying it by the effective surface area of the unit, a constant, resulting in the same shape distribution for each hydrostratigraphic unit.

When cumulative percent is expressed in terms of probability, sorption coefficients for all five radionuclides (in terms of log $K_D$) plot in a straight line over much of the range of interest. This suggests a log-normal distribution is appropriate for all five radioelements. To varying degrees, however, all five show a deviation from the straight line at the lower values. This is due to a small population of high pH, high carbonate, and high salinity waters collected at Franklin Lake Playa (see pg. 58, for example). There is also some deviation at the higher values, due to a suite of high pH, low carbonate samples collected mostly from trenches near the Beatty low-level waste facility (see pg. 58, for example). There are also some high pH, low carbonate chloride brines from Franklin Lake that result in high sorption.

GIS Database - saturated zone water chemistry in the Yucca Mountain region

Objective: create GIS coverages and maps showing variation in the geochemistry (e.g., saturation indices for calcite and cristobalite) of waters in the Yucca Mountain region.

Method: use geochemical data from wells and springs to construct contour maps which can be converted into GIS coverages.

Software
- ARC/INFO GIS software residing on a UNIX based workstation
- ARCVIEW 3.0 map composition software residing on Windows NT PC
- SURFACE III contouring software (currently only MacIntosh version is available)
- EXCEL spreadsheet

Procedure and Results

1. An EXCEL file named YMCHEM was obtained from D. Turner (the PI for the RT KTI) which contained geochemical information on waters sampled from wells and springs in the YM region. The locations of wells and springs were given in UTM coordinates. All sampling locations were located in a region from 500000 to 600000 m east and 4000000 to 4100000 north.

2. The following geochemical parameters contained in file YMCHEM were chosen for construction of GIS converages.

   Equilibrium ionic strength
   Partial pressure of CO2 - PCO2
   Saturation index of calcite
   Saturation index of cristobalite
   Distribution coefficient for neptunium
   Distribution coefficient for uranium

3. The data for these parameters along with well names and locations (UTM coordinates) were cut and pasted into a new file named YMCHEM_1.

   Some wells and springs were sampled several times on several dates. Multiple analyses existed for these wells and springs. In these cases data was averaged to give a single value for each geochemical parameter at each sample location.

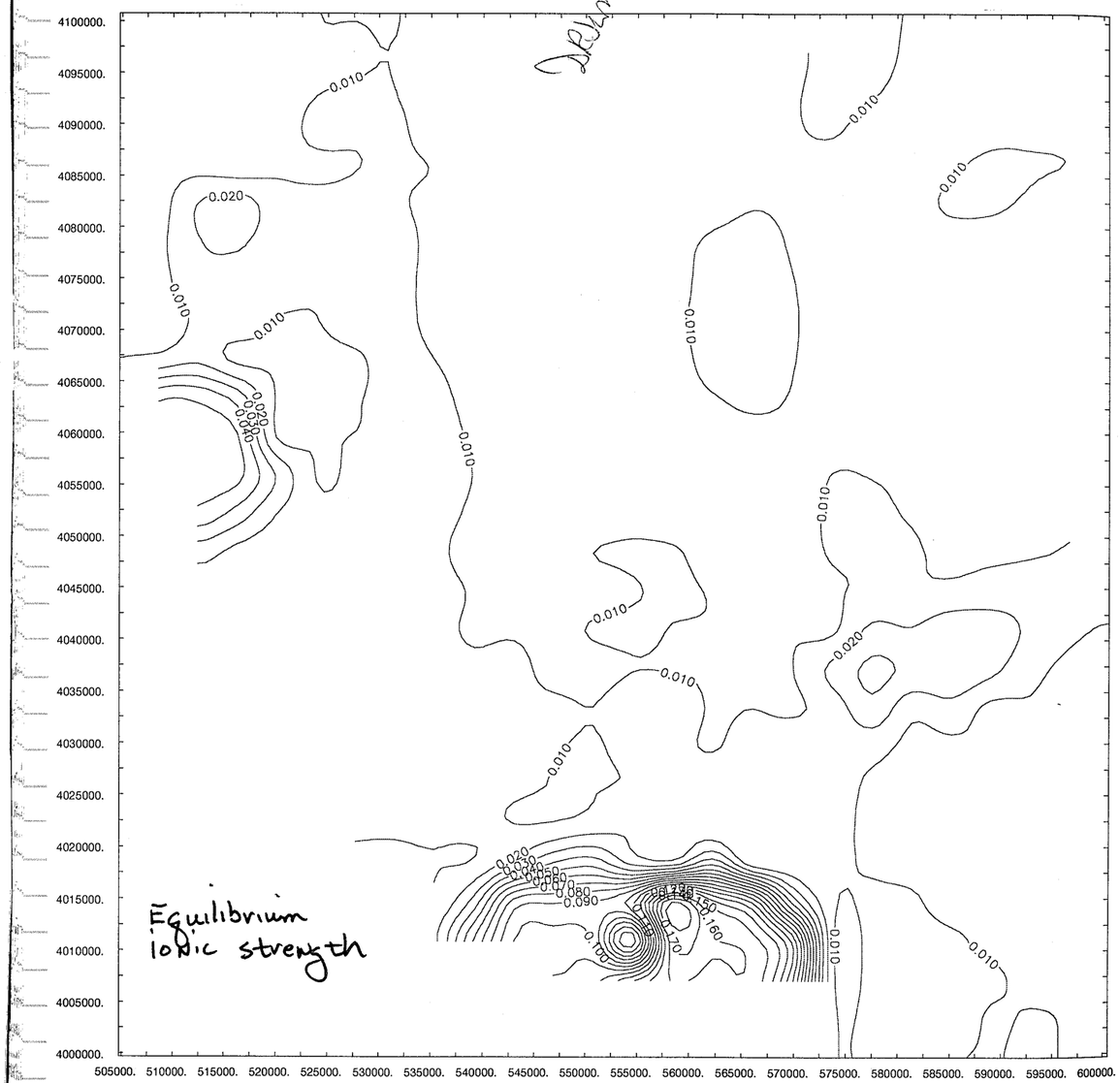
   These averages were placed in a file named YMAVES along with sample locations in UTM coordinates.

4. Contour plots for each geochemical parameter were generated using SURFACE III - a software package developed by the Kansas Geological Survey. SURFACE III was specially designed for plotting and contouring geographic data. SURFACE III is shareware and was downloaded from the Kansas Geological Surveys website on the internet. At this time only a MacIntosh version of software is available.

   SURFACE III allows x, y, z tab delimited data to be read, grided, and contoured. The data contained in YMAVES was placed in several tab delimited files so that a contour plot of each geochemical parameter could be generated. The contour plots were created using the UTM east coordinate of the sample location as the x value, the UTM north coordinate of the location as the y value, and the geochemical parameter value of the sample location as the z value.

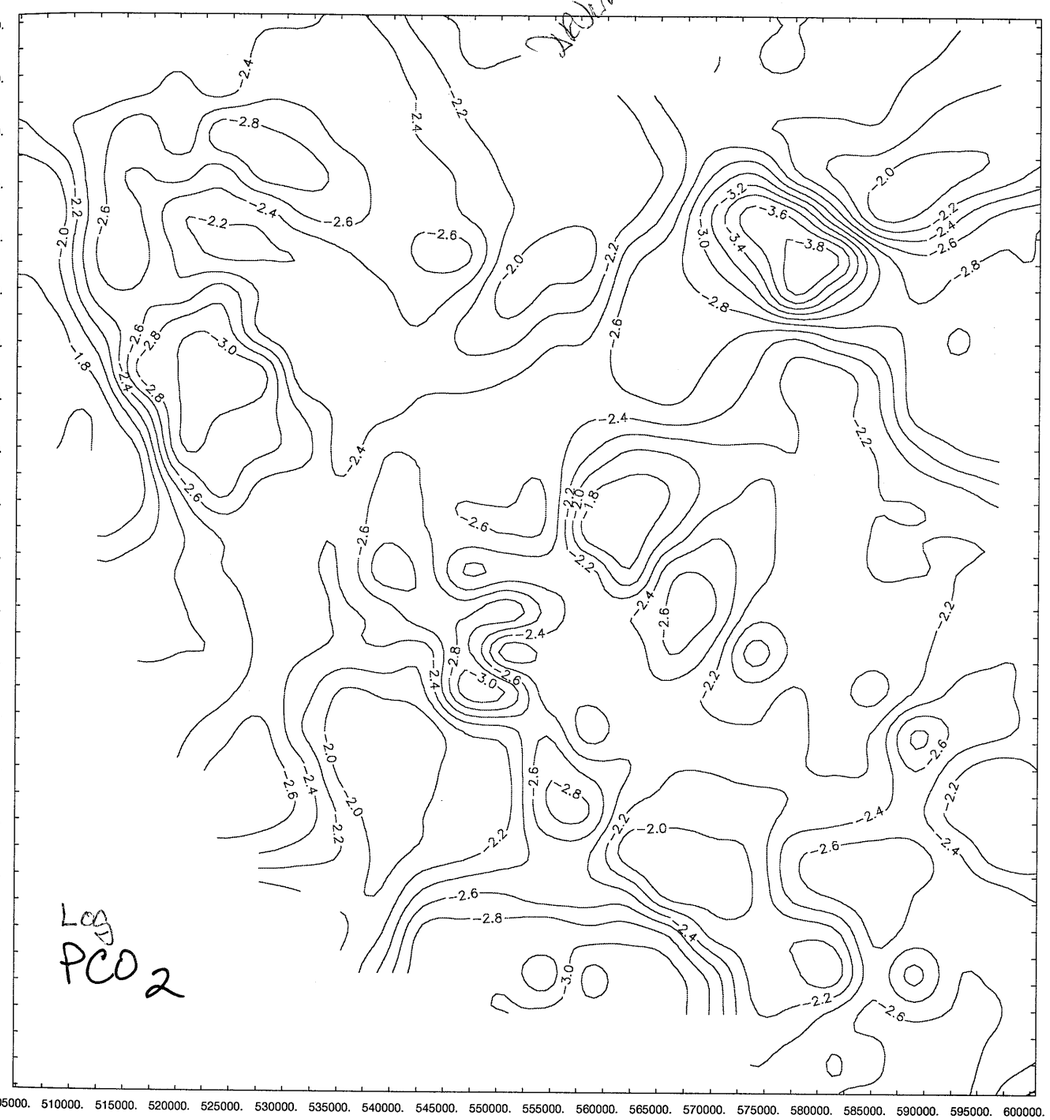
   The contour plots for each geochemical parameter are shown on the following pages.

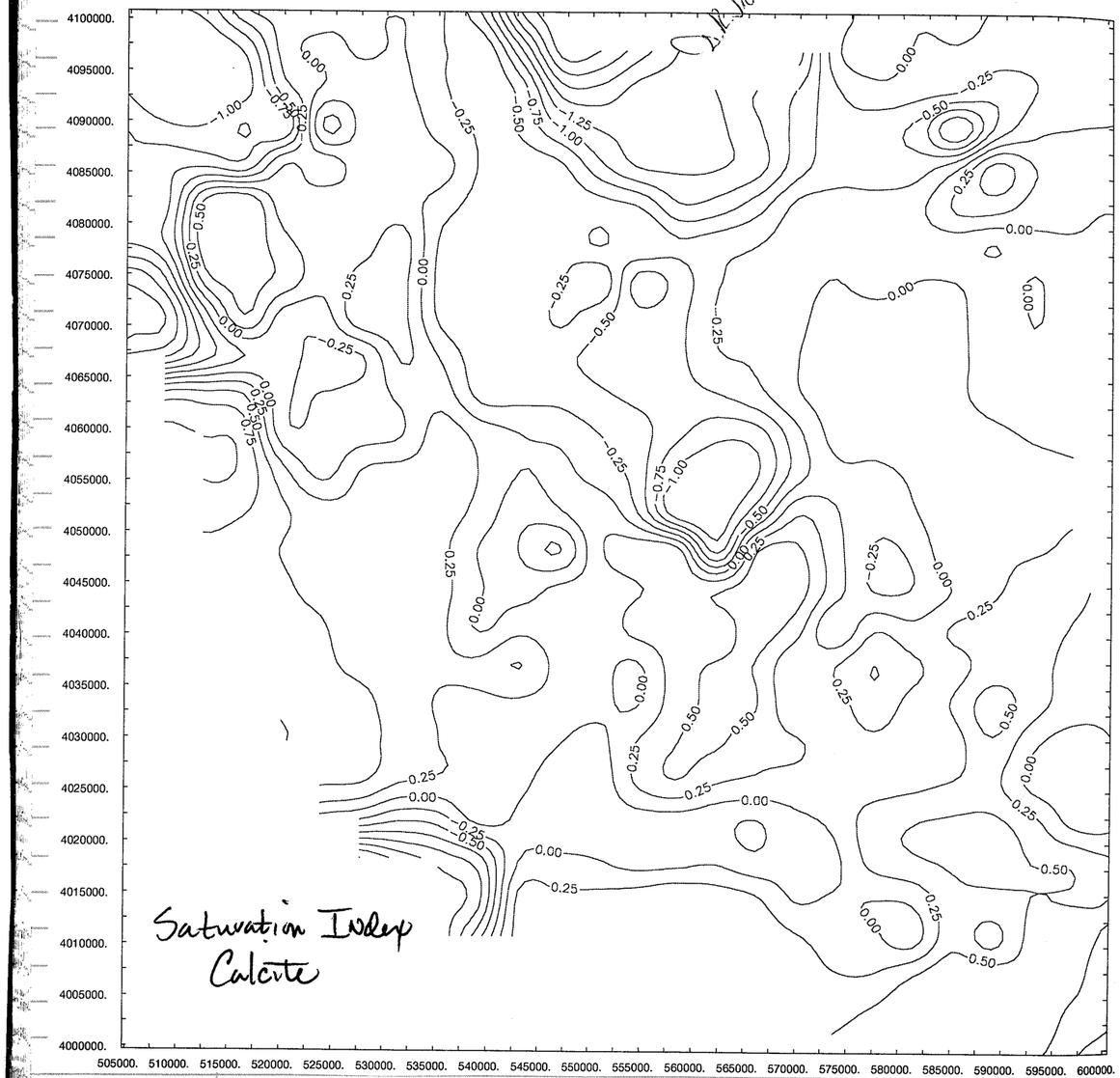
6/15/98 (DRJ)






6/15/98 (DRJ)




4100000.
4095000.
4090000.
4085000.
4080000.
4075000.
4070000.
4065000.
4060000.
4055000.
4050000.
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4040000.
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4025000.
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4015000.
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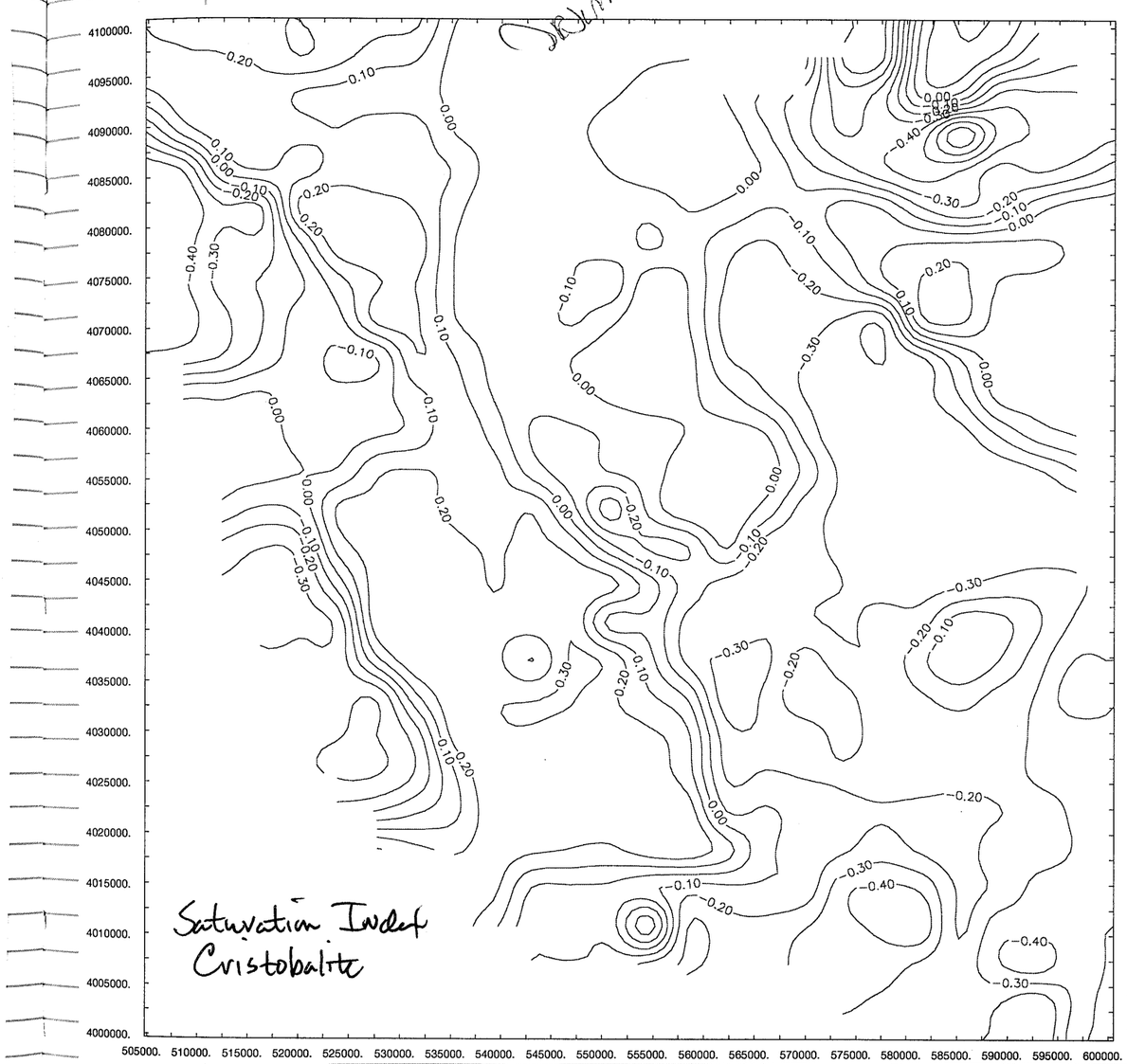
4005000.
4000000.
505000. 510000. 515000. 520000. 525000. 530000. 535000. 540000. 545000. 550000. 555000. 560000. 565000. 570000. 575000. 580000. 585000. 590000. 595000. 600000.
Saturation Index
Calcite


4100000.
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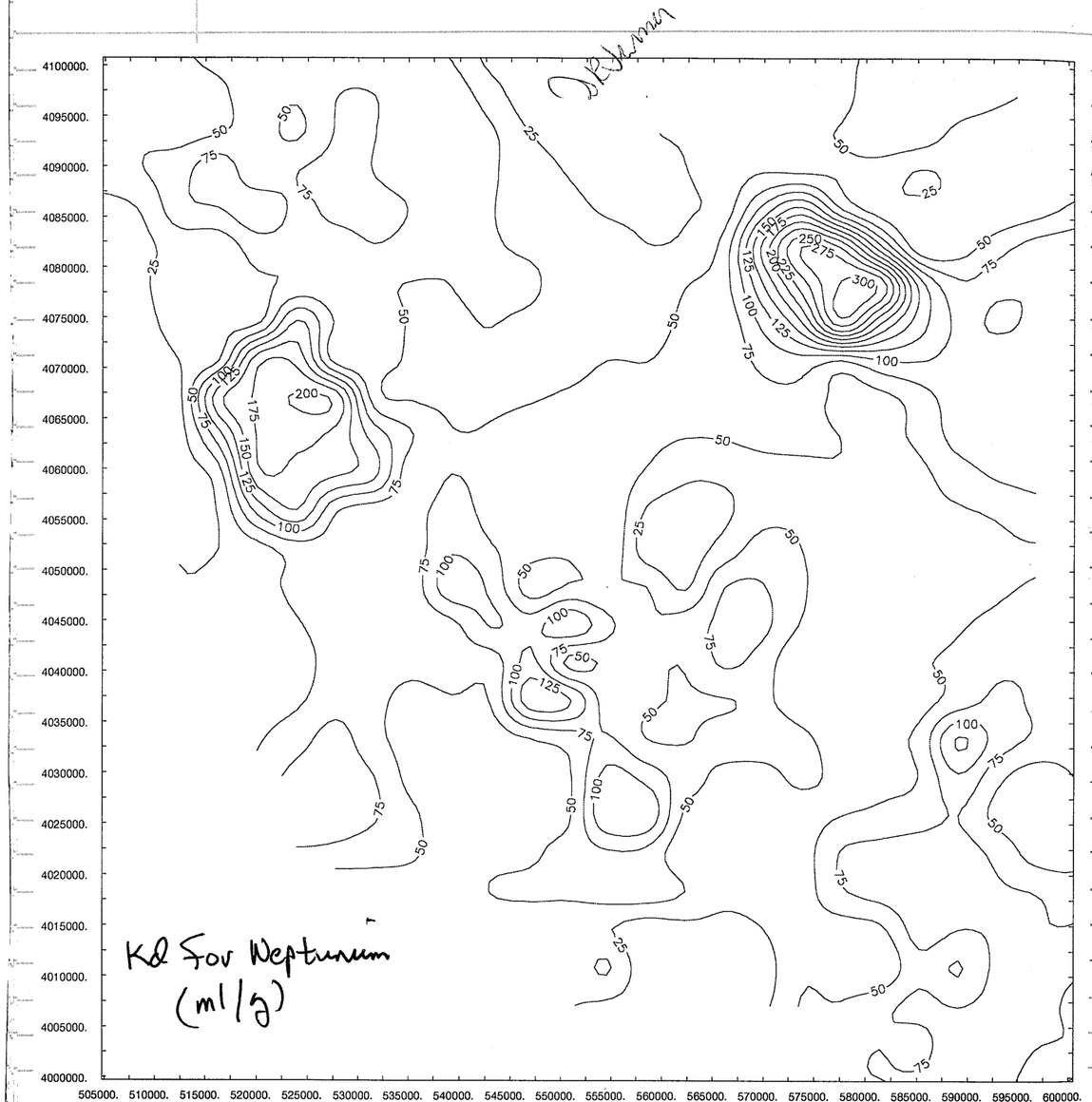
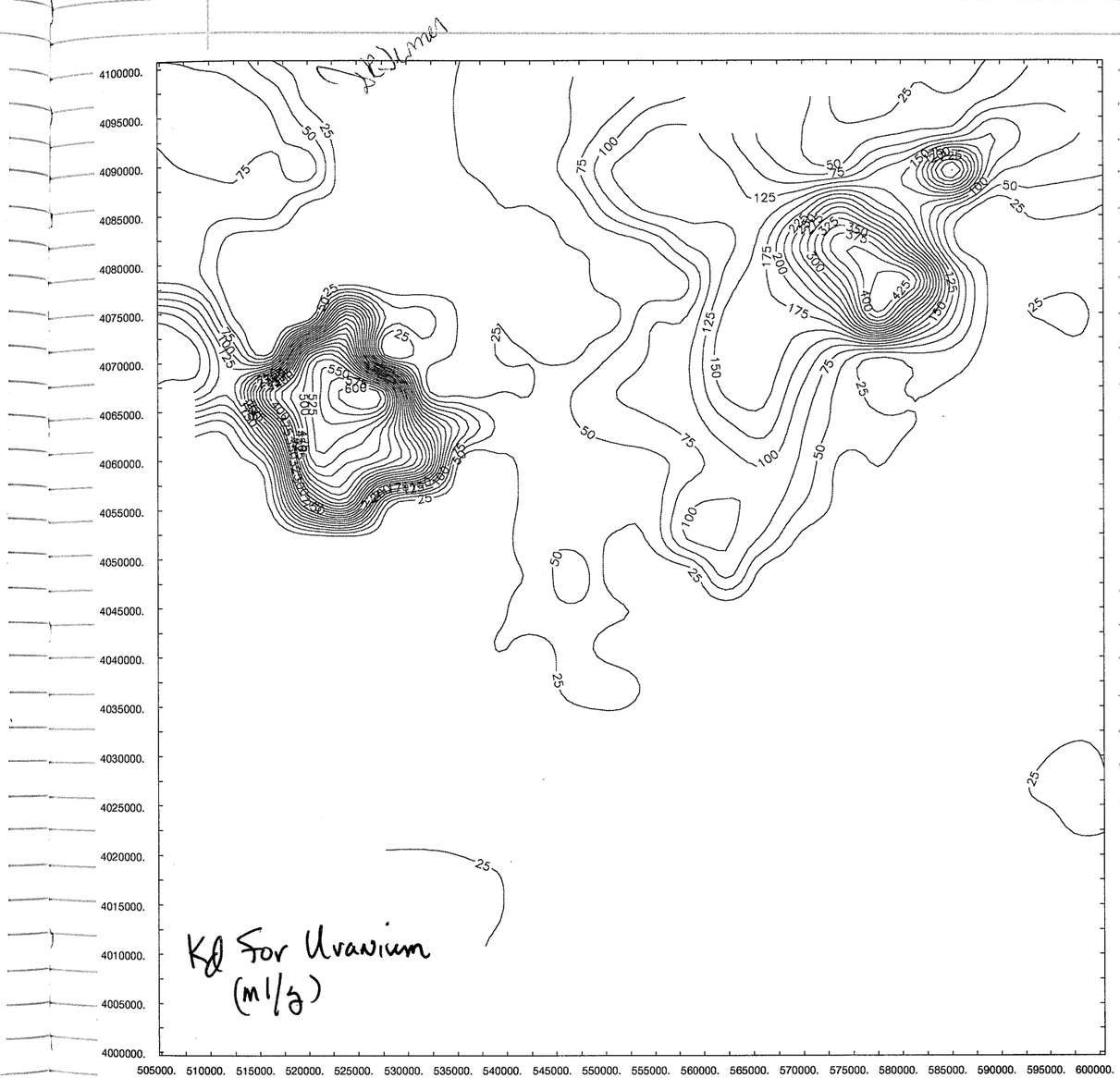
4005000.
4000000.
505000. 510000. 515000. 520000. 525000. 530000. 535000. 540000. 545000. 550000. 555000. 560000. 565000. 570000. 575000. 580000. 585000. 590000. 595000. 600000.
Saturation Index
Cristobalite

6/15/98
DRJ






6/15/98
DRJ



6/15/98 DRS

5. SURFACE III allows contours to be output to files in a format that will allow construction of ARC/INFO coverages of the plots. ARC/INFO uses the GENERATE command to create these coverages.

The contour plot for each geochemical parameter was output to this type of file and coverages were generated using ARC/INFO.

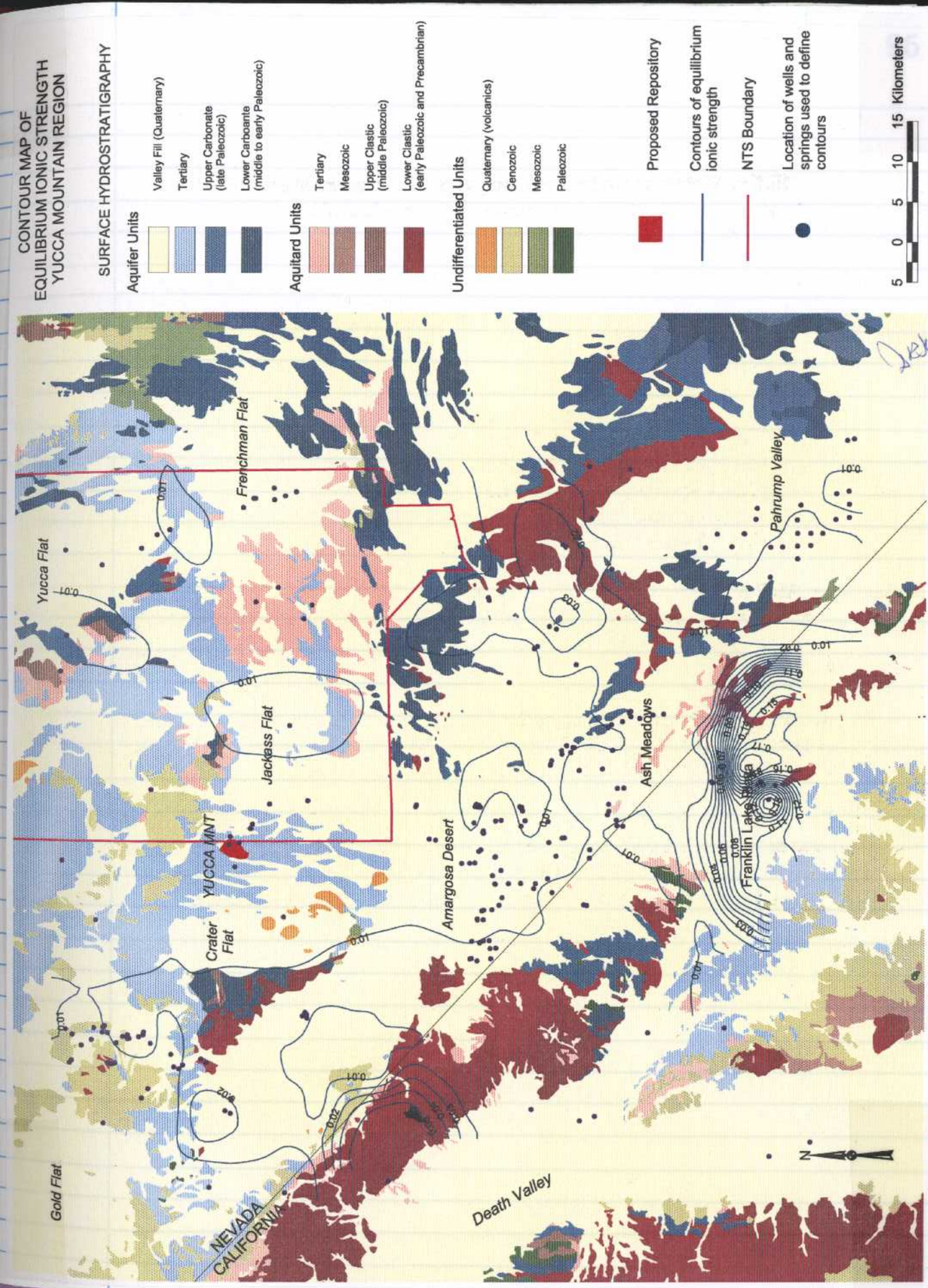
Coverage names were:

eqis_1 - equilibrium ionic strength
kdnp_1 - distribution coefficient for neptunium
kdu_1 - distribution coefficient for uranium
pco2_1 - partial pressure of CO2
sicc_1 - saturation index for calcite
sicrsb_1 - saturation index for cristobalite

6. An ARC/INFO coverage showing well and spring locations was also generated from a file containing the x and y UTM coordinates. This coverage was named wells. The wells coverage also includes the actual values for the geochemical parameters at spring or well locations.

7. Maps showing variation in the geochemical parameters over the YM region were constructed using ARCVIEW 3.0 software. This software allows layering of ARC/INFO coverages and other tools that can be used to construct maps.

Two examples of the types of maps that have been constructed using the geochemical contour coverages are shown on the following pages. In these examples, contours of equilibrium ionic strength are overlain on coverages of surface hydrostratigraphy (see notebook 198, pp. 3 - 29 for information concerning the surface hydrostratigraphic unit coverages).



## Adding TPA sorption coefficient input for Alluvium-SAV

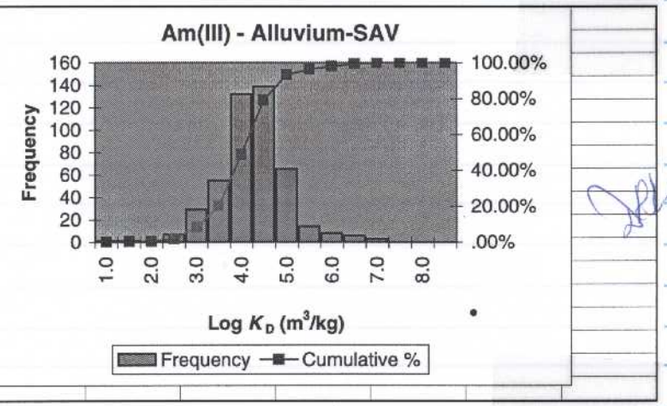
The approach outlined above was used to calculate sorption coefficients for the alluvium unit SAV in TPA, version 3.2. The following input values were used

porosity = 12.5 % (mean between 10 and 15 % in tpa.inp)
aperture = 0.1 micron (r = 0.05 x $10^{-6}$ m)
grain density = 2470 kg/$m^3$ (not a parameter in tpa.inp; unweighted average of all tuff units)

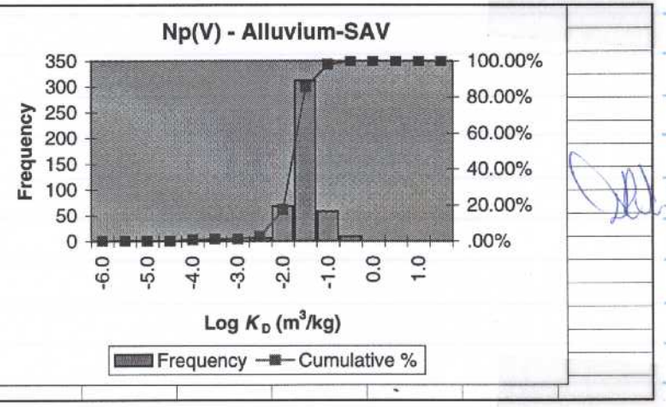
Using these values, $S_r$ = 3.0 $m^2$/g.

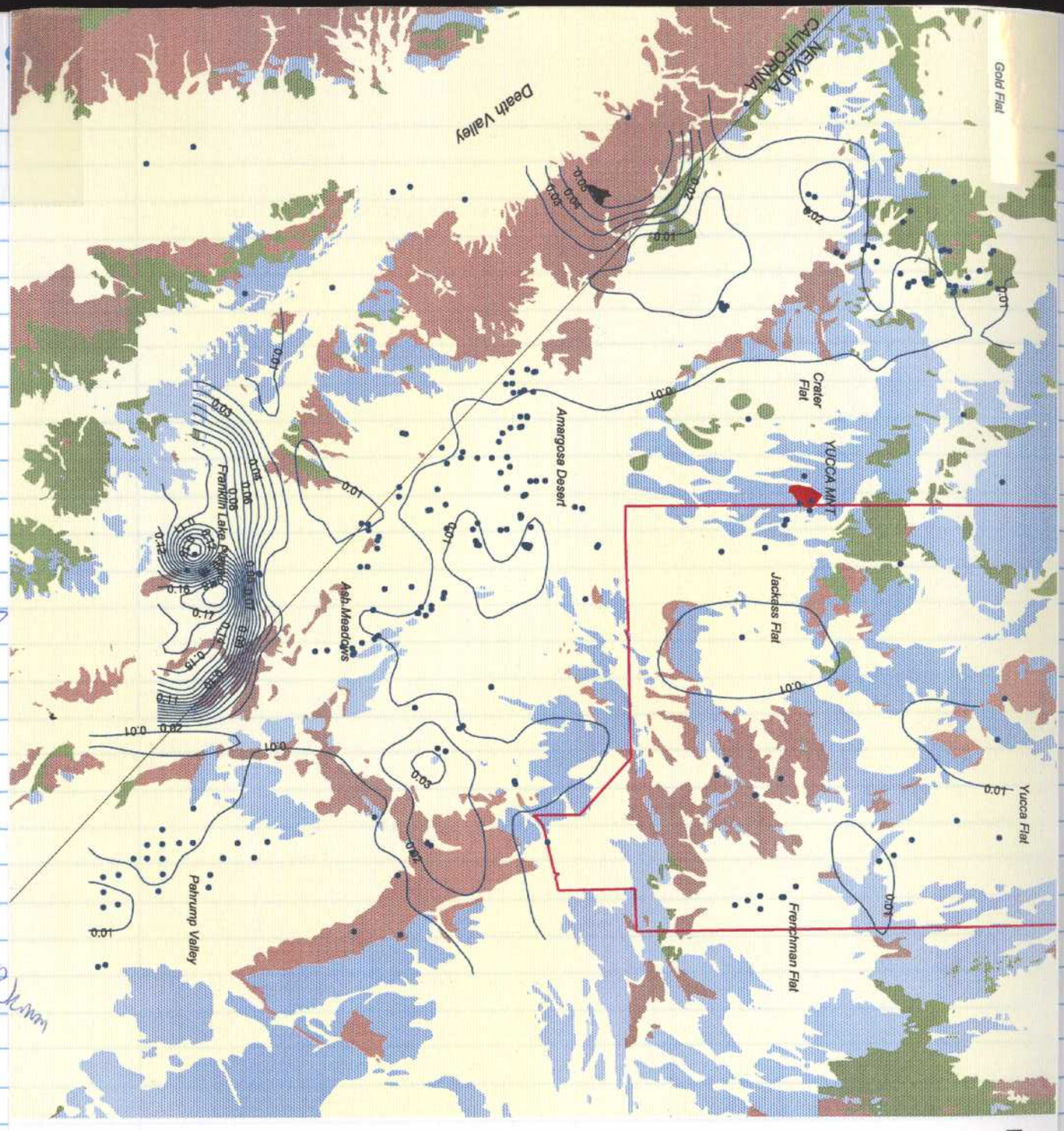
Log $K_D$ values were calculated as discussed above and are shown here

| Alluvium-SAV | Frequency | Cumulative % |
|---|---|---|
| 1.0 | 1 | .22% |
| 1.5 | 1 | .43% |
| 2.0 | 0 | .43% |
| 2.5 | 7 | 1.96% |
| 3.0 | 29 | 8.26% |
| 3.5 | 55 | 20.22% |
| 4.0 | 132 | 48.91% |
| 4.5 | 139 | 79.13% |
| 5.0 | 65 | 93.26% |
| 5.5 | 14 | 96.30% |
| 6.0 | 8 | 98.04% |
| 6.5 | 6 | 99.35% |
| 7.0 | 3 | 100.00% |
| 7.5 | 0 | 100.00% |
| 8.0 | 0 | 100.00% |
| More | 0 | 100.00% |




| Alluvium-SAV | Frequency | Cumulative % |
|---|---|---|
| -6.0 | 0 | .00% |
| -5.5 | 1 | .22% |
| -5.0 | 0 | .22% |
| -4.5 | 0 | .22% |
| -4.0 | 3 | .87% |
| -3.5 | 2 | 1.30% |
| -3.0 | 0 | 1.30% |
| -2.5 | 7 | 2.83% |
| -2.0 | 68 | 17.61% |
| -1.5 | 312 | 85.43% |
| -1.0 | 58 | 98.04% |
| -0.5 | 9 | 100.00% |
| 0.0 | 0 | 100.00% |
| 0.5 | 0 | 100.00% |
| 1.0 | 0 | 100.00% |
| More | 0 | 100.00% |




CONTOUR MAP OF EQUILIBRIUM IONIC STRENGTH YUCCA MOUNTAIN REGION

HYDROSTRATIGRAPHIC UNITS

- Valley Fill
- Aquifers
- Aquitards
- Undifferentiated

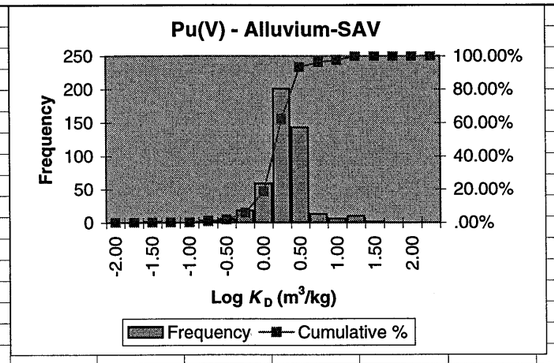
- Proposed Repository
- Contours of equilibrium ionic strength
- NTS Boundary
- Location of wells and springs used to define contours

N

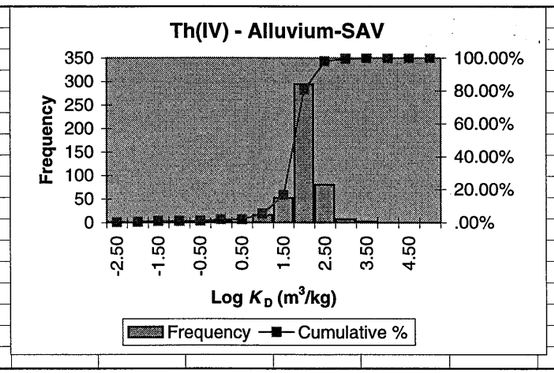
5 0 5 10 15 20 Kilometers

7/7/98

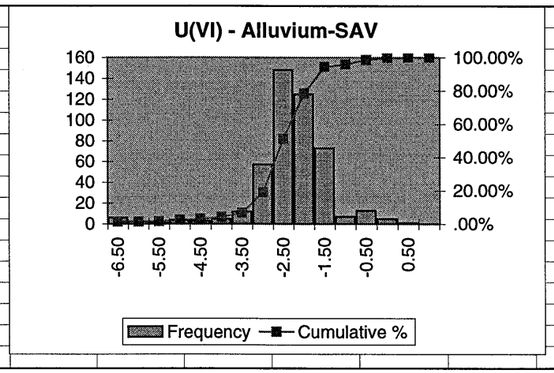
| Alluvium-SAV | Frequency | Cumulative % |
|---|---|---|
| -2.00 | 0 | .00% |
| -1.75 | 0 | .00% |
| -1.50 | 1 | .22% |
| -1.25 | 0 | .22% |
| -1.00 | 0 | .22% |
| -0.75 | 3 | .87% |
| -0.50 | 5 | 1.96% |
| -0.25 | 18 | 5.87% |
| 0.00 | 59 | 18.70% |
| 0.25 | 201 | 62.39% |
| 0.50 | 143 | 93.48% |
| 0.75 | 13 | 96.30% |
| 1.00 | 6 | 97.61% |
| 1.25 | 10 | 99.78% |
| 1.50 | 1 | 100.00% |
| 1.75 | 0 | 100.00% |
| 2.00 | 0 | 100.00% |
| More | 0 | 100.00% |




| Alluvium-SAV | Frequency | Cumulative % |
|---|---|---|
| -2.50 | 1 | .22% |
| -2.00 | 1 | .43% |
| -1.50 | 2 | .87% |
| -1.00 | 0 | .87% |
| -0.50 | 1 | 1.09% |
| 0.00 | 4 | 1.96% |
| 0.50 | 0 | 1.96% |
| 1.00 | 16 | 5.43% |
| 1.50 | 52 | 16.74% |
| 2.00 | 294 | 80.65% |
| 2.50 | 80 | 98.04% |
| 3.00 | 7 | 99.57% |
| 3.50 | 2 | 100.00% |
| 4.00 | 0 | 100.00% |
| 4.50 | 0 | 100.00% |
| More | 0 | 100.00% |




| Alluvium-SAV | Frequency | Cumulative % |
|---|---|---|
| -6.50 | 6 | 1.30% |
| -6.00 | 0 | 1.30% |
| -5.50 | 1 | 1.52% |
| -5.00 | 4 | 2.39% |
| -4.50 | 3 | 3.04% |
| -4.00 | 5 | 4.13% |
| -3.50 | 12 | 6.74% |
| -3.00 | 57 | 19.13% |
| -2.50 | 148 | 51.30% |
| -2.00 | 125 | 78.48% |
| -1.50 | 73 | 94.35% |
| -1.00 | 7 | 95.87% |
| -0.50 | 13 | 98.70% |
| 0.00 | 5 | 99.78% |
| 0.50 | 1 | 100.00% |
| More | 0 | 100.00% |






| Log KD(m3/kg) | Am(III)-TSw | Am(III)-CHnv | Am(III)-CHnz | Am(III)-PPw | Am(III)-UCF | Am(III)-BFw | Am(III)-UFZ | Am(III)-SAV |
|---|---|---|---|---|---|---|---|---|
| Mean | 4.01098789 | 4.49307256 | 4.45167988 | 4.36813383 | 4.38743898 | 3.99574792 | 3.97995365 | 4.02571115 |
| Standard Error | 0.03488939 | 0.03488939 | 0.03488939 | 0.03488939 | 0.03488939 | 0.03488939 | 0.03488939 | 0.03488939 |
| Median | 4.00188867 | 4.48397334 | 4.44258066 | 4.35903461 | 4.37833976 | 3.9866487 | 3.97085443 | 4.01661192 |
| Mode | 3.79964017 | 4.28172484 | 4.24033216 | 4.1567861 | 4.17609126 | 3.7844002 | 3.76860593 | 3.81436342 |
| Standard Deviation | 0.74829408 | 0.74829408 | 0.74829408 | 0.74829408 | 0.74829408 | 0.74829408 | 0.74829408 | 0.74829408 |
| Sample Variance | 0.55994403 | 0.55994403 | 0.55994403 | 0.55994403 | 0.55994403 | 0.55994403 | 0.55994403 | 0.55994403 |
| Kurtosis | 1.92430783 | 1.92430783 | 1.92430783 | 1.92430783 | 1.92430783 | 1.92430783 | 1.92430783 | 1.92430783 |
| Skewness | 0.11843681 | 0.11843681 | 0.11843681 | 0.11843681 | 0.11843681 | 0.11843681 | 0.11843681 | 0.11843681 |
| Range | 5.95820176 | 5.95820176 | 5.95820176 | 5.95820176 | 5.95820176 | 5.95820176 | 5.95820176 | 5.95820176 |
| Minimum | 0.62281817 | 1.10490284 | 1.06351016 | 0.9799641 | 0.99926926 | 0.6075782 | 0.59178393 | 0.63754142 |
| Maximum | 6.58101993 | 7.0631046 | 7.02171192 | 6.93816587 | 6.95747102 | 6.56577996 | 6.5499857 | 6.59574319 |
| Sum | 1845.05443 | 2066.81338 | 2047.77274 | 2009.34156 | 2018.22193 | 1838.04404 | 1830.77868 | 1851.82713 |
| Count | 460 | 460 | 460 | 460 | 460 | 460 | 460 | 460 |
| Confidence Level(95.0%) | 0.06856272 | 0.06856272 | 0.06856272 | 0.06856272 | 0.06856272 | 0.06856272 | 0.06856272 | 0.06856272 |

| Log KD(m3/kg) | Np(V)-TSw | Np(V)-CHnv | Np(V)-CHnz | Np(V)-PPw | Np(V)-UCF | Np(V)-BFw | Np(V)-UFZ | Np(V)-SAV |
|---|---|---|---|---|---|---|---|---|
| Mean | -1.79552265 | -1.31343797 | -1.35483066 | -1.43837671 | -1.41907155 | -1.81076261 | -1.82655688 | -1.78079939 |
| Standard Error | 0.01968626 | 0.01968626 | 0.01968626 | 0.01968626 | 0.01968626 | 0.01968626 | 0.01968626 | 0.01968626 |
| Median | -1.76443882 | -1.28235415 | -1.32374684 | -1.40729289 | -1.38798773 | -1.77967879 | -1.79547306 | -1.74971557 |
| Mode | -1.79988489 | -1.31780022 | -1.3591929 | -1.44273895 | -1.4234338 | -1.81512486 | -1.83091913 | -1.78516163 |
| Standard Deviation | 0.42222331 | 0.42222331 | 0.42222331 | 0.42222331 | 0.42222331 | 0.42222331 | 0.42222331 | 0.42222331 |
| Sample Variance | 0.17827252 | 0.17827252 | 0.17827252 | 0.17827252 | 0.17827252 | 0.17827252 | 0.17827252 | 0.17827252 |
| Kurtosis | 26.5764652 | 26.5764652 | 26.5764652 | 26.5764652 | 26.5764652 | 26.5764652 | 26.5764652 | 26.5764652 |
| Skewness | -3.5561097 | -3.5561097 | -3.5561097 | -3.5561097 | -3.5561097 | -3.5561097 | -3.5561097 | -3.5561097 |
| Range | 5.14041944 | 5.14041944 | 5.14041944 | 5.14041944 | 5.14041944 | 5.14041944 | 5.14041944 | 5.14041944 |
| Minimum | -5.80186766 | -5.31978299 | -5.36117567 | -5.44472173 | -5.42541657 | -5.81710763 | -5.8329019 | -5.78714441 |
| Maximum | -0.66144822 | -0.17936355 | -0.22075623 | -0.30430229 | -0.28499713 | -0.67668819 | -0.69248246 | -0.64672497 |
| Sum | -825.940417 | -604.181467 | -623.222102 | -661.653285 | -652.772914 | -832.950801 | -840.216164 | -819.167719 |
| Count | 460 | 460 | 460 | 460 | 460 | 460 | 460 | 460 |
| Confidence Level(95.0%) | 0.03868637 | 0.03868637 | 0.03868637 | 0.03868637 | 0.03868637 | 0.03868637 | 0.03868637 | 0.03868637 |

| Log KD(m3/kg) | Pu(V)-TSw | Pu(V)-CHnv | Pu(V)-CHnz | Pu(V)-PPw | Pu(V)-UCF | Pu(V)-BFw | Pu(V)-UFZ | Pu(V)-SAV |
|---|---|---|---|---|---|---|---|---|
| Mean | 0.1693902 | 0.65147488 | 0.61008219 | 0.52653614 | 0.54584129 | 0.15415023 | 0.13835597 | 0.18411346 |
| Standard Error | 0.01421027 | 0.01421027 | 0.01421027 | 0.01421027 | 0.01421027 | 0.01421027 | 0.01421027 | 0.01421027 |
| Median | 0.17728195 | 0.65936662 | 0.61797394 | 0.53442788 | 0.55373304 | 0.16204198 | 0.14624771 | 0.1920052 |
| Mode | 0.11242585 | 0.59451052 | 0.55311784 | 0.46957178 | 0.48887694 | 0.09718588 | 0.08139161 | 0.1271491 |
| Standard Deviation | 0.30477639 | 0.30477639 | 0.30477639 | 0.30477639 | 0.30477639 | 0.30477639 | 0.30477639 | 0.30477639 |
| Sample Variance | 0.09288865 | 0.09288865 | 0.09288865 | 0.09288865 | 0.09288865 | 0.09288865 | 0.09288865 | 0.09288865 |
| Kurtosis | 5.05539792 | 5.05539792 | 5.05539792 | 5.05539792 | 5.05539792 | 5.05539792 | 5.05539792 | 5.05539792 |
| Skewness | -0.14772314 | -0.14772314 | -0.14772314 | -0.14772314 | -0.14772314 | -0.14772314 | -0.14772314 | -0.14772314 |
| Range | 2.97414974 | 2.97414974 | 2.97414974 | 2.97414974 | 2.97414974 | 2.97414974 | 2.97414974 | 2.97414974 |
| Minimum | -1.63111006 | -1.14902539 | -1.19041807 | -1.27396412 | -1.25465897 | -1.64635003 | -1.66214429 | -1.6163868 |
| Maximum | 1.34303968 | 1.82512436 | 1.78373167 | 1.70018562 | 1.71949078 | 1.32779972 | 1.31200545 | 1.35776294 |
| Sum | 77.9194926 | 299.678443 | 280.637808 | 242.206624 | 251.086995 | 70.9091079 | 63.643745 | 84.6921907 |
| Count | 460 | 460 | 460 | 460 | 460 | 460 | 460 | 460 |
| Confidence Level(95.0%) | 0.02792525 | 0.02792525 | 0.02792525 | 0.02792525 | 0.02792525 | 0.02792525 | 0.02792525 | 0.02792525 |

7/7/98 (DRJ)

| Log KD(m3/kg) | Th(IV)-TSw | Th(IV)-CHnv | Th(IV)-CHnz | Th(IV)-PPw | Th(IV)-UCF | Th(IV)-BFw | Th(IV)-UFZ | Th(IV)-SAV |
|---|---|---|---|---|---|---|---|---|
| Mean | 1.7107391 | 2.19282377 | 2.15143109 | 2.06788504 | 2.08719019 | 1.69549913 | 1.67970486 | 1.72546235 |
| Standard Error | 0.02716781 | 0.02716781 | 0.02716781 | 0.02716781 | 0.02716781 | 0.02716781 | 0.02716781 | 0.02716781 |
| Median | 1.79194534 | 2.27403002 | 2.23263733 | 2.14909128 | 2.16839644 | 1.77670538 | 1.76091111 | 1.8066686 |
| Mode | 1.90137189 | 2.38345657 | 2.34206388 | 2.25851783 | 2.27782298 | 1.88613193 | 1.87033766 | 1.91609515 |
| Standard Deviation | 0.58268461 | 0.58268461 | 0.58268461 | 0.58268461 | 0.58268461 | 0.58268461 | 0.58268461 | 0.58268461 |
| Sample Variance | 0.33952136 | 0.33952136 | 0.33952136 | 0.33952136 | 0.33952136 | 0.33952136 | 0.33952136 | 0.33952136 |
| Kurtosis | 34.2276103 | 34.2276103 | 34.2276103 | 34.2276103 | 34.2276103 | 34.2276103 | 34.2276103 | 34.2276103 |
| Skewness | -4.41437455 | -4.41437455 | -4.41437455 | -4.41437455 | -4.41437455 | -4.41437455 | -4.41437455 | -4.41437455 |
| Range | 7.71459817 | 7.71459817 | 7.71459817 | 7.71459817 | 7.71459817 | 7.71459817 | 7.71459817 | 7.71459817 |
| Minimum | -4.31729287 | -3.8352082 | -3.87660089 | -3.96014694 | -3.94084178 | -4.33253284 | -4.34832711 | -4.30256962 |
| Maximum | 3.3973053 | 3.87938997 | 3.83799729 | 3.75445123 | 3.77375639 | 3.38206533 | 3.36627106 | 3.41202855 |
| Sum | 786.939985 | 1008.69894 | 989.6583 | 951.227116 | 960.107488 | 779.9296 | 772.664237 | 793.712683 |
| Count | 460 | 460 | 460 | 460 | 460 | 460 | 460 | 460 |
| Confidence Level(95.0%) | 0.05338869 | 0.05338869 | 0.05338869 | 0.05338869 | 0.05338869 | 0.05338869 | 0.05338869 | 0.05338869 |

DRJ 6/30/98

| Log KD(m3/kg) | U(VI)-TSw | U(VI)-CHnv | U(VI)-CHnz | U(VI)-PPw | U(VI)-UCF | U(VI)-BFw | U(VI)-UFZ | U(VI)-SAV |
|---|---|---|---|---|---|---|---|---|
| Mean | -2.56925757 | -2.0871729 | -2.12856558 | -2.21211163 | -2.19280648 | -2.58449754 | -2.60029181 | -2.55453431 |
| Standard Error | 0.04546608 | 0.04546608 | 0.04546608 | 0.04546608 | 0.04546608 | 0.04546608 | 0.04546608 | 0.04546608 |
| Median | -2.53600891 | -2.05392423 | -2.09531692 | -2.17886297 | -2.15955781 | -2.55124887 | -2.56704314 | -2.52128565 |
| Mode | -2.69531764 | -2.21323297 | -2.25462566 | -2.33817171 | -2.31886655 | -2.71055761 | -2.72635188 | -2.68059439 |
| Standard Deviation | 0.97513874 | 0.97513874 | 0.97513874 | 0.97513874 | 0.97513874 | 0.97513874 | 0.97513874 | 0.97513874 |
| Sample Variance | 0.95089556 | 0.95089556 | 0.95089556 | 0.95089556 | 0.95089556 | 0.95089556 | 0.95089556 | 0.95089556 |
| Kurtosis | 12.928374 | 12.928374 | 12.928374 | 12.928374 | 12.928374 | 12.928374 | 12.928374 | 12.928374 |
| Skewness | -2.31839593 | -2.31839593 | -2.31839593 | -2.31839593 | -2.31839593 | -2.31839593 | -2.31839593 | -2.31839593 |
| Range | 9.40703597 | 9.40703597 | 9.40703597 | 9.40703597 | 9.40703597 | 9.40703597 | 9.40703597 | 9.40703597 |
| Minimum | -9.37492959 | -8.89284491 | -8.9342376 | -9.01778365 | -8.99847849 | -9.39016955 | -9.40596382 | -9.36020633 |
| Maximum | 0.03210638 | 0.51419106 | 0.47279837 | 0.38925232 | 0.40855747 | 0.01686641 | 0.00107215 | 0.04682964 |
| Sum | -1181.85848 | -960.099533 | -979.140168 | -1017.57135 | -1008.69098 | -1188.86887 | -1196.13423 | -1175.08578 |
| Count | 460 | 460 | 460 | 460 | 460 | 460 | 460 | 460 |
| Confidence Level(95.0%) | 0.08934745 | 0.08934745 | 0.08934745 | 0.08934745 | 0.08934745 | 0.08934745 | 0.08934745 | 0.08934745 |



4/22/98 (DRJ)

## Effects of Colloids on Radionuclide Transport:

Colloid transport has been identified as an issue of concern Vilks et al. (1998) proposed a method of evaluating the effect of the formation of pseudocolloids on radionuclide transport. This approach is based on the assumption that the sorption of radionuclides onto the natural colloids is reversible, and that the "...amount of radionuclides sorbed on to colloidal material could be significant only if colloid concentrations were high enough to compete with the surface area available to sorption provided by the geologic media, or if sorption or complexation to colloids was stronger than sorption and complexation with the geologic media and dissolved ligands."

The equation developed by Vilks et al. (1998):

$$R_{F,eff} = 1 + \frac{(1 - \varepsilon)*\rho*K_D}{\varepsilon(1 + C*F*K_D)} \quad [1]$$

where: $R_{F,eff}$ = the effective retardation factor (unitless)
- $\varepsilon$ = porosity (assumed to be 0.5 in this exercise)
- $\rho$ = density
- $K_D$ = sorption coefficient for colloid/matrix
- C = colloid concentration
- F = an empirical factor introduced by Vilks (1994) such that

DRJ 6/30/98

$$K_{D,colloid} = F*K_{D,\ geologic\ medium} \quad [2]$$

For a colloid concentration = 0, Equation [1] reduces to the standard expression for the retardation factor:

$$R_F = 1 + \frac{(1 - \varepsilon)*\rho*K_D}{\varepsilon} \quad [3]$$

As demonstrated in Bertetti et al. (1998) and Pabalan et al. (1998), Np(V) and U(VI) sorption on aluminosilicate minerals exhibit pH-dependent behavior that is largely independent of mineral type. The amount of radionuclide sorbed is, instead, mainly a function of surface area. The magnitude of $K_D$ for PA transport calculations can therefore be determined for a given mineral by multiplying the $K_{A'}$ by the effective surface area for that mineral. For example, for quartz, the effective surface area is typically small [A′ = 0.03 $m^2$/g (Bertetti et al., 1998)]. $K_{D,Qz} = K_{A'} \times A' = (5.5\ mL/m^2) \times (0.03\ m^2/g) = 0.2$ mL/g.

In this exercise, it has been assumed that radionuclide sorption on of the colloid expressed in terms of $K_{A'}$ is the same as that on the geologic medium (i.e., $K_{A',colloid} = K_{A',geoloic\ medium}$). This is a reasonable assumption given that natural colloids are typically made up of the same minerals as are found in the host rock. Therefore, combining the expression for $K_{A'}$ with Equation [2] given above:

$$(K_{A',colloid} * A'_{colloid}) = F*(K_{A',geologic\ medium} * A'_{geologic\ medium}) \quad [4]$$

and

$$F = A'_{colloid}/A'_{geologic\ medium} \quad [5]$$

The major difference in the sorptive capacity of the colloids is therefore the greater surface area.

4/22/96 DRJ

Information on colloid concentrations in 23 springs in the Nevada Test Site and Yucca Mountain area has been reported by Kingston and Whitbeck (1991). This information is presented here:

| Kingston and Whitbeck (1991) | K&W91 ID#s | UTM (north) | UTM (east) | Date | aquifer (type) | >1 um (mg/L) | 1>d>0.4 um (mg/L) | 0.4>d>0.1 um (mg/L) | 0.1>d>0.03 um (mg/L) | Total (mg/L) |
|---|---|---|---|---|---|---|---|---|---|---|
| ,UE19c NTS, | 1 | 4124714.9 | 560341.1 | 7/22/87 | Volcanic | 0.13 | 0.23 | 0.23 | 0.23 | 0.69 |
| ,Water Well 20 NTS, | 2 | 4122709.2 | 550624.3 | 7/22/87 | Volcanic | 0.15 | 0.15 | 0.13 | 0.20 | 0.48 |
| ,Well 8 NTS, | 3 | 4113271.2 | 563111.8 | 7/22/87 | Volcanic | 0.13 | 0.25 | 0.18 | 0.30 | 0.73 |
| ,Whiterock Spring NTS, | 4 | 4117486.6 | 577107.5 | 7/22/87 | Volcanic | 0.00 | 129.38 | 15.95 | 0.48 | 145.81 |
| ,UE16d NTS, | 5 | 4103823.5 | 663087.1 | 7/22/87 | Carbonate | 0.10 | 0.13 | 0.03 | 0.20 | 0.36 |
| ,Well A NTS, | 6 | 4099201.6 | 585700.0 | 7/23/87 | Alluvium | 0.43 | 0.05 | 0.05 | 0.21 | 0.31 |
| ,Topopah Spring NTS, | 7 | 4088169.4 | 564956.8 | 7/23/87 | Volcanic | 2.01 | 5.87 | 19.32 | 0.00 | 25.19 |
| ,Well C-1 NTS, | 8 | 4086098.9 | 588233.0 | 7/23/87 | Carbonate | 0.03 | 0.10 | 0.26 | 0.18 | 0.54 |
| ,Well 4 NTS, | 9 | 4084575.7 | 586961.8 | 7/23/87 | Volcanic | 0.30 | 0.23 | 0.16 | 0.33 | 0.72 |
| ,Cane Spring NTS, | 10 | 4073116.9 | 584427.0 | 7/23/87 | Volcanic | 3.89 | 0.08 | 0.08 | 0.20 | 0.36 |
| ,Beatty Well 2, | 11 | 4084343.0 | 521529.3 | 7/24/87 | Alluvium | 0.38 | 0.48 | 4.17 | 1.83 | 6.48 |
| ,Lower Indian Spring, | 12 | 4088589.4 | 519045.2 | 7/24/87 | Volcanic | 0.34 | 0.25 | 0.23 | 0.18 | 0.66 |
| ,Indian Spring Well, | 13 | 4089540.4 | 517064.5 | 7/24/87 | Volcanic | 0.18 | 0.41 | 0.32 | 0.63 | 1.36 |
| ,Lathrop Wells, | 14 | 4055243.0 | 553809.5 | 7/24/87 | Alluvium | 0.43 | 0.13 | 0.23 | 0.18 | 0.54 |
| ,Fairbanks Spring, | 15 | 4036314.5 | 561668.0 | 7/24/87 | Carbonate | 0.28 | 0.05 | 0.17 | 0.17 | 0.39 |
| ,Crystal Pool, | 16 | 4030638.4 | 560762.2 | 7/24/87 | Carbonate | 0.03 | 0.13 | 0.03 | 0.19 | 0.35 |
| ,Indian Springs, | 17 | 4047366.5 | 619311.5 | 7/25/87 | Carbonate | 0.13 | 0.16 | 0.26 | 0.17 | 0.59 |
| ,Cold Creek Spring, | 18 | 4030080.5 | 612699.9 | 7/25/87 | Carbonate | 0.10 | 0.26 | 0.20 | 0.41 | 0.87 |
| ,Ash Springs, | 19 | 4142240.3 | 659956.9 | 7/25/87 | Carbonate | 0.10 | 0.10 | 0.13 | 0.24 | 0.47 |
| ,Pahroc Spring, | 20 | 4171198.8 | 678370.8 | 7/25/87 | Volcanic | 0.18 | 0.58 | 0.48 | 0.24 | 1.30 |
| ,Sidehill Spring, | 21 | 4234070.9 | 527123.0 | 7/26/87 | Volcanic | 0.18 | 0.30 | 0.19 | 0.33 | 0.82 |
| ,Peavine Ranch Well, | 22 | 4269535.0 | 476674.2 | 7/26/87 | Volcanic | 0.68 | 0.18 | 0.20 | 0.13 | 0.51 |
| ,Peavine Canyon Campground Spring, | 23 | 4274168.1 | 473592.3 | 7/26/87 | Volcanic | 0.38 | 0.25 | 0.03 | 0.00 | 0.28 |

The ID numbers were assigned in this exercise to distinguish sample locations. Latitude/longitude locations were converted to UTM coordinates using the conversion formula provided in Snyder (1987).



9/22/96 DRJ

The next stage in the exercise was to determine the sorption coefficients for different radionuclides under the chemical conditions for the water samples. Major element analyses are provided in Kingston and Whitbeck (1991) and are given here:

| Kingston and Whitbeck (1991) | K&W91 ID#s | Ca++ (mg/L) | Mg++ (mg/L) | Na+ (mg/L) | K+ (mg/L) | Cl- (mg/L) | SO4-2 (mg/L) | HCO3- (mg/L) | SiO2 (mg/L) | pH (field) | pH (lab) | Temp (C) | Orig Chemistry Ref. | I.S. | I.S. | Cations | Anions | Charge Balance |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| ,UE19c NTS, | 1 | 13.00 | 0.10 | 141.00 | 0.20 | 7.70 | 0.70 | 0.10 | 400.00 | 30.00 | 7.90 | 31.1 | Blank&Weir(66) | 7.11E-03 | 7.12E-03 | 6.80E-03 | 6.77E-03 | 0.15 |
| ,Water Well 20 NTS, | 2 | 6.18 | 0.28 | 59.40 | 1.78 | 11.80 | 82.60 | 111.00 | 51.00 | 8.23 | 8.03 | 27.0 | King&Whit(91) | 4.44E-03 | 4.41E-03 | 2.96E-03 | 3.87E-03 | -13.34 |
| ,Well 8 NTS, | 3 | 7.91 | 1.15 | 30.30 | 8.39 | 7.60 | 15.80 | 78.10 | 48.00 | | 7.72 | 26.8 | Boughton(86)[mod Perf(95)] | 2.33E-03 | 2.31E-03 | 2.02E-03 | 1.82E-03 | 5.16 |
| ,Whiterock Spring NTS, | 4 | 100.00 | 31.00 | 8.40 | 1.80 | 16.00 | 180.00 | 201.00 | 13.00 | 7.00 | 7.70 | 25.0 | DRI Lab | 1.34E-02 | 1.14E-02 | 7.95E-03 | 7.49E-03 | 2.96 |
| ,UE16d NTS, | 5 | 75.70 | 22.90 | 36.80 | 6.77 | 10.60 | 58.80 | 370.00 | 31.00 | | 7.65 | 23.0 | Boughton(86) | 1.10E-02 | 1.03E-02 | 7.44E-03 | 7.59E-03 | -1.01 |
| ,Well A NTS, | 6 | 22.30 | 6.82 | 48.30 | 9.25 | 6.40 | 20.00 | 209.00 | 78.00 | | 7.79 | 26.9 | Boughton(86) | 5.06E-03 | 4.96E-03 | 4.01E-03 | 4.02E-03 | -0.13 |
| ,Topopah Spring NTS, | 7 | 6.90 | 1.50 | 11.70 | 6.56 | 2.40 | 6.40 | 92.00 | 56.00 | | 6.94 | 16.0 | DRI Lab | 1.45E-03 | 1.36E-03 | 1.14E-03 | 1.15E-03 | -0.06 |
| ,Well C-1 NTS, | 8 | 75.40 | 29.70 | 127.00 | 14.00 | 83.60 | 65.50 | 587.00 | 30.00 | | 6.58 | 36.4 | Boughton(86) | 1.65E-02 | 1.41E-02 | 1.21E-02 | 1.33E-02 | -4.93 |
| ,Well 4 NTS, | 9 | 23.00 | 7.75 | 50.20 | 4.99 | 11.90 | 41.60 | 161.00 | 60.00 | | 8.05 | 38.0 | DRI Lab | 5.29E-03 | 5.11E-03 | 4.10E-03 | 3.84E-03 | 3.22 |
| ,Cane Spring NTS, | 10 | 31.30 | 9.60 | 38.30 | 7.88 | 19.60 | 28.00 | 181.00 | 65.00 | 7.75 | 8.19 | 23.0 | DRI Lab | 5.63E-03 | 5.44E-03 | 4.22E-03 | 4.10E-03 | 1.41 |
| ,Beatty Well 2, | 11 | 29.70 | 4.41 | 227.00 | 9.72 | 77.10 | 174.00 | 376.00 | 63.00 | 6.90 | 7.84 | 22.0 | King&Whit(91) | 1.47E-02 | 1.41E-02 | 1.20E-02 | 1.20E-02 | 0.03 |
| ,Lower Indian Spring, | 12 | 6.65 | 0.69 | 60.70 | 1.39 | 14.90 | 19.40 | 134.00 | 53.00 | 8.66 | 8.38 | 30.0 | King&Whit(91) | 3.44E-03 | 3.21E-03 | 3.06E-03 | 3.02E-03 | 0.72 |
| ,Indian Spring Well, | 13 | 3.62 | 0.40 | 58.50 | 2.12 | 14.00 | 23.70 | 111.00 | 46.00 | 8.13 | 8.20 | 26.0 | King&Whit(91) | 3.11E-03 | 3.20E-03 | 2.81E-03 | 2.71E-03 | 1.90 |
| ,Lathrop Wells, | 14 | 13.90 | 0.87 | 96.30 | 4.16 | 18.40 | 92.00 | 150.00 | 41.00 | 8.20 | | 27.0 | King&Whit(91) | 6.32E-03 | 6.19E-03 | 5.06E-03 | 4.89E-03 | 1.68 |
| ,Fairbanks Spring, | 15 | 51.00 | 18.00 | 71.00 | 8.00 | 22.00 | 80.00 | 300.00 | 20.00 | 7.30 | | 27.0 | Naff(73) | 1.01E-02 | 9.35E-03 | 7.32E-03 | 7.20E-03 | 0.80 |
| ,Crystal Pool, | 16 | 40.00 | 20.00 | 72.00 | 8.60 | 22.00 | 81.00 | 278.00 | 25.00 | 8.20 | | 33.0 | Dud&Lar(76)[mod Perf(95)] | 9.59E-03 | 9.02E-03 | 6.99E-03 | 6.86E-03 | 0.94 |
| ,Indian Springs, | 17 | 46.30 | 24.40 | 4.50 | 1.22 | 3.80 | 16.40 | 281.00 | 13.00 | 8.21 | 8.05 | 25.2 | DRI Lab | 7.13E-03 | 6.87E-03 | 4.55E-03 | 5.05E-03 | -5.30 |
| ,Cold Creek Spring, | 18 | 69.10 | 17.00 | 1.90 | 0.58 | 1.60 | 8.50 | 294.00 | 7.00 | | 8.12 | 10.0 | DRI Lab | 7.50E-03 | 7.34E-03 | 4.94E-03 | 5.04E-03 | -0.96 |
| ,Ash Springs, | 19 | 39.00 | 18.00 | 32.00 | 6.80 | 9.70 | 3.40 | 231.00 | 31.00 | 8.10 | | 31.0 | Eakin(63) | 6.31E-03 | 6.18E-03 | 4.99E-03 | 4.13E-03 | 9.46 |
| ,Pahroc Spring, | 20 | 30.90 | 8.28 | 12.30 | 5.63 | 11.70 | 11.40 | 135.00 | 59.00 | 7.60 | 7.90 | 16.0 | Raker(87) | 4.07E-03 | 3.97E-03 | 2.90E-03 | 2.78E-03 | 2.15 |
| ,Sidehill Spring, | 21 | 25.50 | 4.34 | 24.90 | 5.22 | 9.90 | 14.10 | 136.00 | 48.00 | 6.90 | 7.80 | 18.0 | Raker(87) | 3.79E-03 | 3.53E-03 | 2.85E-03 | 2.80E-03 | 0.79 |
| ,Peavine Ranch Well, | 22 | 30.80 | 7.82 | 16.40 | 1.66 | 6.40 | 26.80 | 127.00 | 38.00 | 6.89 | 7.75 | 12.0 | King&Whit(91) | 4.25E-03 | 3.95E-03 | 2.94E-03 | 2.82E-03 | 2.02 |
| ,Peavine Canyon Campground Spring, | 23 | 27.80 | 6.81 | 15.60 | 1.47 | 5.20 | 19.60 | 125.00 | 33.00 | 6.94 | 7.81 | 11.0 | King&Whit(91) | 3.81E-03 | 3.57E-03 | 2.66E-03 | 2.60E-03 | 1.14 |

It is important to note that a number of these water analyses were not performed on the water sample that was measured for colloid content, but are from earlier reports. To the extent that these analyses are suitable, they can be considered to represent the water chemistry of a given sampling point. These analyses were formatted for use with MINTEQA2 as described above on 60-85 of this scientific notebook. Sorption models of Am(III), Np(V), Pu(V), Th(IV), and U(VI) were prepared.

9/22/98 (DRJ)

```
UE19c  NTS                          ;SampID=1-Well       ;ArcID=1
UTM=4124715.0 North; 560341.1 East; Date=7/22/1987
31.10 MG/L   0.000  0.00000E-01
0 0 1 0 3 0 0 0 1 1 0 0 0
4   1   7
1.000E+00   13.00 0.000 0.000 81
    330  0.000E-01   -7.90 y                    /H+1
    040  1.200E-01   -6.30 y                    /Am+3
    150  0.130E+02   -3.49 y                    /Ca+2
    460  0.100E+00   -5.39 y                    /Mg+2
    500  0.141E+03   -2.21 y                    /Na+1
    410  0.200E+00   -5.29 y                    /K+1
    180  0.770E+01   -3.66 y                    /Cl-1
    732  0.100E+00   -5.98 y                    /SO4-2
    140  0.407E+03   -2.18 y                    /CO3-2
    770  0.188E+02   -3.51 y                    /H4SiO4
    813  0.000E-01    0.00 y                    /ADS1PSIo
    811  4.986E-05   -4.30 y                    /ADS1TYP1

  3   1
    330      7.9000      0.0000                 /H+1
  6   1
    813      0.0000      0.0000                 /ADS1PSIo

  2   3
8113300 >AlO-              0.0000   -9.0500   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 >AlOH2+            0.0000    6.8500   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
8110400 >AlOAm+2           0.0000    4.6600   0.000   0.000 2.00 0.00 0.00   0.0000
 0.00 4   1.000 811    1.000 040   -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
```

Am(III)-$\gamma$Al(OH)$_3$ sorption Kingston + Whitbeck(91) DLM

```
UE19c  NTS                          ;SampID=1-Well       ;ArcID=1
UTM=4124715.0 North; 560341.1 East; Date=7/22/1987
31.10 MG/L   0.000  0.00000E-01
0 0 1 0 3 0 0 0 1 1 0 0 0
4   1   7
1.000E+00   13.00 0.000 0.000 81
    330  0.000E-01   -7.90 y                    /H+1
    642  1.200E-01   -6.36 y                    /PuO2+1
    150  0.130E+02   -3.49 y                    /Ca+2
    460  0.100E+00   -5.39 y                    /Mg+2
    500  0.141E+03   -2.21 y                    /Na+1
    410  0.200E+00   -5.29 y                    /K+1
    180  0.770E+01   -3.66 y                    /Cl-1
    732  0.100E+00   -5.98 y                    /SO4-2
    140  0.407E+03   -2.18 y                    /CO3-2
    770  0.188E+02   -3.51 y                    /H4SiO4
    813  0.000E-01    0.00 y                    /ADS1PSIo
    811  4.986E-05   -4.30 y                    /ADS1TYP1

  3   1
    330      7.9000      0.0000                 /H+1
  6   1
    813      0.0000      0.0000                 /ADS1PSIo

  2   3
8113300 >AlO-              0.0000   -9.0500   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 >AlOH2+            0.0000    6.8500   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
8116420 >AlOPuO2           0.0000   -2.1800   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 3   1.000 811    1.000 642   -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
```

Pu(V)-$\gamma$-Al(OH)$_3$ Sorption Kingston + Whitbeck DLM



9/22/98 (DRJ)

```
UE19c  NTS                          ;SampID=1-Well       ;ArcID=1
UTM=4124715.0 North; 560341.1 East; Date=7/22/1987
31.10 MG/L   0.000  0.00000E-01
0 0 1 0 3 0 0 0 1 1 0 0 0
4   1   7
1.000E+00   13.00 0.000 0.000 81
    330  0.000E-01   -7.90 y                    /H+1
    866  2.300E-01   -6.01 y                    /Th+4
    150  0.130E+02   -3.49 y                    /Ca+2
    460  0.100E+00   -5.39 y                    /Mg+2
    500  0.141E+03   -2.21 y                    /Na+1
    410  0.200E+00   -5.29 y                    /K+1
    180  0.770E+01   -3.66 y                    /Cl-1
    732  0.100E+00   -5.98 y                    /SO4-2
    140  0.407E+03   -2.18 y                    /CO3-2
    770  0.188E+02   -3.51 y                    /H4SiO4
    813  1.000E-07   -7.00 y                    /ADS1PSIo
    811  4.986E-05   -4.30 y                    /ADS1TYP1

  3   1
    330      7.9000      0.0000                 /H+1
  6   1
    813      0.0000      0.0000                 /ADS1PSIo

  2   3
8113300 >AlO-              0.0000   -9.0500   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 >AlOH2+            0.0000    6.8500   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
8118660 >AlOTh+3           0.0000   15.3000   0.000   0.000 3.00 0.00 0.00   0.0000
 0.00 4   1.000 811    1.000 866   -1.000 330    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
```

Th(IV)-$\gamma$Al(OH)$_3$ Kingston + Whitbeck(91) DLM

```
UE19c  NTS                          ;SampID=1-Well       ;ArcID=1
UTM=4124715.0 North; 560341.1 East; Date=7/22/1987
31.10 MG/L   0.000  0.00000E-01
0 0 1 0 3 0 0 0 1 1 0 0 0
4   1   7
1.000E+00    9.70 0.000 0.000 81
    330  0.000E-01   -7.90 y                    /H+1
    893  2.700E-01   -6.00 y                    /uo2+2
    150  0.130E+02   -3.49 y                    /Ca+2
    460  0.100E+00   -5.39 y                    /Mg+2
    500  0.141E+03   -2.21 y                    /Na+1
    410  0.200E+00   -5.29 y                    /K+1
    180  0.770E+01   -3.66 y                    /Cl-1
    732  0.100E+00   -5.98 y                    /SO4-2
    140  0.407E+03   -2.18 y                    /CO3-2
    770  0.188E+02   -3.51 y                    /H4SiO4
    813  0.000E-01    0.00 y                    /ADS1PSIo
    811  1.687E-05   -5.57 y                    /ADS1TYP1
    812  2.033E-05   -5.23 y                    /ADS1TYP2

  2   1
8933301   -13.0000    18.0940                  /uo2(oh)2
  3   1
    330      7.9000      0.0000                 /H+1
  6   1
    813      0.0000      0.0000                 /ADS1PSIo

  2   5
8123300 >SiO-              0.0000   -7.2000   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
8128930 >SiOUO2+           0.0000    2.6000   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 4   1.000 812    1.000 893   -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
8113300 >AlO-              0.0000   -9.7300   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 >AlOH2+            0.0000    8.3300   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
8118930 >AlOUO2+           0.0000    2.7000   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 4   1.000 811    1.000 893   -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
```

U(VI) - montmorillonite sorption Kingston + Whitbeck(91) DLM

No $XO{\cdot}(UO_2)_2(OH)_5^-$ surface complex. Insignificant contribution @ $10^{-6}$ M U total. Leads to instability in MINTEQA2 runs for natural groundwater.

9/22/98
DRJ

```
UE19c  NTS                                ;SampID=1-Well          ;ArcID=1
UTM=4124715.0 North; 560341.1 East; Date=7/22/1987
31.10 MG/L    0.000   0.00000E-01
0 0 1 0 3 0 0 0 1 1 0 0 0
4    1    7
1.00E+00     9.70 0.000 0.000 81
     330  0.000E-01    -7.90 y                    /H+1
     150  0.130E+02    -3.49 y                    /Ca+2
     460  0.100E+00    -5.39 y                    /Mg+2
     500  0.141E+03    -2.21 y                    /Na+1
     410  0.200E+00    -5.29 y                    /K+1
     180  0.770E+01    -3.66 y                    /Cl-1
     732  0.100E+00    -5.98 y                    /SO4-2
     140  0.407E+03    -2.18 y                    /CO3-2
     770  0.188E+02    -3.51 y                    /H4SiO4
     552  2.690E-01    -6.00 y                    /npo2+
     813  0.000E-01     0.00 y                    /ADS1PSIo
     811  1.687E-05    -4.77 y                    /ADS1TYP1
     812  2.033E-05    -4.69 y                    /ADS1TYP2
  2    4
5523300    -10.0000     10.5015                   /npo2(oh)
5521400      4.6000     12.7951                   /npo2(co3)-1
5521401      7.0000      7.1390                   /npo2(co3)2-3
5521402      8.5000      6.2630                   /npo2(co3)3-5
  3    1
     330      7.9000      0.0000                   /H+1
  6    1
     813      0.0000      0.0000                   /ADS1PSIo
  2    6
5523301 npo2(oh)2-          0.0000   -22.4000    0.000    0.000-1.00 4.00 0.00    0.0000
 0.00 3   -2.000 330     1.000 552     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  0.000    0    0.000    0    0.000    0
8113300 >AlO-               0.0000    -9.7300    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 >AlOH2+             0.0000     8.3300    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
8115520 >AlONpO2OH-         0.0000   -13.7900    0.000    0.000-1.00 0.00 0.00    0.0000
 0.00 5    1.000 811     1.000 552     1.000    2   -2.000 330   -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
8123300 >SiO-               0.0000    -7.2000    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
8125520 >SiOHNpO2+          0.0000     4.0500    0.000    0.000 1.00 0.00 0.00    0.0000
 0.00 3    1.000 812     1.000 552     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
```

Np(V)-meta-schoepite
Kingston + Whitbeck (91)

DLM

The result of the MINTEQA2 calculations gives the following $K_A$ values:

| Kingston and Whitbeck (1991) | K&W91 ID#s | pH | P(CO2) | I.S. | log(#colloid part.) | SI(Gyp) | SI(Crsb) | SI(Cc) | Ka'-Am (mL/m2) | Ka'-Np (mL/m2) | Ka'-Pu (mL/m2) | Ka'-Th (mL/m2) | Ka'-U (mL/m2) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| UE19c NTS, | 1 | 7.90 | -2.252 | 7.12E-03 | 6.758 | -5.000 | -0.207 | 0.232 | 2027748.1 | 4.7 | 397.3 | 9042.1 | 0.2 |
| Water Well 20 NTS, | 2 | 8.23 | -3.153 | 4.41E-03 | 6.850 | -2.346 | 0.072 | -0.352 | 34413322.2 | 13.9 | 1251.6 | 13762.7 | 4.3 |
| Well 8 NTS, | 3 | 7.72 | -2.798 | 2.31E-03 | 6.922 | -2.859 | 0.054 | -0.842 | 7517240.3 | 7.6 | 782.1 | 17302.4 | 17.1 |
| Whiterock Spring NTS, | 4 | 7.00 | -1.774 | 1.14E-02 | 6.611 | -1.027 | -0.485 | -0.312 | 249406.5 | 1.9 | 165.3 | 55528.1 | 4.4 |
| UE16d NTS, | 5 | 7.65 | -2.112 | 1.03E-02 | 6.652 | -1.576 | -0.082 | 0.544 | 1499605.4 | 5.1 | 385.1 | 38376.2 | 0.4 |
| Well A NTS, | 6 | 7.79 | -2.449 | 4.96E-03 | 6.832 | -2.418 | 0.264 | 0.049 | 3769078.1 | 6.8 | 581.6 | 17535.5 | 1.6 |
| Topopah Spring NTS, | 7 | 6.94 | -2.305 | 1.36E-03 | 6.954 | -3.236 | 0.274 | -2.012 | 670614.9 | 1.7 | 175.7 | 125859.1 | 53.5 |
| Well C-1 NTS, | 8 | 6.58 | -0.931 | 1.41E-02 | 6.521 | -1.616 | -0.268 | -0.337 | 17202.8 | 0.8 | 62.3 | 21007.2 | 0.6 |
| Well 4 NTS, | 9 | 8.05 | -2.755 | 5.11E-03 | 6.826 | -2.122 | -0.001 | 0.358 | 7455319.4 | 6.4 | 756.0 | 3069.6 | 1.5 |
| Cane Spring NTS, | 10 | 7.54 | -2.361 | 5.44E-03 | 6.815 | -2.362 | 0.338 | -0.288 | 2938306.9 | 5.4 | 488.5 | 114863.0 | 4.9 |
| Beatty Well 2, | 11 | 7.75 | -2.204 | 1.41E-02 | 6.519 | -2.127 | 0.226 | 0.187 | 2059338.3 | 5.6 | 408.8 | 37097.7 | 0.3 |
| Lower Indian Spring, | 12 | 6.90 | -1.866 | 3.21E-03 | 6.891 | -1.549 | 0.165 | -1.676 | 2357351.1 | 1.5 | 150.5 | 61278.5 | 12.8 |
| Indian Spring Well, | 13 | 8.66 | -3.563 | 3.20E-03 | 6.891 | -2.870 | -0.033 | -0.081 | 108651645.8 | 17.0 | 1570.3 | 7335.0 | 2.3 |
| Lathrop Wells, | 14 | 8.13 | -2.935 | 6.19E-03 | 6.789 | -3.075 | -0.008 | -0.011 | 18587234.7 | 11.2 | 965.8 | 16832.4 | 2.2 |
| Fairbanks Spring, | 15 | 7.30 | -1.842 | 9.35E-03 | 6.682 | -1.998 | -0.326 | -0.025 | 456803.0 | 3.0 | 262.2 | 27514.3 | 1.2 |
| Crystal Pool, | 16 | 8.20 | -2.708 | 9.02E-03 | 6.693 | -1.591 | -0.320 | 0.838 | 7684529.8 | 6.0 | 597.1 | 5702.8 | 0.3 |
| Indian Springs, | 17 | 8.21 | -2.759 | 6.87E-03 | 6.767 | -1.707 | -0.497 | 0.854 | 11446914.0 | 9.4 | 673.9 | 18140.4 | 0.4 |
| Cold Creek Spring, | 18 | 8.12 | -2.785 | 7.34E-03 | 6.750 | -2.272 | -0.543 | 0.746 | 1874312 1.7 | 14.3 | 811.7 | 224540.2 | 0.6 |
| Ash Springs, | 19 | 8.10 | -2.693 | 6.18E-03 | 6.790 | -2.362 | -0.196 | 0.686 | 8061172.9 | 7.4 | 674.4 | 8109.2 | 0.7 |
| Pahroc Spring, | 20 | 7.60 | -2.542 | 3.97E-03 | 6.865 | -3.009 | -0.196 | -0.329 | 4919649.7 | 6.2 | 590.5 | 106016.7 | 9.5 |
| Sidehill Spring, | 21 | 6.90 | -1.892 | 3.53E-03 | 6.880 | -2.479 | 0.296 | 0.065 | 283833.5 | 1.6 | 151.1 | 119385.0 | 15.1 |
| Peavine Ranch Well, | 22 | 6.89 | -1.967 | 3.95E-03 | 6.866 | -2.451 | 0.178 | -1.145 | 380492.2 | 1.5 | 148.8 | 336776.3 | 21.6 |
| Peavine Canyon Campground Spring, | 23 | 6.94 | -2.023 | 3.57E-03 | 6.879 | -2.106 | 0.165 | -1.199 | 488009.8 | 1.7 | 166.9 | 370127.0 | 22.2 |

The ionic strength is the equilibrium speciated ionic strength is calculated by MINTEQA2, as are PCO2, and the saturation indices (SI) for calcite, cristobalite, and gypsum. Particle concentration is generated using the empirical relationship of Triay (1998) (log [coll] = 7.0 - 34* I.S.(molal)).

| | Average | Max | Min |
|---|---|---|---|
| | mL/g | mL/g | mL/g |
| Am(III) | 137097053.0 | 1412471396.0 | 223636.4 |
| Np(V) | 59.4 | 164.7 | 8.2 |
| Pu(V) | 6905.6 | 20413.6 | 810.3 |
| Th(IV) | 992070.3 | 4811650.5 | 39905.1 |
| U(VI) | 74.9 | 519.1 | 2.0 |

| | Average | Max | Min |
|---|---|---|---|
| | m3/kg | m3/kg | m3/kg |
| Am(III) | 137097.053 | 1412471.400 | 223.636 |
| Np(V) | 0.059 | 0.165 | 0.008 |
| Pu(V) | 6.906 | 20.414 | 0.810 |
| Th(IV) | 992.070 | 4811.650 | 39.905 |
| U(VI) | 0.075 | 0.519 | 0.002 |



9/22/98
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9/22/98
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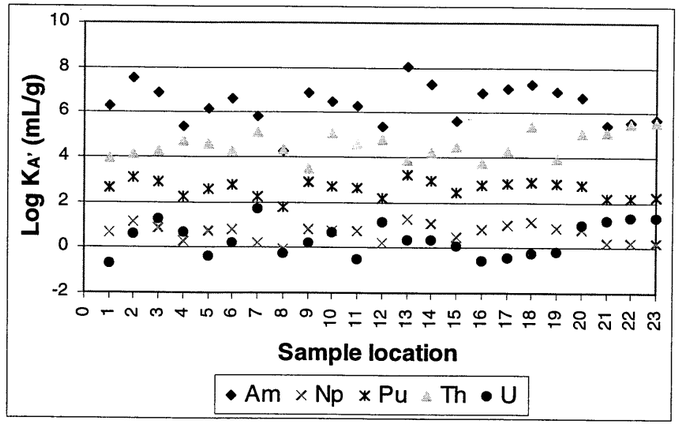
The calculated log $K_{A'}$ values are plotted here:




The next step is to determine the effective surface area of the colloid fraction relative to the geologic medium. This was done by assuming that the colloidal particles were spheres with a radius in the midpoint of a given size fraction. Mineral density was assumed to be related to the lithology of the aquifer:

$\rho_{volcanic}$ = 2,650 kg/m$^3$
$\rho_{carbonate}$= 2,700 kg/m$^3$
$\rho_{alluvium}$ = 2,500 kg/m$^3$

| Kingston and Whitbeck (1991) | K&W91 IDNs | aquifer | Density (g/mL) | >1 um (mg/L) | Surface Area (m2/L, r=0.5um) | Surface Area (m2/g, r=0.5um) | 1>d>0.4 um (mg/L) | Surface Area (m2/L, r=0.35um) | Surface Area (m2/g, r=0.35 um) | 0.4>d>0.1 um (mg/L) | Surface Area (m2/L, r=0.125um) | Surface Area (m2/g, r=0.125 um) | 0.1>d>0.03 um (mg/L) | Surface Area (m2/L, r=0.065um) | Surface Area (m2/g, r=0.065 um) | Total (mg/L) | Surface Area (m2/L) | Surface Area (m2/g) | F(Viks et al., 1998) coli SA/2 m2/g |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Testing UTM Conversion | | | | | | | | | | | | | | | | | | | |
| UE19c NTS. | 1 | Volcanic | 2.65 | 0.13 | 2.94E-04 | 2.26E+00 | 0.23 | 1.52E-03 | 6.60E+00 | 0.23 | 3.33E-02 | 1.45E+02 | 0.23 | 2.37E-01 | 1.03E+03 | 0.69 | 0.27 | 1184.34 | 592.17 |
| Water Well 20 NTS. | 2 | Volcanic | 2.65 | 0.15 | 3.40E-04 | 2.26E+00 | 0.15 | 9.90E-04 | 6.60E+00 | 0.13 | 1.88E-02 | 1.45E+02 | 0.20 | 2.06E-01 | 1.03E+03 | 0.48 | 0.23 | 1184.34 | 592.17 |
| Well 8 NTS. | 3 | Volcanic | 2.65 | 0.13 | 2.94E-04 | 2.26E+00 | 0.25 | 1.65E-03 | 6.60E+00 | 0.18 | 2.61E-02 | 1.45E+02 | 0.30 | 3.09E-01 | 1.03E+03 | 0.73 | 0.34 | 1184.34 | 592.17 |
| Whiterock Spring NTS. | 4 | Volcanic | 2.65 | 0.00 | 0.00E+00 | 0.00E+00 | 129.38 | 8.54E-01 | 6.60E+00 | 15.95 | 2.31E+00 | 1.45E+02 | 0.48 | 4.95E-01 | 1.03E+03 | 145.81 | 3.66 | 1182.07 | 591.04 |
| UE16d NTS. | 5 | Carbonate | 2.70 | 0.10 | 2.22E-04 | 2.22E+00 | 0.13 | 8.42E-04 | 6.48E+00 | 0.03 | 4.27E-03 | 1.42E+02 | 0.20 | 2.02E-01 | 1.01E+03 | 0.36 | 0.21 | 1162.40 | 581.20 |
| Well A NTS. | 6 | Alluvium | 2.50 | 0.43 | 1.03E-03 | 2.40E+00 | 0.05 | 3.50E-04 | 7.00E+00 | 0.05 | 7.68E-03 | 1.54E+02 | 0.21 | 2.29E-01 | 1.09E+03 | 0.31 | 0.24 | 1295.40 | 627.70 |
| Topopah Spring NTS. | 7 | Volcanic | 2.65 | 2.01 | 4.55E-03 | 2.26E+00 | 5.87 | 3.87E-02 | 6.60E+00 | 19.32 | 2.80E+00 | 1.45E+02 | 0.00 | 0.00E+00 | 0.00E+00 | 25.19 | 2.84 | 153.77 | 76.89 |
| Well C-1 NTS. | 8 | Carbonate | 2.70 | 0.03 | 6.67E-05 | 2.22E+00 | 0.10 | 6.48E-04 | 6.48E+00 | 0.26 | 3.70E-02 | 1.42E+02 | 0.18 | 1.82E-01 | 1.01E+03 | 0.54 | 0.22 | 1162.40 | 581.20 |
| Well 4 NTS. | 9 | Volcanic | 2.65 | 0.30 | 6.79E-04 | 2.26E+00 | 0.23 | 1.52E-03 | 6.60E+00 | 0.16 | 2.32E-02 | 1.45E+02 | 0.33 | 3.40E-01 | 1.03E+03 | 0.72 | 0.37 | 1184.34 | 592.17 |
| Cane Spring NTS. | 10 | Volcanic | 2.65 | 3.89 | 8.81E-03 | 2.26E+00 | 0.08 | 5.28E-04 | 6.60E+00 | 0.08 | 1.16E-02 | 1.45E+02 | 0.20 | 2.06E-01 | 1.03E+03 | 0.36 | 0.23 | 1184.34 | 592.17 |
| Beatty Well 2. | 11 | Alluvium | 2.50 | 0.38 | 9.12E-04 | 2.40E+00 | 0.48 | 3.36E-03 | 7.00E+00 | 4.17 | 6.41E-01 | 1.54E+02 | 1.83 | 2.00E+00 | 1.09E+03 | 6.48 | 2.64 | 1295.40 | 627.70 |
| Lower Indian Spring. | 12 | Volcanic | 2.65 | 0.34 | 7.70E-04 | 2.26E+00 | 0.25 | 1.65E-03 | 6.60E+00 | 0.23 | 3.53E-02 | 1.45E+02 | 0.18 | 1.86E-01 | 1.03E+03 | 0.66 | 0.22 | 1184.34 | 592.17 |
| Indian Spring Well. | 13 | Volcanic | 2.65 | 0.18 | 4.08E-04 | 2.26E+00 | 0.41 | 2.71E-03 | 6.60E+00 | 0.32 | 4.64E-02 | 1.45E+02 | 0.63 | 6.49E-01 | 1.03E+03 | 1.36 | 0.70 | 1184.34 | 592.17 |
| Lathrop Wells. | 14 | Alluvium | 2.50 | 0.43 | 1.03E-03 | 2.40E+00 | 0.13 | 9.10E-04 | 7.00E+00 | 0.23 | 3.33E-02 | 1.45E+02 | 0.17 | 1.72E-01 | 1.01E+03 | 0.54 | 0.23 | 1295.40 | 627.70 |
| Fairbanks Spring. | 15 | Carbonate | 2.70 | 0.28 | 6.22E-04 | 2.22E+00 | 0.05 | 3.24E-04 | 6.48E+00 | 0.03 | 4.27E-03 | 1.42E+02 | 0.19 | 1.92E-01 | 1.01E+03 | 0.35 | 0.20 | 1162.40 | 581.20 |
| Crystal Pool. | 16 | Carbonate | 2.70 | 0.03 | 6.67E-05 | 2.22E+00 | 0.13 | 8.42E-04 | 6.48E+00 | 0.03 | 4.27E-03 | 1.42E+02 | 0.17 | 1.72E-01 | 1.01E+03 | 0.39 | 0.20 | 1162.40 | 581.20 |
| Indian Springs. | 17 | Carbonate | 2.70 | 0.13 | 2.89E-04 | 2.22E+00 | 0.16 | 1.04E-03 | 6.48E+00 | 0.26 | 3.70E-02 | 1.42E+02 | 0.17 | 1.72E-01 | 1.01E+03 | 0.59 | 0.21 | 1162.40 | 581.20 |
| Cold Creek Spring. | 18 | Carbonate | 2.70 | 0.10 | 2.22E-04 | 2.22E+00 | 0.26 | 1.68E-03 | 6.48E+00 | 0.20 | 2.84E-02 | 1.42E+02 | 0.41 | 4.15E-01 | 1.01E+03 | 0.87 | 0.45 | 1162.40 | 581.20 |
| Ash Springs. | 19 | Carbonate | 2.70 | 0.10 | 2.22E-04 | 2.22E+00 | 0.10 | 6.48E-04 | 6.48E+00 | 0.13 | 1.85E-02 | 1.42E+02 | 0.24 | 2.43E-01 | 1.01E+03 | 0.47 | 0.26 | 1162.40 | 581.20 |
| Pahroo Spring. | 20 | Volcanic | 2.65 | 0.18 | 4.08E-04 | 2.26E+00 | 0.58 | 3.83E-03 | 6.60E+00 | 0.48 | 6.96E-02 | 1.45E+02 | 0.24 | 2.47E-01 | 1.03E+03 | 1.30 | 0.32 | 1184.34 | 592.17 |
| Sidehill Spring. | 21 | Volcanic | 2.65 | 0.18 | 4.08E-04 | 2.26E+00 | 0.30 | 1.98E-03 | 6.60E+00 | 0.19 | 2.75E-02 | 1.45E+02 | 0.33 | 3.40E-01 | 1.03E+03 | 0.82 | 0.37 | 1184.34 | 592.17 |
| Paavina Ranch Well. | 22 | Volcanic | 2.65 | 0.68 | 1.54E-03 | 2.26E+00 | 0.18 | 1.19E-03 | 6.60E+00 | 0.20 | 2.90E-02 | 1.45E+02 | 0.13 | 1.34E-01 | 1.03E+03 | 0.51 | 0.17 | 1184.34 | 592.17 |
| Paavina Canyon Campground Spring. | 23 | Volcanic | 2.65 | 0.38 | 8.60E-04 | 2.26E+00 | 0.25 | 1.65E-03 | 6.60E+00 | 0.03 | 4.35E-03 | 1.45E+02 | 0.000 | 0.00E+00 | 0.00E+00 | 0.28 | 0.011 | 153.77 | 76.89 |



9/22/98
DRJ

uming a surface area of 2 m$^2$/g for the geologic medium. This is the lower limit of the range point of view of the effects of colloid transport, can be considered to be conservative (i.e.,

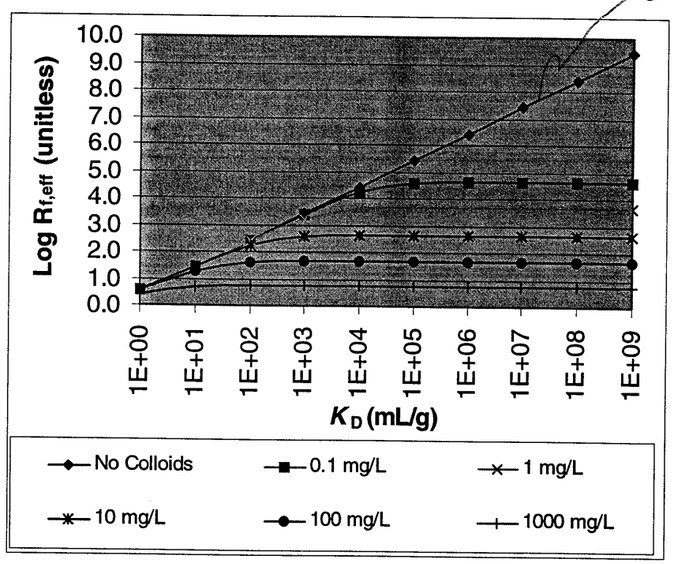
The final column of this table is the F factor in Equation [2] assuming a surface area of 2 m$^2$/g for the geologic medium. This is the lower limit of the range reported for the volcanic tuffs at Yucca Mountain, and from the point of view of the effects of colloid transport, can be considered to be conservative (i.e., higher values for F suggest greater impacts of colloid transport.

9/22/98 DRJ

Using Equation [1], a general reference model was drawn for F = 590:

| porosity (m3/m3) = 0.5 | | | | | | | |
|---|---|---|---|---|---|---|---|
| tuff density(kg/m3) = 2650 | | Log Rf (unitless) | | | | | |
| F = 590 | | Colloid Conc. (mg/L) | | | | | |
| | | 0 | 0.1 | 1 | 10 | 100 | 1000 |
| Log KD (mL/g) | KD (m3/kg) = | | | | | | |
| | 0.000 | 0 | 0 | 0 | 0 | 0 | 0 |
| 1 | 0.001 | 0.562 | 0.562 | 0.562 | 0.560 | 0.544 | 0.426 |
| 10 | 0.010 | 1.439 | 1.439 | 1.437 | 1.415 | 1.247 | 0.685 |
| 100 | 0.100 | 2.425 | 2.422 | 2.400 | 2.224 | 1.596 | 0.734 |
| 1000 | 1.000 | 3.423 | 3.399 | 3.222 | 2.586 | 1.655 | 0.739 |
| 10000 | 10.000 | 4.423 | 4.222 | 3.585 | 2.646 | 1.661 | 0.740 |
| 100000 | 100.000 | 5.423 | 4.584 | 3.645 | 2.653 | 1.662 | 0.740 |
| 1000000 | 1000.000 | 6.423 | 4.645 | 3.652 | 2.653 | 1.662 | 0.740 |
| 10000000 | 10000.000 | 7.423 | 4.652 | 3.652 | 2.653 | 1.662 | 0.740 |
| 100000000 | 100000.000 | 8.423 | 4.652 | 3.652 | 2.653 | 1.662 | 0.740 |
| 1000000000 | 1000000.000 | 9.423 | 4.652 | 3.652 | 2.653 | 1.662 | 0.740 |
| 10000000000 | 10000000.000 | 10.423 | 4.652 | 3.652 | 2.653 | 1.662 | 0.740 |

A plot of these results is given here:




C=0 colloid

$R_{F,eff} = R_F = 1 + \frac{\rho K_D}{\phi \varepsilon}$

DRJ 9/22/98

F = 590

$\rho$ = 2650 kg/m$^3$

$\varepsilon$ = 0.5

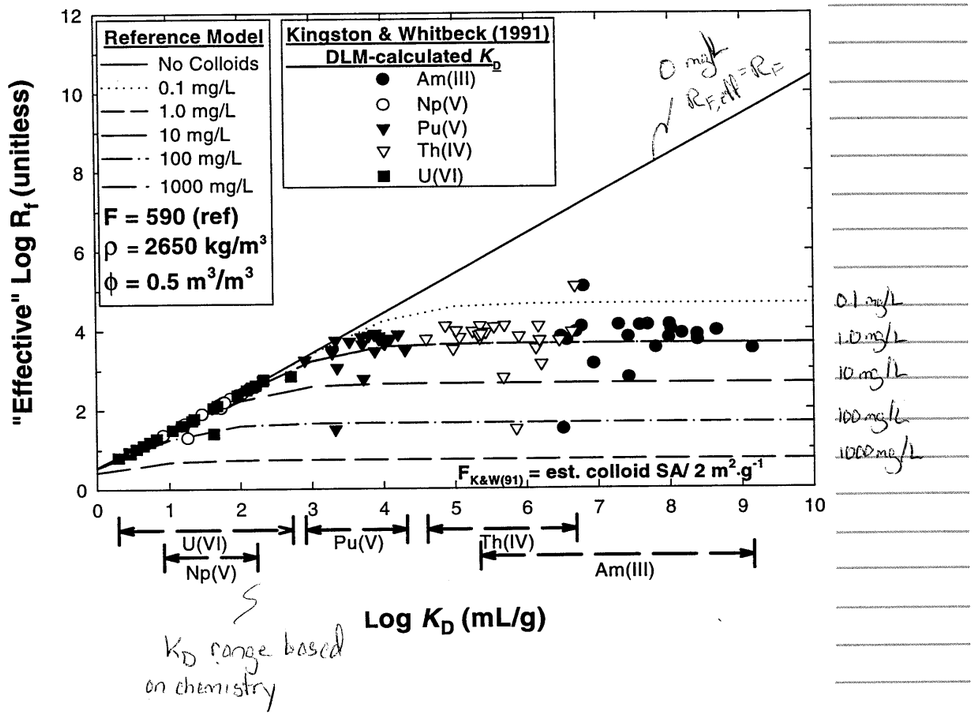
It can be noted that for colloid concentration = 0 mg/L, the model produces a straight line that is the standard $R_F$. As colloid concentration increases, the effective retardation factor decreases. As the radionuclide sorption coefficient increases, the effect is more pronounced, but for a given colloid concentration, the effect disappears above a certain threshold value.



9/22/98 DRJ

Taking the information provided above, the effect was calculated for each sample, using the radionuclide sorption coefficient calculated for the reported water chemistry, the colloid concentration, and the empirical parameter F based on assuming a spherical boundary. This was superimposed on the reference model (note: reference model used a constant value of F = 590, so the comparison to the site-specific calculation is not direct). The results are plotted here:

The horizontal lines plotted along the x-axis demonstrate the minimum and maximum values for the caluclated sorption coefficient, as indicated. Extrapolating these extrema vertically to interesection with




$K_D$ range based on chemistry

the model results for $R_F$ with no colloids indicates the likely extremes in the retardation factor. As can be seen, the effect is calculated to be most significant for the highly sorbing radionuclides Am(III) and Th(IV), reducing $R_{F,eff}$ by almost 5 orders of magnitude over the colloid-free case . The effect is somewhat less pronounced for Pu(V), and almost nonexistent for Np(V) and U(VI) except at the very highest reported colloid concentrations (C = 145 mg/L), where reduction is at most a half an order of magnitude.

5/22/98 DBS

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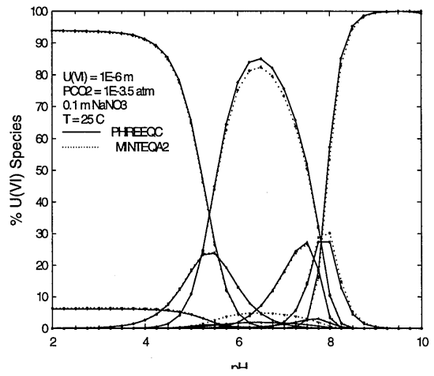
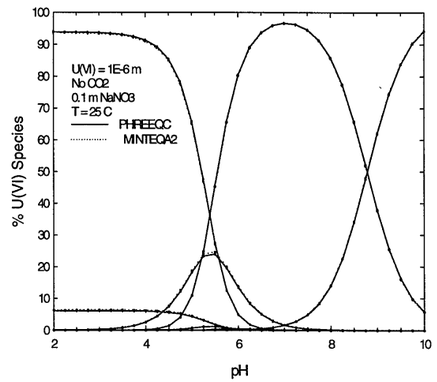
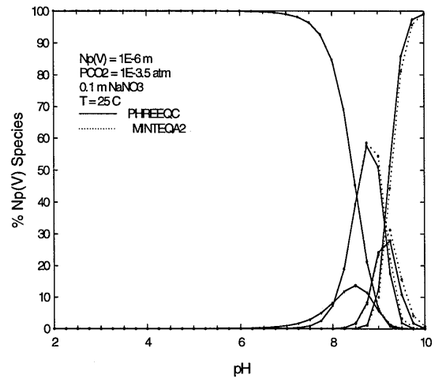
**Modifying the thermodynamic database for the PHREEQC geochemical speciation code.**

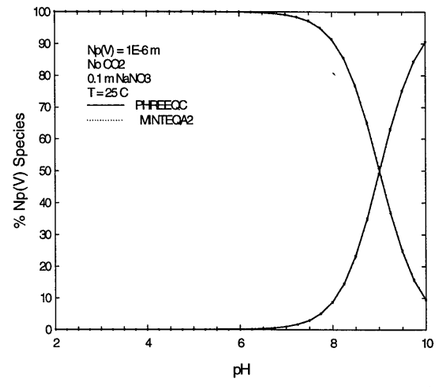
4/13/99

Radionuclide thermodynamic data (solid, aqueous, and redox) from EQ3/6 (Data0.com.r16, 26Jun92 release) was added to the PHREEQC database for the following elements: Am, Co, Cs, Eu, Np, Pu, Ra, Ru, Sn, Sr, Tc, Th, U, and Zr. The initial database was the MINTEQ.DAT database [Based on MINTEQA2, Version 3.11 (Allison et al., 1991)] provided with the PHREEQC, Version 1.6 distribution. A petition for exemption from qualificatino for the original MINTEQA2 data is included below. The data were alphabetized and about 600 chemical reactions involving radioelements were added. The thermodynamic data are consistent with the MINTEQA2 geochemical database developed and discussed in Turner (1993). Where the MINTEQ.DAT already had data (e.g., Sr, U), these data were replaced with the EQ3/6 values. PHREEQC was benchmarked for U(6+) and Np(5+) aqueous speciation against MINTEQA2, Version 3.11, and the data seem to produce consistent results. There are some minor differences, but these are more likely to be due to differences in the way that MINTEQA2 and PHREEQC handle activity coefficients than mistakes in the thermo data.



Two electronic files are included on a 3.25" floppy disk included in this scientific notebook. One (MINTEQA2.DAT) is the complete database (MINTEQ.DAT + new data). The second (MINRAD95.DAT) is just the new radionuclide data. These are the data that were used in preparing two earlier reports (Turner, 1993; 1995). Hardcopies of the database are also included in this scientific notebook. Original references for the data sources as listed in EQ3/6 are included below.

4/13/99 DRL

| AQUEOUS SPECIES | LOGK | REF |
|---|---|---|
| Am(CO3)2- | | 95NEA/1 |
| AmCO3+ | | 95NEA/1 |
| Am(CO3)3 -3 | | 95NEA/1 |
| AmNO3 +2 | | 95NEA/1 |
| Am(OH) +2 | | 95NEA/1 |
| Am(OH)2+ | | 95NEA/1 |
| Am(OH)3 (aq) | | 95NEA/1 |
| Am(SO4)+ | | 95NEA/1 |
| Am(SO4)2- | | 95NEA/1 |
| AmCl +2 | | 95NEA/1 |
| AmF +2 | | 95NEA/1 |
| AmF2+ | | 95NEA/1 |
| Am(H2PO4) +2 | | 95NEA/1 |
| Am(CO3)5 -6 | | 95NEA/1 |
| Co(HS)2 (aq) | | 74NAU/RYZ |
| Co(OH)2 (aq) | | 76BAE/MES |
| Co(OH)4 -2 | | 76SMI/MAR |
| Co2(OH)3+ | | 76BAE/MES |
| Co4(OH)4 +4 | | 76SMI/MAR |
| CoBr2 (aq) | | 82WAG/EVA |
| CoCl+ | | 74NAU/RYZ |
| CoHS+ | | 74NAU/RYZ |
| CoI2 (aq) | | 82WAG/EVA |
| CoNO3+ | | 76SMI/MAR |
| CoOH+ | | SUPCRT91 |
| CoS2O3 (aq) | | 74NAU/RYZ |
| CoSeO4 (aq) | | 76SMI/MAR |
| CoSO4 (aq) | | 82WAG/EVA |
| CsBr | | SUPCRT91 |
| CsCl | | SUPCRT91 |
| Cs+ | | SUPCRT91 |
| Eu(CO3)- | | 87RAR2 |
| Eu(CO3)3 -3 | | 87RAR2 |
| Eu(HCO3) +2 | | 87RAR2 |
| EuOH(CO3)2 -2 | | 87RAR2 |
| Eu(OH)2+ | | 87RAR2 |
| Eu(OH)2CO3 -1 | | 87RAR2 |
| Eu(OH)3 (aq) | | 87RAR2 |
| Eu(OH)4- | | 87RAR2 |
| EuOHCO3 (aq) | | 87RAR2 |
| Eu(SO4)2- | | 85RAR2 |
| Eu2(OH)2 +4 | | 87RAR2 |
| EuBr +2 | | 85RAR2 |
| EuBr2+ | | 85RAR2 |
| EuBrO3 +2 | | 85RAR2 |
| EuCl +2 | | 85RAR2 |
| EuCl2+ | | 85RAR2 |
| EuCO3+ | | 87RAR2 |
| EuF +2 | | 85RAR2 |
| EuF2+ | | 85RAR2 |
| EuIO3 +2 | | 85RAR2 |
| EuNO3 +2 | | 85RAR2 |
| EuOH +2 | | 87RAR2 |
| EuSO4+ | | 85RAR2 |
| NpH2PO4++ | | 84LEM |
| Np(H2PO4)2+ | | 84LEM |
| Np(H2PO4)3(aq) | | 84LEM |
| NpOH++ | | 84LEM |
| Np(CO3)5-6 | | 84LEM |
| NpHPO4++ | | 84LEM |
| Np(HPO4)2(aq) | | 84LEM |
| Np(HPO4)3(-2) | | 84LEM |
| Np(HPO4)4(-4) | | 84LEM |
| Np(HPO4)5(-6) | | 84LEM |
| NpOH+++ | | 84LEM |
| Np(OH)2++ | | 84LEM |
| Np(OH)3+ | | 84LEM |
| Np(OH)4(aq) | | 84LEM |
| NpSO4++ | | 84LEM |
| Np(SO4)2(aq) | | 84LEM |
| NpCl+++ | | 84LEM |
| NpCl2++ | | 84LEM |
| NpF+++ | | 84LEM |
| NpF2++ | | 84LEM |
| NpO2OH(aq) | | 84LEM |
| NpO2CO3-1 | | 84LEM |
| NpO2(CO3)2-3 | | 84LEM |
| NpO2(CO3)3-5 | | 84LEM |
| NpO2Cl(aq) | | 84LEM |
| NpO2F(aq) | | 84LEM |
| NpO2HPO4-1 | | 84LEM |
| NpO2H2PO4(aq) | | 84LEM |
| NpO2SO4-1 | | 84LEM |
| NpO2OH+ | | 84LEM |
| (NpO2)2(OH)2++ | | 84LEM |
| (NpO2)3(OH)5+ | | 84LEM |
| NpO2(CO3)2-2 | | 84LEM |
| NpO2(CO3)3-4 | | 84LEM |
| NpO2HPO4(aq) | | 84LEM |
| NpO2H2PO4+1 | | 84LEM |
| NpO2SO4(aq) | | 84LEM |
| NpO2Cl+ | | 84LEM |
| NpO2F+ | | 84LEM |
| NpO2F2(aq) | | 84LEM |
| PuH2PO4++ | | 80LEM/TRE |
| PuOH++ | | 80LEM/TRE |
| PuSO4+ | | 92PAL/SIL |
| Pu(SO4)2- | | 80LEM/TRE |
| PuHPO4++ | | 80LEM/TRE |
| Pu(HPO4)2(aq) | | 80LEM/TRE |
| Pu(HPO4)3(-2) | | 80LEM/TRE |
| Pu(HPO4)4(-4) | | 80LEM/TRE |
| PuOH+++ | | 80LEM/TRE |
| Pu(OH)2++ | | 80LEM/TRE |
| Pu(OH)3+ | | 80LEM/TRE |
| Pu(OH)4(aq) | | 80LEM/TRE |
| PuSO4++ | | 80LEM/TRE |
| Pu(SO4)2(aq) | | 80LEM/TRE |
| Pu(SO4)3-2 | | 80LEM/TRE |
| PuF+++ | | 84NAS/CLE |
| PuF2++ | | 84NAS/CLE |
| PuF3+ | | 84NAS/CLE |
| PuF4(aq) | | 84NAS/CLE |
| PuO2OH(aq) | | 80LEM/TRE |
| PuO2OH+ | | 80LEM/TRE |
| (PuO2)2(OH)2++ | | 80LEM/TRE |
| (PuO2)3(OH)5+ | | 80LEM/TRE |
| PuO2(CO3)2-2 | | 80LEM/TRE |
| PuO2H2PO4+1 | | 80LEM/TRE |
| PuO2SO4(aq) | | 80LEM/TRE |
| PuO2Cl+ | | 80LEM/TRE |
| PuO2F+ | | 80LEM/TRE |
| PuO2F2(aq) | | 80LEM/TRE |
| PuO2F3-1 | | 80LEM/TRE |
| PuO2F4-2 | | 80LEM/TRE |
| RuCl +2 | | 85RAR1 |
| RuCl2+ | | 85RAR1 |
| RuCl3 (aq) | | 85RAR1 |
| RuCl4- | | 85RAR1 |
| RuCl5 -2 | | 85RAR1 |
| RuCl6 -3 | | 85RAR1 |
| RuOH +2 | | 85RAR1 |
| Ru(OH)2+ | | 85RAR1 |
| RuSO4+ | | 85RAR1 |
| Ru(SO4)2- | | 85RAR1 |
| RuCl+ | | 85RAR1 |
| RuSO4 (aq) | | 85RAR1 |
| Ru(OH)2Cl+ | | 85RAR1 |
| Ru(OH)2Cl2 (aq) | | 85RAR1 |
| Ru(OH)2SO4 (aq) | | 85RAR1 |
| Ru4(OH)12 +4 | | 85RAR1 |
| Sn(OH)2 (aq) | | 84JAC/HEL |
| Sn(OH)3- | | 84JAC/HEL |
| SnOH+ | | 84JAC/HEL |
| SnCl+ | | 84JAC/HEL |
| SnCl2 (aq) | | 84JAC/HEL |
| SnCl3- | | 84JAC/HEL |
| SnF +2 | | 84JAC/HEL |
| SnF2 (aq) | | 84JAC/HEL |
| SnF3- | | 84JAC/HEL |
| Sn(OH)2 +2 | | 84JAC/HEL |
| Sn(OH)3+ | | 84JAC/HEL |
| Sn(OH)4 (aq) | | 82WAG/EVA |
| SnOH +3 | | 84JAC/HEL |
| SnSO4 +2 | | 82WAG/EVA |
| SrCl+ | | SUPCRT91 |
| SrCO3 (aq) | | SUPCRT91 |
| SrF+ | | SUPCRT91 |
| SrH2PO4+ | | 76SMI/MAR |
| SrHPO4 | | 76SMI/MAR |
| SrNO3+ | | 76SMI/MAR |
| SrOH+ | | 76BAE/MES |
| SrP2O7 -2 | | 76SMI/MAR |
| SrPO4- | | 76SMI/MAR |
| SrSO4 (aq) | | 83REA |
| ThH3PO4 +4 | | 80LAN/HER |
| ThH2PO4 +3 | | 80LAN/HER |
| Th(H2PO4)2 +2 | | 80LAN/HER |
| Th(HPO4)2 (aq) | | 80LAN/HER |
| Th(HPO4)3 -2 | | 80LAN/HER |
| Th(OH)2 +2 | | 80LAN/HER |
| Th(OH)3+ | | 80LAN/HER |
| Th(OH)4 (aq) | | 76BAE/MES |
| Th(SO4)2 (aq) | | 80LAN/HER |
| Th(SO4)3 -2 | | 80LAN/HER |
| Th(SO4)4 -4 | | 80LAN/HER |
| Th2(OH)2 +6 | | 80LAN/HER |
| Th4(OH)8 +8 | | 80LAN/HER |
| Th6(OH)15 +9 | | 80LAN/HER |
| ThCl +3 | | 80LAN/HER |
| ThCl2 +2 | | 80LAN/HER |
| ThCl3+ | | 80LAN/HER |
| ThCL4 (aq) | | 80LAN/HER |
| ThF +3 | | 80LAN/HER |
| ThF2 +2 | | 80LAN/HER |
| ThF3+ | | 80LAN/HER |
| ThF4 (aq) | | 80LAN/HER |
| ThOH +3 | | 82WAG/EVA |
| ThSO4 +2 | | 80LAN/HER |
| UOH +3 | | 92NEA |
| U(OH)2 +2 | | 90NEA |
| U(OH)3+ | | 90NEA |
| U(OH)4 (aq) | | 90NEA |
| U(OH)5- | | 90NEA |
| U6(OH)15 | | 92NEA |
| UF +3 | | 92NEA |
| UF2 +2 | | 92NEA |
| UF3+ | | 92NEA |
| UF4 (aq) | | 92NEA |
| UF5- | | 92NEA |
| UF6 -2 | | 92NEA |
| UCl +3 | | 92NEA |
| UBr +3 | | 92NEA |
| UI +3 | | 92NEA |
| UF2 +2 | | 95NEA/2 |
| UNO3 +3 | | 92NEA |
| U(NO3)2 +2 | | 92NEA |
| USO4 +2 | | 92NEA |
| U(SO4)2 (aq) | | 92NEA |
| UO2(CO3)3 -5 | | 92NEA |
| UO2OH+ | | 92NEA |
| UO2(CO3)2 (aq) | | 92NEA |
| UO2(OH)3- | | 92NEA |
| UO2(OH)4 -2 | | 92NEA |
| (UO2)2OH +3 | | 92NEA |
| (UO2)2(OH)2 +2 | | 92NEA |
| (UO2)3(OH)4 +2 | | 92NEA |
| (UO2)3(OH)5+ | | 92NEA |
| (UO2)3(OH)7- | | 92NEA |
| (UO2)4(OH)7+ | | 92NEA |
| U02F+ | | 92NEA |
| U02F2 (aq) | | 92NEA |
| U02F3- | | 92NEA |
| U02F4 -2 | | 92NEA |
| U02CL+ | | 92NEA |
| U02Cl2 (aq) | | 92NEA |
| U02Br+ | | 92NEA |
| U02CO3 (aq) | | 95NEA/2 |
| U02(CO3)2 -2 | | 92NEA |
| U02(CO3)4 -4 | | 92NEA |
| (UO2)2(CO3)6 -6 | | 92NEA |
| (UO2)11(CO3)6(OH)12 -2 | | 90NEA |
| (UO2)2CO3(OH)3- | | 90NEA |
| U02OHCO2+ | | 90NEA |
| U02NO3+ | | 92NEA |
| U02SO4 (aq) | | 92NEA |
| U02(SO4)2 -2 | | 92NEA |
| U02HPO4 (aq) | | 90NEA |
| U02H2PO4+ | | 90NEA |
| U02(H2PU4)2 (aq) | | 90NEA |
| U02(H2PO4)(H3PO4)+ | | 90NEA |
| U02H3PO4 +2 | | 90NEA |
| U02PO4- | | 90NEA |
| U02H3SiO4 | | 90NEA |
| Zr(OH)3+ | | 74NAU/RYZ |
| Zr(OH)4 (aq) | | 74NAU/RYZ |
| Zr(SO4)2 (aq) | | 74NAU/RYZ |
| Zr(SO4)3 -2 | | 74NAU/RYZ |
| ZrF +3 | | 74NAU/RYZ |
| ZrF2 +2 | | 74NAU/RYZ |
| ZrF3+ | | 74NAU/RYZ |
| ZrF4 (aq) | | 74NAU/RYZ |
| ZrF5- | | 74NAU/RYZ |
| ZrF6 -2 | | 74NAU/RYZ |
| ZrOH +3 | | 74NAU/RYZ |
| ZrSO4 +2 | | 74NAU/RYZ |
| Zr(OH)2 +2 | | 74NAU/RYZ |

| SOLIDS: | LOGK | REF |
|---|---|---|
| Am (c) | | 95NEA/1 |
| Am(OH)3 (am) | | 95NEA/1 |
| Am(OH)3 (c) | | 95NEA/1 |
| Am2O3 | | 95NEA/1 |
| AmOHCO3 (s) | | 95NEA/1 |
| Am2(CO3)3 | | 95NEA/1 |
| AmBr3 | | 95NEA/1 |
| AmOBr | | 95NEA/1 |
| AmCl3 | | 95NEA/1 |
| AmOCl | | 95NEA/1 |
| AmF3 | | 95NEA/1 |
| AmI3 | | 95NEA/1 |
| AmO2 | | 95NEA/1 |
| AmP4 | | 95NEA/1 |
| Co(c) | | 79ROB/HEM |
| CoS | | 74NAU/RYZ |
| Co(OH)2 | | 76BAE/MES |
| CoFe2O4 | | 74NAU/RYZ |
| CoO | | 82WAG/EVA |
| CoCO3 | | 84SVE |
| CoCl2 | | 82WAG/EVA |
| CoCl2:2H2O | | 82WAG/EVA |
| CoCl2:6H2O | | 82WAG/EVA |
| CoF2 | | 82WAG/EVA |
| CoF3 | | 79KUB/ALC |
| Co(NO3)2 | | 65GAR/CHR |
| CoSO4 | | 82WAG/EVA |
| CoSO4:3CoOH2 | | 82WAG/EVA |
| CoSO4:6H2O | | 82WAG/EVA |
| CoSO4:H2O | | 74NAU/RYZ |
| CoSeO3 | | 76SMI/MAR |
| Co2SiO4 | | |
| 82WAG/EVA,74NAU/RYZ | | |
| Co3(PO4)2 | | 82WAG/EVA |
| CoHPO4 | | 82WAG/EVA |
| Co3(AsO4)2 | | 82WAG/EVA |
| Cs(c) | | 89COX/WAG |
| Cs2U2O7 | | 90NEA |
| Cs2U4O12 | | 90NEA |
| Eu(c) | | 85RAR2 |
| EuS | | 85RAR2 |
| Eu(OH)2Cl | | 85RAR2 |
| Eu(OH)3 | | 87RAR2 |
| Eu2O3(cubic) | | 85RAR2 |
| Eu2O3(mono) | | 85RAR2 |
| Eu3O4 | | 85RAR2 |
| EuO | | 85RAR2 |
| EuOCl | | 87RAR2 |
| EuBr3 | | 85RAR2 |
| EuCl2 | | 87RAR2 |
| EuCl3 | | 85RAR2 |
| EuCl3:6H2O | | 85RAR2 |
| EuF3:5H2O | | 85RAR2 |
| Eu(IO3)3:2H2O | | 85RAR2 |
| Eu2(CO3)3:3H2O | | 87RAR2 |
| Eu(NO3)3:6H2O | | 85RAR2 |
| Eu2(SO4)3:8H2O | | 85RAR2 |
| EuSO4 | | 85RAR2 |



| | | | | |
|---|---|---|---|---|
| Np(c) | 84LEM | UCl4 | 90NEA | PuO2+/Pu+4 |
| NaNpO2CO3:3.5H2O | 84LEM | UBr2Cl2 | 90NEA | PuO2+2/Pu+4 |
| Np(OH)4 | 84LEM | UOCl2 | 90NEA | Ru+2/RuO4-2 |
| NpO2 | 84LEM | U2O2Cl5 | 90NEA | Ru+3/RuO4-2 |
| Np(HPO4)2 | 84LEM | UF4 (c) | 90NEA | Ru(OH)2+2/RuO4-2 |
| NpO2(OH) (am) | 84LEM | UF4:2.5H2O | 90NEA | RuO4-/RuO4-2 |
| Np2O5 | 84LEM | U2F9 | 90NEA | Sn+2/Sn+4 |
| NpO2(OH)2 | 84LEM | U4F17 | 89NEA | Tc+3/TcO4- |
| | | UClF3 | 90NEA | TcO+2/TcO4- |
| Pu(OH)3 | 80LEM/TRE | UCl2F2 | 90NEA | TcO4-3/TcO4- |
| Beta-Pu2O3 | 80LEM/TRE | UCl3F | 90NEA | TcO4-2/TcO4- |
| PuF3 | 80LEM/TRE | UOF2 | 90NEA | Co+2/Co+3 |
| Pu(c) | 86MOR | UOF2:H2O | 90NEA | |
| Pu(OH)4 | 80LEM/TRE | UOFOH | 90NEA | |
| PuO2 | 80LEM/TRE | UI4 | 90NEA | |
| PuF4 | 80LEM/TRE | UCl3I3 | 90NEA | |
| Pu(HPO4)2 | 80LEM/TRE | UCl2I2 | 90NEA | |
| PuO2(OH) (am) | 80LEM/TRE | UCl3I | 90NEA | |
| PuO2(OH)2 | 80LEM/TRE | U(CO3)2 | 90NEA | |
| PuO2(HPO4) | 80LEM/TRE | U(OH)2SO4 | 90NEA | |
| | | U(SO4)2 | 90NEA | |
| Ra (c) | 82WAG/EVA | U(SO4)2:4H2O | 90NEA | |
| Ra(NO3)2 | 82WAG/EVA | U(SO4)2:8H2O | 90NEA | |
| RaCl2:2H2O | 82WAG/EVA | U(HPO4)2:4H2O | 90NEA | |
| RaSO4 | 82WAG | Coffinite | 90NEA | |
| | | Na3UO4 | 90NEA | |
| Ru(c) | 85RAR1 | UBr5 | 90NEA | |
| Ru(OH)3:H2O | 85RAR1 | UOBr3 | 90NEA | |
| RuO2:2H2O | 85RAR1 | UCl5 | 90NEA | |
| RuO2 | 85RAR1 | UOCl3 | 90NEA | |
| RuBr3 | 85RAR1 | UO2Cl | 90NEA | |
| RuCl3 | 85RAR1 | U5O12Cl | 90NEA | |
| RuI3 | 85RAR1 | Alpha-UF5 | 90NEA | |
| | | Beta-UF5 | 90NEA | |
| Sn(c) | SUPCRT91 | UPO5 | 90NEA | |
| Sn2S3(Ottemanite) | 79KUB/ALC | Beta-UO2(OH)2 | 90NEA | |
| Sn3S4 | 79KUB/ALC | Schoepite | 90NEA | |
| Sn(OH)2 | 82WAG/EVA | Dehyd-Schoep(.393) | 88OHA/LEW | |
| Romarchite(SnO) | SUPCRT91 | Dehyd-Schoep(.648) | 88OHA/LEW | |
| Cassiterite(SnO2) | SUPCRT91 | Dehyd-Schoep(.850) | 88OHA/LEW | |
| SnBr2 | 79KUB/ALC | Dehyd-Schoep(.900) | 90NEA | |
| SnBr4 | 82WAG/EVA | Dehyd-Schoep(1.00) | 88OHA/LEW | |
| SnCl2 | 79KUB/ALC | Uraninite | 90NEA | |
| Sn(SO4)2 | 79KUB/ALC | Alpha-UO3 | 90NEA | |
| Sn(SO4) | 79KUB/ALC | Beta-UO3 | 90NEA | |
| SnSe | 79KUB/ALC | Gamma-UO3 | 90NEA | |
| SnSe2 | 79KUB/ALC | Gummite | 78LAN | |
| | | K2UO4 | 90NEA | |
| Sr(c) | 79ROB/HEM | Li2UO4 | 90NEA | |
| Sr(NO3)2 | 79ROB/HEM | Na2U2O7 | 90NEA | |
| Sr(NO3)2:4H2O | 82WAG/EVA | Alpha-Na2UO4 | 90NEA | |
| Sr(OH)2 | 85CHA/DAV | BaUO4 | 90NEA | |
| Sr2SiO4 | 77BAR/KNA | CaUO4 | 90NEA | |
| SrSiO3 | 82WAG/EVA | MgUO4 | 90NEA | |
| SrBr2 | 82WAG/EVA | NaUO3 | 90NEA | |
| SrBr2:H2O | 82WAG/EVA | NaUO2(CO3)3 | 90NEA | |
| SrBr2:6H2O | 82WAG/EVA | Rb2UO4 | 90NEA | |
| SrCl2 | 82WAG/EVA | Alpha-SrUO4 | 90NEA | |
| SrCl2:H2O | 82WAG/EVA | UO2Br2 | 90NEA | |
| SrCl2:2H2O | 82WAG/EVA | UO2Br2:H2O | 90NEA | |
| SrCl2:6H2O | 82WAG/EVA | UO2Br2:3H2O | 90NEA | |
| SrI2 | 79KUB/ALC | UO2BrOH:2H2O | 90NEA | |
| SrF2 | 76SMI/MAR | UCl6 | 90NEA | |
| SrHPO4 | 82WAG/EVA | UO2Cl2 | 90NEA | |
| SrO | 82WAG/EVA | UO2Cl2:H2O | 90NEA | |
| SrS | 82WAG/EVA | UO2Cl2:3H2O | 90NEA | |
| SrZrO3 | 74NAU/RYZ | UO2ClOH:2H2O | 90NEA | |
| Strontianite | SUPCRT91 | (UO2)2Cl3 | 90NEA | |
| Celestite | SUPCRT91 | UF6 | 90NEA | |
| | | UO2FOH | 90NEA | |
| KTcO4 | 83RAR | UO2FOH:H2O | 90NEA | |
| NaTcO4 | 83RAR | UO2FOH:2H2O | 90NEA | |
| Tc(OH)2 | 83RAR | UO2F2 | 90NEA | |
| Tc(OH)3 | 83RAR | UO2F2:3H2O | 90NEA | |
| Tc3O4 | 83RAR | U2O3F6 | 90NEA | |
| TcS2 | 83RAR | U3O5F8 | 90NEA | |
| TcOH | 83RAR | UOF4 | 90NEA | |
| TcO2:2H2O (am) | 83RAR | Rutherfordine | 95NEA/2 | |
| Tc4O7 | 83RAR | UO2(NO3)2 | 90NEA | |
| TcS3 | 83RAR | UO2(NO3)2:H2O | 90NEA | |
| TcO3 | 83RAR | UO2(NO3)2:2H2O | 90NEA | |
| Tc(c) | 83RAR | UO2(NO3)2:3H2O | 90NEA | |
| Tc2S7 | 83RAR | UO2(NO3)2:6H2O | 90NEA | |
| | | UO2SO4 | 90NEA | |
| Th(c) | 89COX/WAG | UO2SO4:H2O | 64OWE/MAY | |
| Th2S3 | 82WAG/EVA | UO2SO4:2.5H2O | 64OWE/MAY | |
| Th7S12 | 82WAG/EVA | UO2SO4:3H2O | 64OWE/MAY | |
| ThS2 | 82WAG/EVA | UO2SO4:3.5H2O | 64OWE/MAY | |
| Th(OH)4 | 74NAU/RYZ | (UO2)3(PO4)2 | 90NEA | |
| ThO2 | 89COX/WAG | (UO2)3(PO4)2:4H2O | 90NEA | |
| ThBr4 | 82WAG/EVA | (UO2)P2O7 | 90NEA | |
| ThCl4 | 80LAN/HER | Parsonsite | 78RIC/NRI | |
| ThF4 | 80LAN/HER | UO2(NO3)2 | 90NEA | |
| ThF4:2.5H2O | 82WAG/EVA | UO2HPO4 | 84TRI | |
| ThI4 | 82WAG/EVA | UO2HPO4:4H2O | 90NEA | |
| Th(NO3)4:5H2O | 82WAG/EVA | UP2O7:20H2O | 90NEA | |
| Th(SO4)2 | 82WAG/EVA | UO2(AsO3)2 | 90NEA | |
| Th2Se3 | 74MIL | (UO2)2As2O7 | 90NEA | |
| | | (UO2)3(AsO4)2 | 90NEA | |
| Autunite | 90SVE | K(UO2)AsO4 | 82WAG/EVA | |
| H-Autunite | 90NEA | Boltwoodite | 82HEM | |
| K-Autunite | 90SVE | Haiweeite | 82HEM | |
| Na-Autunite | 90SVE | Kasolite | 82HEM | |
| Sr-Autunite | 78LAN | Sklodowskite | 82HEM | |
| USb2 | | Soddyite | 82HEM | |
| U3Sb4 | | Weeksite | 82HEM | |
| Ningyoite | 78LAN | Tyuyamunite | 78LAN | |
| Uramphite | 78LAN | Carnotite | 78LAN | |
| Saleeite | 90SVE | | | |
| Uranocirite | 78LAN | Zr(c) | 79ROB/HEM | |
| Bassetite | 78LAN | Baddelyite | 79ROB/HEM | |
| Torbernite | 90SVE | Zircon | 79ROB/HEM | |
| Przhevalskite | 78LAN | | | |
| Uranophane | 78LAN | | | |
| UBr2Cl | 90NEA | REDOX | | |
| UBr3 | 90NEA | SPECIES | LOGK | REF |
| UCl3 | 90NEA | | | |
| UBrCl2 | 90NEA | Eu+3/Eu+2 | SUPCRT91 | |
| UOCl | 90NEA | U+3/UO2+2 | 90NEA | |
| UF3 | 90NEA | U+4/UO2+2 | 90NEA | |
| UI3 | 90NEA | UO2+/UO2+2 | 90NEA | |
| UO2 (am) | 90NEA | Am+4/Am+3 | 95NEA/1 | |
| U4O9 (c) | 78LAN | AmO2+/Am+3 | 95NEA/1 | |
| U3O8 (c) | 90NEA | AmO2+2/Am+3 | 95NEA/1 | |
| UBr4 | 90NEA | Np+3/Np+4 | 84LEM | |
| UOBr2 | 90NEA | NpO2+/Np+4 | 84LEM | |
| UBr3Cl | 90NEA | NpO2+2/Np++4 | 84LEM | |
| UBrCl3 | 90NEA | Pu+3/Pu+4 | 80LEM/TRE | |

4/13/99 DRL

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**Memorandum**

**To:** Wesley C. Patrick (Technical Director)
and Bruce E. Mabrito (Director of Quality Assurance)

**From:** David R. Turner

**Subject:** Exemption for qualification of data in the MINTEQA2/PRODEFA2 software package

**Date:** May 7, 1992

The MINTEQA2/PRODEFA2 geochemical speciation code is under continuing development at the Environmental Research Laboratory of the U. S. Environmental Protection Agency in Athens, Georgia. Version 3.0 will be used in research and technical assistance activities at the Center for Nuclear Waste Regulatory Analyses, and it is anticipated that updated versions will be incorporated and evaluated as they become available. The PRODEFA2 code is the preprocessor used to prepare input files for the MINTEQA2 code, and as such does not directly use any geochemical data. As it is currently constructed, the MINTEQA2 code uses extensive databases to provide the information necessary in calculating equilibrium species distribution between liquid, solid, and gas phases from well established thermodynamic principles. The purpose of this memorandum is to petition for exclusion and exemption of these existing data from qualification requirements under Quality Assurance Procedure QAP-015.

Section 5.1.3 in QAP-015 provides for the exclusion of existing data from qualification if "The existing data were generated by the DOE or its contractors and the purpose of the Center activity or project is to provide an independent evaluation of that data" and/or "The existing data are being used as a basis of comparison in confirmatory research or other evaluations". The original MINTEQ code was developed at Pacific Northwest Laboratory and funded in part by the DOE. Much of the original data are based on the U. S. Geological Survey's WATEQ3 code, which has been used extensively in the scientific community and is well documented. At CNWRA, the MINTEQA2 database has also been expanded to include radioelement data from the EQ3/6 software package, also developed by the DOE. In addition, many of the data in the MINTEQA2 database (such as molecular weights and species charge) "... are accepted in the scientific and engineering community as established fact.", the third criteria justifying exclusion from qualification (Section 5.1.3).

Section 5.3 in QAP-015 also permits exemption of existing data from qualification where "In certain circumstances, programmatic requirements and constrains or other factors may make it necessary to use data which are not qualified". If such data are used in Center reports, a clear statement on the qualification status of the data is to be provided. Progress in numerous research and technical assistance activities at the CNWRA requires the use of geochemical data. While some of the data in the MINTEQA2 database are recognized by the scientific and engineering community as uncertain, they represent the current best estimates in the evolving state of geochemical data. Even though activities at CNWRA may address the state-of-the-art in geochemical data in narrowly defined areas, it is beyond the scope of the CNWRA program and resources to do so for all of the data in the MINTEQA2/PRODEFA2 package, which currently includes data for over 1200 species involving more than 125 components.

| Concurrence | Approval | Approval |
|---|---|---|
| 5/8/92 | 5/8/92 | 5/8/92 |
| John L. Russell | Wesley C. Patrick | Bruce E. Mabrito |
| Element Manager | Technical Director | Director of Quality Assurance |

4/13/99
DRL

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TITLE Test Example, Speciation of Uranium, 1e-6 molal UO2+2,PCO2=1e-3.5
SOLUTION 1
        -units  mmol/kgw
        pH      2.0
        U(+6)   0.001 as UO2
        Na      100.    charge
        N(+5)   100.   as NO3
# Model definitions
PHASES 1 # Do not change this number it is used by the program!
        Fix_H+
        H+ = H+
        log_k  0.0
END
#
#   UO2+2 = 1e-6
#
SELECTED_OUTPUT
        -file uranco2.123
        -molalities     UO2+2 UO2NO3+ UO2OH+ UO2(OH)2 UO2(OH)3- UO2(OH)4-2 \
                        (UO2)2(OH)+3 (UO2)2(OH)2+2 (UO2)3(OH)4+2 (UO2)3(OH)5+ \
                        (UO2)3(OH)7- (UO2)4(OH)7+ UO2CO3 UO2(CO3)2-2 UO2(CO3)3-4\
                        (UO2)3(CO3)6-6 (UO2)11(CO3)6(OH)12-2 (UO2)2CO3(OH)3-
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -2.0   NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -2.25  NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -2.50  NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -2.75  NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -3.0   NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -3.25  NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -3.50  NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -3.75  NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -4.00  NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -4.25  NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -4.50  NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -4.75  NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -5.0   NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -5.25  NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -5.5   NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -5.75  NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -6.0   NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -6.25  NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -6.5   NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -6.75  NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -7.0   NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -7.25  NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -7.5   NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -7.75  NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -8.0   NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -8.25  NaOH    10.0
        CO2(g)   -3.5   1.0
```

$U(VI) = 1e-6\,m$

$P_{CO_2} = 1e-3.5\,atm$

$0.1\,m\ NaNO_3$

PHREEQC input file

4/13/99
DRJ



PHREEQC Results
U(vi) = 1e-6m
$P_{CO_2}$ = 1e-3.5 atm
0.1 m $NaNO_3$

| U(total) | ph | pe | ionic_strength | H2O | UO2+2_m | UO2+2_% | UO2NO3+_m | UO2NO3+_% | UO2OH+_m | UO2OH+_% | UO2(OH)2_m | UO2(OH)2_% | UO2(OH)3-_m | UO2(OH)3-_% | UO2(OH)4-2_m | UO2(OH)4-2_% | (UO2)2(OH)+3_m | (UO2)2(OH)+3_% | (UO2)2(OH)3+2_m | (UO2)2(OH)2+2_% | (UO2)3(OH)4+2_m | (UO2)3(OH)4+2_% | (UO2)3(OH)5+_m | (UO2)3(OH)5+_% | (UO2)3(OH)7-_m | (UO2)3(OH)7-_% |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1.00E-06 | 2.00 | 16.402695 | 0.100001 | 1.000000 | 9.38E-07 | 93.83 | 6.14E-08 | 6.14 | 2.60E-10 | 0.03 | 1.56E-13 | 0.00 | 2.54E-20 | 0.00 | 8.65E-32 | 0.00 | 1.90E-13 | 0.00 | 6.82E-15 | 0.00 | 1.13E-23 | 0.00 | 1.17E-25 | 0.00 | 3.99E-37 | 0.00 |
| | 2.25 | 16.140683 | 0.099991 | 1.000095 | 9.38E-07 | 93.81 | 6.14E-08 | 6.14 | 4.62E-10 | 0.05 | 4.92E-13 | 0.00 | 1.43E-19 | 0.00 | 8.65E-31 | 0.00 | 3.37E-13 | 0.00 | 2.15E-14 | 0.00 | 1.13E-22 | 0.00 | 2.08E-24 | 0.00 | 2.24E-35 | 0.00 |
| | 2.50 | 15.875308 | 0.099986 | 1.000149 | 9.38E-07 | 93.77 | 6.14E-08 | 6.14 | 8.21E-10 | 0.08 | 1.56E-12 | 0.00 | 8.02E-19 | 0.00 | 8.64E-30 | 0.00 | 5.99E-13 | 0.00 | 6.81E-14 | 0.00 | 1.13E-21 | 0.00 | 3.69E-23 | 0.00 | 1.26E-33 | 0.00 |
| | 2.75 | 15.609172 | 0.099983 | 1.000179 | 9.37E-07 | 93.70 | 6.13E-08 | 6.13 | 1.46E-09 | 0.15 | 4.92E-12 | 0.00 | 4.51E-18 | 0.00 | 8.64E-29 | 0.00 | 1.06E-12 | 0.00 | 2.15E-13 | 0.00 | 1.13E-20 | 0.00 | 6.56E-22 | 0.00 | 7.06E-32 | 0.00 |
| | 3.00 | 15.342836 | 0.099981 | 1.000196 | 9.36E-07 | 93.59 | 6.12E-08 | 6.12 | 2.59E-09 | 0.26 | 1.55E-11 | 0.00 | 2.53E-17 | 0.00 | 8.63E-28 | 0.00 | 1.89E-12 | 0.00 | 6.78E-13 | 0.00 | 1.12E-19 | 0.00 | 1.16E-20 | 0.00 | 3.96E-30 | 0.00 |
| | 3.25 | 15.128237 | 0.099980 | 1.000206 | 9.34E-07 | 93.40 | 6.11E-08 | 6.11 | 4.60E-09 | 0.46 | 4.90E-11 | 0.00 | 1.42E-16 | 0.00 | 8.61E-27 | 0.00 | 3.34E-12 | 0.00 | 2.14E-12 | 0.00 | 1.12E-18 | 0.00 | 2.05E-19 | 0.00 | 2.21E-28 | 0.00 |
| | 3.50 | 14.843645 | 0.099980 | 1.000211 | 9.31E-07 | 93.06 | 6.09E-08 | 6.09 | 8.15E-09 | 0.82 | 1.54E-10 | 0.02 | 7.96E-16 | 0.00 | 8.58E-26 | 0.00 | 5.90E-12 | 0.00 | 6.71E-12 | 0.00 | 1.10E-17 | 0.00 | 3.61E-18 | 0.00 | 1.23E-26 | 0.00 |
| | 3.75 | 14.647279 | 0.099979 | 1.000214 | 9.24E-07 | 92.43 | 6.05E-08 | 6.05 | 1.44E-08 | 1.44 | 4.85E-10 | 0.05 | 4.44E-15 | 0.00 | 8.52E-25 | 0.00 | 1.03E-11 | 0.00 | 2.09E-11 | 0.00 | 1.08E-16 | 0.00 | 6.29E-17 | 0.00 | 6.78E-25 | 0.00 |
| | 4.00 | 14.283352 | 0.099978 | 1.000216 | 9.13E-07 | 91.30 | 5.97E-08 | 5.97 | 2.53E-08 | 2.53 | 1.51E-09 | 0.15 | 2.47E-14 | 0.00 | 8.42E-24 | 0.00 | 1.80E-11 | 0.00 | 6.46E-11 | 0.01 | 1.04E-15 | 0.00 | 1.08E-15 | 0.00 | 3.67E-23 | 0.00 |
| | 4.25 | 14.150145 | 0.099979 | 1.000217 | 8.92E-07 | 89.22 | 5.84E-08 | 5.84 | 4.39E-08 | 4.39 | 4.68E-09 | 0.47 | 1.36E-13 | 0.00 | 8.23E-23 | 0.00 | 3.05E-11 | 0.01 | 1.95E-10 | 0.04 | 9.72E-15 | 0.00 | 1.79E-14 | 0.00 | 1.93E-21 | 0.00 |
| | 4.50 | 13.824425 | 0.099979 | 1.000217 | 8.53E-07 | 85.35 | 5.59E-08 | 5.59 | 7.48E-08 | 7.48 | 1.42E-08 | 1.42 | 7.30E-13 | 0.00 | 7.87E-22 | 0.00 | 4.99E-11 | 0.01 | 5.64E-10 | 0.11 | 8.51E-14 | 0.00 | 2.79E-13 | 0.00 | 9.49E-20 | 0.00 |
| | 4.75 | 13.521996 | 0.099979 | 1.000218 | 7.82E-07 | 78.18 | 5.12E-08 | 5.12 | 1.22E-07 | 12.18 | 4.10E-08 | 4.10 | 3.76E-12 | 0.00 | 7.21E-21 | 0.00 | 7.40E-11 | 0.01 | 1.50E-09 | 0.30 | 6.54E-13 | 0.00 | 3.81E-12 | 0.00 | 4.10E-18 | 0.00 |
| | 5.00 | 13.306306 | 0.099979 | 1.000218 | 6.57E-07 | 65.66 | 4.30E-08 | 4.30 | 1.82E-07 | 18.19 | 1.09E-07 | 10.89 | 1.78E-11 | 0.00 | 6.05E-20 | 0.00 | 9.29E-11 | 0.02 | 3.34E-09 | 0.67 | 3.88E-12 | 0.00 | 4.01E-11 | 0.01 | 1.37E-16 | 0.00 |
| | 5.25 | 13.151706 | 0.099980 | 1.000218 | 4.72E-07 | 47.16 | 3.09E-08 | 3.09 | 2.32E-07 | 23.23 | 2.47E-07 | 24.74 | 7.17E-11 | 0.01 | 4.35E-19 | 0.00 | 8.52E-11 | 0.02 | 5.45E-09 | 1.09 | 1.44E-11 | 0.00 | 2.64E-10 | 0.08 | 2.85E-15 | 0.00 |
| | 5.50 | 12.902534 | 0.099980 | 1.000218 | 2.70E-07 | 27.05 | 1.77E-08 | 1.77 | 2.37E-07 | 23.69 | 4.49E-07 | 44.86 | 2.31E-10 | 0.02 | 2.49E-18 | 0.00 | 4.98E-11 | 0.01 | 5.66E-09 | 1.13 | 2.71E-11 | 0.01 | 8.87E-10 | 0.27 | 3.02E-14 | 0.00 |
| | 5.75 | 12.638809 | 0.099982 | 1.000218 | 1.23E-07 | 12.28 | 8.03E-09 | 0.80 | 1.91E-07 | 19.12 | 6.44E-07 | 64.39 | 5.90E-10 | 0.06 | 1.13E-17 | 0.00 | 1.83E-11 | 0.00 | 3.69E-09 | 0.74 | 2.53E-11 | 0.01 | 1.47E-09 | 0.44 | 1.59E-13 | 0.00 |
| | 6.00 | 12.324706 | 0.099984 | 1.000218 | 4.67E-08 | 4.67 | 3.06E-09 | 0.31 | 1.29E-07 | 12.95 | 7.75E-07 | 77.54 | 1.26E-09 | 0.13 | 4.31E-17 | 0.00 | 4.71E-12 | 0.00 | 1.69E-09 | 0.34 | 1.40E-11 | 0.00 | 1.45E-09 | 0.43 | 4.93E-13 | 0.00 |
| | 6.25 | 12.142740 | 0.099989 | 1.000218 | 1.60E-08 | 1.60 | 1.05E-09 | 0.10 | 7.87E-08 | 7.87 | 8.39E-07 | 83.86 | 2.43E-09 | 0.24 | 1.47E-16 | 0.00 | 9.79E-13 | 0.00 | 6.26E-10 | 0.13 | 5.60E-12 | 0.00 | 1.03E-09 | 0.31 | 1.11E-12 | 0.00 |
| | 6.50 | 11.885466 | 0.099997 | 1.000219 | 5.12E-09 | 0.51 | 3.35E-10 | 0.03 | 4.49E-08 | 4.49 | 8.50E-07 | 84.97 | 4.38E-09 | 0.44 | 4.72E-16 | 0.00 | 1.79E-13 | 0.00 | 2.03E-10 | 0.04 | 1.84E-12 | 0.00 | 6.02E-10 | 0.18 | 2.05E-12 | 0.00 |
| | 6.75 | 11.542520 | 0.100012 | 1.000218 | 1.56E-09 | 0.16 | 1.02E-10 | 0.01 | 2.44E-08 | 2.44 | 8.20E-07 | 82.03 | 7.52E-09 | 0.75 | 1.44E-15 | 0.00 | 2.96E-14 | 0.00 | 5.99E-11 | 0.01 | 5.24E-13 | 0.00 | 3.05E-10 | 0.09 | 3.28E-12 | 0.00 |
| | 7.00 | 11.402450 | 0.100038 | 1.000218 | 4.56E-10 | 0.05 | 2.98E-11 | 0.00 | 1.26E-08 | 1.26 | 7.56E-07 | 75.56 | 1.23E-08 | 1.23 | 4.20E-15 | 0.00 | 4.47E-15 | 0.00 | 1.61E-11 | 0.00 | 1.29E-13 | 0.00 | 1.34E-10 | 0.04 | 4.56E-12 | 0.00 |
| | 7.25 | 11.018002 | 0.100084 | 1.000218 | 1.25E-10 | 0.01 | 8.20E-12 | 0.00 | 6.17E-09 | 0.62 | 6.57E-07 | 65.70 | 1.90E-08 | 1.90 | 1.16E-14 | 0.00 | 6.01E-16 | 0.00 | 3.84E-12 | 0.00 | 2.69E-14 | 0.00 | 4.95E-11 | 0.01 | 5.33E-12 | 0.00 |
| | 7.50 | 10.781573 | 0.100168 | 1.000218 | 3.13E-11 | 0.00 | 2.05E-12 | 0.00 | 2.74E-09 | 0.27 | 5.20E-07 | 51.96 | 2.68E-08 | 2.68 | 2.89E-14 | 0.00 | 6.69E-17 | 0.00 | 7.60E-13 | 0.00 | 4.21E-15 | 0.00 | 1.38E-11 | 0.00 | 4.69E-12 | 0.00 |
| | 7.75 | 10.522566 | 0.100321 | 1.000218 | 6.16E-12 | 0.00 | 4.02E-13 | 0.00 | 9.58E-10 | 0.10 | 3.23E-07 | 32.26 | 2.96E-08 | 2.96 | 5.68E-14 | 0.00 | 4.59E-18 | 0.00 | 9.27E-14 | 0.00 | 3.19E-16 | 0.00 | 1.85E-12 | 0.00 | 2.00E-12 | 0.00 |
| | 8.00 | 10.322041 | 0.100598 | 1.000218 | 6.16E-13 | 0.00 | 4.02E-14 | 0.00 | 1.70E-10 | 0.02 | 1.02E-07 | 10.19 | 1.66E-08 | 1.66 | 5.68E-14 | 0.00 | 8.17E-20 | 0.00 | 2.93E-15 | 0.00 | 3.18E-18 | 0.00 | 3.29E-14 | 0.00 | 1.12E-13 | 0.00 |
| | 8.25 | 10.148062 | 0.101107 | 1.000219 | 2.88E-14 | 0.00 | 1.87E-15 | 0.00 | 1.41E-11 | 0.00 | 1.50E-08 | 1.50 | 4.36E-09 | 0.44 | 2.65E-14 | 0.00 | 3.17E-22 | 0.00 | 2.02E-17 | 0.00 | 3.23E-21 | 0.00 | 5.93E-17 | 0.00 | 6.39E-16 | 0.00 |
| | 8.50 | 9.883421 | 0.102074 | 1.000220 | 1.01E-15 | 0.00 | 6.54E-17 | 0.00 | 8.77E-13 | 0.00 | 1.66E-09 | 0.17 | 8.56E-10 | 0.09 | 9.29E-15 | 0.00 | 6.91E-25 | 0.00 | 7.80E-20 | 0.00 | 1.38E-24 | 0.00 | 4.49E-20 | 0.00 | 1.53E-18 | 0.00 |
| | 8.75 | 9.567515 | 0.103999 | 1.000224 | 3.23E-17 | 0.00 | 2.08E-18 | 0.00 | 4.97E-14 | 0.00 | 1.57E-10 | 0.02 | 1.53E-10 | 0.02 | 2.97E-15 | 0.00 | 1.26E-27 | 0.00 | 2.51E-22 | 0.00 | 4.47E-28 | 0.00 | 2.57E-23 | 0.00 | 2.77E-21 | 0.00 |
| | 9.00 | 9.313535 | 0.108104 | 1.000236 | 9.88E-19 | 0.00 | 6.27E-20 | 0.00 | 2.67E-15 | 0.00 | 1.59E-11 | 0.00 | 2.61E-11 | 0.00 | 9.10E-16 | 0.00 | 2.10E-30 | 0.00 | 7.32E-25 | 0.00 | 1.24E-31 | 0.00 | 1.26E-26 | 0.00 | 4.29E-24 | 0.00 |
| | 9.25 | 9.051275 | 0.117731 | 1.000278 | 2.85E-20 | 0.00 | 1.75E-21 | 0.00 | 1.33E-16 | 0.00 | 1.40E-12 | 0.00 | 4.13E-12 | 0.00 | 2.62E-16 | 0.00 | 3.09E-33 | 0.00 | 1.85E-27 | 0.00 | 2.77E-35 | 0.00 | 4.89E-30 | 0.00 | 5.26E-27 | 0.00 |
| | 9.50 | 8.811089 | 0.143631 | 1.000431 | 7.15E-22 | 0.00 | 4.05E-23 | 0.00 | 5.59E-18 | 0.00 | 1.03E-13 | 0.00 | 5.49E-13 | 0.00 | 6.56E-17 | 0.00 | 3.45E-36 | 0.00 | 3.41E-30 | 0.00 | 3.74E-39 | 0.00 | 1.11E-33 | 0.00 | 3.78E-30 | 0.00 |
| | 9.75 | 8.516815 | 0.231576 | 1.001115 | 1.26E-23 | 0.00 | 5.81E-25 | 0.00 | 1.48E-19 | 0.00 | 4.71E-15 | 0.00 | 4.68E-14 | 0.00 | 1.15E-17 | 0.00 | 1.87E-39 | 0.00 | 2.70E-33 | 0.00 | 0.00E+00 | 0.00 | 6.29E-38 | 0.00 | 6.73E-34 | 0.00 |
| | 10.00 | 8.382695 | 0.766213 | 1.007189 | 8.53E-26 | 0.00 | 2.22E-27 | 0.00 | 1.01E-21 | 0.00 | 5.77E-17 | 0.00 | 1.15E-15 | 0.00 | 7.33E-19 | 0.00 | 0.00E+00 | 0.00 | 2.11E-37 | 0.00 | 0.00E+00 | 0.00 | 0.00E+00 | 0.00 | 2.47E-39 | 0.00 |

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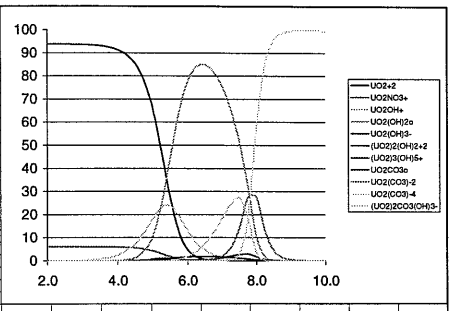
| (UO2)4(OH)7+_m | (UO2)4(OH)7+_% | UO2CO3_m | UO2CO3_% | UO2(CO3)2-2_m | UO2(CO3)2-2_% | UO2(CO3)3-4_m | UO2(CO3)3-4_% | (UO2)3(CO3)6-6_m | (UO2)3(CO3)6-6_% | (UO2)11(CO3)6(OH | (UO2)11(CO3)6(OH | (UO2)2CO3(OH)3-_ | (UO2)2CO3(OH)3-_% | Total_m | Total_% |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1.65E-34 | 0.00 | 3.35E-15 | 0.00 | 4.16E-25 | 0.00 | 8.67E-37 | 0.00 | 0.00E+00 | 0.00 | 0.00E+00 | 0.00 | 3.85E-28 | 0.00 | 1.00E-06 | 100.00 |
| 9.28E-33 | 0.00 | 1.06E-14 | 0.00 | 4.16E-24 | 0.00 | 2.74E-35 | 0.00 | 0.00E+00 | 0.00 | 0.00E+00 | 0.00 | 6.84E-25 | 0.00 | 1.00E-06 | 99.99 |
| 5.21E-31 | 0.00 | 3.35E-14 | 0.00 | 4.16E-23 | 0.00 | 8.66E-34 | 0.00 | 0.00E+00 | 0.00 | 0.00E+00 | 0.00 | 1.22E-23 | 0.00 | 1.00E-06 | 99.99 |
| 2.92E-29 | 0.00 | 1.06E-13 | 0.00 | 4.16E-22 | 0.00 | 2.74E-33 | 0.00 | 0.00E+00 | 0.00 | 0.00E+00 | 0.00 | 2.16E-22 | 0.00 | 1.00E-06 | 99.98 |
| 1.64E-27 | 0.00 | 3.35E-13 | 0.00 | 4.15E-21 | 0.00 | 8.65E-31 | 0.00 | 0.00E+00 | 0.00 | 0.00E+00 | 0.00 | 3.83E-21 | 0.00 | 1.00E-06 | 99.98 |
| 9.12E-26 | 0.00 | 1.06E-12 | 0.00 | 4.14E-20 | 0.00 | 2.73E-29 | 0.00 | 0.00E+00 | 0.00 | 0.00E+00 | 0.00 | 6.78E-20 | 0.00 | 1.00E-06 | 99.98 |
| 5.06E-24 | 0.00 | 3.33E-12 | 0.00 | 4.13E-19 | 0.00 | 8.60E-28 | 0.00 | 0.00E+00 | 0.00 | 0.00E+00 | 0.00 | 1.20E-18 | 0.00 | 1.00E-06 | 99.98 |
| 2.77E-22 | 0.00 | 1.05E-11 | 0.00 | 4.10E-18 | 0.00 | 2.70E-26 | 0.00 | 0.00E+00 | 0.00 | 0.00E+00 | 0.00 | 2.10E-17 | 0.00 | 1.00E-06 | 99.98 |
| 1.48E-20 | 0.00 | 3.26E-11 | 0.00 | 4.05E-17 | 0.00 | 8.44E-25 | 0.00 | 0.00E+00 | 0.00 | 0.00E+00 | 0.00 | 3.64E-16 | 0.00 | 1.00E-06 | 99.98 |
| 7.60E-19 | 0.00 | 1.01E-10 | 0.01 | 3.96E-16 | 0.00 | 2.61E-23 | 0.00 | 0.00E+00 | 0.00 | 0.00E+00 | 0.00 | 6.19E-15 | 0.00 | 1.00E-06 | 99.98 |
| 3.58E-17 | 0.00 | 3.05E-10 | 0.03 | 3.78E-15 | 0.00 | 7.89E-22 | 0.00 | 2.94E-38 | 0.00 | 0.00E+00 | 0.00 | 1.01E-13 | 0.00 | 9.99E-07 | 99.98 |
| 1.42E-15 | 0.00 | 8.84E-10 | 0.09 | 3.47E-14 | 0.00 | 2.28E-20 | 0.00 | 2.26E-35 | 0.00 | 0.00E+00 | 0.00 | 1.50E-12 | 0.00 | 9.98E-07 | 99.98 |
| 3.96E-14 | 0.00 | 2.35E-09 | 0.23 | 2.91E-13 | 0.00 | 6.07E-19 | 0.00 | 1.34E-32 | 0.00 | 0.00E+00 | 0.00 | 1.88E-11 | 0.00 | 9.96E-07 | 99.98 |
| 5.93E-13 | 0.00 | 5.33E-09 | 0.53 | 2.09E-12 | 0.00 | 1.38E-17 | 0.00 | 4.96E-30 | 0.00 | 0.00E+00 | 0.00 | 1.73E-10 | 0.03 | 9.94E-07 | 99.98 |
| 3.61E-12 | 0.00 | 9.67E-09 | 0.97 | 1.20E-11 | 0.00 | 2.50E-16 | 0.00 | 9.36E-28 | 0.00 | 2.77E-39 | 0.00 | 1.01E-09 | 0.20 | 9.91E-07 | 99.98 |
| 8.61E-12 | 0.00 | 1.39E-08 | 1.39 | 5.44E-11 | 0.01 | 3.59E-15 | 0.00 | 8.75E-26 | 0.00 | 4.67E-37 | 0.00 | 3.70E-09 | 0.74 | 9.89E-07 | 99.98 |
| 1.02E-11 | 0.00 | 1.67E-08 | 1.67 | 2.07E-10 | 0.02 | 4.32E-14 | 0.00 | 4.83E-24 | 0.00 | 1.14E-35 | 0.00 | 9.55E-09 | 1.91 | 9.86E-07 | 99.98 |
| 7.83E-12 | 0.00 | 1.81E-08 | 1.81 | 7.09E-10 | 0.07 | 4.67E-13 | 0.00 | 1.93E-22 | 0.00 | 8.54E-35 | 0.00 | 1.99E-08 | 3.97 | 9.77E-07 | 99.98 |
| 4.64E-12 | 0.00 | 1.83E-08 | 1.83 | 2.27E-09 | 0.23 | 4.73E-12 | 0.00 | 6.36E-21 | 0.00 | 3.12E-34 | 0.00 | 3.63E-08 | 7.26 | 9.52E-07 | 99.98 |
| 2.27E-12 | 0.00 | 1.77E-08 | 1.77 | 6.94E-09 | 0.69 | 4.57E-11 | 0.00 | 1.81E-19 | 0.00 | 6.69E-34 | 0.00 | 6.01E-08 | 12.02 | 9.39E-07 | 99.98 |
| 9.18E-13 | 0.00 | 1.63E-08 | 1.63 | 2.02E-08 | 2.02 | 4.21E-10 | 0.04 | 4.48E-18 | 0.00 | 8.57E-34 | 0.00 | 9.07E-08 | 18.14 | 9.09E-07 | 99.98 |
| 2.95E-13 | 0.00 | 1.42E-08 | 1.42 | 5.56E-08 | 5.56 | 3.66E-09 | 0.37 | 9.32E-17 | 0.00 | 5.82E-34 | 0.00 | 1.22E-07 | 24.39 | 8.78E-07 | 99.98 |
| 6.49E-14 | 0.00 | 1.12E-08 | 1.12 | 1.39E-07 | 13.90 | 2.90E-08 | 2.90 | 1.46E-15 | 0.00 | 1.39E-34 | 0.00 | 1.36E-07 | 27.13 | 8.64E-07 | 99.98 |
| 5.43E-15 | 0.00 | 6.95E-09 | 0.70 | 2.73E-07 | 27.31 | 1.81E-07 | 18.06 | 1.11E-14 | 0.00 | 2.33E-36 | 0.00 | 9.30E-08 | 18.60 | 9.07E-07 | 99.98 |
| 3.04E-17 | 0.00 | 2.20E-09 | 0.22 | 2.73E-07 | 27.31 | 5.73E-07 | 57.28 | 1.12E-14 | 0.00 | 0.00E+00 | 0.00 | 1.65E-08 | 3.30 | 9.83E-07 | 99.98 |
| 8.09E-21 | 0.00 | 3.24E-10 | 0.03 | 1.28E-07 | 12.76 | 8.51E-07 | 85.12 | 1.15E-15 | 0.00 | 0.00E+00 | 0.00 | 6.39E-10 | 0.13 | 9.99E-07 | 99.98 |
| 6.75E-25 | 0.00 | 3.58E-11 | 0.00 | 4.47E-08 | 4.47 | 9.53E-07 | 95.25 | 5.06E-17 | 0.00 | 0.00E+00 | 0.00 | 1.38E-11 | 0.00 | 1.00E-06 | 99.98 |
| 3.89E-29 | 0.00 | 3.60E-12 | 0.00 | 1.43E-08 | 1.43 | 9.85E-07 | 98.51 | 1.74E-18 | 0.00 | 0.00E+00 | 0.00 | 2.50E-13 | 0.00 | 1.00E-06 | 99.98 |
| 1.82E-33 | 0.00 | 3.43E-13 | 0.00 | 4.38E-09 | 0.44 | 9.95E-07 | 99.53 | 5.42E-20 | 0.00 | 0.00E+00 | 0.00 | 4.05E-15 | 0.00 | 1.00E-06 | 99.98 |
| 6.22E-38 | 0.00 | 3.02E-14 | 0.00 | 1.26E-09 | 0.13 | 9.98E-07 | 99.85 | 1.57E-21 | 0.00 | 0.00E+00 | 0.00 | 5.64E-17 | 0.00 | 1.00E-06 | 99.97 |
| 0.00E+00 | 0.00 | 2.22E-15 | 0.00 | 3.16E-10 | 0.03 | 9.99E-07 | 99.93 | 3.96E-23 | 0.00 | 0.00E+00 | 0.00 | 5.52E-19 | 0.00 | 1.00E-06 | 99.96 |
| 0.00E+00 | 0.00 | 1.02E-16 | 0.00 | 5.56E-11 | 0.01 | 9.99E-07 | 99.88 | 6.98E-25 | 0.00 | 0.00E+00 | 0.00 | 2.15E-21 | 0.00 | 9.99E-07 | 99.89 |
| 0.00E+00 | 0.00 | 1.27E-18 | 0.00 | 3.65E-12 | 0.00 | 9.93E-07 | 99.29 | 4.66E-27 | 0.00 | 0.00E+00 | 0.00 | 6.55E-25 | 0.00 | 9.93E-07 | 99.29 |



122
4/13/04
KP-1

MINTEQAD Results
0.1m $NaNO_3$
U(VI) = 1e-6m
$P_{CO_2}$ = 1e-3.5 atm

| U(total) | ph | | | | UO2+2_m | UO2+2_% | UO2NO3+_m | UO2NO3+_% | UO2OH+_m | UO2OH+_% | UO2(OH)2_m | UO2(OH)2_% | UO2(OH)3-_m | UO2(OH)3-_% | UO2(OH)4-2_m | UO2(OH)4-2_% | (UO2)2(OH)+3_m | (UO2)2(OH)+3_% | (UO2)2(OH)3+2_m | (UO2)2(OH)2+2_% | (UO2)3(OH)4+2_m | (UO2)3(OH)4+2_% | (UO2)3(OH)5+_m | (UO2)3(OH)5+_% | (UO2)3(OH)7-_m | (UO2)3(OH)7-_% |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1.00E-06 | 2.00 | | | | 9.37E-07 | 93.70 | 6.33E-08 | 6.33 | 2.66E-10 | 0.03 | 1.53E-13 | 0.00 | 2.55E-20 | 0.00 | 8.63E-32 | 0.00 | 2.21E-13 | 0.00 | 7.12E-15 | 0.00 | 1.19E-23 | 0.00 | 1.20E-25 | 0.00 | 4.06E-37 | 0.00 |
| | 2.25 | | | | 9.36E-07 | 93.60 | 6.37E-08 | 6.37 | 4.75E-10 | 0.05 | 4.88E-13 | 0.00 | 1.44E-19 | 0.00 | 8.62E-31 | 0.00 | 3.92E-13 | 0.00 | 2.27E-14 | 0.00 | 1.21E-22 | 0.00 | 2.18E-24 | 0.00 | 2.34E-35 | 0.00 |
| | 2.50 | | | | 9.35E-07 | 93.50 | 6.40E-08 | 6.40 | 8.47E-10 | 0.08 | 1.55E-12 | 0.00 | 8.14E-19 | 0.00 | 8.62E-30 | 0.00 | 6.95E-13 | 0.00 | 7.20E-14 | 0.00 | 1.22E-21 | 0.00 | 3.91E-23 | 0.00 | 1.33E-33 | 0.00 |
| | 2.75 | | | | 9.34E-07 | 93.40 | 6.41E-08 | 6.41 | 1.51E-09 | 0.15 | 4.92E-12 | 0.00 | 4.58E-18 | 0.00 | 8.61E-29 | 0.00 | 1.23E-12 | 0.00 | 2.28E-13 | 0.00 | 1.22E-20 | 0.00 | 6.99E-22 | 0.00 | 7.53E-32 | 0.00 |
| | 3.00 | | | | 9.33E-07 | 93.30 | 6.42E-08 | 6.42 | 2.68E-09 | 0.27 | 1.56E-11 | 0.00 | 2.58E-17 | 0.00 | 8.60E-28 | 0.00 | 2.19E-12 | 0.00 | 7.20E-13 | 0.00 | 1.22E-19 | 0.00 | 1.24E-20 | 0.00 | 4.24E-30 | 0.00 |
| | 3.25 | | | | 9.31E-07 | 93.10 | 6.41E-08 | 6.41 | 4.76E-09 | 0.48 | 4.91E-11 | 0.00 | 1.45E-16 | 0.00 | 8.59E-27 | 0.00 | 3.87E-12 | 0.00 | 2.27E-12 | 0.00 | 1.22E-18 | 0.00 | 2.20E-19 | 0.00 | 2.37E-28 | 0.00 |
| | 3.50 | | | | 9.28E-07 | 92.80 | 6.39E-08 | 6.39 | 8.44E-09 | 0.84 | 1.55E-10 | 0.02 | 8.11E-16 | 0.00 | 8.54E-26 | 0.00 | 6.83E-12 | 0.00 | 7.12E-12 | 0.00 | 1.20E-17 | 0.00 | 3.88E-18 | 0.00 | 1.32E-26 | 0.00 |
| | 3.75 | | | | 9.21E-07 | 92.10 | 6.34E-08 | 6.34 | 1.49E-08 | 1.49 | 4.86E-10 | 0.05 | 4.53E-15 | 0.00 | 8.49E-25 | 0.00 | 1.20E-11 | 0.00 | 2.22E-11 | 0.00 | 1.18E-16 | 0.00 | 6.76E-17 | 0.00 | 7.28E-25 | 0.00 |
| | 4.00 | | | | 9.09E-07 | 90.90 | 6.26E-08 | 6.26 | 2.62E-08 | 2.62 | 1.52E-09 | 0.15 | 2.51E-14 | 0.00 | 8.38E-24 | 0.00 | 2.08E-11 | 0.00 | 6.85E-11 | 0.01 | 1.13E-15 | 0.00 | 1.16E-15 | 0.00 | 3.94E-23 | 0.00 |
| | 4.25 | | | | 8.88E-07 | 88.80 | 6.12E-08 | 6.12 | 4.54E-08 | 4.54 | 4.69E-09 | 0.47 | 1.38E-13 | 0.00 | 8.18E-23 | 0.00 | 3.52E-11 | 0.01 | 2.07E-10 | 0.04 | 1.06E-14 | 0.00 | 1.92E-14 | 0.00 | 2.06E-21 | 0.00 |
| | 4.50 | | | | 8.48E-07 | 84.80 | 5.84E-08 | 5.84 | 7.72E-08 | 7.72 | 1.42E-08 | 1.42 | 7.42E-13 | 0.00 | 7.81E-22 | 0.00 | 5.71E-11 | 0.01 | 5.96E-10 | 0.12 | 9.21E-14 | 0.00 | 2.97E-13 | 0.00 | 1.01E-19 | 0.00 |
| | 4.75 | | | | 7.75E-07 | 77.50 | 5.34E-08 | 5.34 | 1.29E-07 | 12.90 | 4.09E-08 | 4.09 | 3.81E-12 | 0.00 | 7.14E-21 | 0.00 | 8.47E-11 | 0.02 | 1.57E-09 | 0.31 | 7.02E-13 | 0.00 | 4.03E-12 | 0.00 | 4.34E-18 | 0.00 |
| | 5.00 | | | | 6.47E-07 | 64.70 | 4.46E-08 | 4.46 | 1.86E-07 | 18.60 | 1.09E-07 | 10.90 | 1.79E-11 | 0.00 | 5.99E-20 | 0.00 | 1.05E-10 | 0.02 | 3.47E-09 | 0.69 | 4.09E-12 | 0.00 | 4.18E-11 | 0.01 | 1.42E-16 | 0.00 |
| | 5.25 | | | | 4.61E-07 | 46.10 | 3.18E-08 | 3.18 | 2.36E-07 | 23.60 | 2.44E-07 | 24.40 | 7.16E-11 | 0.01 | 4.25E-19 | 0.00 | 9.51E-11 | 0.02 | 5.58E-09 | 1.12 | 1.48E-11 | 0.00 | 2.69E-10 | 0.08 | 2.90E-15 | 0.00 |
| | 5.50 | | | | 2.63E-07 | 26.30 | 1.81E-08 | 1.81 | 2.39E-07 | 23.90 | 4.39E-07 | 43.90 | 2.30E-10 | 0.02 | 2.42E-18 | 0.00 | 5.47E-11 | 0.01 | 5.71E-09 | 1.14 | 2.73E-11 | 0.01 | 8.81E-10 | 0.26 | 3.00E-14 | 0.00 |
| | 5.75 | | | | 1.18E-07 | 11.80 | 8.16E-09 | 0.82 | 1.92E-07 | 19.20 | 6.26E-07 | 62.60 | 5.82E-10 | 0.06 | 1.09E-17 | 0.00 | 1.98E-11 | 0.00 | 3.67E-09 | 0.73 | 2.51E-11 | 0.01 | 1.44E-09 | 0.43 | 1.55E-13 | 0.00 |
| | 6.00 | | | | 4.50E-08 | 4.50 | 3.10E-09 | 0.31 | 1.29E-07 | 12.90 | 7.51E-07 | 75.10 | 1.24E-09 | 0.12 | 4.14E-17 | 0.00 | 5.08E-12 | 0.00 | 1.67E-09 | 0.33 | 1.37E-11 | 0.00 | 1.40E-09 | 0.42 | 4.77E-13 | 0.00 |
| | 6.25 | | | | 1.54E-08 | 1.54 | 1.06E-09 | 0.11 | 7.86E-08 | 7.86 | 8.12E-07 | 81.20 | 2.39E-09 | 0.24 | 1.42E-16 | 0.00 | 1.05E-12 | 0.00 | 6.16E-10 | 0.12 | 5.48E-12 | 0.00 | 9.93E-10 | 0.30 | 1.07E-12 | 0.00 |
| | 6.50 | | | | 4.92E-09 | 0.49 | 3.39E-10 | 0.03 | 4.48E-08 | 4.48 | 8.23E-07 | 82.30 | 4.31E-09 | 0.43 | 4.54E-16 | 0.00 | 1.93E-13 | 0.00 | 2.01E-10 | 0.04 | 1.80E-12 | 0.00 | 5.81E-10 | 0.17 | 1.98E-12 | 0.00 |
| | 6.75 | | | | 1.50E-09 | 0.15 | 1.04E-10 | 0.01 | 2.43E-08 | 2.43 | 7.95E-07 | 79.50 | 7.40E-09 | 0.74 | 1.39E-15 | 0.00 | 3.20E-14 | 0.00 | 5.93E-11 | 0.01 | 5.14E-13 | 0.00 | 2.95E-10 | 0.09 | 3.16E-12 | 0.00 |
| | 7.00 | | | | 4.39E-10 | 0.04 | 3.02E-11 | 0.00 | 1.26E-08 | 1.26 | 7.33E-07 | 73.30 | 1.21E-08 | 1.21 | 4.04E-15 | 0.00 | 4.83E-15 | 0.00 | 1.59E-11 | 0.00 | 1.27E-13 | 0.00 | 1.30E-10 | 0.04 | 4.43E-12 | 0.00 |
| | 7.25 | | | | 1.21E-10 | 0.01 | 8.32E-12 | 0.00 | 6.18E-09 | 0.62 | 6.38E-07 | 63.80 | 1.88E-08 | 1.88 | 1.11E-14 | 0.00 | 6.51E-16 | 0.00 | 3.82E-12 | 0.00 | 2.66E-14 | 0.00 | 4.82E-11 | 0.01 | 5.19E-12 | 0.00 |
| | 7.50 | | | | 3.02E-11 | 0.00 | 2.08E-12 | 0.00 | 2.75E-09 | 0.28 | 5.05E-07 | 50.50 | 2.64E-08 | 2.64 | 2.79E-14 | 0.00 | 7.26E-17 | 0.00 | 7.57E-13 | 0.00 | 4.17E-15 | 0.00 | 1.35E-11 | 0.00 | 4.58E-12 | 0.00 |
| | 7.75 | | | | 6.01E-12 | 0.00 | 4.14E-13 | 0.00 | 9.71E-10 | 0.10 | 3.17E-07 | 31.70 | 2.95E-08 | 2.95 | 5.53E-14 | 0.00 | 5.09E-18 | 0.00 | 9.44E-14 | 0.00 | 3.27E-16 | 0.00 | 1.87E-12 | 0.00 | 2.02E-12 | 0.00 |
| | 8.00 | | | | 6.31E-13 | 0.00 | 4.34E-14 | 0.00 | 1.81E-10 | 0.02 | 1.05E-07 | 10.50 | 1.74E-08 | 1.74 | 5.81E-14 | 0.00 | 9.99E-20 | 0.00 | 3.29E-15 | 0.00 | 3.78E-18 | 0.00 | 3.86E-14 | 0.00 | 1.31E-13 | 0.00 |
| | 8.25 | | | | 3.09E-14 | 0.00 | 2.13E-15 | 0.00 | 1.58E-11 | 0.00 | 1.63E-08 | 1.63 | 4.80E-09 | 0.48 | 2.85E-14 | 0.00 | 4.27E-22 | 0.00 | 2.50E-17 | 0.00 | 4.45E-21 | 0.00 | 8.07E-17 | 0.00 | 8.69E-16 | 0.00 |
| | 8.50 | | | | 1.11E-15 | 0.00 | 7.62E-17 | 0.00 | 1.01E-12 | 0.00 | 1.85E-09 | 0.19 | 9.68E-10 | 0.10 | 1.02E-14 | 0.00 | 9.78E-25 | 0.00 | 1.02E-19 | 0.00 | 2.05E-24 | 0.00 | 6.59E-20 | 0.00 | 2.24E-18 | 0.00 |
| | 8.75 | | | | 3.62E-17 | 0.00 | 2.48E-18 | 0.00 | 5.83E-14 | 0.00 | 1.90E-10 | 0.02 | 1.77E-10 | 0.02 | 3.33E-15 | 0.00 | 1.85E-27 | 0.00 | 3.41E-22 | 0.00 | 7.05E-28 | 0.00 | 4.03E-23 | 0.00 | 4.34E-21 | 0.00 |
| | 9.00 | | | | 1.14E-18 | 0.00 | 7.72E-20 | 0.00 | 3.24E-15 | 0.00 | 1.87E-11 | 0.00 | 3.11E-11 | 0.00 | 1.05E-15 | 0.00 | 3.25E-30 | 0.00 | 1.05E-24 | 0.00 | 2.15E-31 | 0.00 | 2.18E-26 | 0.00 | 7.42E-24 | 0.00 |
| | 9.25 | | | | 3.45E-20 | 0.00 | 2.31E-21 | 0.00 | 1.73E-16 | 0.00 | 1.77E-12 | 0.00 | 5.25E-12 | 0.00 | 3.19E-16 | 0.00 | 1.05E-27 | 0.00 | 3.41E-22 | 0.00 | 7.05E-28 | 0.00 | 4.03E-23 | 0.00 | 4.34E-21 | 0.00 |
| | 9.50 | | | | 9.81E-22 | 0.00 | 6.34E-23 | 0.00 | 8.51E-18 | 0.00 | 1.53E-13 | 0.00 | 8.18E-13 | 0.00 | 9.04E-17 | 0.00 | 5.35E-33 | 0.00 | 3.03E-27 | 0.00 | 5.86E-35 | 0.00 | 1.04E-29 | 0.00 | 1.12E-26 | 0.00 |
| | 9.75 | | | | 2.40E-23 | 0.00 | 1.43E-24 | 0.00 | 3.48E-19 | 0.00 | 1.08E-14 | 0.00 | 1.06E-13 | 0.00 | 2.21E-17 | 0.00 | 8.46E-39 | 0.00 | 1.30E-32 | 0.00 | 1.55E-42 | 0.00 | 7.98E-37 | 0.00 | 8.59E-33 | 0.00 |
| | 10.00 | | | | 4.74E-25 | 0.00 | 2.41E-26 | 0.00 | 1.08E-20 | 0.00 | 5.58E-16 | 0.00 | 1.04E-14 | 0.00 | 4.37E-18 | 0.00 | 6.09E-42 | 0.00 | 1.37E-35 | 0.00 | 6.73E-47 | 0.00 | 7.08E-41 | 0.00 | 2.41E-36 | 0.00 |

122
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TITLE Test Example, Speciation of Neptunium, 1e-6 molal Np

SOLUTION 1
        -units  mmol/kgw
        pH      2.0
        Np(+5)  0.001 as NpO2
        Na      100.    charge
        N(+5)   100.   as NO3
```
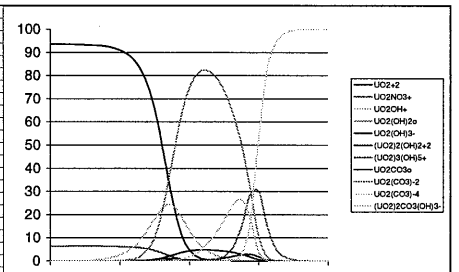

| (UO2)4(OH)7+_m | (UO2)4(OH)7+_% | UO2CO3_m | UO2CO3_% | UO2(CO3)2-2_m | UO2(CO3)2-2_% | UO2(CO3)3-4_m | UO2(CO3)3-4_% | (UO2)3(CO3)6-6_m | (UO2)3(CO3)6-6_% | (UO2)11(CO3)6(OH | (UO2)11(CO3)6(OH | (UO2)2CO3(OH)3-_ | (UO2)2CO3(OH)3-_% | Total_m | Total_% |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1.71E-34 | 0.00 | 8.89E-15 | 0.00 | 4.47E-25 | 0.00 | 8.38E-37 | 0.00 | 3.64E-68 | 0.00 | 1.00E-100 | 0.00 | 3.90E-26 | 0.00 | 1.00E-06 | 100.06 |
| 9.87E-33 | 0.00 | 2.83E-14 | 0.00 | 4.47E-24 | 0.00 | 2.58E-35 | 0.00 | 3.45E-65 | 0.00 | 1.00E-100 | 0.00 | 7.04E-25 | 0.00 | 1.00E-06 | 100.02 |
| 5.64E-31 | 0.00 | 9.00E-14 | 0.00 | 4.47E-23 | 0.00 | 8.03E-34 | 0.00 | 3.34E-62 | 0.00 | 1.00E-100 | 0.00 | 1.26E-23 | 0.00 | 1.00E-06 | 99.99 |
| 3.19E-29 | 0.00 | 2.85E-13 | 0.00 | 4.46E-22 | 0.00 | 2.52E-32 | 0.00 | 3.28E-59 | 0.00 | 3.03E-99 | 0.00 | 2.25E-22 | 0.00 | 1.00E-06 | 99.96 |
| 1.80E-27 | 0.00 | 9.03E-13 | 0.00 | 4.46E-21 | 0.00 | 7.91E-31 | 0.00 | 3.23E-56 | 0.00 | 3.03E-93 | 0.00 | 4.00E-21 | 0.00 | 1.00E-06 | 99.99 |
| 1.01E-25 | 0.00 | 2.85E-12 | 0.00 | 4.45E-20 | 0.00 | 2.49E-29 | 0.00 | 3.20E-53 | 0.00 | 2.98E-87 | 0.00 | 7.09E-20 | 0.00 | 1.00E-06 | 99.99 |
| 5.58E-24 | 0.00 | 8.99E-12 | 0.00 | 4.43E-19 | 0.00 | 7.83E-28 | 0.00 | 3.15E-50 | 0.00 | 2.87E-81 | 0.00 | 1.25E-18 | 0.00 | 1.00E-06 | 100.05 |
| 3.05E-22 | 0.00 | 2.82E-11 | 0.00 | 4.40E-18 | 0.00 | 2.46E-26 | 0.00 | 3.08E-47 | 0.00 | 2.67E-75 | 0.00 | 2.20E-17 | 0.00 | 1.00E-06 | 99.99 |
| 1.63E-20 | 0.00 | 8.81E-11 | 0.01 | 4.34E-17 | 0.00 | 7.67E-25 | 0.00 | 2.96E-44 | 0.00 | 2.32E-69 | 0.00 | 3.81E-16 | 0.00 | 9.99E-07 | 99.96 |
| 8.34E-19 | 0.00 | 2.72E-10 | 0.03 | 4.24E-16 | 0.00 | 2.37E-23 | 0.00 | 2.76E-41 | 0.00 | 1.79E-63 | 0.00 | 6.46E-15 | 0.00 | 1.00E-06 | 100.00 |
| 3.91E-17 | 0.00 | 8.22E-10 | 0.08 | 4.05E-15 | 0.00 | 7.15E-22 | 0.00 | 2.40E-38 | 0.00 | 1.08E-57 | 0.00 | 1.05E-13 | 0.00 | 9.99E-07 | 99.99 |
| 1.53E-15 | 0.00 | 2.37E-09 | 0.24 | 3.70E-14 | 0.00 | 2.06E-20 | 0.00 | 1.83E-35 | 0.00 | 3.99E-52 | 0.00 | 1.56E-12 | 0.00 | 9.98E-07 | 100.00 |
| 4.19E-14 | 0.00 | 6.28E-09 | 0.63 | 3.09E-13 | 0.00 | 5.45E-19 | 0.00 | 1.07E-32 | 0.00 | 5.54E-47 | 0.00 | 1.93E-11 | 0.00 | 9.96E-07 | 99.92 |
| 6.09E-13 | 0.00 | 1.41E-08 | 1.41 | 2.20E-12 | 0.00 | 1.23E-17 | 0.00 | 3.87E-30 | 0.00 | 1.34E-42 | 0.00 | 1.75E-10 | 0.04 | 9.93E-07 | 99.85 |
| 3.59E-12 | 0.00 | 2.54E-08 | 2.54 | 1.25E-11 | 0.00 | 2.21E-16 | 0.00 | 7.11E-28 | 0.00 | 2.70E-39 | 0.00 | 1.00E-09 | 0.20 | 9.92E-07 | 100.10 |
| 8.39E-12 | 0.00 | 3.63E-08 | 3.63 | 5.66E-11 | 0.01 | 3.16E-15 | 0.00 | 6.53E-26 | 0.00 | 4.25E-37 | 0.00 | 3.64E-09 | 0.73 | 9.90E-07 | 100.02 |
| 9.76E-12 | 0.00 | 4.36E-08 | 4.36 | 2.15E-10 | 0.02 | 3.79E-14 | 0.00 | 3.58E-24 | 0.00 | 1.01E-35 | 0.00 | 9.32E-09 | 1.86 | 9.86E-07 | 99.94 |
| 7.48E-12 | 0.00 | 4.71E-08 | 4.71 | 7.34E-10 | 0.07 | 4.09E-13 | 0.00 | 1.43E-22 | 0.00 | 7.46E-35 | 0.00 | 1.93E-08 | 3.86 | 9.78E-07 | 100.02 |
| 4.44E-12 | 0.00 | 4.77E-08 | 4.77 | 2.35E-09 | 0.24 | 4.15E-12 | 0.00 | 4.70E-21 | 0.00 | 2.73E-34 | 0.00 | 3.53E-08 | 7.06 | 9.64E-07 | 100.02 |
| 2.18E-12 | 0.00 | 4.61E-08 | 4.61 | 7.19E-09 | 0.72 | 4.01E-11 | 0.00 | 1.34E-19 | 0.00 | 5.93E-34 | 0.00 | 5.87E-08 | 11.74 | 9.41E-07 | 100.01 |
| 8.85E-13 | 0.00 | 4.25E-08 | 4.25 | 2.10E-08 | 2.10 | 3.70E-10 | 0.04 | 3.32E-18 | 0.00 | 7.68E-34 | 0.00 | 8.87E-08 | 17.74 | 9.11E-07 | 99.99 |
| 2.85E-13 | 0.00 | 3.70E-08 | 3.70 | 5.77E-08 | 5.77 | 3.22E-09 | 0.32 | 6.93E-17 | 0.00 | 5.26E-34 | 0.00 | 1.19E-07 | 23.80 | 8.80E-07 | 99.92 |
| 6.31E-14 | 0.00 | 2.93E-08 | 2.93 | 1.44E-07 | 14.40 | 2.55E-08 | 2.55 | 1.09E-15 | 0.00 | 1.28E-34 | 0.00 | 1.33E-07 | 26.60 | 8.66E-07 | 99.90 |
| 5.51E-15 | 0.00 | 1.84E-08 | 1.84 | 2.87E-07 | 28.70 | 1.60E-07 | 16.00 | 8.55E-15 | 0.00 | 2.41E-36 | 0.00 | 9.34E-08 | 18.68 | 9.06E-07 | 99.97 |
| 3.77E-17 | 0.00 | 6.11E-09 | 0.61 | 3.01E-07 | 30.10 | 5.33E-07 | 53.30 | 9.93E-15 | 0.00 | 4.12E-41 | 0.00 | 1.83E-08 | 3.66 | 9.81E-07 | 99.93 |
| 1.22E-20 | 0.00 | 9.46E-10 | 0.09 | 1.48E-07 | 14.80 | 8.29E-07 | 82.90 | 1.18E-15 | 0.00 | 1.61E-49 | 0.00 | 7.82E-10 | 0.16 | 1.00E-06 | 100.06 |
| 1.13E-24 | 0.00 | 1.07E-10 | 0.01 | 5.30E-08 | 5.30 | 9.44E-07 | 94.40 | 5.48E-17 | 0.00 | 2.01E-59 | 0.00 | 1.78E-11 | 0.00 | 1.00E-06 | 100.00 |
| 7.10E-29 | 0.00 | 1.10E-11 | 0.00 | 1.73E-08 | 1.73 | 9.82E-07 | 98.20 | 1.93E-18 | 0.00 | 8.62E-70 | 0.00 | 3.35E-13 | 0.00 | 1.00E-06 | 99.97 |
| 3.79E-33 | 0.00 | 1.09E-12 | 0.00 | 5.43E-09 | 0.54 | 9.95E-07 | 99.50 | 6.22E-20 | 0.00 | 2.36E-80 | 0.00 | 5.81E-15 | 0.00 | 1.00E-06 | 100.05 |
| 1.71E-37 | 0.00 | 1.03E-13 | 0.00 | 1.65E-09 | 0.17 | 9.98E-07 | 99.80 | 1.90E-21 | 0.00 | 4.12E-91 | 0.00 | 9.29E-17 | 0.00 | 1.00E-06 | 99.97 |
| 5.52E-42 | 0.00 | 8.88E-15 | 0.00 | 4.69E-10 | 0.05 | 1.00E-06 | 100.00 | 5.43E-23 | 0.00 | 1.00E-100 | 0.00 | 1.26E-18 | 0.00 | 1.00E-06 | 100.05 |
| 8.10E-47 | 0.00 | 6.26E-16 | 0.00 | 1.15E-10 | 0.01 | 1.00E-06 | 100.00 | 1.33E-24 | 0.00 | 1.00E-100 | 0.00 | 1.15E-20 | 0.00 | 1.00E-06 | 100.01 |
| 3.83E-52 | 0.00 | 3.24E-17 | 0.00 | 2.27E-11 | 0.00 | 1.00E-06 | 100.00 | 2.63E-26 | 0.00 | 1.00E-100 | 0.00 | 6.07E-23 | 0.00 | 1.00E-06 | 100.00 |




DRJ

```
TITLE Test Example, Speciation of Neptunium, 1e-6 molal NpO2+,PCO2=1e-3.5

SOLUTION 1
        -units  mmol/kgw
        pH      2.0
        Np(+5)  0.001 as NpO2
        Na      100.    charge
        N(+5)   100.  as NO3
# Model definitions
PHASES 1 # Do not change this number it is used by the program!
        Fix_H+
        H+ = H+
        log_k  0.0
END
#
#  NpO2+ = 1e-6
#
SELECTED_OUTPUT
        -file npco2.123
        -molalities     NpO2+ NpO2NO3 NpO2(NO3)2- NpO2OH NpO2CO3- NpO2(CO3)2-3 \
                        NpO2(CO3)3-5
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -2.0   NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -2.25  NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -2.50  NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -2.75  NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -3.0   NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -3.25  NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -3.50  NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -3.75  NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -4.00  NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -4.25  NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -4.50  NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -4.75  NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -5.0   NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -5.25  NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -5.5   NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -5.75  NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -6.0   NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -6.25  NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -6.5   NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -6.75  NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -7.0   NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -7.25  NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -7.5   NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -7.75  NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -8.0   NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -8.25  NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -8.50  NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -8.75  NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -9.0   NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -9.25  NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -9.50  NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -9.75  NaOH    10.0
        CO2(g)   -3.5   1.0
END
USE solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -10.0  NaOH    10.0
        CO2(g)   -3.5   1.0
END
```

Np(V) = 1e-6 m

$P_{CO_2}$ = 1e-3.5 atm

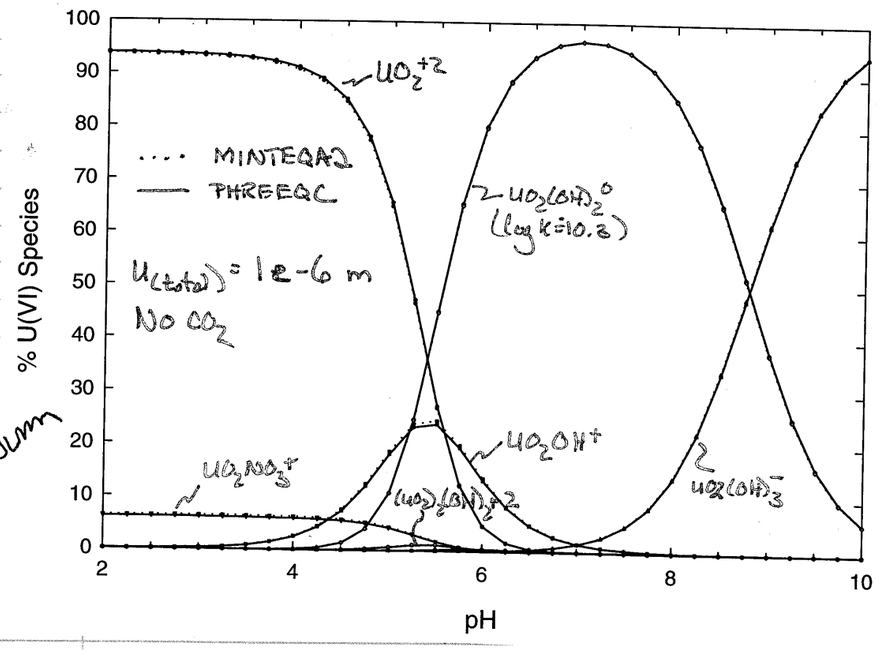
0.1 m $NaNO_3$

PHREEQC Input File

4/13/99

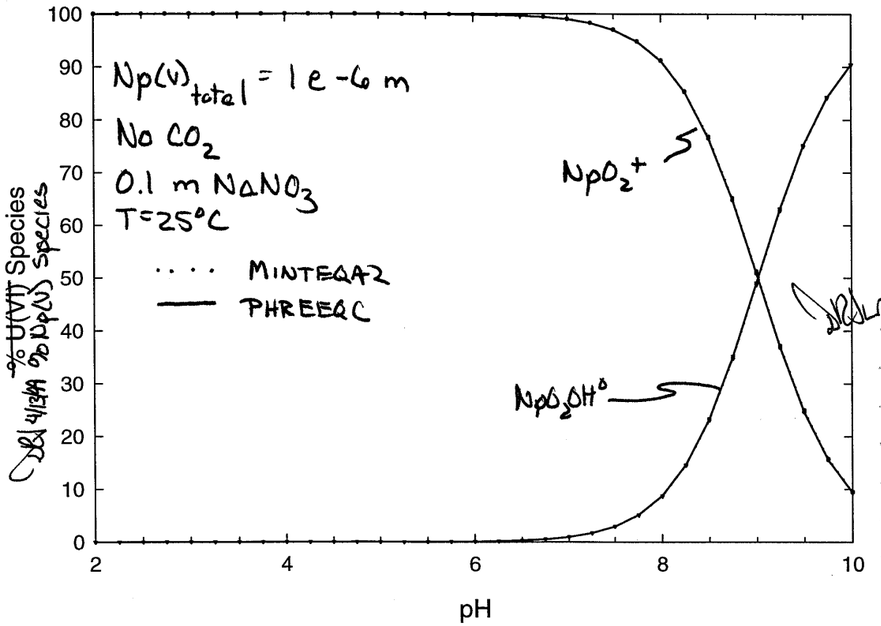
DLH

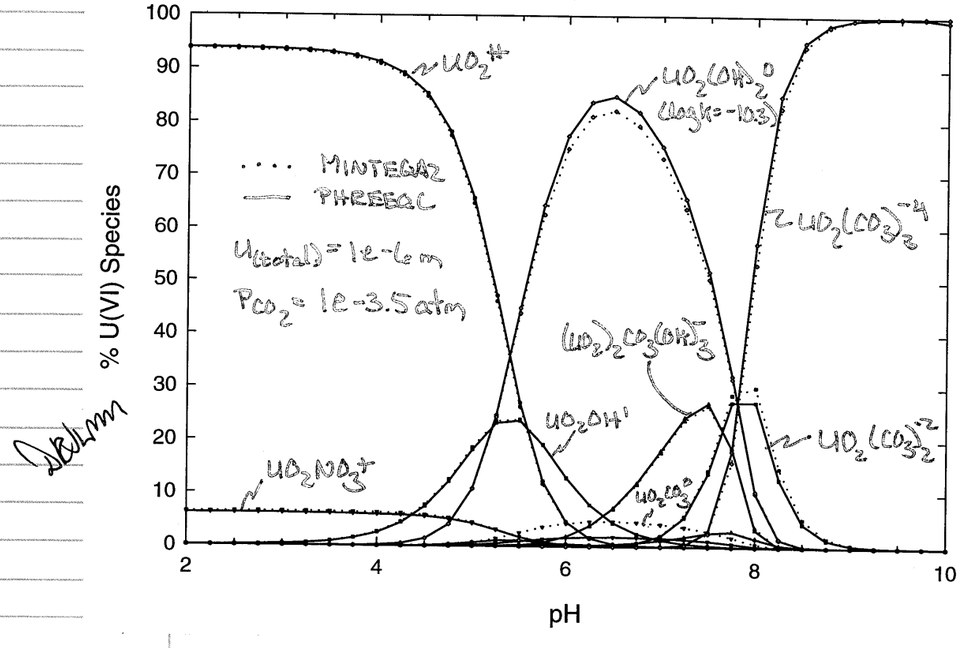
4/13/99 DRL

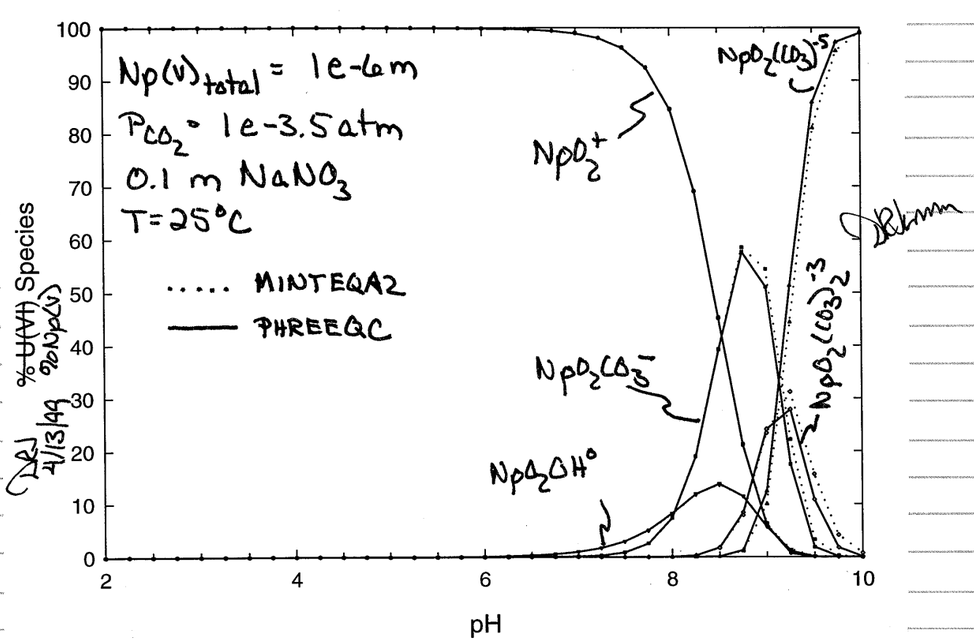





4/13/99 DRL



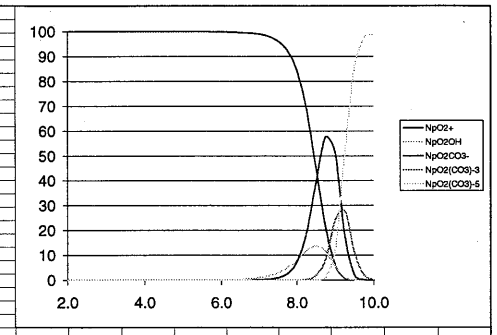



4/13/99
DRL

DRLumm

PHREEQC results
0.1 m NaHCO3
Np(V) = 1e-6 m
$P_{CO_2}$ = 1e-3.5 atm

| Np(total) | ph | pe | ionic_strength | H2O | NpO2+_m | NpO2+_% | NpO2OH_m | NpO2OH_% | NpO2CO3-_m | NpO2CO3-_% | NpO2(CO3)2-3_m | NpO2(CO3)2-3_% | NpO2(CO3)3-5_m | NpO2(CO3)3-5_% | Total_m | Total_% |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1.00E-06 | 2.00 | 16.393642 | 0.1 | 1 | 1.00E-06 | 99.99 | 9.65E-14 | 0.00 | 8.68E-20 | 0.00 | 3.87E-34 | 0.00 | 0.00E+00 | 0.00 | 1.00E-06 | 99.99 |
| | 2.25 | 16.145592 | 0.09999 | 1.000095 | 1.00E-06 | 99.99 | 1.72E-13 | 0.00 | 2.74E-19 | 0.00 | 3.87E-33 | 0.00 | 0.00E+00 | 0.00 | 1.00E-06 | 99.99 |
| | 2.50 | 15.896584 | 0.099985 | 1.000149 | 1.00E-06 | 99.98 | 3.05E-13 | 0.00 | 8.68E-19 | 0.00 | 3.87E-32 | 0.00 | 0.00E+00 | 0.00 | 1.00E-06 | 99.98 |
| | 2.75 | 15.647501 | 0.099982 | 1.000179 | 1.00E-06 | 99.98 | 5.43E-13 | 0.00 | 2.74E-18 | 0.00 | 3.87E-31 | 0.00 | 0.00E+00 | 0.00 | 1.00E-06 | 99.98 |
| | 3.00 | 15.397523 | 0.09998 | 1.000196 | 1.00E-06 | 99.98 | 9.65E-13 | 0.00 | 8.68E-18 | 0.00 | 3.87E-30 | 0.00 | 0.00E+00 | 0.00 | 1.00E-06 | 99.98 |
| | 3.25 | 15.147801 | 0.099979 | 1.000206 | 1.00E-06 | 99.98 | 1.72E-12 | 0.00 | 2.74E-17 | 0.00 | 3.87E-29 | 0.00 | 0.00E+00 | 0.00 | 1.00E-06 | 99.98 |
| | 3.50 | 14.897953 | 0.099979 | 1.000211 | 1.00E-06 | 99.98 | 3.05E-12 | 0.00 | 8.68E-17 | 0.00 | 3.87E-28 | 0.00 | 1.76E-39 | 0.00 | 1.00E-06 | 99.98 |
| | 3.75 | 14.647963 | 0.099979 | 1.000214 | 1.00E-06 | 99.98 | 5.43E-12 | 0.00 | 2.74E-16 | 0.00 | 3.87E-27 | 0.00 | 5.58E-38 | 0.00 | 1.00E-06 | 99.98 |
| | 4.00 | 14.399272 | 0.099978 | 1.000216 | 1.00E-06 | 99.98 | 9.65E-12 | 0.00 | 8.68E-16 | 0.00 | 3.87E-26 | 0.00 | 1.76E-36 | 0.00 | 1.00E-06 | 99.98 |
| | 4.25 | 14.152464 | 0.099978 | 1.000217 | 1.00E-06 | 99.98 | 1.72E-11 | 0.00 | 2.74E-15 | 0.00 | 3.87E-25 | 0.00 | 5.58E-35 | 0.00 | 1.00E-06 | 99.98 |
| | 4.50 | 13.897925 | 0.099978 | 1.000217 | 1.00E-06 | 99.98 | 3.05E-11 | 0.00 | 8.68E-15 | 0.00 | 3.87E-24 | 0.00 | 1.76E-33 | 0.00 | 1.00E-06 | 99.98 |
| | 4.75 | 13.513957 | 0.099979 | 1.000218 | 1.00E-06 | 99.97 | 5.43E-11 | 0.01 | 2.74E-14 | 0.00 | 3.87E-23 | 0.00 | 5.58E-32 | 0.00 | 1.00E-06 | 99.98 |
| | 5.00 | 13.385178 | 0.099979 | 1.000218 | 1.00E-06 | 99.97 | 9.65E-11 | 0.01 | 8.68E-14 | 0.00 | 3.87E-22 | 0.00 | 1.76E-30 | 0.00 | 1.00E-06 | 99.98 |
| | 5.25 | 13.110218 | 0.099979 | 1.000218 | 1.00E-06 | 99.96 | 1.72E-10 | 0.02 | 2.74E-13 | 0.00 | 3.87E-21 | 0.00 | 5.58E-29 | 0.00 | 1.00E-06 | 99.98 |
| | 5.50 | 12.834621 | 0.09998 | 1.000218 | 9.99E-07 | 99.95 | 3.05E-10 | 0.03 | 8.68E-13 | 0.00 | 3.86E-20 | 0.00 | 1.76E-27 | 0.00 | 1.00E-06 | 99.98 |
| | 5.75 | 12.524259 | 0.099982 | 1.000218 | 9.99E-07 | 99.92 | 5.42E-10 | 0.05 | 2.74E-12 | 0.00 | 3.86E-19 | 0.00 | 5.57E-26 | 0.00 | 1.00E-06 | 99.98 |
| | 6.00 | 12.386202 | 0.099984 | 1.000218 | 9.99E-07 | 99.88 | 9.64E-10 | 0.10 | 8.67E-12 | 0.00 | 3.86E-18 | 0.00 | 1.76E-24 | 0.00 | 1.00E-06 | 99.98 |
| | 6.25 | 12.106396 | 0.099989 | 1.000218 | 9.98E-07 | 99.80 | 1.71E-09 | 0.17 | 2.74E-11 | 0.00 | 3.86E-17 | 0.00 | 5.57E-23 | 0.00 | 1.00E-06 | 99.98 |
| | 6.50 | 11.767377 | 0.099997 | 1.000218 | 9.97E-07 | 99.67 | 3.04E-09 | 0.30 | 8.65E-11 | 0.01 | 3.85E-16 | 0.00 | 1.76E-21 | 0.00 | 1.00E-06 | 99.98 |
| | 6.75 | 11.649644 | 0.100012 | 1.000218 | 9.94E-07 | 99.41 | 5.40E-09 | 0.54 | 2.73E-10 | 0.03 | 3.85E-15 | 0.00 | 5.55E-20 | 0.00 | 1.00E-06 | 99.98 |
| | 7.00 | 11.393544 | 0.100038 | 1.000218 | 9.89E-07 | 98.94 | 9.55E-09 | 0.96 | 8.59E-10 | 0.09 | 3.83E-14 | 0.00 | 1.75E-18 | 0.00 | 1.00E-06 | 99.98 |
| | 7.25 | 11.1383 | 0.100084 | 1.000218 | 9.80E-07 | 98.03 | 1.68E-08 | 1.68 | 2.69E-09 | 0.27 | 3.79E-13 | 0.00 | 5.48E-17 | 0.00 | 1.00E-06 | 99.98 |
| | 7.50 | 10.899594 | 0.100168 | 1.000218 | 9.62E-07 | 96.21 | 2.94E-08 | 2.94 | 8.35E-09 | 0.84 | 3.73E-12 | 0.00 | 1.70E-15 | 0.00 | 1.00E-06 | 99.98 |
| | 7.75 | 10.650611 | 0.100318 | 1.000218 | 9.24E-07 | 92.42 | 5.02E-08 | 5.02 | 2.54E-08 | 2.54 | 3.58E-11 | 0.00 | 5.19E-14 | 0.00 | 1.00E-06 | 99.98 |
| | 8.00 | 10.397812 | 0.100592 | 1.000218 | 8.45E-07 | 84.46 | 8.15E-08 | 8.15 | 7.33E-08 | 7.33 | 3.28E-10 | 0.03 | 1.51E-12 | 0.00 | 1.00E-06 | 99.98 |
| | 8.25 | 10.144723 | 0.101098 | 1.000219 | 6.89E-07 | 68.95 | 1.18E-07 | 11.82 | 1.89E-07 | 18.93 | 2.69E-09 | 0.27 | 3.94E-11 | 0.00 | 1.00E-06 | 99.97 |
| | 8.50 | 9.858539 | 0.102065 | 1.00022 | 4.51E-07 | 45.14 | 1.38E-07 | 13.75 | 3.92E-07 | 39.18 | 1.77E-08 | 1.77 | 8.33E-10 | 0.08 | 9.99E-07 | 99.92 |
| | 8.75 | 9.41726 | 0.103991 | 1.000224 | 2.10E-07 | 21.01 | 1.14E-07 | 11.38 | 5.76E-07 | 57.65 | 8.36E-08 | 8.36 | 1.28E-08 | 1.28 | 9.97E-07 | 99.66 |
| | 9.00 | 8.932342 | 0.108098 | 1.000236 | 5.88E-08 | 5.88 | 5.64E-08 | 5.64 | 5.10E-07 | 51.04 | 2.41E-07 | 24.09 | 1.23E-07 | 12.35 | 9.90E-07 | 98.99 |
| | 9.25 | 8.56942 | 0.117731 | 1.000278 | 6.37E-09 | 0.64 | 1.08E-08 | 1.08 | 1.75E-07 | 17.47 | 2.78E-07 | 27.83 | 5.13E-07 | 51.32 | 9.83E-07 | 98.33 |
| | 9.50 | 8.352124 | 0.143635 | 1.000431 | 2.12E-10 | 0.02 | 6.25E-10 | 0.06 | 1.84E-08 | 1.84 | 1.08E-07 | 10.80 | 8.58E-07 | 85.83 | 9.86E-07 | 98.56 |
| | 9.75 | 8.226519 | 0.231582 | 1.001115 | 2.36E-12 | 0.00 | 1.17E-11 | 0.00 | 6.45E-10 | 0.06 | 1.77E-08 | 1.77 | 9.73E-07 | 97.29 | 9.91E-07 | 99.12 |
| | 10.00 | 8.193827 | 0.766221 | 1.007189 | 3.35E-15 | 0.00 | 2.56E-14 | 0.00 | 2.86E-12 | 0.00 | 7.02E-10 | 0.07 | 9.90E-07 | 99.00 | 9.91E-07 | 99.07 |

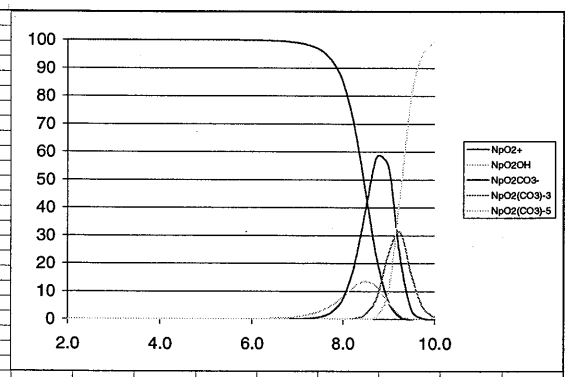



MINTEQA2 Results

0.1 m $NaHCO_3$
Np(V) = 1e-6 m
$P_{CO_2}$ = 1e-3.5 atm

DRLumm

| Np(total) | ph | NpO2+_m | NpO2+_% | NpO2OH_m | NpO2OH_% | NpO2CO3-_m | NpO2CO3-_% | NpO2(CO3)2-3_m | NpO2(CO3)2-3_% | NpO2(CO3)3-5_m | NpO2(CO3)3-5_% | Total_m | Total_% |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1.00E-06 | 2.00 | 1.00E-06 | 100.00 | 9.44E-14 | 0.00 | 8.68E-20 | 0.00 | 3.78E-34 | 0.00 | 1.65E-48 | 0.00 | 1.00E-06 | 100.00 |
| | 2.25 | 1.00E-06 | 100.00 | 1.68E-13 | 0.00 | 2.74E-19 | 0.00 | 3.72E-33 | 0.00 | 4.97E-47 | 0.00 | 1.00E-06 | 100.00 |
| | 2.50 | 1.00E-06 | 100.00 | 3.00E-13 | 0.00 | 8.68E-19 | 0.00 | 3.68E-32 | 0.00 | 1.53E-45 | 0.00 | 1.00E-06 | 100.00 |
| | 2.75 | 1.00E-06 | 100.00 | 5.34E-13 | 0.00 | 2.74E-18 | 0.00 | 3.66E-31 | 0.00 | 4.74E-44 | 0.00 | 1.00E-06 | 100.00 |
| | 3.00 | 1.00E-06 | 100.00 | 9.50E-13 | 0.00 | 8.68E-18 | 0.00 | 3.65E-30 | 0.00 | 1.49E-42 | 0.00 | 1.00E-06 | 100.00 |
| | 3.25 | 1.00E-06 | 100.00 | 1.69E-12 | 0.00 | 2.74E-17 | 0.00 | 3.64E-29 | 0.00 | 4.67E-41 | 0.00 | 1.00E-06 | 100.00 |
| | 3.50 | 1.00E-06 | 100.00 | 3.01E-12 | 0.00 | 8.68E-17 | 0.00 | 3.64E-28 | 0.00 | 1.47E-39 | 0.00 | 1.00E-06 | 100.00 |
| | 3.75 | 1.00E-06 | 100.00 | 5.34E-12 | 0.00 | 2.74E-16 | 0.00 | 3.64E-27 | 0.00 | 4.65E-38 | 0.00 | 1.00E-06 | 100.00 |
| | 4.00 | 1.00E-06 | 100.00 | 9.50E-12 | 0.00 | 8.68E-16 | 0.00 | 3.64E-26 | 0.00 | 1.47E-36 | 0.00 | 1.00E-06 | 100.00 |
| | 4.25 | 1.00E-06 | 100.00 | 1.69E-11 | 0.00 | 2.74E-15 | 0.00 | 3.64E-25 | 0.00 | 4.64E-35 | 0.00 | 1.00E-06 | 100.00 |
| | 4.50 | 1.00E-06 | 100.00 | 3.01E-11 | 0.00 | 8.68E-15 | 0.00 | 3.64E-24 | 0.00 | 1.47E-33 | 0.00 | 1.00E-06 | 100.00 |
| | 4.75 | 1.00E-06 | 100.00 | 5.35E-11 | 0.01 | 2.74E-14 | 0.00 | 3.64E-23 | 0.00 | 4.64E-32 | 0.00 | 1.00E-06 | 100.01 |
| | 5.00 | 1.00E-06 | 100.00 | 9.50E-11 | 0.01 | 8.68E-14 | 0.00 | 3.64E-22 | 0.00 | 1.47E-30 | 0.00 | 1.00E-06 | 100.01 |
| | 5.25 | 1.00E-06 | 100.00 | 1.69E-10 | 0.02 | 2.74E-13 | 0.00 | 3.64E-21 | 0.00 | 4.64E-29 | 0.00 | 1.00E-06 | 100.02 |
| | 5.50 | 1.00E-06 | 100.00 | 3.00E-10 | 0.03 | 8.68E-13 | 0.00 | 3.64E-20 | 0.00 | 1.47E-27 | 0.00 | 1.00E-06 | 100.03 |
| | 5.75 | 9.99E-07 | 99.90 | 5.34E-10 | 0.05 | 2.74E-12 | 0.00 | 3.63E-19 | 0.00 | 4.64E-26 | 0.00 | 1.00E-06 | 99.95 |
| | 6.00 | 9.99E-07 | 99.90 | 9.50E-10 | 0.10 | 8.67E-12 | 0.00 | 3.63E-18 | 0.00 | 1.47E-24 | 0.00 | 1.00E-06 | 100.00 |
| | 6.25 | 9.98E-07 | 99.80 | 1.69E-09 | 0.17 | 2.74E-11 | 0.00 | 3.63E-17 | 0.00 | 4.63E-23 | 0.00 | 1.00E-06 | 99.97 |
| | 6.50 | 9.97E-07 | 99.70 | 3.00E-09 | 0.30 | 8.65E-11 | 0.01 | 3.63E-16 | 0.00 | 1.46E-21 | 0.00 | 1.00E-06 | 100.01 |
| | 6.75 | 9.94E-07 | 99.40 | 5.32E-09 | 0.53 | 2.73E-10 | 0.03 | 3.62E-15 | 0.00 | 4.62E-20 | 0.00 | 1.00E-06 | 99.96 |
| | 7.00 | 9.90E-07 | 99.00 | 9.41E-09 | 0.94 | 8.59E-10 | 0.09 | 3.60E-14 | 0.00 | 1.45E-18 | 0.00 | 1.00E-06 | 100.03 |
| | 7.25 | 9.81E-07 | 98.10 | 1.66E-08 | 1.66 | 2.69E-09 | 0.27 | 3.57E-13 | 0.00 | 4.56E-17 | 0.00 | 1.00E-06 | 100.03 |
| | 7.50 | 9.63E-07 | 96.30 | 2.89E-08 | 2.89 | 8.36E-09 | 0.84 | 3.50E-12 | 0.00 | 1.42E-15 | 0.00 | 1.00E-06 | 100.03 |
| | 7.75 | 9.25E-07 | 92.50 | 4.94E-08 | 4.94 | 2.54E-08 | 2.54 | 3.37E-11 | 0.00 | 4.31E-14 | 0.00 | 1.00E-06 | 99.98 |
| | 8.00 | 8.46E-07 | 84.60 | 8.04E-08 | 8.04 | 7.34E-08 | 7.34 | 3.08E-10 | 0.03 | 1.25E-12 | 0.00 | 1.00E-06 | 100.01 |
| | 8.25 | 6.91E-07 | 69.10 | 1.17E-07 | 11.70 | 1.90E-07 | 19.00 | 2.52E-09 | 0.25 | 3.24E-11 | 0.00 | 1.00E-06 | 100.06 |
| | 8.50 | 4.53E-07 | 45.30 | 1.36E-07 | 13.60 | 3.93E-07 | 39.30 | 1.66E-08 | 1.66 | 6.78E-10 | 0.07 | 9.99E-07 | 99.93 |
| | 8.75 | 2.13E-07 | 21.30 | 1.14E-07 | 11.40 | 5.85E-07 | 58.50 | 7.85E-08 | 7.85 | 1.03E-08 | 1.03 | 1.00E-06 | 100.08 |
| | 9.00 | 6.27E-08 | 6.27 | 5.94E-08 | 5.94 | 5.44E-07 | 54.40 | 2.34E-07 | 23.40 | 9.95E-08 | 9.95 | 1.00E-06 | 99.96 |
| | 9.25 | 8.11E-09 | 0.81 | 1.36E-08 | 1.36 | 2.22E-07 | 22.20 | 3.12E-07 | 31.20 | 4.44E-07 | 44.40 | 1.00E-06 | 99.97 |
| | 9.50 | 3.77E-10 | 0.04 | 1.11E-09 | 0.11 | 3.28E-08 | 3.28 | 1.56E-07 | 15.60 | 8.10E-07 | 81.00 | 1.00E-06 | 100.03 |
| | 9.75 | 8.44E-12 | 0.00 | 4.29E-11 | 0.00 | 2.32E-09 | 0.23 | 4.13E-08 | 4.13 | 9.56E-07 | 95.60 | 1.00E-06 | 99.97 |
| | 10.00 | 1.08E-13 | 0.00 | 9.09E-13 | 0.00 | 9.37E-11 | 0.01 | 7.24E-09 | 0.72 | 9.93E-07 | 99.30 | 1.00E-06 | 100.03 |



4/13/99 RJ



```
SOLUTION_MASTER_SPECIES
##########################################################
#               essential definitions                    #
##########################################################
#
#element species       alk     gfw_formula     element_gfw
#
Alkalinity      CO3-2    1.0    61.0173          61.0173
E               e-       0.0     0.0              0.0
H               H+      -1.0     1.008            1.008
H(0)            H2       0.0     1.008
H(+1)           H+      -1.0     1.008
O               H2O      0.0    16.00            16.00
O(-2)           H2O      0.0    16.00            16.00
O(0)            O2       0.0    16.00            16.00
##########################################################
Ag              Ag+      0.0   107.868           107.868
Al              Al+3     0.0    26.9815           26.9815
Am              Am+3     0.0   243.0614          243.0614
Am(+3)          Am+3     0.0   243.0614
Am(+4)          Am+4     0.0   243.0614
Am(+5)          AmO2+    0.0   243.0614
Am(+6)          AmO2+2   0.0   243.0614
As              H3AsO4  -1.0    74.9216           74.9216
As(+3)          H3AsO3   0.0    74.9216
As(+5)          H3AsO4  -1.0    74.9216
B               H3BO3    0.0    10.81             10.81
Ba              Ba+2     0.0   137.34            137.34
Be              Be+2     0.0     9.0122            9.0122
Br              Br-      0.0    79.904            79.904
C               CO3-2    2.0    61.0173           12.011
C(+4)           CO3-2    2.0    61.0173
#C(-4)           CH4     0.0    16.042
Ca              Ca+2     0.0    40.08             40.08
Cd              Cd+2     0.0   112.399           112.399
Cl              Cl-      0.0    35.453            35.453
Co              Co+2     0.0    58.9332           58.9332
Co(+2)          Co+2     0.0    58.9332
Co(+3)          Co+3     0.0    58.9332
Cr              CrO4-2   0.0    51.996            51.996
Cr(+2)          Cr+2     0.0    51.996
Cr(+3)          Cr(OH)2+ 0.0    51.996
Cr(+6)          CrO4-2   0.0    51.996
Cs              Cs+      0.0   132.9054          132.9054
Cu              Cu+2     0.0    63.546            63.546
Cu(+1)          Cu+      0.0    63.546
Cu(+2)          Cu+2     0.0    63.546
Eu              Eu+3     0.0   151.965           151.965
Eu(+2)          Eu+2     0.0   151.965
Eu(+3)          Eu+3     0.0   151.635
F               F-       0.0    18.9984           18.9984
Fe              Fe+3     0.0    55.847            55.847
Fe(+2)          Fe+2     0.0    55.847
Fe(+3)          Fe+3    -2.0    55.847
Hg              Hg(OH)2  0.0   200.59            200.59
Hg(+2)          Hg(OH)2  0.0   200.59
Hg(+1)          Hg2+2    0.0   200.59
Hg(+0)          Hg       0.0   200.59
I               I-       0.0   126.904           126.904
K               K+       0.0    39.102            39.102
Li              Li+      0.0     6.939             6.939
Mg              Mg+2     0.0    24.312            24.312
Mn              Mn+3     0.0    54.938            54.938
Mn(+2)          Mn+2     0.0    54.938
Mn(+3)          Mn+3     0.0    54.938
Mn(+6)          MnO4-2   0.0    54.938
Mn(+7)          MnO4-    0.0    54.938
N               NO3-     0.0    14.0067           14.0067
#N(0)            N2      0.0    14.0067
N(-3)           NH4+     0.0    14.0067
N(+3)           NO2-     0.0    14.0067
N(+5)           NO3-     0.0    14.0067
Na              Na+      0.0    22.9898           22.9898
Ni              Ni+2     0.0    58.71             58.71
Np              NpO2+    0.0   243.0614          243.0614
Np(+3)          Np+3     0.0   243.0614
Np(+4)          Np+4     0.0   243.0614
Np(+5)          NpO2+    0.0   243.0614
Np(+6)          NpO2+2   0.0   243.0614
P               PO4-3    2.0    30.9738           30.9738
Pb              Pb+2     0.0   207.19            207.19
Pu              Pu+4     0.0   244.0000          244.0000
Pu(+3)          Pu+3     0.0   244.0000
Pu(+4)          Pu+4     0.0   244.0000
Pu(+5)          PuO2+    0.0   244.0000
Pu(+6)          PuO2+2   0.0   244.0000
Ra              Ra+2     0.0   226.025           226.025
Rb              Rb+      0.0    85.4699           85.4699
Ru              RuO4-2   0.0   101.0700          101.0700
Ru(+2)          Ru+2     0.0   101.0700
Ru(+3)          Ru+3     0.0   101.0700
Ru(+4)          Ru(OH)2+2 0.0  101.0700
Ru(+6)          RuO4-2   0.0   101.0700
Ru(+7)          RuO4-    0.0   101.0700
S               SO4-2    0.0    96.0616           32.064
S(-2)           HS-      1.0    32.064
S(+6)           SO4-2    0.0    96.0616
Sb              Sb(OH)6- 6.0   172.772           172.772
Sb(+3)          Sb(OH)3  3.0   172.772
Sb(+5)          Sb(OH)6- 0.0   172.772
Se              SeO4-2   0.0    78.96             78.96
Se(-2)          HSe-     0.0    78.96
Se(+4)          SeO3-2   0.0    78.96
Se(+6)          SeO4-2   0.0    78.96
Si              H4SiO4   0.0    96.1155           28.0843
Sn              Sn+4     0.0   118.710           118.710
Sn(+2)          Sn+2     0.0   118.710
Sn(+4)          Sn+4     0.0   118.710
Sr              Sr+2     0.0    87.62             87.62
Tc              TcO4-    0.0    98.0000           98.0000
Tc(+3)          Tc+3     0.0    98.0000
Tc(+4)          TcO+2    0.0    98.0000
Tc(+5)          TcO4-3   0.0    98.0000
Tc(+6)          TcO4-2   0.0    98.0000
Tc(+7)          TcO4-    0.0    98.0000
Th              Th+4     0.0   232.0381          232.0381
Tl              Tl(OH)3  0.0   204.37            204.37
Tl(+1)          Tl+      0.0   204.37
Tl(+3)          Tl(OH)3  0.0   204.37
U               UO2+2    0.0   238.0290          238.0290
U(+3)           U+3      0.0   238.0290
U(+4)           U+4      0.0   238.0290
U(+5)           UO2+     0.0   238.0290
U(+6)           UO2+2    0.0   238.0290
V               VO2+     0.0    50.94             50.94
V(+2)           V+2      0.0    50.94
V(+3)           V+3      0.0    50.94
V(+4)           VO+2     0.0    50.94
V(+5)           VO2+     0.0    50.94
Zn              Zn+2     0.0    65.37             65.37
Zr              Zr+4     0.0    91.224            91.224
##########################################################
#MINTEQA2 ORGANIC LIGANDS                                 #
##########################################################
Acetate         Acetate-         0     59.05   59.05
Benzoate        Benzoate-        0    121.12  121.12
Butanoate       Butanoate-       0     87.043  87.043
Citrate         Citrate-3        0    189.06  189.06
Cyanide         Cyanide-         0     26.018  26.018
Cyanate         Cyanate-         0     42.017  42.017
Diethylamine    Diethylamine     0     73      73
Dimethylamine   Dimethylamine    0     45.028  45.028
Edta            Edta-4           0    276     276
Ethylenediamine Ethylenediamine  0     60.12   60.12
Formate         Formate-         0     45.02   45.02
Four_methylpyridine Four_methylpyridine 0  94   94
Glutamate       Glutamate-2      0    145.13  145.13
Glycine         Glycine-         0     74.07   74.07
Hexylamine      Hexylamine       0    101     101
Isobutyrate     Isobutyrate-     0     87.043  87.043
Isophthalate    Isophthalate-2   0    164.12  164.12
Isopropylamine  Isopropylamine   0     59.04   59.04
Isovalerate     Isovalerate-     0    101.13  101.13
Methylamine     Methylamine      0     31.018  31.018
Nbutylamine     Nbutylamine      0     73      73
Npropylamine    Npropylamine     0     59.04   59.04
Nta             Nta-3            0    188.06  188.06
Para_acetate    Para_acetate-    0    134.14  134.14
Phthalate       Phthalate-2      0    164.13  164.13
Propanoate      Propanoate-      0     73.032  73.032
Salicylate      Salicylate-2     0    136.12  136.12
Tartrate        Tartrate-2       0    148.09  148.09
Three_methylpyridine Three_methylpyridine 0  94   94
Tributylphosphate Tributylphosphate 0  265.97  265.97
Trimethylamine  Trimethylamine   0     59.04   59.04
Two_methylpyridine Two_methylpyridine 0  94   94
Valerate        Valerate-        0    101.13  101.13

SOLUTION_SPECIES
##########################################################
#               essential definitions                    #
##########################################################
e- = e-
        log_k   0
        delta_h 0       kcal

H+ = H+
        log_k   0
        delta_h 0       kcal
        -gamma  9.0  0.0

H2O = H2O
        log_k   0
        delta_h 0       kcal

2H2O = O2 + 4H+ + 4e-
        log_k   -83.12
        delta_h 133.83  kcal

2H+ + 2e- = H2
        log_k   -3.15
        delta_h -1.759  kcal

CO3-2 = CO3-2
        log_k   0
        delta_h 0       kcal
        -gamma  5.4  0.0

##########################################################
Ag+ = Ag+
        log_k   0
        delta_h 0       kcal

Al+3 = Al+3
        log_k   0
        delta_h 0       kcal
        -gamma  9.0  0.0

Am+3 = Am+3
        log_k   0
        delta_h 0       kcal
        -gamma  5.0  0.0

Am+3 = Am+4 + e-
        log_k   -44.2105
        delta_h 50.359  kcal
        -gamma  5.5  0.0

Am+3 + 2H2O = AmO2+ + 4H+ + 2e-
        log_k   -58.3742
        delta_h 91.802  kcal
        -gamma  4.0  0.0

Am+3 + 2H2O = AmO2+2 + 4H+ + 3e-
        log_k   -85.3545
        delta_h 128.489 kcal
        -gamma  4.5  0.0

H3AsO4 = H3AsO4
        log_k   0
        delta_h 0       kcal

H3AsO4 + 2e- + 2H+ = H3AsO3 + H2O
        log_k   19.444
        delta_h -30.015 kcal

H3BO3 = H3BO3
        log_k   0
        delta_h 0       kcal

Ba+2 = Ba+2
        log_k   0
        delta_h 0       kcal
        -gamma  5.0  0.0

Be+2 = Be+2
        log_k   0
        delta_h 0       kcal

Br- = Br-
        log_k   0
        delta_h 0       kcal
        -gamma  4.0  0.0

Ca+2 = Ca+2
        log_k   0
        delta_h 0       kcal
        -gamma  6.0  .165

Cd+2 = Cd+2
        log_k   0
        delta_h 0       kcal

Cl- = Cl-
        log_k   0
        delta_h 0       kcal
        -gamma  3.0  .015

Co+2 = Co+2
        log_k   0
        delta_h 0       kcal
        -gamma  4.5  0.0

Co+2 = Co+3 + e-
        log_k   -32.9891
        delta_h 35.9    kcal
        -gamma  5.0  0.0

CrO4-2 = CrO4-2
        log_k   0
        delta_h 0       kcal
        -gamma  4.0  0.0

Cr(OH)2+ + 2h+ + e- = Cr+2 + 2H2O
        log_k   2.947
        delta_h 6.36    kcal

CrO4-2 + 6H+ + 3e- = Cr(OH)2+ + 2H2O
        log_k   67.376
        delta_h -103    kcal

Cs+ = Cs+
        log_k   0
        delta_h 0       kcal
        -gamma  4.0  0.0

Cu+2 = Cu+2
        log_k   0
        delta_h 0       kcal
        -gamma  2.5  0.0

Cu+2 + e- = Cu+
        log_k   2.72
        delta_h 1.65    kcal
        -gamma  2.5  0.0

Eu+3 = Eu+3
        log_k   0
        delta_h 0       kcal
        -gamma  5.0  0.0

Eu+3 + e- = Iu+2
        log_k   -6.0069
        delta_h 18.60   kcal
        -gamma  4.5  0.0

F- = F-
        log_k   0
        delta_h 0       kcal
        -gamma  3.5  0.0

Fe+3 = Fe+3
        log_k   0
        delta_h 0       kcal
        -gamma  9.0  0.0

Fe+3 + e- = Ie+2
        log_k   13.032
        delta_h -10     kcal
        -gamma  6.0  0.0

Hg(OH)2 = Hg(OH)2
        log_k   0
        delta_h 0       kcal

2Hg(OH)2 + 4H+ + 2e- = Hg2+2 + 4H2O
        log_k   42.987
        delta_h -63.59  kcal
        -gamma  4.0  0.0

0.5Hg2+2 + e- = Hg
        log_k   6.9316
        delta_h -16.605 kcal

I- = I-
        log_k   0
        delta_h 0       kcal

K+ = K+
        log_k   0
        delta_h 0       kcal
        -gamma  3.0  .015

Li+ = Li+
```

```
        log_k     0
        delta_h   0        kcal
        -gamma    6.0  0.0

Mg+2 = Mg+2
        log_k     0
        delta_h   0        kcal
        -gamma    6.5  .20

Mn+2 + 4H2O = MnO4- + 8H+ + 5e-
        log_k   -127.824
        delta_h  176.62    kcal
        -gamma    3.0   0

Mn+2 + 4H2O = MnO4-2 + 8H+ + 4e-
        log_k   -118.44
        delta_h  150.02    kcal
        -gamma    5.0   0

Mn+3 = Mn+3
        log_k     0
        delta_h   0        kcal
        -gamma    9.0  0.0

Mn+3 + e- = Mn+2
        log_k     25.507
        delta_h   25.76    kcal
        -gamma    6.0  0.0

NO3- = NO3-
        log_k     0
        delta_h   0        kcal
        -gamma    3.0  0.0

NO3- + 2H+ + 2e- = NO2- + H2O
        log_k     28.57
        delta_h  -43.76    kcal

NO3- + 10H+ + 8e- = NH4+ + 3H2O
        log_k    119.077
        delta_h -187.055   kcal
        -gamma    2.5  0.0

Na+ = Na+
        log_k     0
        delta_h   0        kcal
        -gamma    4.0  .075

Ni+2 = Ni+2
        log_k     0
        delta_h   0        kcal

NpO2+ = NpO2+
        log_k     0
        delta_h   0        kcal
        -gamma    4.0  0.0

NpO2+ + 4H+ + 2e- = Np+3 + 2H2O
        log_k     13.40
        delta_h  -28.8424  kcal
        -gamma    5.5  0.0

NpO2+ + 4H+ + e- = Np+4 + 2H2O
        log_k     10.91
        delta_h  -35.7497  kcal
        -gamma    5.5  0.0

NpO2+ = NpO2+2 + e-
        log_k    -20.88
        delta_h   28.1071  kcal
        -gamma    4.5  0.0

PO4-3 = PO4-3
        log_k     0
        delta_h   0        kcal
        -gamma    5.0  0.0

Pb+2 = Pb+2
        log_k     0
        delta_h   0        kcal

Pu+4 = Pu+4
        log_k     0
        delta_h   0        kcal
        -gamma    5.5  0.0

Pu+4 + e- = Pu+3
        log_k     16.9975
        delta_h  -13.303   kcal
        -gamma    5.0  0.0

Pu+4 + 2H2O = PuO2+ + 4H+ + e-
        log_k    -18.6027
        delta_h   46.269   kcal
        -gamma    4.0  0.0

Pu+4 + 2H2O = PuO2+2 + 4H+ + 2e-
        log_k    -34.8819
        delta_h   68.354   kcal
        -gamma    4.5  0.0

Ra+2 = Ra+2
        log_k     0
        delta_h   0        kcal
        -gamma    4.5  0.0

Rb+ = Rb+
        log_k     0
        delta_h   0        kcal

RuO4-2 = RuO4-2
        log_k     0
        delta_h   0        kcal
        -gamma    4.0   0

RuO4-2 + 8H+ + 4e- = Ru+2 + 4H2O
        log_k     86.1793
        delta_h   0        kcal
        -gamma    4.5   0

RuO4-2 + 8H+ + 3e- = Ru+3 + 4H2O
        log_k     82.1286
        delta_h   0        kcal
        -gamma    5.0  0.0

RuO4-2 + 6H+ + 2e- = Ru(OH)2+2 + 2H2O
        log_k     68.2561
        delta_h   0        kcal
        -gamma    4.0  0.0

RuO4-2 = RuO4- + e-
        log_k     9.9022
        delta_h   29.562   kcal
        -gamma    4.0  0.0

SO4-2 = SO4-2
        log_k     0
        delta_h   0        kcal
        -gamma    4.0  -.04

SO4-2 + 9H+ + 8e- = HS- + 4H2O
        log_k     33.66
        delta_h  -60.14    kcal
        -gamma    3.5  0.0

Sb(OH)6- = Sb(OH)6-
        log_k     0
        delta_h   0        kcal

Sb(OH)6- + 2e- + 3H+ = Sb(OH)3 + 3H2O
        log_k     25.7791
        delta_h   0        kcal

SeO4-2 = SeO4-2
        log_k     0
        delta_h   0        kcal
        -gamma    4.0  0.0

HSeO3- + 6e- + 6H+ = HSe- + 3H2O
        log_k     35.38
        delta_h  -78.17    kcal

SeO4-2 + 2e- + 3H+ = HSeO3- + H2O
        log_k     36.319
        delta_h  -48.095   kcal

H4SiO4 = H4SiO4
        log_k     0
        delta_h   0        kcal

Sn+4 = Sn+4
        log_k     0
        delta_h   0        kcal
        -gamma    5.5  0.0

Sn+4 + 2e- = Sn+2
        log_k     5.3072
        delta_h   -9.327   kcal
        -gamma    6.0  0.0

Sr+2 = Sr+2
        log_k     0
        delta_h   0        kcal
        -gamma    5.0  0.0

TcO4- = TcO4-
        log_k     0
        delta_h   0        kcal
        -gamma    4.0   0

TcO4- + 8H+ + 4e- = Tc+3 + 4H2O
        log_k     38.4043
        delta_h   0        kcal
        -gamma    5.0   0

TcO4- + 6H+ + 3e- = TcO+2 + 3H2O
        log_k     33.0078
        delta_h   0        kcal
        -gamma    4.5  0.0

TcO4- + 2e- = TcO4-3
        log_k    -20.2798
        delta_h   0        kcal
        -gamma    4.0  0.0

TcO4- + e- = TcO4-2
        log_k    -10.3151
        delta_h   0        kcal
        -gamma    4.0  0.0

Th+4 = Th+4
        log_k     0
        delta_h   0        kcal
        -gamma    5.5  0.0

Tl(OH)3 = Tl(OH)3
        log_k     0
        delta_h   0        kcal

Tl(OH)3 + 2e- + 3H+ = Tl+ + 3H2O
        log_k     48.0178
        delta_h   0        kcal

UO2+2 = UO2+2
        log_k     0
        delta_h   0        kcal
        -gamma    4.0  0.0

UO2+2 + 3e- + 4H+ = U+3 + 2H2O
        log_k    -0.5316
        delta_h  -9.984    kcal
        -gamma    5.0  0.0

UO2+2 + 2e- + 4H+ = U+4 + 2H2O
        log_k     9.0644
        delta_h  -34.384   kcal
        -gamma    5.5  0.0

UO2+2 + e- = UO2+
        log_k     1.4883
        delta_h   -1.43    kcal
        -gamma    4.0  0.0

VO2+ = VO2+
        log_k     0
        delta_h   0        kcal

VO2+ + e- + 2H+ = VO+2 + H2O
        log_k     16.93
        delta_h   -29.32   kcal

VO2+ + 2e- + 4H+ = V+3 + 2H2O
        log_k     22.61
        delta_h   -44.23   kcal

VO2+ + 3e- + 4H+ = V+2 + 2H2O
        log_k     18.38
        delta_h   -35.33   kcal

Zn+2 = Zn+2
        log_k     0
        delta_h   0        kcal
        -gamma    6.0  0.0

Zr+4 = Zr+4
        log_k     0
        delta_h   0        kcal
        -gamma    5.5  0.0

Acetate- = Acetate-
        log_k     0
        delta_h   0        kcal

Benzoate- = Benzoate-
        log_k     0
        delta_h   0        kcal

Butanoate- = Butanoate-
        log_k     0
        delta_h   0        kcal

Citrate-3 = Citrate-3
        log_k     0
        delta_h   0        kcal

Cyanate- = Cyanate-
        log_k     0
        delta_h   0        kcal

Cyanide- = Cyanide-
        log_k     0
        delta_h   0        kcal

Diethylamine = Diethylamine
        log_k     0
        delta_h   0        kcal

Dimethylamine = Dimethylamine
        log_k     0
        delta_h   0        kcal

Edta-4 = Edta-4
        log_k     0
        delta_h   0        kcal

Ethylenediamine = Ethylenediamine
        log_k     0
        delta_h   0        kcal

Formate- = Formate-
        log_k     0
        delta_h   0        kcal

Four_methylpyridine = Four_methylpyridine
        log_k     0
        delta_h   0        kcal

Glutamate-2 = Glutamate-2
        log_k     0
        delta_h   0        kcal

Glycine- = Glycine-
        log_k     0
        delta_h   0        kcal

Hexylamine = Hexylamine
        log_k     0
        delta_h   0        kcal

Isobutyrate- = Isobutyrate-
        log_k     0
        delta_h   0        kcal

Isophthalate-2 = Isophthalate-2
        log_k     0
        delta_h   0        kcal

Isopropylamine = Isopropylamine
        log_k     0
        delta_h   0        kcal

Isovalerate- = Isovalerate-
        log_k     0
        delta_h   0        kcal

Methylamine = Methylamine
        log_k     0
        delta_h   0        kcal

Nbutylamine = Nbutylamine
        log_k     0
        delta_h   0        kcal

Npropylamine = Npropylamine
        log_k     0
        delta_h   0        kcal

Nta-3 = Nta-3
        log_k     0
        delta_h   0        kcal

Para_acetate- = Para_acetate-
        log_k     0
        delta_h   0        kcal

Phthalate-2 = Phthalate-2
        log_k     0
        delta_h   0        kcal

Propanoate- = Propanoate-
        log_k     0
        delta_h   0        kcal

Salicylate-2 = Salicylate-2
        log_k     0
        delta_h   0        kcal

Tartrate-2 = Tartrate-2
        log_k     0
        delta_h   0        kcal

Three_methylpyridine = Three_methylpyridine
        log_k     0
        delta_h   0        kcal

Tributylphosphate = Tributylphosphate
        log_k     0
        delta_h   0        kcal

Trimethylamine = Trimethylamine
        log_k     0
        delta_h   0        kcal

Two_methylpyridine = Two_methylpyridine
        log_k     0
        delta_h   0        kcal

Valerate- = Valerate-
        log_k     0
        delta_h   0        kcal

SOLUTION_SPECIES

H2O = OH- + H+
        log_k    -13.998
        delta_h  13.345  kcal
        -gamma   3.5    0
CO3-2 + H+ = HCO3-
        log_k     10.33
        delta_h   -3.617   kcal
        -gamma    5.4     0
        -analytical -6.498     0.02379     2902.39

CO3-2 + 2H+ = H2CO3
        log_k     16.681
        delta_h   -2.247  kcal

Cr(OH)2+ = CrO2- + 2H+
        log_k    -17.7456
        delta_h   0        kcal

F- + H+ = HF
        log_k     3.169
        delta_h   3.46     kcal

2F- + H+ = HF2-
        log_k     3.749
        delta_h   4.55     kcal
        -gamma    3.5      0

2F- + 2H+ = H2F2
        log_k     6.768
        delta_h   0        kcal

Hg(OH)2 + 2H+ = Hg+2 + 2H2O
        log_k     6.097
        delta_h  -11.06  kcal

PO4-3 + H+ = HPO4-2
        log_k     12.346
        delta_h   -3.53    kcal
        -gamma    5.0      0

PO4-3 + 2H+ = H2PO4-
        log_k     19.553
        delta_h   -4.52    kcal
        -gamma    5.4      0

PO4-3 + 3H+ = H3PO4
        log_k     21.7
        delta_h   0        kcal

HS- + H+ = H2S
        log_k     6.994
        delta_h   -5.3     kcal
        -analytical -11.17     0.02386     3279.0

HS- = S-2 + H+
        log_k    -12.918
        delta_h   12.1     kcal
        -gamma    5.0      0

HS- = S2-2 + H+
        log_k    -14.528
        delta_h   11.4     kcal
        -no_check
        -mass_balance S(-2)2

HS- = S3-2 + H+
        log_k    -13.282
        delta_h   10.4     kcal
        -no_check
        -mass_balance S(-2)3

HS- = S4-2 + H+
        log_k     -9.829
        delta_h    9.7     kcal
        -no_check
        -mass_balance S(-2)4

HS- = S5-2 + H+
        log_k     -9.595
        delta_h    9.3     kcal
        -no_check
        -mass_balance S(-2)5

HS- = S6-2 + H+
        log_k     -9.881
        delta_h    0       kcal
        -no_check
        -mass_balance S(-2)6

SO4-2 + H+ = HSO4-
        log_k     1.987
        delta_h   4.91     kcal
        -gamma    4.5      0
        -analytical -5.3505     0.0183412   557.2461

HSe- = Se-2 + H+
        log_k    -14.9529
        delta_h   11.5     kcal

HSe- + H+ = H2Se
        log_k     3.8115
        delta_h   0.8      kcal

HSeO3- = SeO3-2 + H+
        log_k     -8.48
        delta_h    1.28    kcal

HSeO3- + H+ = H2SeO3
        log_k     2.65
        delta_h   1.69     kcal

SeO4-2 + H+ = HSeO4-
        log_k     1.9058
        delta_h   4.2      kcal

H4SiO4 = H3SiO4- + H+
        log_k     -9.93
        delta_h   8.935    kcal
        -gamma    4.0      0
        -analytical 6.368      -0.016346   -3405.9

H4SiO4 = H2SiO4-2 + 2H+
        log_k    -21.619
        delta_h   29.714   kcal
        -gamma    5.4      0
        -analytical 39.478     -0.065927   -12355.1

H4SiO4 + 6F- + 4H+ = SiF6-2 + 4H2O
        log_k     30.18
        delta_h  -16.26    kcal
        -gamma    5.0      0

Ag+ + Br- = AgBr
        log_k     4.24
        delta_h   0        kcal

Ag+ + 2Br- = AgBr2-
        log_k     7.28
        delta_h   0        kcal

Ag+ + 3Br- = AgBr3-2
        log_k     8.71
        delta_h   0        kcal

Ag+ + Cl- = AgCl
        log_k     3.27
        delta_h   -2.68    kcal

Ag+ + 2Cl- = AgCl2-
        log_k     5.27
        delta_h   -3.93    kcal

Ag+ + 3Cl- = AgCl3-2
        log_k     5.29
        delta_h   0        kcal

Ag+ + 4Cl- = AgCl4-3
        log_k     5.51
        delta_h   0        kcal

Ag+ + F- = AgF
        log_k     0.36
        delta_h   -2.83    kcal

Ag+ + I- = AgI
        log_k     6.6
        delta_h   0        kcal

Ag+ + 2I- = AgI2-
        log_k     10.68
        delta_h   0        kcal

Ag+ + 3I- = AgI3-2
        log_k     13.37
        delta_h   -27.03   kcal

Ag+ + 4I- = AgI4-3
        log_k     14.08
        delta_h   0        kcal

Ag+ + 2NO2- = Ag(NO2)2-
        log_k     2.22
        delta_h   0        kcal

Ag+ + NO3- = AgNO3
        log_k    -0.29
        delta_h   0        kcal
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Ag+ + H2O = AgOH + H+
        log_k    -12.0
        delta_h    0        kcal

Ag+ + 2H2O = Ag(OH)2- + 2H+
        log_k    -24.0
        delta_h    0        kcal

Ag+ + HS- = AgHS
        log_k     14.05
        delta_h    0        kcal

Ag+ + 2HS- = Ag(HS)2-
        log_k     18.45
        delta_h    0        kcal

Ag+ + 2HS- = Ag(S4)2-3 + 2H+
        log_k      0.991
        delta_h    0        kcal
        -gamma    22.0      0
        -no_check
        -mass_balance Ag(S(-2)4)2

Ag+ + 2HS- = AgS4S5-3 + 2H+
        log_k      0.68
        delta_h    0        kcal
        -gamma    24.0      0
        -no_check
        -mass_balance AgS(-2)4S(-2)5

Ag+ + 2HS- = Ag(HS)S4-2 + H+
        log_k     10.431
        delta_h    0        kcal
        -gamma    15.0      0
        -no_check
        -mass_balance Ag(HS(-2))S(-2)4

Ag+ + SO4-2 = AgSO4-
        log_k      1.29
        delta_h    1.49     kcal

Ag+ + 2HSe- + H2O = AgOH(Se)2-4 + 3H+
        log_k    -18.6237
        delta_h    0        kcal

2Ag+ + HSe- = Ag2Se + H+
        log_k     34.0677
        delta_h    0        kcal

Ag+ + HSeO3- = AgSeO3- + H+
        log_k     -5.5985
        delta_h    0        kcal

Ag+ + 2HSeO3- = Ag(SeO3)2-3 + 2H+
        log_k    -13.2
        delta_h    0        kcal

Al+3 + F- = AlF+2
        log_k      7.01
        delta_h    0        kcal
        -gamma     5.4      0

Al+3 + 2F- = AlF2+
        log_k     12.75
        delta_h   20.0      kcal
        -gamma     5.4      0

Al+3 + 3F- = AlF3
        log_k     17.02
        delta_h    2.5      kcal

Al+3 + 4F- = AlF4-
        log_k     19.72
        delta_h    0        kcal
        -gamma     4.5      0

Al+3 + H2O = AlOH+2 + H+
        log_k     -4.99
        delta_h   11.899    kcal
        -gamma     5.4      0

Al+3 + 2H2O = Al(OH)2+ + 2H+
        log_k    -10.1
        delta_h    0        kcal
        -gamma     5.4      0

Al+3 + 3H2O = Al(OH)3 + 3H+
        log_k    -16.0
        delta_h    0        kcal

Al+3 + 4H2O = Al(OH)4- + 4H+
        log_k    -23.0
        delta_h   44.06     kcal
        -gamma     4.5      0

Al+3 + SO4-2 = AlSO4+
        log_k      3.02
        delta_h    2.15     kcal
        -gamma     4.5      0

Al+3 + 2SO4-2 = Al(SO4)2-
        log_k      4.92
        delta_h    2.84     kcal
        -gamma     4.5      0

Am+3 + CO3-2 = AmCO3+
        log_k      7.8005
        delta_h    3.568    kcal
        -gamma     4.0      0

Am+3 + 2CO3-2 = Am(CO3)2-
        log_k     12.3009
        delta_h    2.428    kcal
        -gamma     4.0      0

Am+3 + 3CO3-2 = Am(CO3)3-3
        log_k     15.2012
        delta_h    0        kcal
        -gamma     4.0      0

Am+3 + Cl- = AmCl+2
        log_k      1.0502
        delta_h   -3.733    kcal
        -gamma     4.5      0

Am+3 + F- = AmF+2
        log_k      3.4001
        delta_h    4.543    kcal
        -gamma     4.5      0

Am+3 + 2F- = AmF2+
        log_k      5.8004
        delta_h    4.398    kcal
        -gamma     4.0      0

Am+3 + NO3- = AmNO3+2
        log_k      1.3300
        delta_h    0        kcal
        -gamma     4.5      0

Am+3 + H2O = AmOH+2 + H+
        log_k     -6.4003
        delta_h   13.798    kcal
        -gamma     4.5      0

Am+3 + 2H2O = Am(OH)2+ + 2H+
        log_k    -14.1008
        delta_h   18.728    kcal
        -gamma     4.0      0

Am+3 + 3H2O = Am(OH)3 + 3H+
        log_k    -25.7015
        delta_h   22.512    kcal
        -gamma     3.0      0

Am+3 + SO4-2 = AmSO4+
        log_k      3.8502
        delta_h    5.029    kcal
        -gamma     4.0      0

Am+3 + 2SO4-2 = Am(SO4)2-
        log_k      5.4004
        delta_h   10.607    kcal
        -gamma     4.0      0

Am+3 + PO4-3 + 2H+ = AmH2PO4+2
        log_k     22.5634
        delta_h    0        kcal
        -gamma     4.5      0

Am+4 + 5CO3-2 = Am(CO3)5-6
        log_k     12.629
        delta_h    0        kcal
        -gamma     4.0      0

H3AsO3 = H2AsO3- + H+
        log_k     -9.228
        delta_h    6.56     kcal

H3AsO3 = HAsO3-2 + 2H+
        log_k    -21.33
        delta_h   14.199    kcal

H3AsO3 = AsO3-3 + 3H+
        log_k    -34.744
        delta_h   20.25     kcal

H3AsO3 + H+ = H4AsO3+
        log_k     -0.305
        delta_h    0        kcal

H3AsO4 = H2AsO4- + H+
        log_k     -2.243
        delta_h   -1.69     kcal

H3AsO4 = HAsO4-2 + 2H+
        log_k     -9.001
        delta_h   -0.92     kcal

H3AsO4 = AsO4-3 + 3H+
        log_k    -20.597
        delta_h    3.43     kcal

H3BO3 = H2BO3- + H+
        log_k     -9.24
        delta_h    3.224    kcal
        -gamma     2.5      0
        -analytical 24.3919    0.012078   -1343.9
-13.2258

H3BO3 + F- = BF(OH)3-
        log_k     -0.399
        delta_h    1.85     kcal
        -gamma     2.5      0

H3BO3 + 2F- + H+ = BF2(OH)2- + H2O
        log_k      7.63
        delta_h    1.635    kcal
        -gamma     2.5      0

H3BO3 + 3F- + 2H+ = BF3OH- + 2H2O
        log_k     13.667
        delta_h   -1.58     kcal
        -gamma     2.5      0

H3BO3 + 4F- + 3H+ = BF4- + 3H2O
        log_k     20.274
        delta_h   -1.795    kcal
        -gamma     2.5      0

Ba+2 + H2O = BaOH+ + H+
        log_k    -13.358
        delta_h   15.095    kcal
        -gamma     5.0      0

Ca+2 + CO3-2 = CaCO3
        log_k      3.15
        delta_h    4.03     kcal
        -analytical -27.393    0.05617    4114.0

Ca+2 + CO3-2 + H+ = CaHCO3+
        log_k     11.33
        delta_h    1.79     kcal
        -gamma     6.0      0

Ca+2 + F- = CaF+
        log_k      0.94
        delta_h    3.798    kcal
        -gamma     5.0      0

Ca+2 + H2O = CaOH+ + H+
        log_k    -12.598
        delta_h   14.535    kcal
        -gamma     6.0      0

Ca+2 + PO4-3 = CaPO4-
        log_k      6.459
        delta_h    3.1      kcal
        -gamma     5.4      0

Ca+2 + PO4-3 + H+ = CaHPO4
        log_k     15.085
        delta_h   -0.23     kcal

Ca+2 + PO4-3 + 2H+ = CaH2PO4+
        log_k     20.96
        delta_h   -1.12     kcal
        -gamma     5.4      0

Ca+2 + SO4-2 = CaSO4
        log_k      2.309
        delta_h    1.47     kcal

Cd+2 + Br- = CdBr+
        log_k      2.17
        delta_h   -0.81     kcal

Cd+2 + 2Br- = CdBr2
        log_k      2.899
        delta_h    0        kcal

Cd+2 + CO3-2 = CdCO3
        log_k      5.399
        delta_h    0        kcal

Cd+2 + 3CO3-2 = Cd(CO3)3-4
        log_k      6.22
        delta_h    0        kcal

Cd+2 + CO3-2 + H+ = CdHCO3+
        log_k     12.4
        delta_h    0        kcal

Cd+2 + Cl- = CdCl+
        log_k      1.98
        delta_h    0.59     kcal

Cd+2 + 2Cl- = CdCl2
        log_k      2.6
        delta_h    1.24     kcal

Cd+2 + 3Cl- = CdCl3-
        log_k      2.399
        delta_h    3.9      kcal

Cd+2 + F- = CdF+
        log_k      1.1
        delta_h    0        kcal

Cd+2 + 2F- = CdF2
        log_k      1.5
        delta_h    0        kcal

Cd+2 + I- = CdI+
        log_k      2.15
        delta_h   -2.37     kcal

Cd+2 + 2I- = CdI2
        log_k      3.59
        delta_h    0        kcal

Cd+2 + NO3- = CdNO3+
        log_k      0.399
        delta_h   -5.2      kcal

Cd+2 + H2O = CdOH+ + H+
        log_k    -10.08
        delta_h   13.1      kcal

Cd+2 + 2H2O = Cd(OH)2 + 2H+
        log_k    -20.35
        delta_h    0        kcal

Cd+2 + 3H2O = Cd(OH)3- + 3H+
        log_k    -33.3
        delta_h    0        kcal

Cd+2 + 4H2O = Cd(OH)4-2 + 4H+
        log_k    -47.35
        delta_h    0        kcal

2Cd+2 + H2O = Cd2OH+3 + H+
        log_k     -9.39
        delta_h   10.899    kcal

Cd+2 + H2O + Cl- = CdOHCl + H+
        log_k     -7.404
        delta_h    4.355    kcal

Cd+2 + HS- = CdHS+
        log_k     10.17
        delta_h    0        kcal

Cd+2 + 2HS- = Cd(HS)2
        log_k     16.53
        delta_h    0        kcal

Cd+2 + 3HS- = Cd(HS)3-
        log_k     18.71
        delta_h    0        kcal

Cd+2 + 4HS- = Cd(HS)4-2
        log_k     20.9
        delta_h    0        kcal

Cd+2 + SO4-2 = CdSO4
        log_k      2.46
        delta_h    1.08     kcal

Cd+2 + 2SO4-2 = Cd(SO4)2-2
        log_k      3.5
        delta_h    0        kcal

Cd+2 + 2HSeO3- = Cd(SeO3)2-2 + 2H+
        log_k    -11.189
        delta_h    0        kcal

Cd+2 + SeO4-2 = CdSeO4
        log_k      2.2415
        delta_h    0        kcal

Co+2 + 2Br- = CoBr2
        log_k     -0.0358
        delta_h   -0.135    kcal
        -gamma     3.0      0

Co+2 + Cl- = CoCl+
        log_k      0.1547
        delta_h   41.066    kcal
        -gamma     4.0      0

Co+2 + 2I- = CoI2
        log_k     -0.0944
        delta_h    0.759    kcal
        -gamma     3.0      0

Co+2 + NO3- = CoNO3+
        log_k      0.2000
        delta_h    0        kcal
        -gamma     4.0      0

Co+2 + H2O = CoOH+ + H+
        log_k    -10.0149
        delta_h   13.732    kcal
        -gamma     4.0      0

Co+2 + 2H2O = Co(OH)2 + 2H+
        log_k    -18.8000
        delta_h    0        kcal
        -gamma     3.0      0

Co+2 + 4H2O = Co(OH)4-2 + 4H+
        log_k    -45.7804
        delta_h    0        kcal
        -gamma     4.0      0

2Co+2 + 3H2O = Co2(OH)3+ + 3H+
        log_k    -11.2000
        delta_h    0        kcal
        -gamma     4.0      0

4Co+2 + 4H2O = Co4(OH)4+4 + 4H+
        log_k    -30.3804
        delta_h    0        kcal
        -gamma     5.5      0
        -analytical -9.448     0.03709    2902.39

Co+2 + HS- = CoHS+
        log_k      5.9813
        delta_h    0        kcal
        -gamma     4.0      0

Co+2 + 2HS- = Co(HS)2
        log_k      9.0306
        delta_h    0        kcal
        -gamma     3.0      0

Co+2 + SO4-2 = CoSO4
        log_k      0.0436
        delta_h    0.094    kcal
        -gamma     3.0      0

Co+2 + SeO4-2 = CoSeO4
        log_k      2.7000
        delta_h    0        kcal
        -gamma     3.0      0

Cr(OH)2+ + Br- + 2H+ = CrBr+2 + 2H2O
        log_k      7.5519
        delta_h  -11.211    kcal

Cr(OH)2+ + Cl- + 2H+ = CrCl+2 + 2H2O
        log_k      9.3683
        delta_h  -13.847    kcal

Cr(OH)2+ + 2Cl- + 2H+ = CrCl2+ + 2H2O
        log_k      8.658
        delta_h   -9.374    kcal

Cr(OH)2+ + 2Cl- + H+ = CrOHCl2 + H2O
        log_k      2.9627
        delta_h    0        kcal

Cr(OH)2+ + F- + 2H+ = CrF+2 + 2H2O
        log_k     14.5424
        delta_h  -16.789    kcal

Cr(OH)2+ + I- + 2H+ = CrI+2 + 2H2O
        log_k      4.8289
        delta_h    0        kcal

Cr(OH)2+ + 6NH4+ = Cr(NH3)6+3 + 4H+ + 2H2O
        log_k    -32.5709
        delta_h    0        kcal

Cr(OH)2+ + 5NH4+ = Cr(NH3)5OH+2 + 4H+ + H2O
        log_k    -30.2759
        delta_h    0        kcal

Cr(OH)2+ + 4NH4+ = Cr(NH3)4(OH)2+ + 4H+
        log_k    -29.8574
        delta_h    0        kcal

Cr(OH)2+ + 6NH4+ + Cl- = Cr(NH3)6Cl+2 + 2H2O + 4H+
        log_k    -31.7932
        delta_h    0        kcal

Cr(OH)2+ + 6NH4+ + Br- = Cr(NH3)6Br+2 + 4H+ + 2H2O
        log_k    -31.887
        delta_h    0        kcal

Cr(OH)2+ + 6NH4+ + I- = Cr(NH3)6I+2 + 4H+ + 2H2O
        log_k    -32.008
        delta_h    0        kcal

Cr(OH)2+ + NO3- + 2H+ = CrNO3+2 + 2H2O
        log_k      8.2094
        delta_h  -15.64     kcal

Cr(OH)2+ + 2H+ = Cr+3 + 2H2O
        log_k      9.62
        delta_h  -20.14     kcal

Cr(OH)2+ + H+ = Cr(OH)+2 + H2O
        log_k      5.62
        delta_h    0        kcal

Cr(OH)2+ + H2O = Cr(OH)3 + H+
        log_k     -7.13
        delta_h    0        kcal

Cr(OH)2+ + 2H2O = Cr(OH)4- + 2H+
        log_k    -18.15
        delta_h    0        kcal

Cr(OH)2+ + 4H+ + PO4-3 = CrH2PO4+2 + 2H2O
        log_k     31.9068
        delta_h    0        kcal

Cr(OH)2+ + SO4-2 + 2H+ = CrSO4+ + 2H2O
        log_k     10.9654
        delta_h  -12.62     kcal

Cr(OH)2+ + SO4-2 + H+ = CrOHSO4 + H2O
        log_k      8.2754
        delta_h    0        kcal

2Cr(OH)2+ + SO4-2 + 2H+ = Cr2(OH)2SO4+2 + 2H2O
        log_k     16.155
        delta_h    0        kcal

CrO4-2 + H+ = HCrO4-
        log_k      6.5089
        delta_h    0.9      kcal

CrO4-2 + 2H+ = H2CrO4
        log_k      5.6513
        delta_h    0        kcal

2CrO4-2 + 2H+ = Cr2O7-2 + H2O
        log_k     14.5571
        delta_h   -2.995    kcal

CrO4-2 + Cl- + 2H+ = CrO3Cl- + H2O
        log_k      7.3086
        delta_h    0        kcal

CrO4-2 + 4H+ + PO4-3 = CrO3H2PO4- + H2O
        log_k     29.3634
        delta_h    0        kcal

CrO4-2 + 3H+ + PO4-3 = CrO3HPO4-2 + H2O
        log_k     26.6806
        delta_h    0        kcal

CrO4-2 + SO4-2 + 2H+ = CrO3SO4-2 + H2O
        log_k      8.9937
        delta_h    0        kcal

CrO4-2 + Na+ = NaCrO4-
        log_k      0.6963
        delta_h    0        kcal

CrO4-2 + K+ = KCrO4-
        log_k      0.799
        delta_h    0        kcal

Cs+ + Br- = CsBr
        log_k     -0.2712
        delta_h    2.62     kcal
        -gamma     3.0      0

Cs+ + Cl- = CsCl
        log_k     -0.1385
        delta_h    0.653    kcal
        -gamma     3.0      0

Cs+ + I- = CsI
        log_k      0.2639
        delta_h   -1.57     kcal
        -gamma     3.0      0

Cu+ + 2Cl- = CuCl2-
        log_k      5.5
        delta_h   -0.42     kcal
        -gamma     4.0      0

Cu+ + 3Cl- = CuCl3-2
        log_k      5.7
        delta_h    0.26     kcal
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        -gamma      5.0     0

Cu+ + 2HS- = Cu(S4)2-3 + 2H+
        log_k       3.39
        delta_h     0       kcal
        -gamma     23.0     0
        -no_check
        -mass_balance Cu(S(-2)4)2

Cu+ + 2HS- = CuS4S5-3 + 2H+
        log_k       2.66
        delta_h     0       kcal
        -gamma     25.0     0
        -no_check
        -mass_balance CuS(-2)4S(-2)5

Cu+2 + CO3-2 = CuCO3
        log_k       6.73
        delta_h     0       kcal

Cu+2 + 2CO3-2 = Cu(CO3)2-2
        log_k       9.83
        delta_h     0       kcal

Cu+2 + CO3-2 + H+ = CuHCO3+
        log_k      13.0
        delta_h     0       kcal

Cu+2 + Cl- = CuCl+
        log_k       0.43
        delta_h     8.65    kcal
        -gamma      4.0     0

Cu+2 + 2Cl- = CuCl2
        log_k       0.16
        delta_h    10.56    kcal

Cu+2 + 3Cl- = CuCl3-
        log_k      -2.29
        delta_h    13.69    kcal
        -gamma      4.0     0

Cu+2 + 4Cl- = CuCl4-2
        log_k      -4.59
        delta_h     7.78    kcal
        -gamma      5.0     0

Cu+2 + F- = CuF+
        log_k       1.26
        delta_h     1.62    kcal

Cu+2 + H2O = CuOH+ + H+
        log_k      -8.0
        delta_h     0       kcal
        -gamma      4.0     0

Cu+2 + 2H2O = Cu(OH)2 + 2H+
        log_k     -13.68
        delta_h     0       kcal

Cu+2 + 3H2O = Cu(OH)3- + 3H+
        log_k     -26.899
        delta_h     0       kcal

Cu+2 + 4H2O = Cu(OH)4-2 + 4H+
        log_k     -39.6
        delta_h     0       kcal

2Cu+2 + 2H2O = Cu2(OH)2+2 + 2H+
        log_k     -10.359
        delta_h    17.539   kcal
        -analytical 2.497       0.0         -3833.0

Cu+2 + 3HS- = Cu(HS)3-
        log_k      25.899
        delta_h     0       kcal

Cu+2 + SO4-2 = CuSO4
        log_k       2.31
        delta_h     1.22    kcal

Eu+3 + Br- = EuBr+2
        log_k       0.5572
        delta_h     0       kcal
        -gamma      4.5     0

Eu+3 + 2Br- = EuBr2+
        log_k       0.2145
        delta_h     0       kcal
        -gamma      4.0     0

Eu+3 + CO3-2 = EuCO3+
        log_k       7.8005
        delta_h     0       kcal
        -gamma      4.0     0

Eu+3 + 2CO3-2 = Eu(CO3)2-
        log_k      12.2583
        delta_h     0       kcal
        -gamma      4.0     0

Eu+3 + 3CO3-2 = Eu(CO3)3-3
        log_k      14.1709
        delta_h     0       kcal
        -gamma      4.0     0

Eu+3 + CO3-2 + H+ = Eu(HCO3)+2
        log_k      11.9225
        delta_h     0       kcal
        -gamma      4.5     0

Eu+3 + CO3-2 + H2O = EuOHCO3 + H+
        log_k       1.8347
        delta_h     0       kcal
        -gamma      3.0     0

Eu+3 + 2CO3-2 + H2O = EuOH(CO3)2-2 + H+
        log_k       5.4816
        delta_h     0       kcal
        -gamma      4.0     0

Eu+3 + CO3-2 + 2H2O = Eu(OH)2CO3- + 2H+
        log_k      -7.5174
        delta_h     0       kcal
        -gamma      4.0     0

Eu+3 + Cl- = EuCl+2
        log_k       0.6915
        delta_h     0.023   kcal
        -gamma      4.5     0

Eu+3 + 2Cl- = EuCl2+
        log_k       0.2553
        delta_h     0       kcal
        -gamma      4.0     0

Eu+3 + F- = EuF+2
        log_k       3.6416
        delta_h     0       kcal
        -gamma      4.5     0

Eu+3 + 2F- = EuF2+
        log_k       6.0854
        delta_h     0       kcal
        -gamma      4.0     0

Eu+3 + NO3- = EuNO3+2
        log_k       1.0392
        delta_h     0       kcal
        -gamma      4.5     0

Eu+3 + H2O = EuOH+2 + H+
        log_k      -7.8214
        delta_h     0       kcal
        -gamma      4.5     0

Eu+3 + 2H2O = Eu(OH)2+ + 2H+
        log_k     -14.8609
        delta_h     0       kcal
        -gamma      4.0     0

Eu+3 + 3H2O = Eu(OH)3 + 3H+
        log_k     -24.1253
        delta_h     0       kcal
        -gamma      3.0     0

Eu+3 + 4H2O = Eu(OH)4- + 4H+
        log_k     -36.5958
        delta_h     0       kcal
        -gamma      4.0     0

2Eu+3 + 2H2O = Eu2(OH)2+4 + 2H+
        log_k      -6.9182
        delta_h     0       kcal
        -gamma      5.5     0

Eu+3 + SO4-2 = EuSO4+
        log_k       3.9029
        delta_h     4.192   kcal
        -gamma      4.0     0

Eu+3 + 2SO4-2 = Eu(SO4)2-
        log_k       5.4693
        delta_h     6.129   kcal
        -gamma      4.0     0

Fe+2 + H2O = FeOH+ + H+
        log_k      -9.5
        delta_h    13.199   kcal
        -gamma      5.0     0

Fe+2 + 2H2O = Fe(OH)2 + 2H+
        log_k     -20.57
        delta_h    28.565   kcal

Fe+2 + 3H2O = Fe(OH)3- + 3H+
        log_k     -31.0
        delta_h    30.3     kcal
        -gamma      5.0     0

Fe+2 + PO4-3 + H+ = FeHPO4
        log_k      15.95
        delta_h     0       kcal

Fe+2 + PO4-3 + 2H+ = FeH2PO4+
        log_k      22.253
        delta_h     0       kcal
        -gamma      5.4     0

Fe+2 + 2HS- = Fe(HS)2
        log_k       8.95
        delta_h     0       kcal

Fe+2 + 3HS- = Fe(HS)3-
        log_k      10.987
        delta_h     0       kcal

Fe+2 + SO4-2 = FeSO4
        log_k       2.25
        delta_h     3.23    kcal

Fe+3 + Cl- = FeCl+2
        log_k       1.48
        delta_h     5.6     kcal
        -gamma      5.0     0

Fe+3 + 2Cl- = FeCl2+
        log_k       2.13
        delta_h     0       kcal
        -gamma      5.0     0

Fe+3 + 3Cl- = FeCl3
        log_k       1.13
        delta_h     0       kcal

Fe+3 + F- = FeF+2
        log_k       6.199
        delta_h     2.699   kcal
        -gamma      5.0     0

Fe+3 + 2F- = FeF2+
        log_k      10.8
        delta_h     4.8     kcal
        -gamma      5.0     0

Fe+3 + 3F- = FeF3
        log_k      14.0
        delta_h     5.399   kcal

Fe+3 + H2O = FeOH+2 + H+
        log_k      -2.19
        delta_h    10.399   kcal
        -gamma      5.0     0

Fe+3 + 2H2O = Fe(OH)2+ + 2H+
        log_k      -5.67
        delta_h     0       kcal
        -gamma      5.4     0

Fe+3 + 3H2O = Fe(OH)3 + 3H+
        log_k     -13.6
        delta_h     0       kcal

Fe+3 + 4H2O = Fe(OH)4- + 4H+
        log_k     -21.6
        delta_h     0       kcal
        -gamma      5.4     0

2Fe+3 + 2H2O = Fe2(OH)2+4 + 2H+
        log_k      -2.95
        delta_h    13.5     kcal

3Fe+3 + 4H2O = Fe3(OH)4+5 + 4H+
        log_k      -6.3
        delta_h    14.3     kcal

Fe+3 + PO4-3 + H+ = FeHPO4+
        log_k      17.78
        delta_h    -7.3     kcal
        -gamma      5.4     0

Fe+3 + PO4-3 + 2H+ = FeH2PO4+2
        log_k      24.98
        delta_h     0       kcal
        -gamma      5.4     0

Fe+3 + SO4-2 = FeSO4+
        log_k       3.92
        delta_h     3.91    kcal
        -gamma      5.0     0

Fe+3 + 2SO4-2 = Fe(SO4)2-
        log_k       5.42
        delta_h     4.6     kcal

Fe+3 + HSeO3- = FeHSeO3+2
        log_k       3.61
        delta_h     0       kcal

Hg(OH)2 + Br- + 2H+ = HgBr+ + 2H2O
        log_k      15.8347
        delta_h     0       kcal

Hg(OH)2 + 2Br- + 2H+ = HgBr2 + 2H2O
        log_k      23.6065
        delta_h   -30.832   kcal

Hg(OH)2 + 2H+ + 3Br- = HgBr3- + 2H2O
        log_k      25.7857
        delta_h     0       kcal

Hg(OH)2 + 2H+ + 4Br- = HgBr4-2 + 2H2O
        log_k      27.0633
        delta_h     0       kcal

Hg(OH)2 + Br- + Cl- + 2H+ = HgBrCl + 2H2O
        log_k      22.0145
        delta_h     0       kcal

Hg(OH)2 + Br- + I- + 2H+ = HgBrI + 2H2O
        log_k      27.1212
        delta_h     0       kcal

Hg(OH)2 + Br- + 3I- + 2H+ = HgBrI3-2 + 2H2O
        log_k      34.2135
        delta_h     0       kcal

Hg(OH)2 + 2Br- + 2I- + 2H+ = HgBr2I2-2 + 2H2O
        log_k      32.3994
        delta_h     0       kcal

Hg(OH)2 + 3Br- + I- + 2H+ = HgBr3I-2 + 2H2O
        log_k      30.1528
        delta_h     0       kcal

Hg(OH)2 + Br- + H+ = HgBrOH + H2O
        log_k      11.598
        delta_h     0       kcal

Hg(OH)2 + Cl- + 2H+ = HgCl+ + 2H2O
        log_k      12.85
        delta_h     0       kcal

Hg(OH)2 + 2Cl- + 2H+ = HgCl2 + 2H2O
        log_k      19.2203
        delta_h     0       kcal

Hg(OH)2 + 3Cl- + 2H+ = HgCl3- + 2H2O
        log_k      20.1226
        delta_h     0       kcal

Hg(OH)2 + 4Cl- + 2H+ = HgCl4-2 + 2H2O
        log_k      20.5338
        delta_h     0       kcal

Hg(OH)2 + Cl- + I- + 2H+ = HgClI + 2H2O
        log_k      25.3532
        delta_h     0       kcal

Hg(OH)2 + Cl- + H+ = HgClOH + H2O
        log_k       9.317
        delta_h   -12.482   kcal

Hg(OH)2 + F- + 2H+ = HgF+ + 2H2O
        log_k       8.0848
        delta_h     0       kcal

Hg(OH)2 + I- + 2H+ = HgI+ + 2H2O
        log_k      18.8949
        delta_h     0       kcal

Hg(OH)2 + 2I- + 2H+ = HgI2 + 2H2O
        log_k      30.1081
        delta_h   -44.522   kcal

Hg(OH)2 + 3I- + 2H+ = HgI3- + 2H2O
        log_k      33.7935
        delta_h   -47.943   kcal

Hg(OH)2 + 4I- + 2H+ = HgI4-2 + 2H2O
        log_k      35.7858
        delta_h     0       kcal

Hg(OH)2 + NH4+ + H+ = HgNH3+2 + 2H2O
        log_k       5.6139
        delta_h     0       kcal

Hg(OH)2 + 2NH4+ = Hg(NH3)2+2 + 2H2O
        log_k       5.0341
        delta_h     0       kcal

Hg(OH)2 + 3NH4+ = Hg(NH3)3+2 + H+ + 2H2O
        log_k      -3.2493
        delta_h     0       kcal

Hg(OH)2 + 4NH4+ = Hg(NH3)4+2 + 2H+ + 2H2O
        log_k     -11.7307
        delta_h     0       kcal

Hg(OH)2 + NO3- + 2H+ = HgNO3+ + 2H2O
        log_k       6.4503
        delta_h     0       kcal

Hg(OH)2 + 2NO3- + 2H+ = Hg(NO3)2 + 2H2O
        log_k       4.7791
        delta_h     0       kcal

Hg(OH)2 + H+ = HgOH+ + H2O
        log_k       2.6974
        delta_h     0       kcal

Hg(OH)2 + H2O = Hg(OH)3- + H+
        log_k     -15.0042
        delta_h     0       kcal

Hg(OH)2 + 2HS- = HgS2-2 + 2H2O
        log_k      31.2398
        delta_h     0       kcal

Hg(OH)2 + 2HS- + 2H+ = Hg(HS)2 + 2H2O
        log_k      43.8178
        delta_h     0       kcal

Hg(OH)2 + SO4-2 + 2H+ = HgSO4 + 2H2O
        log_k       7.4911
        delta_h     0       kcal

K+ + PO4-3 + H+ = KHPO4-
        log_k      12.64
        delta_h     0       kcal
        -gamma      5.4     0

K+ + SO4-2 = KSO4-
        log_k       0.85
        delta_h     2.25    kcal
        -gamma      5.4     0
        -analytical 3.106       0.00        -673.6

Li+ + SO4-2 = LiSO4-
        log_k       0.64
        delta_h     0       kcal
        -gamma      5.0     0

Mg+2 + CO3-2 = MgCO3
        log_k       2.98
        delta_h     2.022   kcal
        -analytical 0.991       0.00667

Mg+2 + CO3-2 + H+ = MgHCO3+
        log_k      11.4
        delta_h    -2.43    kcal
        -gamma      4.0     0

Mg+2 + F- = MgF+
        log_k       1.82
        delta_h     4.674   kcal
        -gamma      4.5     0

Mg+2 + H2O = MgOH+ + H+
        log_k     -11.79
        delta_h    15.935   kcal
        -gamma      6.5     0
        -analytical -3.53       0.00513     -2917.1

Mg+2 + PO4-3 + 2H+ = MgH2PO4+
        log_k      21.066
        delta_h    -1.12    kcal
        -gamma      5.4     0

Mg+2 + PO4-3 = MgPO4-
        log_k       6.589
        delta_h     3.1     kcal
        -gamma      5.4     0

Mg+2 + PO4-3 + H+ = MgHPO4
        log_k      15.22
        delta_h    -0.23    kcal

Mg+2 + SO4-2 = MgSO4
        log_k       2.25
        delta_h     1.399   kcal

Mn+2 + CO3-2 + H+ = MnHCO3+
        log_k      11.6
        delta_h     0       kcal
        -gamma      5.0     0

Mn+2 + Cl- = MnCl+
        log_k       0.607
        delta_h     0       kcal
        -gamma      5.0     0

Mn+2 + 2Cl- = MnCl2
        log_k       0.041
        delta_h     0       kcal

Mn+2 + 3Cl- = MnCl3-
        log_k      -0.305
        delta_h     0       kcal
        -gamma      5.0     0

Mn+2 + F- = MnF+
        log_k       0.85
        delta_h     0       kcal
        -gamma      5.0     0

Mn+2 + 2NO3- = Mn(NO3)2
        log_k       0.6
        delta_h    -0.396   kcal

Mn+2 + H2O = MnOH+ + H+
        log_k     -10.59
        delta_h    14.399   kcal
        -gamma      5.0     0

Mn+2 + 3H2O = Mn(OH)3- + 3H+
        log_k     -34.8
        delta_h     0       kcal
        -gamma      5.0     0

Mn+2 + SO4-2 = MnSO4
        log_k       2.26
        delta_h     2.17    kcal

Mn+2 + HSe- = MnSe + H+
        log_k      -6.7435
        delta_h     0       kcal

Mn+2 + SeO4-2 = MnSeO4
        log_k       2.4188
        delta_h     3.46    kcal

Na+ + CO3-2 + H+ = NaHCO3
        log_k      10.08
        delta_h     0       kcal

Na+ + CO3-2 = NaCO3-
        log_k       1.268
        delta_h     8.911   kcal
        -gamma      5.4     0

Na+ + F- = NaF
        log_k      -0.79
        delta_h     0       kcal

Na+ + H2O = NaOH + H+
        log_k     -14.180

Na+ + PO4-3 + H+ = NaHPO4-
        log_k      12.636
        delta_h     0       kcal
        -gamma      5.4     0

Na+ + SO4-2 = NaSO4-
        log_k       0.7
        delta_h     1.12    kcal
        -gamma      5.4     0

NH4+ = NH3 + H+
        log_k      -9.252
        delta_h    12.48    kcal
        -analytical 0.6322      -0.001225   -2835.76

NH4+ + SO4-2 = NH4SO4-
        log_k       1.11
        delta_h     0       kcal
        -gamma      5.0     0

Ni+2 + Br- = NiBr+
        log_k       0.5
        delta_h     0       kcal

Ni+2 + CO3-2 = NiCO3
        log_k       6.87
        delta_h     0       kcal

Ni+2 + 2CO3-2 = Ni(CO3)2-2
        log_k      10.11
        delta_h     0       kcal

Ni+2 + CO3-2 + H+ = NiHCO3+
        log_k      12.47
        delta_h     0       kcal

Ni+2 + Cl- = NiCl+
        log_k       0.399
        delta_h     0       kcal

Ni+2 + 2Cl- = NiCl2
        log_k       0.96
        delta_h     0       kcal
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Ni+2 + F- = NiF+
        log_k     1.3
        delta_h   0        kcal

Ni+2 + H2O = NiOH+ + H+
        log_k     -9.86
        delta_h   12.42    kcal

Ni+2 + 2H2O = Ni(OH)2 + 2H+
        log_k     -19.0
        delta_h   0        kcal

Ni+2 + 3H2O = Ni(OH)3- + 3H+
        log_k     -30.0
        delta_h   0        kcal

Ni+2 + SO4-2 = NiSO4
        log_k     2.29
        delta_h   1.52     kcal

Ni+2 + 2SO4-2 = Ni(SO4)2-2
        log_k     1.02
        delta_h   0        kcal

Ni+2 + SeO4-2 = NiSeO4
        log_k     2.6387
        delta_h   3.5      kcal

Np+3 + H2O = NpOH+2 + H+
        log_k     -7.0000
        delta_h   11.976   kcal
        -gamma    4.5      0

Np+3 + PO4-3 + 2H+ = NpH2PO4+2
        log_k     21.9300
        delta_h   -11.888  kcal
        -gamma    4.5      0

Np+3 + 2PO4-3 + 4H+ = Np(H2PO4)2+
        log_k     42.7500
        delta_h   -27.057  kcal
        -gamma    4.0      0

Np+3 + 3PO4-3 + 6H+ = Np(H2PO4)3
        log_k     64.1800
        delta_h   -45.253  kcal
        -gamma    3.0      0

Np+4 + 5CO3-2 = Np(CO3)5-6
        log_k     38.3000
        delta_h   4.599    kcal
        -gamma    4.0      0

Np+4 + Cl- = NpCl+3
        log_k     0.2000
        delta_h   4.873    kcal
        -gamma    5.0      0

Np+4 + 2Cl- = NpCl2+2
        log_k     -0.1000
        delta_h   22.614   kcal
        -gamma    4.5      0

Np+4 + F- = NpF+3
        log_k     8.7000
        delta_h   -0.818   kcal
        -gamma    5.0      0

Np+4 + 2F- = NpF2+2
        log_k     15.4000
        delta_h   1.449    kcal
        -gamma    4.5      0

Np+4 + H2O = NpOH+3 + H+
        log_k     -1.0000
        delta_h   12.192   kcal
        -gamma    5.0      0

Np+4 + 2H2O = Np(OH)2+2 + 2H+
        log_k     -2.8000
        delta_h   18.42    kcal
        -gamma    4.5      0

Np+4 + 3H2O = Np(OH)3+ + 3H+
        log_k     -5.8000
        delta_h   23.792   kcal
        -gamma    4.0      0

Np+4 + 4H2O = Np(OH)4 + 4H+
        log_k     -9.6000
        delta_h   26.193   kcal
        -gamma    3.0      0

Np+4 + 5H2O = Np(OH)5- + 5H+
        log_k     -14.3000
        delta_h   29.109   kcal
        -gamma    4.0      0

Np+4 + PO4-3 + H+ = NpHPO4+2
        log_k     25.2200
        delta_h   -1.71    kcal
        -gamma    4.5      0

Np+4 + 2PO4-3 + 2H+ = Np(HPO4)2
        log_k     48.0400
        delta_h   -15.449  kcal
        -gamma    3.0      0

Np+4 + 3PO4-3 + 3H+ = Np(HPO4)3-2
        log_k     70.3700
        delta_h   -21.533  kcal
        -gamma    4.0      0

Np+4 + 4PO4-3 + 4H+ = Np(HPO4)4-4
        log_k     92.4900
        delta_h   -30.085  kcal
        -gamma    4.0      0

Np+4 + 5PO4-3 + 5H+ = Np(HPO4)5-6
        log_k     113.6100
        delta_h   -37.532  kcal
        -gamma    4.0      0

Np+4 + SO4-2 = NpSO4+2
        log_k     5.5000
        delta_h   4.959    kcal
        -gamma    4.5      0

Np+4 + 2SO4-2 = Np(SO4)2
        log_k     9.9000
        delta_h   9.565    kcal
        -gamma    3.0      0

NpO2+ + CO3-2 = NpO2CO3-
        log_k     4.6000
        delta_h   13.018   kcal
        -gamma    4.0      0

NpO2+ + 2CO3-2 = NpO2(CO3)2-3
        log_k     7.0000
        delta_h   6.876    kcal
        -gamma    4.0      0

NpO2+ + 3CO3-2 = NpO2(CO3)3-5
        log_k     8.5000
        delta_h   6.237    kcal
        -gamma    4.0      0

NpO2+ + Cl- = NpO2Cl
        log_k     -0.4000
        delta_h   3.696    kcal
        -gamma    3.0      0

NpO2+ + F- = NpO2F
        log_k     1.0000
        delta_h   8.19     kcal
        -gamma    3.0      0

NpO2+ + H2O = NpO2OH + H+
        log_k     -8.9000
        delta_h   10.427   kcal
        -gamma    3.0      0

NpO2+ + PO4-3 + 2H+ = NpO2H2PO4
        log_k     20.1300
        delta_h   16.844   kcal
        -gamma    3.0      0

NpO2+ + PO4-3 + H+ = NpO2HPO4-
        log_k     15.8200
        delta_h   8.405    kcal
        -gamma    4.0      0

NpO2+ + SO4-2 = NpO2SO4-
        log_k     0.4000
        delta_h   4.576    kcal
        -gamma    4.0      0

NpO2+2 + 2CO3-2 = NpO2(CO3)2-2
        log_k     14.0000
        delta_h   6.662    kcal
        -gamma    4.0      0

NpO2+2 + 3CO3-2 = NpO2(CO3)3-4
        log_k     20.4000
        delta_h   -9.783   kcal
        -gamma    4.0      0

NpO2+2 + Cl- = NpO2Cl+
        log_k     -0.2000
        delta_h   2.871    kcal
        -gamma    4.0      0

NpO2+2 + F- = NpO2F+
        log_k     4.6000
        delta_h   0.215    kcal
        -gamma    4.0      0

NpO2+2 + 2F- = NpO2F2
        log_k     7.8000
        delta_h   0.63     kcal
        -gamma    3.0      0

NpO2+2 + H2O = NpO2OH+ + H+
        log_k     -5.2000
        delta_h   10.368   kcal
        -gamma    4.0      0

2NpO2+2 + 2H2O = (NpO2)2(OH)2+2 + 2H+
        log_k     -6.4000
        delta_h   10.921   kcal
        -gamma    4.5      0

3NpO2+2 + 5H2O = (NpO2)3(OH)5+ + 5H+
        log_k     -17.5000
        delta_h   26.937   kcal
        -gamma    4.0      0

NpO2+2 + PO4-3 + 2H+ = NpO2H2PO4+
        log_k     21.8300
        delta_h   -36.956  kcal
        -gamma    4.0      0

NpO2+2 + PO4-3 + H+ = NpO2HPO4
        log_k     20.5200
        delta_h   -5.061   kcal
        -gamma    3.0      0

NpO2+2 + SO4-2 = NpO2SO4
        log_k     3.3000
        delta_h   4.753    kcal
        -gamma    3.0      0

Pb+2 + Br- = PbBr+
        log_k     1.77
        delta_h   2.88     kcal

Pb+2 + 2Br- = PbBr2
        log_k     1.44
        delta_h   0        kcal

Pb+2 + 2CO3-2 = Pb(CO3)2-2
        log_k     10.64
        delta_h   0        kcal

Pb+2 + CO3-2 + H+ = PbHCO3+
        log_k     13.2
        delta_h   0        kcal

Pb+2 + Cl- = PbCl+
        log_k     1.6
        delta_h   4.38     kcal

Pb+2 + 2Cl- = PbCl2
        log_k     1.8
        delta_h   1.08     kcal

Pb+2 + 3Cl- = PbCl3-
        log_k     1.699
        delta_h   2.17     kcal

Pb+2 + 4Cl- = PbCl4-2
        log_k     1.38
        delta_h   3.53     kcal

Pb+2 + F- = PbF+
        log_k     1.25
        delta_h   0        kcal

Pb+2 + 2F- = PbF2
        log_k     2.56
        delta_h   0        kcal

Pb+2 + 3F- = PbF3-
        log_k     3.42
        delta_h   0        kcal

Pb+2 + 4F- = PbF4-2
        log_k     3.1
        delta_h   0        kcal

Pb+2 + I- = PbI+
        log_k     1.94
        delta_h   0        kcal

Pb+2 + 2I- = PbI2
        log_k     3.199
        delta_h   0        kcal

Pb+2 + NO3- = PbNO3+
        log_k     1.17
        delta_h   0        kcal

Pb+2 + H2O = PbOH+ + H+
        log_k     -7.71
        delta_h   0        kcal

Pb+2 + 2H2O = Pb(OH)2 + 2H+
        log_k     -17.12
        delta_h   0        kcal

Pb+2 + 3H2O = Pb(OH)3- + 3H+
        log_k     -28.06
        delta_h   0        kcal

2Pb+2 + H2O = Pb2OH+3 + H+
        log_k     -6.36
        delta_h   0        kcal

3Pb+2 + 4H2O = Pb3(OH)4+2 + 4H+
        log_k     -23.88
        delta_h   26.5     kcal

Pb+2 + 2HS- = Pb(HS)2
        log_k     15.27
        delta_h   0        kcal

Pb+2 + 3HS- = Pb(HS)3-
        log_k     16.57
        delta_h   0        kcal

Pb+2 + SO4-2 = PbSO4
        log_k     2.75
        delta_h   0        kcal

Pb+2 + CO3-2 = PbCO3
        log_k     7.24
        delta_h   0        kcal

Pb+2 + 4H2O = Pb(OH)4-2 + 4H+
        log_k     -39.699
        delta_h   0        kcal

Pb+2 + 2SO4-2 = Pb(SO4)2-2
        log_k     3.47
        delta_h   0        kcal

Pu+3 + Cl- = PuCl+2
        log_k     0.0017
        delta_h   0        kcal
        -gamma    4.5      0

Pu+3 + H2O = PuOH+2 + H+
        log_k     -7.9680
        delta_h   12.79    kcal
        -gamma    4.5      0

Pu+3 + PO4-3 + 2H+ = PuH2PO4+2
        log_k     22.0035
        delta_h   3.322    kcal
        -gamma    4.5      0

Pu+3 + SO4-2 = PuSO4+
        log_k     3.4935
        delta_h   3.492    kcal
        -gamma    4.0      0

Pu+3 + 2SO4-2 = Pu(SO4)2-
        log_k     3.39
        delta_h   0        kcal
        -gamma    4.0      0

Pu+4 + Cl- = PuCl+3
        log_k     0.1435
        delta_h   3.984    kcal
        -gamma    5.0      0

Pu+4 + F- = PuF+3
        log_k     8.4600
        delta_h   5.091    kcal
        -gamma    5.0      0

Pu+4 + 2F- = PuF2+2
        log_k     15.4000
        delta_h   0        kcal
        -gamma    4.5      0

Pu+4 + 3F- = PuF3+
        log_k     5.300
        delta_h   0        kcal
        -gamma    4.0      0

Pu+4 + 4F- = PuF4
        log_k     4.2000
        delta_h   0        kcal
        -gamma    3.0      0

Pu+4 + H2O = PuOH+3 + H+
        log_k     -0.5048
        delta_h   11.516   kcal
        -gamma    5.0      0

Pu+4 + 2H2O = Pu(OH)2+2 + 2H+
        log_k     -2.3235
        delta_h   17.77    kcal
        -gamma    4.5      0

Pu+4 + 3H2O = Pu(OH)3+ + 3H+
        log_k     -5.2810
        delta_h   23.084   kcal
        -gamma    4.0      0

Pu+4 + 4H2O = Pu(OH)4 + 4H+
        log_k     -9.5174
        delta_h   26.08    kcal
        -gamma    3.0      0

Pu+4 + 5H2O = Pu(OH)5- + 5H+
        log_k     -14.9802
        delta_h   30.037   kcal
        -gamma    4.0      0

Pu+4 + PO4-3 + H+ = PuHPO4+2
        log_k     25.3321
        delta_h   6.12     kcal
        -gamma    4.5      0

Pu+4 + 2PO4-3 + 2H+ = Pu(HPO4)2
        log_k     48.4919
        delta_h   -0.83    kcal
        -gamma    3.0      0

Pu+4 + 3PO4-3 + 3H+ = Pu(HPO4)3-2
        log_k     70.4253
        delta_h   -12.092  kcal
        -gamma    4.0      0

Pu+4 + 4PO4-3 + 4H+ = Pu(HPO4)4-4
        log_k     92.5339
        delta_h   -32.572  kcal
        -gamma    4.0      0

Pu+4 + SO4-2 = PuSO4+2
        log_k     5.7710
        delta_h   2.95     kcal
        -gamma    4.5      0

Pu+4 + 2SO4-2 = Pu(SO4)2
        log_k     10.2456
        delta_h   9.806    kcal
        -gamma    3.0      0

PuO2+ + H2O = PuO2OH + H+
        log_k     -9.6323
        delta_h   16.486   kcal
        -gamma    3.0      0

PuO2+2 + CO3-2 = PuO2CO3
        log_k     12.7000
        delta_h   0        kcal

PuO2+2 + 2CO3-2 = PuO2(CO3)2-2
        log_k     14.9148
        delta_h   5.485    kcal
        -gamma    4.0      0

PuO2+2 + 3CO3-2 = PuO2(CO3)3-4
        log_k     18.5000
        delta_h   -9.304   kcal

PuO2+2 + Cl- = PuO2Cl+
        log_k     -0.2084
        delta_h   2.78     kcal
        -gamma    4.0      0

PuO2+2 + F- = PuO2F+
        log_k     5.6674
        delta_h   -1.241   kcal
        -gamma    4.0      0

PuO2+2 + 2F- = PuO2F2
        log_k     10.9669
        delta_h   -3.69    kcal
        -gamma    3.0      0

PuO2+2 + 3F- = PuO2F3-
        log_k     15.9160
        delta_h   -7.016   kcal
        -gamma    4.0      0

PuO2+2 + 4F- = PuO2F4-2
        log_k     18.7628
        delta_h   -9.54    kcal
        -gamma    3.0      0

PuO2+2 + H2O = PuO2OH+ + H+
        log_k     -5.6379
        delta_h   10.823   kcal
        -gamma    4.0      0

PuO2+2 + 2H2O = PuO2(OH)2 + 2H+
        log_k     -11.9000
        delta_h   0        kcal

PuO2+2 + 3H2O = PuO2(OH)3- + 3H+
        log_k     -20.7000
        delta_h   0        kcal

2PuO2+2 + H2O = (PuO2)2(OH)+3 + H+
        log_k     -4.3000
        delta_h   207.367  kcal

2PuO2+2 + 2H2O = (PuO2)2(OH)2+2 + 2H+
        log_k     -8.2626
        delta_h   13.83    kcal
        -gamma    4.5      0

3PuO2+2 + 5H2O = (PuO2)3(OH)5+ + 5H+
        log_k     -21.6550
        delta_h   33.335   kcal
        -gamma    4.0      0

PuO2+2 + PO4-3 + 2H+ = PuO2H2PO4+
        log_k     23.5277
        delta_h   -5.1     kcal
        -gamma    4.0      0

PuO2+2 + SO4-2 = PuO2SO4
        log_k     3.2658
        delta_h   4.8      kcal
        -gamma    3.0      0

Ru+2 + Cl- = RuCl+
        log_k     -0.4887
        delta_h   0        kcal
        -gamma    4.0      0

Ru+2 + SO4-2 = RuSO4
        log_k     2.3547
        delta_h   0        kcal
        -gamma    3.0      0

Ru+3 + Cl- = RuCl+2
        log_k     2.1742
        delta_h   0        kcal
        -gamma    4.5      0

Ru+3 + 2Cl- = RuCl2+
        log_k     3.7527
        delta_h   0        kcal
        -gamma    4.0      0

Ru+3 + 3Cl- = RuCl3
        log_k     4.2976
        delta_h   0        kcal
        -gamma    3.0      0

Ru+3 + 4Cl- = RuCl4-
        log_k     4.1418
        delta_h   0        kcal
        -gamma    4.0      0

Ru+3 + 5Cl- = RuCl5-2
        log_k     3.8457
        delta_h   0        kcal
        -gamma    4.0      0

Ru+3 + 6Cl- = RuCl6-3
        log_k     3.4446
        delta_h   0        kcal
        -gamma    4.0      0

Ru+3 + H2O = RuOH+2 + H+
        log_k     -2.2392
        delta_h   0        kcal
        -gamma    4.5      0

Ru+3 + 2H2O = Ru(OH)2+ + 2H+
        log_k     -3.5148
        delta_h   0        kcal
        -gamma    4.0      0

Ru+3 + SO4-2 = RuSO4+
        log_k     1.9518
        delta_h   0        kcal
        -gamma    4.0      0

Ru+3 + 2SO4-2 = Ru(SO4)2-
        log_k     3.0627
        delta_h   0        kcal
        -gamma    4.0      0

4Ru(OH)2+2 + 4H2O = Ru4(OH)12+4 + 4H+
        log_k     7.1960
        delta_h   0        kcal
        -gamma    5.5      0

Ru(OH)2+2 + Cl- = Ru(OH)2Cl+
        log_k     1.3858
        delta_h   0        kcal
        -gamma    4.0      0
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Ru(OH)2+2 + 2Cl- = Ru(OH)2Cl2
        log_k       1.8081
        delta_h     0          kcal
        -gamma      3.0        0

Ru(OH)2+2 + 3Cl- = Ru(OH)2Cl3-
        log_k       1.6172
        delta_h     0          kcal
        -gamma      4.0        0

Ru(OH)2+2 + 4Cl- = Ru(OH)2Cl4-2
        log_k       2.7052
        delta_h     0          kcal
        -gamma      4.0        0

Ru(OH)2+2 + SO4-2 = Ru(OH)2SO4
        log_k       1.7941
        delta_h     0          kcal
        -gamma      3.0        0

Sb(OH)3 = HSbO2 + H2O
        log_k       -0.0073
        delta_h     -0.015     kcal

Sb(OH)3 + H+ = SbO+ + 2H2O
        log_k       0.9228
        delta_h     1.97       kcal

Sb(OH)3 = SbO2- + H2O + H+
        log_k       -11.8011
        delta_h     16.775     kcal

Sb(OH)3 + F- + H+ = SbOF + 2H2O
        log_k       6.1864
        delta_h     0          kcal

Sb(OH)3 + H+ = Sb(OH)2+ + H2O
        log_k       1.3853
        delta_h     0          kcal

Sb(OH)3 + H2O = Sb(OH)4- + H+
        log_k       -12.0429
        delta_h     16.695     kcal

Sb(OH)3 + F- + H+ = Sb(OH)2F + H2O
        log_k       6.1937
        delta_h     0          kcal

2Sb(OH)3 + 4HS- + 2H+ = Sb2S4-2 + 6H2O
        log_k       49.3005
        delta_h     -75.68     kcal

Sb(OH)6- = SbO3- + 3H2O
        log_k       2.9319
        delta_h     0          kcal

Sb(OH)6- + 2H+ = SbO2+ + 4H2O
        log_k       2.3895
        delta_h     0          kcal

Sn+2 + Cl- = SnCl+
        log_k       1.0500
        delta_h     2.511      kcal
        -gamma      4.0        0

Sn+2 + 2Cl- = SnCl2
        log_k       1.7100
        delta_h     2.931      kcal
        -gamma      3.0        0

Sn+2 + 3Cl- = SnCl3-
        log_k       1.6900
        delta_h     5.173      kcal
        -gamma      4.0        0

Sn+2 + F- = SnF+
        log_k       4.0800
        delta_h     -1.056     kcal
        -gamma      4.0        0

Sn+2 + 2F- = SnF2
        log_k       6.6800
        delta_h     -0.063     kcal
        -gamma      3.0        0

Sn+2 + 3F- = SnF3-
        log_k       9.4600
        delta_h     -7.346     kcal
        -gamma      4.0        0

Sn+2 + H2O = SnOH+ + H+
        log_k       -3.9851
        delta_h     4.943      kcal
        -gamma      4.0        0

Sn+2 + 2H2O = Sn(OH)2 + 2H+
        log_k       -7.9102
        delta_h     10.05      kcal
        -gamma      3.0        0

Sn+2 + 3H2O = Sn(OH)3- + 3H+
        log_k       -17.4053
        delta_h     22.633     kcal
        -gamma      4.0        0

Sn+4 + H2O = SnOH+3 + H+
        log_k       0.6049
        delta_h     -1.196     kcal
        -gamma      5.0        0

Sn+4 + 2H2O = Sn(OH)2+2 + 2H+
        log_k       -0.1902
        delta_h     -0.482     kcal
        -gamma      4.5        0

Sn+4 + 3H2O = Sn(OH)3+ + 3H+
        log_k       0.5147
        delta_h     -1.887     kcal
        -gamma      4.0        0

Sn+4 + 4H2O = Sn(OH)4 + 4H+
        log_k       0.8496
        delta_h     -2.642     kcal
        -gamma      3.0        0

Sn+4 + SO4-2 = SnSO4+2
        log_k       -3.1094
        delta_h     0          kcal
        -gamma      4.5        0

Sn+4 + 2SO4-2 = Sn(SO4)2
        log_k       -0.8072
        delta_h     0          kcal
        -gamma      3.0        0

Sr+2 + CO3-2 = SrCO3
        log_k       2.8653
        delta_h     0          kcal

Sr+2 + Cl- = SrCl+
        log_k       -0.2485
        delta_h     0          kcal
        -gamma      4.0        0

Sr+2 + F- = SrF+
        log_k       0.1393
        delta_h     0          kcal
        -gamma      4.0        0

Sr+2 + NO3- = SrNO3+
        log_k       0.800
        delta_h     0          kcal
        -gamma      4.0        0

Sr+2 + H2O = SrOH+ + H+
        log_k       -13.29
        delta_h     0          kcal
        -gamma      4.0        0

Sr+2 + PO4-3 = SrPO4-
        log_k       5.48
        delta_h     0          kcal
        -gamma      4.0        0

Sr+2 + PO4-3 + H+ = SrHPO4
        log_k       14.406
        delta_h     0          kcal
        -gamma      3.0        0

Sr+2 + PO4-3 + 2H+ = SrH2PO4+
        log_k       20.2834
        delta_h     0          kcal
        -gamma      4.0        0

Sr+2 + 2PO4-3 + 2H+ = SrP2O7-2 + H2O
        log_k       1.6561
        delta_h     0          kcal
        -gamma      4.0        0

Sr+2 + SO4-2 = SrSO4
        log_k       2.30
        delta_h     0          kcal
        -gamma      3.0        0

TcO+2 + H2O = TcOOH+ + H+
        log_k       -1.3355
        delta_h     0          kcal
        -gamma      4.0        0

TcO+2 + 2H2O = TcO(OH)2 + 2H+
        log_k       -3.3221
        delta_h     0          kcal
        -gamma      3.0        0

2TcO+2 + 4H2O = (TcO)2(OH)4 + 4H+
        log_k       -0.1271
        delta_h     0          kcal
        -gamma      3.0        0

TcO4-2 + H+ = HTcO4-
        log_k       8.7070
        delta_h     0          kcal

TcO4-2 + 2H+ = H2TcO4
        log_k       9.0050
        delta_h     0          kcal

TcO4- + H+ = HTcO4
        log_k       1.1600
        delta_h     0          kcal

Th+4 + Cl- = ThCl+3
        log_k       0.9533
        delta_h     0.019      kcal
        -gamma      5.0        0

Th+4 + 2Cl- = ThCl2+2
        log_k       0.6755
        delta_h     20.906     kcal
        -gamma      4.5        0

Th+4 + 3Cl- = ThCl3+
        log_k       1.4972
        delta_h     15.769     kcal
        -gamma      4.0        0

Th+4 + 4Cl- = ThCl4
        log_k       1.0728
        delta_h     0          kcal
        -gamma      3.0        0

Th+4 + F- = ThF+3
        log_k       7.8722
        delta_h     -1.161     kcal
        -gamma      5.0        0

Th+4 + 2F- = ThF2+2
        log_k       14.0881
        delta_h     -1.851     kcal
        -gamma      4.5        0

Th+4 + 3F- = ThF3+
        log_k       18.7353
        delta_h     -2.787     kcal
        -gamma      4.0        0

Th+4 + 4F- = ThF4
        log_k       22.1511
        delta_h     -3.533     kcal
        -gamma      3.0        0

Th+4 + H2O = ThOH+3 + H+
        log_k       -3.8874
        delta_h     5.982      kcal
        -gamma      5.0        0

Th+4 + 2H2O = Th(OH)2+2 + 2H+
        log_k       -7.1071
        delta_h     14.023     kcal
        -gamma      4.5        0

Th+4 + 3H2O = Th(OH)3+ + 3H+
        log_k       -11.7000
        delta_h     20.348     kcal

Th+4 + 4H2O = Th(OH)4 + 4H+
        log_k       -15.9000
        delta_h     27.24      kcal
        -gamma      3.0        0

2Th+4 + 2H2O = Th2(OH)2+6 + 2H+
        log_k       -6.4624
        delta_h     15.23      kcal
        -gamma      6.0        0

4Th+4 + 8H2O = Th4(OH)8+8 + 8H+
        log_k       -21.7581
        delta_h     58.619     kcal
        -gamma      6.0        0

6Th+4 + 15H2O = Th6(OH)15+9 + 15H+
        log_k       -37.7046
        delta_h     109.531    kcal
        -gamma      6.0        0

Th+4 + 2PO4-3 + 2H+ = Th(HPO4)2
        log_k       47.3372
        delta_h     -10.287    kcal
        -gamma      3.0        0

Th+4 + 3PO4-3 + 3H+ = Th(HPO4)3-2
        log_k       68.1545
        delta_h     -19.66     kcal
        -gamma      4.0        0

Th+4 + PO4-3 + 2H+ = ThH2PO4+3
        log_k       24.0276
        delta_h     11.59      kcal
        -gamma      5.0        0

Th+4 + 2PO4-3 + 4H+ = Th(H2PO4)2+2
        log_k       47.8503
        delta_h     -6.44      kcal
        -gamma      4.5        0

Th+4 + PO4-3 + 3H+ = ThH3PO4+4
        log_k       23.4412
        delta_h     12.38      kcal
        -gamma      5.5        0

Th+4 + SO4-2 = ThSO4+2
        log_k       5.3140
        delta_h     3.91       kcal
        -gamma      4.5        0

Th+4 + 2SO4-2 = Th(SO4)2
        log_k       9.6167
        delta_h     7.709      kcal
        -gamma      3.0        0

Th+4 + 3SO4-2 = Th(SO4)3-2
        log_k       10.4010
        delta_h     11.88      kcal
        -gamma      4.0        0

Th+4 + 4SO4-2 = Th(SO4)4-4
        log_k       8.3999
        delta_h     13.37      kcal
        -gamma      4.0        0

Tl+ + Br- = TlBr
        log_k       0.9477
        delta_h     -2.461     kcal

Tl+ + 2Br- = TlBr2-
        log_k       0.9719
        delta_h     2.998      kcal

Tl+ + Br- + Cl- = TlBrCl-
        log_k       0.8165
        delta_h     0          kcal

Tl+ + Cl- = TlCl
        log_k       0.6824
        delta_h     -1.147     kcal

Tl+ + 2Cl- = TlCl2-
        log_k       0.2434
        delta_h     0          kcal

Tl+ + F- = TlF
        log_k       -0.4251
        delta_h     0          kcal

Tl+ + I- = TlI
        log_k       1.4279
        delta_h     0          kcal

Tl+ + 2I- = TlI2-
        log_k       1.8588
        delta_h     0          kcal

Tl+ + I- + Br- = TlIBr-
        log_k       2.185
        delta_h     0          kcal

Tl+ + NO2- = TlNO2
        log_k       0.9969
        delta_h     0          kcal

Tl+ + NO3- = TlNO3
        log_k       0.3665
        delta_h     -0.65      kcal

Tl+ + H2O = TlOH + H+
        log_k       -13.1717
        delta_h     13.935     kcal

Tl+ + HS- = TlHS
        log_k       1.8178
        delta_h     0          kcal

2Tl+ + HS- = Tl2HS+
        log_k       7.6979
        delta_h     0          kcal

2Tl+ + 3HS- + H2O = Tl2OH(HS)3-2 + H+
        log_k       1.0044
        delta_h     0          kcal

2Tl+ + 2HS- + 2H2O = Tl2(OH)2(HS)2-2 + 2H+
        log_k       -11.0681
        delta_h     0          kcal

Tl+ + SO4-2 = TlSO4-
        log_k       1.  1.3853
        delta_h     -0.22      kcal

Tl(OH)3 + 3H+ = Tl+3 + 3H2O
        log_k       4.7424
        delta_h     0          kcal

Tl(OH)3 + Br- + 3H+ = TlBr+2 + 3H2O
        log_k       14.2221
        delta_h     0          kcal

Tl(OH)3 + 2Br- + 3H+ = TlBr2+ + 3H2O
        log_k       21.5761
        delta_h     0          kcal

Tl(OH)3 + 3Br- + 3H+ = TlBr3 + 3H2O
        log_k       27.0244
        delta_h     0          kcal

Tl(OH)3 + 4Br- + 3H+ = TlBr4- + 3H2O
        log_k       31.1533
        delta_h     0          kcal

Tl(OH)3 + Cl- + 3H+ = TlCl+2 + 3H2O
        log_k       12.2342
        delta_h     0          kcal

Tl(OH)3 + 2Cl- + 3H+ = TlCl2+ + 3H2O
        log_k       18.0402
        delta_h     0          kcal

Tl(OH)3 + 3Cl- + 3H+ = TlCl3 + 3H2O
        log_k       21.4273
        delta_h     0          kcal

Tl(OH)3 + 4Cl- + 3H+ = TlCl4- + 3H2O
        log_k       24.2281
        delta_h     0          kcal

Tl(OH)3 + Cl- + 2H+ = TlOHCl+ + 2H2O
        log_k       10.629
        delta_h     0          kcal

Tl(OH)3 + 4I- + 3H+ = TlI4- + 3H2O
        log_k       34.7596
        delta_h     0          kcal

Tl(OH)3 + NO3- + 3H+ = TlNO3+2 + 3H2O
        log_k       7.0073
        delta_h     0          kcal

Tl(OH)3 + 2H+ = TlOH+2 + 2H2O
        log_k       3.577
        delta_h     0          kcal

Tl(OH)3 + H+ = Tl(OH)2+ + H2O
        log_k       2.1183
        delta_h     0          kcal

Tl(OH)3 + H2O = Tl(OH)4- + H+
        log_k       -10.2545
        delta_h     0          kcal

U+4 + Br- = UBr+3
        log_k       1.4250
        delta_h     0          kcal
        -gamma      5.0        0

U+4 + 4CO3-2 = U(CO3)4-4
        log_k       32.8272
        delta_h     0          kcal
        -gamma      4.0        0

U+4 + 5CO3-2 = U(CO3)5-6
        log_k       33.9000
        delta_h     -4.766     kcal
        -gamma      4.0        0

U+4 + Cl- = UCl+3
        log_k       1.7082
        delta_h     -4.537     kcal
        -gamma      5.0        0

U+4 + F- = UF+3
        log_k       9.2413
        delta_h     -1.336     kcal
        -gamma      5.0        0

U+4 + 2F- = UF2+2
        log_k       16.1403
        delta_h     -0.903     kcal
        -gamma      4.5        0

U+4 + 3F- = UF3+
        log_k       21.4818
        delta_h     0.036      kcal
        -gamma      4.0        0

U+4 + 4F- = UF4
        log_k       25.3412
        delta_h     -0.972     kcal
        -gamma      3.0        0

U+4 + 5F- = UF5-
        log_k       26.8110
        delta_h     4.38       kcal
        -gamma      4.0        0

U+4 + 6F- = UF6-2
        log_k       28.8414
        delta_h     3.29       kcal
        -gamma      4.0        0

U+4 + I- = UI+3
        log_k       1.2152
        delta_h     0          kcal
        -gamma      5.0        0

U+4 + NO3- = UNO3+3
        log_k       1.4514
        delta_h     0          kcal
        -gamma      5.0        0

U+4 + 2NO3- = U(NO3)2+2
        log_k       2.2617
        delta_h     0          kcal
        -gamma      4.5        0

U+4 + H2O = UOH+3 + H+
        log_k       -0.5381
        delta_h     11.205     kcal
        -gamma      5.0        0

U+4 + 2H2O = U(OH)2+2 + 2H+
        log_k       -2.270
        delta_h     20.434     kcal

U+4 + 3H2O = U(OH)3+ + 3H+
        log_k       -4.935
        delta_h     26.651     kcal

U+4 + 4H2O = U(OH)4 + 4H+
        log_k       -4.5577
        delta_h     28.798     kcal

U+4 + 5H2O = U(OH)5- + 5H+
        log_k       -13.120
        delta_h     30.245     kcal

6U+4 + 15H2O = U6(OH)15+9 + 15H+
        log_k       -17.229
        delta_h     0          kcal

U+4 + SO4-2 = USO4+2
        log_k       6.5016
        delta_h     36.961     kcal
        -gamma      4.5        0

U+4 + 2SO4-2 = U(SO4)2
        log_k       10.3507
        delta_h     7.946      kcal
        -gamma      3.0        0

UO2+ + 3CO3-2 = UO2(CO3)3-5
        log_k       7.3898
        delta_h     0          kcal
        -gamma      4.0        0

UO2+2 + Br- = UO2Br+
        log_k       0.1731
        delta_h     0          kcal
        -gamma      4.0        0

UO2+2 + CO3-2 = UO2CO3
        log_k       9.6700
        delta_h     1.202      kcal
        -gamma      3.0        0

UO2+2 + 2CO3-2 = UO2(CO3)2-2
        log_k       16.9698
        delta_h     4.297      kcal
        -gamma      4.0        0

UO2+2 + 3CO3-2 = UO2(CO3)3-4
        log_k       21.5846
        delta_h     -9.281     kcal
        -gamma      4.0        0

3UO2+2 + 6CO3-2 = (UO2)3(CO3)6-6
        log_k       53.9127
        delta_h     -16.323    kcal
        -gamma      4.0        0

11UO2+2 + 6CO3-2 + 12H2O = (UO2)11(CO3)6(OH)12-2 +
12H+
        log_k       36.2277
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        delta_h     0        kcal
        -gamma      4.0      0

2UO2+2 + CO3-2 + 3H2O = (UO2)2CO3(OH)3- + 3H+
        log_k      -0.8969
        delta_h   -14.394    kcal
        -gamma      4.0      0

3UO2+2 + CO3-2 + 4H2O = (UO2)3CO2(OH)5+ + 3H+
        log_k       0.7066
        delta_h     0        kcal
        -gamma      4.0      0

UO2+2 + Cl- = UO2Cl+
        log_k       0.1567
        delta_h     1.921    kcal
        -gamma      4.0      0

UO2+2 + 2Cl- = UO2Cl2
        log_k      -1.1257
        delta_h     3.593    kcal
        -gamma      3.0      0

UO2+2 + F- = UO2F+
        log_k       5.0497
        delta_h     0.413    kcal
        -gamma      4.0      0

UO2+2 + 2F- = UO2F2
        log_k       8.5394
        delta_h     0.513    kcal
        -gamma      3.0      0

UO2+2 + 3F- = UO2F3-
        log_k      10.7800
        delta_h     0.575    kcal
        -gamma      4.0      0

UO2+2 + 4F- = UO2F4-2
        log_k      11.5403
        delta_h     0.088    kcal
        -gamma      4.0      0

UO2+2 + H2O = UO2OH+ + H+
        log_k      -5.2080
        delta_h    10.325    kcal

UO2+2 + 2H2O = UO2(OH)2 + 2H+
        log_k     -10.3221
        delta_h    18.094    kcal
        -gamma      3.0      0

UO2+2 + 3H2O = UO2(OH)3- + 3H+
        log_k     -19.2222
        delta_h     0        kcal
        -gamma      4.0      0

UO2+2 + 4H2O = UO2(OH)4-2 + 4H+
        log_k     -33.0294
        delta_h     0        kcal
        -gamma      4.0      0

2UO2+2 + H2O = (UO2)2(OH)+3 + H+
        log_k      -2.7091
        delta_h     0        kcal
        -gamma      5.0      0

2UO2+2 + 2H2O = (UO2)2(OH)2+2 + 2H+
        log_k      -5.6368
        delta_h     0        kcal
        -gamma      4.5      0

3UO2+2 + 4H2O = (UO2)3(OH)4+2 + 4H+
        log_k     -11.9312
        delta_h     0        kcal
        -gamma      4.5      0

3UO2+2 + 5H2O = (UO2)3(OH)5+ + 5H+
        log_k     -15.5895
        delta_h    23.224    kcal
        -gamma      4.0      0

3UO2+2 + 7H2O = (UO2)3(OH)7- + 7H+
        log_k     -31.0542
        delta_h     0        kcal
        -gamma      4.0      0

4UO2+2 + 7H2O = (UO2)4(OH)7+ + 7H+
        log_k     -21.954
        delta_h     0        kcal
        -gamma      4.0      0

UO2+2 + NO3- = UO2NO3+
        log_k       0.2801
        delta_h     0        kcal
        -gamma      4.0      0

UO2+2 + PO4-3 + H+ = UO2HPO4
        log_k      21.2298
        delta_h    -2.03     kcal
        -gamma      3.0      0

UO2+2 + PO4-3 + 2H+ = UO2H2PO4+
        log_k      23.9926
        delta_h    -3.66     kcal
        -gamma      4.0      0

UO2+2 + 2PO4-3 + 4H+ = UO2(H2PO4)2
        log_k      46.6163
        delta_h    79.15     kcal
        -gamma      3.0      0

UO2+2 + 2PO4-3 + 5H+ = UO2(H2PO4)(H3PO4)+
        log_k      47.4362
        delta_h     0        kcal
        -gamma      4.0      0

UO2+2 + PO4-3 + 3H+ = UO2H3PO4+2
        log_k      23.6405
        delta_h     0        kcal
        -gamma      4.5      0

UO2+2 + PO4-3 = UO2PO4-
        log_k      14.8528
        delta_h     0        kcal
        -gamma      4.0      0

UO2+2 + SO4-2 = UO2SO4
        log_k       3.0632
        delta_h     4.738    kcal
        -gamma      3.0      0

UO2+2 + 2SO4-2 = UO2(SO4)2-2
        log_k       3.9796
        delta_h     8.523    kcal
        -gamma      4.0      0

V+2 + H2O = VOH+ + H+
        log_k      -5.64
        delta_h     0        kcal

V+3 + H2O = VOH+2 + H+
        log_k      -2.3
        delta_h 9.35     kcal

V+3 + 2H2O = V(OH)2+ + 2H+
        log_k      -5.83
        delta_h     0        kcal

V+3 + 3H2O = V(OH)3 + 3H+
        log_k     -11.02
        delta_h     0        kcal

2V+3 + 2H2O = V2(OH)2+4 + 2H+
        log_k      -3.75
        delta_h     0        kcal

2V+3 + 3H2O = V2(OH)3+3 + 3H+
        log_k      -7.5
        delta_h     0        kcal

V+3 + SO4-2 = VSO4+
        log_k       1.44
        delta_h     0        kcal

VO+2 + 2H2O = V(OH)3+ + H+
        log_k      -5.67
        delta_h     0        kcal

2VO+2 + 2H2O = H2V2O4+2 + 2H+
        log_k      -6.44
        delta_h     0        kcal

VO+2 + Cl- = VOCl+
        log_k       0.02
        delta_h     0        kcal

VO+2 + F- = VOF+
        log_k       3.34
        delta_h     1.9      kcal

VO+2 + 2F- = VOF2
        log_k       5.74
        delta_h     3.5      kcal

VO+2 + 3F- = VOF3-
        log_k       7.3
        delta_h     4.9      kcal

VO+2 + 4F- = VOF4-2
        log_k       8.11
        delta_h     6.4      kcal

VO+2 + SO4-2 = VOSO4
        log_k       2.45
        delta_h     3.72     kcal

VO2+ + 2H2O = H3VO4 + H+
        log_k      -3.3
        delta_h    10.63     kcal

VO2+ + 2H2O = H2VO4- + 2H+
        log_k      -7.09
        delta_h    11.33     kcal

VO2+ + 2H2O = HVO4-2 + 3H+
        log_k     -15.15
        delta_h    14.93     kcal

VO2+ + 2H2O = VO4-3 + 4H+
        log_k     -28.4
        delta_h    19.53     kcal

2VO2+ + 3H2O = V2O7-4 + 6H+
        log_k     -29.08
        delta_h     0        kcal

2VO2+ + 3H2O = HV2O7-3 + 5H+
        log_k     -16.32
        delta_h     0        kcal

2VO2+ + 3H2O = H3V2O7- + 3H+
        log_k      -3.79
        delta_h     0        kcal

3VO2+ + 3H2O = V3O9-3 + 6H+
        log_k     -15.88
        delta_h     0        kcal

4VO2+ + 4H2O = V4O12-4 + 8H+
        log_k     -20.79
        delta_h     0        kcal

10VO2+ + 8H2O = V10O28-6 + 16H+
        log_k     -17.53
        delta_h     0        kcal

10VO2+ + 8H2O = HV10O28-5 + 15H+
        log_k     -11.35
        delta_h    21.52     kcal

10VO2+ + 8H2O = H2V10O28-4 + 14H+
        log_k      -7.71
        delta_h     0        kcal

VO2+ + F- = VO2F
        log_k       3.12
        delta_h     0        kcal

VO2+ + 2F- = VO2F2-
        log_k       5.67
        delta_h     0        kcal

VO2+ + 3F- = VO2F3-2
        log_k       6.97
        delta_h     0        kcal

VO2+ + 4F- = VO2F4-3
        log_k       7.07
        delta_h     0        kcal

VO2+ + NO3- = VO2NO3
        log_k      -0.43
        delta_h     0        kcal

VO2+ + SO4-2 = VO2SO4-
        log_k       1.71
        delta_h     0        kcal

Zn+2 + Br- = ZnBr+
        log_k      -0.58
        delta_h     0        kcal

Zn+2 + 2Br- = ZnBr2
        log_k      -0.98
        delta_h     0        kcal

Zn+2 + CO3-2 = ZnCO3
        log_k       5.3
        delta_h     0        kcal

Zn+2 + 2CO3-2 = Zn(CO3)2-2
        log_k       9.63
        delta_h     0        kcal

Zn+2 + CO3-2 + H+ = ZnHCO3+
        log_k      12.4
        delta_h     0        kcal

Zn+2 + Cl- = ZnCl+
        log_k       0.43
        delta_h     7.79     kcal
        -gamma      4.0      0

Zn+2 + 2Cl- = ZnCl2
        log_k       0.45
        delta_h     8.5      kcal

Zn+2 + 3Cl- = ZnCl3-
        log_k       0.5
        delta_h     9.56     kcal
        -gamma      4.0      0

Zn+2 + 4Cl- = ZnCl4-2
        log_k       0.199
        delta_h    10.96     kcal
        -gamma      5.0      0

Zn+2 + F- = ZnF+
        log_k       1.15
        delta_h     2.22     kcal

Zn+2 + I- = ZnI+
        log_k      -2.91
        delta_h     0        kcal

Zn+2 + 2I- = ZnI2
        log_k      -1.69
        delta_h     0        kcal

Zn+2 + H2O = ZnOH+ + H+
        log_k      -8.96
        delta_h    13.399    kcal

Zn+2 + 2H2O = Zn(OH)2 + 2H+
        log_k     -16.899
        delta_h     0        kcal

Zn+2 + 3H2O = Zn(OH)3- + 3H+
        log_k     -28.399
        delta_h     0        kcal

Zn+2 + 4H2O = Zn(OH)4-2 + 4H+
        log_k     -41.199
        delta_h     0        kcal

Zn+2 + H2O + Cl- = ZnOHCl + H+
        log_k      -7.48
        delta_h     0        kcal

Zn+2 + 2HS- = Zn(HS)2
        log_k      14.94
        delta_h     0        kcal

Zn+2 + 3HS- = Zn(HS)3-
        log_k      16.1
        delta_h     0        kcal

Zn+2 + SO4-2 = ZnSO4
        log_k       2.37
        delta_h     1.36     kcal

Zn+2 + 2SO4-2 = Zn(SO4)2-2
        log_k       3.28
        delta_h     0        kcal

Zn+2 + SeO4-2 = ZnSeO4
        log_k       2.2019
        delta_h     0        kcal

Zn+2 + 2SeO4-2 = Zn(SeO4)2-2
        log_k      -0.0704
        delta_h     0        kcal

Zr+4 + F- = ZrF+3
        log_k       8.5835
        delta_h     0        kcal
        -gamma      5.0      0

Zr+4 + 2F- = ZrF2+2
        log_k      15.7377
        delta_h     0        kcal
        -gamma      4.5      0

Zr+4 + 3F- = ZrF3+
        log_k      21.2792
        delta_h     0        kcal
        -gamma      4.0      0

Zr+4 + 4F- = ZrF4
        log_k      25.9411
        delta_h     0        kcal
        -gamma      3.0      0

Zr+4 + 5F- = ZrF5-
        log_k      30.3098
        delta_h     0        kcal
        -gamma      4.0      0

Zr+4 + 6F- = ZrF6-2
        log_k      34.0188
        delta_h     0        kcal
        -gamma      4.0      0

Zr+4 + H2O = ZrOH+3 + H+
        log_k       0.0457
        delta_h     0        kcal
        -gamma      5.0      0

Zr+4 + 2H2O = Zr(OH)2+2 + 2H+
        log_k       0.2385
        delta_h     0        kcal
        -gamma      4.5      0

Zr+4 + 3H2O = Zr(OH)3+ + 3H+
        log_k      -0.6693
        delta_h     0        kcal
        -gamma      4.0      0

Zr+4 + 4H2O = Zr(OH)4 + 4H+
        log_k      -1.4666
        delta_h     0        kcal
        -gamma      3.0      0

Zr+4 + SO4-2 = ZrSO4+2
        log_k       3.6064
        delta_h     0        kcal
        -gamma      4.5      0

Zr+4 + 2SO4-2 = Zr(SO4)2
        log_k       6.2965
        delta_h     0        kcal
        -gamma      3.0      0

Zr+4 + 3SO4-2 = Zr(SO4)3-2
        log_k       7.3007
        delta_h     0        kcal
        -gamma      4.0      0

Acetate- + H+ = HAcetate
        log_k       4.76
        delta_h 0        kcal
        -gamma  0        0.06

Ag+ + Methylamine = AgMethylamine+
        log_k       3.18
        delta_h 0        kcal

Ag+ + Nta-3 = AgNta-2
        log_k       5.36
        delta_h 0        kcal

Ag+ + Edta-4 = AgEdta-3
        log_k       7.355
        delta_h 0        kcal

Ag+ + 2Edta-4 = AgEdta2-7
        log_k      11.355
        delta_h 0        kcal

Ag+ + 2Nbutylamine = AgNbutylamine2+
        log_k       7.77
        delta_h 0        kcal

Ag+ + Acetate- = AgAcetate
        log_k       0.73
        delta_h 0        kcal

Ag+ + 2Acetate- = AgAcetate2-
        log_k       0.64
        delta_h 0        kcal

Ag+ + Glycine- = AgGlycine
        log_k       3.51
        delta_h 0        kcal

Ag+ + 2Glycine- = AgGlycine2-
        log_k       3.38
        delta_h 0        kcal

Ag+ + Ethylenediamine = AgEthylenediamine+
        log_k       4.7
        delta_h 0        kcal

Ag+ + 2Ethylenediamine = AgEthylenediamine2+
        log_k       7.7
        delta_h 0        kcal

Ag+ + Ethylenediamine + H+ = AgEthylenediamineH+2
        log_k       7.31
        delta_h 0        kcal

Ag+ + Isopropylamine = AgIsopropylamine+
        log_k       3.19
        delta_h 0        kcal

Ag+ + Npropylamine = AgNpropylamine+
        log_k       3.47
        delta_h 0        kcal

Ag+ + 2Four_methylpyridine = AgFour_methylpyridine2+
        log_k       4.67
        delta_h 0        kcal

Ag+ + Diethylamine = AgDiethylamine+
        log_k       3.965
        delta_h 0        kcal

Ag+ + 2Diethylamine = AgDiethylamine2+
        log_k       7.02
        delta_h 0        kcal

Ag+ + Four_methylpyridine = AgFour_methylpyridine+
        log_k       2.21
        delta_h 0        kcal

Ag+ + 2Methylamine = AgMethylamine2+
        log_k       7.14
        delta_h 0        kcal

Ag+ + Hexylamine = AgHexylamine+
        log_k       3.66
        delta_h 0        kcal

Ag+ + 2Hexylamine = AgHexylamine2+
        log_k       7.35
        delta_h 0        kcal

Ag+ + Two_methylpyridine = AgTwo_methylpyridine+
        log_k       2.32
        delta_h 0        kcal

Ag+ + 2Isopropylamine = AgIsopropylamine2+
        log_k       6.85
        delta_h 0        kcal

Ag+ + Nbutylamine = AgNbutylamine+
        log_k       3.55
        delta_h 0        kcal

Ag+ + 2Npropylamine = AgNpropylamine2+
        log_k       7.51
        delta_h 0        kcal

Ag+ + Glutamate-2 = AgGlutamate-
        log_k       3.79
        delta_h 0        kcal

Ag+ + 2Glutamate-2 = AgGlutamate2-3
        log_k       6.55
        delta_h 0        kcal

Ag+ + 2Three_methylpyridine =
AgThree_methylpyridine2+
        log_k       4.46
        delta_h 0        kcal

Ag+ + Three_methylpyridine = AgThree_methylpyridine+
        log_k       2.2
        delta_h 0        kcal

Ag+ + 2Two_methylpyridine = AgTwo_methylpyridine2+
        log_k       4.68
        delta_h 0        kcal

Ag+ + Edta-4 + H+ = AgHEdta-2
        log_k       3.36
        delta_h 0        kcal

2Ag+ + 2Ethylenediamine = Ag2Ethylenediamine2+2
        log_k      12.73
        delta_h 0        kcal

2Ag+ + Ethylenediamine = Ag2Ethylenediamine+2
        log_k       1.43
        delta_h 0        kcal

Al+3 + Edta-4 + H+ = AlHEdta
        log_k      21.6
        delta_h 0        kcal

Al+3 + Edta-4 = AlEdta-
        log_k      18.9
        delta_h 0        kcal

Ba+2 + Salicylate-2 = BaSalicylate
        log_k       0.21
        delta_h 0        kcal

Ba+2 + Glycine- = BaGlycine+
        log_k       0.77
        delta_h 0        kcal

Ba+2 + Citrate-3 = BaCitrate-
        log_k       4.06
        delta_h 0        kcal

Ba+2 + Fe+3 + 6Cyanide- = BaFe(Cyanide)6-
        log_k      55.4356
        delta_h -69.68   kcal

Ba+2 + Edta-4 = BaEdta-2
        log_k       8
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        delta_h 0       kcal

Ba+2 + Phthalate-2 = BaPhthalate
        log_k   2.33
        delta_h 0       kcal

Ba+2 + Citrate-3 + H+ = BaCitrateH
        log_k   2.7
        delta_h 0       kcal

Ba+2 + Citrate-3 + 2H+ = BaCitrateH2+
        log_k   1.27
        delta_h 0       kcal

Ba+2 + Acetate- = BaAcetate+
        log_k   1.07
        delta_h 0       kcal

Ba+2 + Tartrate-2 = BaTartrate
        log_k   2.54
        delta_h 0       kcal

Ba+2 + Propanoate- = BaPropanoate+
        log_k   0.34
        delta_h 0       kcal

Ba+2 + Butanoate- = BaButanoate+
        log_k   0.94
        delta_h 0       kcal

Ba+2 + Glutamate-2 = BaGlutamate
        log_k   1.28
        delta_h 0       kcal

Benzoate- + Zn+2 = ZnBenzoate+
        log_k   1.4
        delta_h 0       kcal

Benzoate- + Mg+2 = MgBenzoate+
        log_k   0.1
        delta_h 0       kcal

Benzoate- + H+ = HBenzoate
        log_k   4.2
        delta_h 0       kcal

Benzoate- + Pb+2 = PbBenzoate+
        log_k   2.5
        delta_h 0       kcal

Benzoate- + Ca+2 = CaBenzoate+
        log_k   0.2
        delta_h 0       kcal

Benzoate- + Cd+2 = CdBenzoate+
        log_k   1.9
        delta_h 0       kcal

Benzoate- + Ni+2 = NiBenzoate+
        log_k   1.4
        delta_h 0       kcal

Benzoate- + Cu+2 = CuBenzoate+
        log_k   2.1
        delta_h 0       kcal

2Benzoate- + Cd+2 = CdBenzoate2
        log_k   1.65
        delta_h 0       kcal

Butanoate- + Fe+3 = FeButanoate+2
        log_k   5.56
        delta_h 0       kcal

Ca+2 + Phthalate-2 = CaPhthalate
        log_k   2.42
        delta_h 0       kcal

Ca+2 + Propanoate- = CaPropanoate+
        log_k   0.5
        delta_h 0       kcal

Ca+2 + Citrate-3 = CaCitrate-
        log_k   4.73
        delta_h 0       kcal

Ca+2 + H+ + Fe+2 + 6Cyanide- + e- =
CaHFe(Cyanide)6-2
        log_k   52.7097
        delta_h -82     kcal

Ca+2 + Isophthalate-2 = CaIsophthalate
        log_k   2
        delta_h 0       kcal

Ca+2 + Acetate- = CaAcetate+
        log_k   1.18
        delta_h 0       kcal

Ca+2 + Citrate-3 + H+ = CaCitrateH
        log_k   3.02
        delta_h 0       kcal

Ca+2 + Citrate-3 + 2H+ = CaCitrateH2+
        log_k   1.29
        delta_h 0       kcal

Ca+2 + Butanoate- = CaButanoate+
        log_k   0.51
        delta_h 0       kcal

Ca+2 + Ethylenediamine = CaEthylenediamine+2
        log_k   0.1
        delta_h 0       kcal

Ca+2 + Edta-4 + H+ = CaHEdta-
        log_k   16
        delta_h 0       kcal

Ca+2 + Edta-4 = CaEdta-2
        log_k   12.4
        delta_h 0       kcal

Cd+2 + Three_methylpyridine =
CdThree_methylpyridine+2
        log_k   1.62
        delta_h 0       kcal

Cd+2 + 2Nta-3 = CdNta2-4
        log_k   14.3
        delta_h 0       kcal

Cd+2 + Ethylenediamine = CdEthylenediamine+2
        log_k   5.61
        delta_h 0       kcal

Cd+2 + 3Glycine- = CdGlycine3-
        log_k   10.7
        delta_h 0       kcal

Cd+2 + 2Three_methylpyridine =
CdThree_methylpyridine2+2
        log_k   2.8
        delta_h 0       kcal

Cd+2 + Phthalate-2 = CdPhthalate
        log_k   2.5
        delta_h 0       kcal

Cd+2 + 2Glutamate-2 = CdGlutamate2-2
        log_k   2.78
        delta_h 0       kcal

Cd+2 + Glutamate-2 = CdGlutamate
        log_k   4.78
        delta_h 0       kcal

Cd+2 + 2Glycine- = CdGlycine2
        log_k   8.4
        delta_h 0       kcal

Cd+2 + Glycine- = CdGlycine+
        log_k   4.8
        delta_h 0       kcal

Cd+2 + 3Three_methylpyridine =
CdThree_methylpyridine3+2
        log_k   3.6
        delta_h 0       kcal

Cd+2 + 4Four_methylpyridine =
CdFour_methylpyridine4+2
        log_k   4
        delta_h 0       kcal

Cd+2 + 4Three_methylpyridine =
CdThree_methylpyridine4+2
        log_k   4
        delta_h 0       kcal

Cd+2 + 2Phthalate-2 = CdPhthalate2-2
        log_k   2.88
        delta_h 0       kcal

Cd+2 + 4Isopropylamine = CdIsopropylamine4+2
        log_k   6.9
        delta_h 0       kcal

Cd+2 + 3Isopropylamine = CdIsopropylamine3+2
        log_k   6.07
        delta_h 0       kcal

Cd+2 + 2Isopropylamine = CdIsopropylamine2+2
        log_k   4.57
        delta_h 0       kcal

Cd+2 + Isopropylamine = CdIsopropylamine+2
        log_k   2.55
        delta_h 0       kcal

Cd+2 + Tartrate-2 = CdTartrate
        log_k   3.9
        delta_h 0       kcal
        -gamma  0       0.02

Cd+2 + 3Four_methylpyridine =
CdFour_methylpyridine3+2
        log_k   2.9
        delta_h 0       kcal

Cd+2 + Four_methylpyridine = CdFour_methylpyridine+2
        log_k   1.51
        delta_h 0       kcal

Cd+2 + 2Npropylamine = CdNpropylamine2+2
        log_k   4.64
        delta_h 0       kcal

Cd+2 + Npropylamine = CdNpropylamine+2
        log_k   2.62
        delta_h 0       kcal

Cd+2 + 4Butanoate- = CdButanoate4-2
        log_k   1.98
        delta_h 0       kcal

Cd+2 + 3Butanoate- = CdButanoate3-
        log_k   2.34
        delta_h 0       kcal

Cd+2 + 2Butanoate- = CdButanoate2
        log_k   1.98
        delta_h 0       kcal

Cd+2 + 2Four_methylpyridine =
CdFour_methylpyridine2+2
        log_k   2.5
        delta_h 0       kcal

Cd+2 + 3Propanoate- = CdPropanoate3-
        log_k   2.345
        delta_h 0       kcal

Cd+2 + 2Propanoate- = CdPropanoate2
        log_k   1.86
        delta_h 0       kcal

Cd+2 + Propanoate- = CdPropanoate+
        log_k   1.19
        delta_h 0       kcal

Cd+2 + 4Diethylamine = CdDiethylamine4+2
        log_k   7.31
        delta_h 0       kcal

Cd+2 + 3Diethylamine = CdDiethylamine3+2
        log_k   6.36
        delta_h 0       kcal

Cd+2 + 2Diethylamine = CdDiethylamine2+2
        log_k   4.86
        delta_h 0       kcal

Cd+2 + Phthalate-2 + H+ = CdPhthalateH+
        log_k   5.88
        delta_h 0       kcal

Cd+2 + Nta-3 = CdNta-
        log_k   9.4
        delta_h 0       kcal

Cd+2 + Edta-4 = CdEdta-2
        log_k   16.275
        delta_h 0       kcal

Cd+2 + Diethylamine = CdDiethylamine+2
        log_k   2.62
        delta_h 0       kcal

Cd+2 + 4Acetate- = CdAcetate4-2
        log_k   2.04
        delta_h 0       kcal

Cd+2 + 3Acetate- = CdAcetate3-
        log_k   2.17
        delta_h 0       kcal

Cd+2 + 2Acetate- = CdAcetate2
        log_k   3.15
        delta_h 0       kcal

Cd+2 + Edta-4 + H+ = CdHEdta-
        log_k   2.9
        delta_h 0       kcal

Cd+2 + 2Citrate-3 = CdCitrate2-4
        log_k   5.34
        delta_h 0       kcal

Cd+2 + Citrate-3 + H+ = CdHCitrate
        log_k   3.37
        delta_h 0       kcal

Cd+2 + Citrate-3 + 2H+ = CdH2Citrate+
        log_k   2.05
        delta_h 0       kcal

Cd+2 + Citrate-3 = CdCitrate-
        log_k   5.3
        delta_h 0       kcal

Cd+2 + Butanoate- = CdButanoate+
        log_k   1.25
        delta_h 0       kcal

Cd+2 + Isovalerate- = CdIsovalerate+
        log_k   1.34
        delta_h 0       kcal

Cd+2 + 2Isovalerate- = CdIsovalerate2
        log_k   2.3
        delta_h 0       kcal

Cd+2 + 3Isovalerate- = CdIsovalerate3-
        log_k   2.5
        delta_h 0       kcal

Cd+2 + 3Npropylamine = CdNpropylamine3+2
        log_k   6.03
        delta_h 0       kcal

Cd+2 + Acetate- = CdAcetate+
        log_k   1.93
        delta_h 0       kcal
        -gamma  0       0.01

Cd+2 + 4Propanoate- = CdPropanoate4-2
        log_k   1.98
        delta_h 0       kcal

Cd+2 + 4Isovalerate- = CdIsovalerate4-2
        log_k   2
        delta_h 0       kcal

Cd+2 + 2Ethylenediamine = CdEthylenediamine2+2
        log_k   10.34
        delta_h 0       kcal

Cd+2 + 3Ethylenediamine = CdEthylenediamine3+2
        log_k   12.26
        delta_h 0       kcal

Cr(OH)2+ + Propanoate- + 2H+ = CrPropanoate+2 + 2H2O
        log_k   14.32
        delta_h 0       kcal

Cr(OH)2+ + 2Propanoate- + 2H+ = CrPropanoate2+ +
2H2O
        log_k   16.66
        delta_h 0       kcal
Cr(OH)2+ + 2Phthalate-2 + 2H+ = CrPhthalate2- + 2H2O
        log_k   19.62
        delta_h 0       kcal

Cr(OH)2+ + 2Acetate- + 2H+ = CrAcetate2+ + 2H2O
        log_k   16.68
        delta_h 0       kcal

Cr(OH)2+ + Acetate- + 2H+ = CrAcetate+2 + 2H2O
        log_k   14.25
        delta_h 0       kcal

Cr(OH)2+ + 3Phthalate-2 + 2H+ = CrPhthalate3-3 +
2H2O
        log_k   22.1
        delta_h 0       kcal

Cr(OH)2+ + Phthalate-2 + 2H+ = CrPhthalate+ + 2H2O
        log_k   15.14
        delta_h 0       kcal

Cr(OH)2+ + 3Acetate- + 2H+ = CrAcetate3 + 2H2O
        log_k   19.2
        delta_h 0       kcal

Cr(OH)2+ + 3Propanoate- + 2H+ = CrPropanoate3 + 2H2O
        log_k   19.32
        delta_h 0       kcal

Cr+2 + Acetate- = CrAcetate+
        log_k   1.8
        delta_h 0       kcal

Cr+2 + Edta-4 = CrEdta-2
        log_k   13.61
        delta_h 0       kcal

Cr+2 + Edta-4 + H+ = CrHEdta-
        log_k   6.1
        delta_h 0       kcal

Cr+2 + 2Acetate- = CrAcetate2
        log_k   2.92
        delta_h 0       kcal

Cu+2 + 2Valerate- = CuValerate2
        log_k   3
        delta_h 0       kcal

Cu+2 + Ethylenediamine = CuEthylenediamine+2
        log_k   10.49
        delta_h 0       kcal

Cu+2 + 4Propanoate- = CuPropanoate4-2
        log_k   2.7
        delta_h 0       kcal

Cu+2 + Propanoate- = CuPropanoate+
        log_k   2.22
        delta_h 0       kcal

Cu+2 + Valerate- = CuValerate+
        log_k   2.12
        delta_h 0       kcal

Cu+2 + Phthalate-2 + H+ = CuPhthalateH+
        log_k   6.74
        delta_h 0       kcal
        -gamma  4       0

Cu+2 + 2Isobutyrate- = CuIsobutyrate2
        log_k   2.7
        delta_h 0       kcal

Cu+2 + Isobutyrate- = CuIsobutyrate+
        log_k   2.17
        delta_h 0       kcal

Cu+2 + 4Butanoate- = CuButanoate4-2
        log_k   2.95
        delta_h 0       kcal

Cu+2 + 2Acetate- = CuAcetate2
        log_k   3.63
        delta_h 0       kcal

Cu+2 + Edta-4 + H+ = CuHEdta-
        log_k   11.195
        delta_h 0       kcal

Cu+2 + Phthalate-2 = CuPhthalate
        log_k   4.04
        delta_h 0       kcal

Cu+2 + Isovalerate- = CuIsovalerate+
        log_k   2.08
        delta_h 0       kcal

Cu+2 + Citrate-3 + 2H+ = CuH2Citrate+
        log_k   2.2
        delta_h 0       kcal

Cu+2 + Citrate-3 + H+ = CuHCitrate
        log_k   4.27
        delta_h 0       kcal

Cu+2 + 2Citrate-3 = CuCitrate2-4
        log_k   8.72
        delta_h 0       kcal

Cu+2 + Citrate-3 = CuCitrate-
        log_k   7.26
        delta_h 0       kcal

Cu+2 + 3Butanoate- = CuButanoate3-
        log_k   2.3
        delta_h 0       kcal

Cu+2 + 5Four_methylpyridine =
CuFour_methylpyridine5+2
        log_k   8.3
        delta_h 0       kcal

Cu+2 + 4Four_methylpyridine =
CuFour_methylpyridine4+2
        log_k   8.08
        delta_h 0       kcal

Cu+2 + 3Four_methylpyridine =
CuFour_methylpyridine3+2
        log_k   6.77
        delta_h 0       kcal
Cu+2 + 2Four_methylpyridine =
CuFour_methylpyridine2+2
        log_k   5.16
        delta_h 0       kcal

Cu+2 + Four_methylpyridine = CuFour_methylpyridine+2
        log_k   2.88
        delta_h 0       kcal

Cu+2 + 4Three_methylpyridine =
CuThree_methylpyridine4+2
        log_k   7.2
        delta_h 0       kcal

Cu+2 + 3Three_methylpyridine =
CuThree_methylpyridine3+2
        log_k   6.3
        delta_h 0       kcal

Cu+2 + 2Butanoate- = CuButanoate2
        log_k   2.6
        delta_h 0       kcal

Cu+2 + 2Three_methylpyridine =
CuThree_methylpyridine2+2
        log_k   4.8
        delta_h 0       kcal

Cu+2 + Butanoate- = CuButanoate+
        log_k   2.14
        delta_h 0       kcal

Cu+2 + 3Dimethylamine = CuDimethylamine3+2
        log_k   7.26
        delta_h 0       kcal

Cu+2 + 2Dimethylamine = CuDimethylamine2+2
        log_k   5.66
        delta_h 0       kcal

Cu+2 + Dimethylamine = CuDimethylamine+2
        log_k   3.21
        delta_h 0       kcal

Cu+2 + 2Methylamine = CuMethylamine2+2
        log_k   7.51
        delta_h 0       kcal

Cu+2 + 2Ethylenediamine = CuEthylenediamine2+2
        log_k   19.62
        delta_h 0       kcal

Cu+2 + 3Propanoate- = CuPropanoate3-
        log_k   2.3
        delta_h 0       kcal

Cu+2 + 2Propanoate- = CuPropanoate2
        log_k   2.62
        delta_h 0       kcal

Cu+2 + 2Nta-3 = CuNta2-4
        log_k   17.5
        delta_h 0       kcal

Cu+2 + 4Acetate- = CuAcetate4-2
        log_k   2.9
        delta_h 0       kcal

Cu+2 + 3Acetate- = CuAcetate3-
        log_k   3.1
        delta_h 0       kcal

Cu+2 + Nta-3 = CuNta-
        log_k   13.1
        delta_h 0       kcal

Cu+2 + Edta-4 = CuEdta-2
        log_k   18.785
        delta_h 0       kcal

Cu+2 + 4Methylamine = CuMethylamine4+2
        log_k   12.08
        delta_h 0       kcal

Cu+2 + 3Methylamine = CuMethylamine3+2
        log_k   10.21
        delta_h 0       kcal

Cu+2 + Methylamine = CuMethylamine+2
        log_k   4.11
        delta_h 0       kcal

Cu+2 + Three_methylpyridine =
CuThree_methylpyridine+2
        log_k   2.74
        delta_h 0       kcal

Cyanate- + H+ = HCyanate
        log_k   3.445
        delta_h -2      kcal
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2Cyanate- + Ag+ = Ag(Cyanate)2-
        log_k   5.0034
        delta_h 0       kcal

Cyanide- + 2I- = I2Cyanide- + 2e-
        log_k   -11.848
        delta_h 0       kcal

Cyanide- + Hg(OH)2 + 2H+ = HgCyanide+ + 2H2O
        log_k   24.1738
        delta_h -33.83  kcal

Cyanide- + Cd+2 = CdCyanide+
        log_k   5.32
        delta_h 0       kcal

Cyanide- + Ag+ + H2O = Ag(Cyanide)OH- + H+
        log_k   -0.56
        delta_h 0       kcal

Cyanide- + H+ = HCyanide
        log_k   9.2356
        delta_h -10.4   kcal


2Cyanide- + Ag+ = Ag(Cyanide)2-
        log_k   20.3814
        delta_h -32.675 kcal

2Cyanide- + I- = I(Cyanide)2- + 2e-
        log_k   -11.458
        delta_h 0       kcal
2Cyanide- + Ni+2 = Ni(Cyanide)2
        log_k   14.5864
        delta_h 0       kcal

2Cyanide- + Hg(OH)2 + 2H+ = Hg(Cyanide)2 + 2H2O
        log_k   40.6513
        delta_h -57.24  kcal

2Cyanide- + Cl- + Hg(OH)2 + 2H+ = Hg(Cyanide)2Cl- +
2H2O
        log_k   40.3735
        delta_h 0       kcal

2Cyanide- + Cd+2 = Cd(Cyanide)2
        log_k   10.3703
        delta_h -13     kcal

2Cyanide- + Zn+2 = Zn(Cyanide)2
        log_k   11.071
        delta_h -10.999 kcal

2Cyanide- + Cu+ = Cu(Cyanide)2-
        log_k   24.0272
        delta_h -29.1   kcal

3Cyanide- + Br- + Hg(OH)2 + 2H+ = Hg(Cyanide)3Br-2 +
2H2O
        log_k   44.9415
        delta_h 0       kcal

3Cyanide- + Cl- + Hg(OH)2 + 2H+ = Hg(Cyanide)3Cl-2 +
2H2O
        log_k   43.8332
        delta_h 0       kcal

3Cyanide- + Cu+ = Cu(Cyanide)3-2
        log_k   28.6524
        delta_h -40.2   kcal

3Cyanide- + Zn+2 = Zn(Cyanide)3-
        log_k   16.048
        delta_h -20.199 kcal

3Cyanide- + Ag+ = Ag(Cyanide)3-2
        log_k   21.4002
        delta_h -33.495 kcal

3Cyanide- + Hg(OH)2 + 2H+ = Hg(Cyanide)3- + 2H2O
        log_k   44.4042
        delta_h -64.83  kcal

3Cyanide- + Cd+2 = Cd(Cyanide)3-
        log_k   14.8341
        delta_h -21.6   kcal

3Cyanide- + Ni+2 = Ni(Cyanide)3-
        log_k   22.6346
        delta_h 0       kcal

4Cyanide- + Ni+2 + H+ = NiH(Cyanide)4-
        log_k   36.7482
        delta_h 0       kcal

4Cyanide- + Ni+2 + 2H+ = NiH2Cyanide4
        log_k   41.4576
        delta_h 0       kcal

4Cyanide- + Cd+2 = Cd(Cyanide)4-2
        log_k   18.2938
        delta_h -23.56  kcal

4Cyanide- + Zn+2 = Zn(Cyanide)4-2
        log_k   16.715
        delta_h -25.539 kcal

4Cyanide- + Cu+ = Cu(Cyanide)4-3
        log_k   30.3456
        delta_h -51.4   kcal

4Cyanide- + Hg(OH)2 + 2H+ = Hg(Cyanide)4-2 + 2H2O
        log_k   47.4094
        delta_h -69.93  kcal

4Cyanide- + Ni+2 + 3H+ = NiH3(Cyanide)4+
        log_k   43.9498
        delta_h 0       kcal

4Cyanide- + Ni+2 = Ni(Cyanide)4-2
        log_k   30.1257
        delta_h -43.19  kcal

4Cyanide- + Tl+ = Tl(Cyanide)4- + 2e-
        log_k   -8.0189
        delta_h 0       kcal

6Cyanide- + 2Fe+3 = Fe2(Cyanide)6
        log_k   56.9822
        delta_h 0       kcal

6Cyanide- + Mg+2 + Fe+2 = MgFe(Cyanide)6-2
        log_k   49.4251
        delta_h 0       kcal

6Cyanide- + Mg+2 + Fe+3 = MgFe(Cyanide)6-
        log_k   55.3916
        delta_h -69.31  kcal

6Cyanide- + Fe+2 + Ba+2 = BaFe(Cyanide)6-2
        log_k   49.4032
        delta_h 0       kcal

6Cyanide- + Fe+3 = Fe(Cyanide)6-3
        log_k   52.6283
        delta_h -70.1   kcal

6Cyanide- + 2H+ + Fe+2 = H2Fe(Cyanide)6-2
        log_k   52.445
        delta_h -83.1   kcal

6Cyanide- + Fe+2 + H+ = HFe(Cyanide)6-3
        log_k   49.9969
        delta_h -84.16  kcal

6Cyanide- + Fe+2 = Fe(Cyanide)6-4
        log_k   45.6063
        delta_h -85.8   kcal

6Cyanide- + 2K+ + 2H+ + Fe+2 = K2H2Fe(Cyanide)6
        log_k   52.3058
        delta_h -85.86  kcal

6Cyanide- + 2Ca+2 + Fe+2 = Ca2Fe(Cyanide)6
        log_k   50.9952
        delta_h -83.7   kcal

6Cyanide- + Ca+2 + Fe+2 = CaFe(Cyanide)6-2
        log_k   49.6898
        delta_h -83.1   kcal

6Cyanide- + Ca+2 + Fe+3 = CaFe(Cyanide)6-
        log_k   55.473
        delta_h -69.5   kcal

6Cyanide- + Tl+ + Fe+2 = TlFe(Cyanide)6-3
        log_k   48.7508
        delta_h -84.88  kcal

6Cyanide- + 3K+ + H+ + Fe+2 = K3HFe(Cyanide)6
        log_k   50.2241
        delta_h -85.99  kcal

6Cyanide- + Li+ + Fe+2 = LiFe(Cyanide)6-3
        log_k   47.6858
        delta_h -80.149 kcal

Fe+2 + 3Ethylenediamine = FeEthylenediamine3+2
        log_k   9.68
        delta_h 0       kcal

Fe+2 + Edta-4 = FeEdta-2
        log_k   16.1
        delta_h 0       kcal

Fe+2 + Citrate-3 + H+ = FeCitrateH
        log_k   3.5
        delta_h 0       kcal

Fe+2 + Edta-4 + H2O = FeOHEdta-3 + H+
        log_k   6.4
        delta_h 0       kcal

Fe+2 + Edta-4 + H+ = FeHEdta-
        log_k   19.3
        delta_h 0       kcal

Fe+2 + Citrate-3 = FeCitrate-
        log_k   5.7
        delta_h 0       kcal

Fe+2 + Acetate- = FeAcetate+
        log_k   1.4
        delta_h 0       kcal

Fe+2 + Edta-4 + 2H2O = Fe(OH)2Edta-4 + 2H+
        log_k   -4.3
        delta_h 0       kcal

Fe+2 + 2Ethylenediamine = FeEthylenediamine2+2
        log_k   7.65
        delta_h 0       kcal

Fe+2 + Ethylenediamine = FeEthylenediamine+2
        log_k   4.36
        delta_h 0       kcal

Fe+3 + Edta-4 + 2H2O = Fe(OH)2Edta-3 + 2H+
        log_k   9.7
        delta_h 0       kcal

Fe+3 + Citrate-3 = FeCitrate
        log_k   12.55
        delta_h 0       kcal

Fe+3 + Acetate- = FeAcetate+2
        log_k   3.21
        delta_h 0       kcal

Fe+3 + 2Acetate- = FeAcetate2+
        log_k   6.5
        delta_h 0       kcal

Fe+3 + Edta-4 + H2O = FeOHEdta-2 + H+
        log_k   19.8
        delta_h 0       kcal

Fe+3 + 3Acetate- = FeAcetate3
        log_k   8.3
        delta_h 0       kcal

Fe+3 + Edta-4 + H+ = FeHEdta
        log_k   29.2
        delta_h 0       kcal

Fe+3 + Edta-4 = FeEdta-
        log_k   27.7
        delta_h 0       kcal

Fe+3 + Citrate-3 + H+ = FeCitrateH+
        log_k   19.8
        delta_h 0       kcal

Glutamate-2 + 2H+ = H2Glutamate
        log_k   14.37
        delta_h 0       kcal
        -gamma  0       0.01

Glutamate-2 + H+ = HGlutamate-
        log_k   9.95
        delta_h 0       kcal
        -gamma  0       0.01

Glycine- + H+ = HGlycine
        log_k   9.78
        delta_h 0       kcal
        -gamma  0       0.07

Glycine- + 2H+ = H2Glycine+
        log_k   12.12
        delta_h 0       kcal
        -gamma  0       0.07

H+ + Isovalerate- = IsovalerateH
        log_k   4.781
        delta_h 0       kcal

H+ + Diethylamine = DiethylamineH+
        log_k   10.774
        delta_h 0       kcal

H+ + Butanoate- = ButanoateH
        log_k   4.73
        delta_h 0       kcal

H+ + Trimethylamine = TrimethylamineH+
        log_k   9.8
        delta_h 0       kcal

H+ + Edta-4 = EdtaH-3
        log_k   9.96
        delta_h 0       kcal

H+ + Nta-3 = NtaH-2
        log_k   10.334
        delta_h 0       kcal

H+ + Isobutyrate- = IsobutyrateH
        log_k   4.849
        delta_h 0       kcal

H+ + Formate- = FormateH
        log_k   3.745
        delta_h 0       kcal

H+ + Npropylamine = NpropylamineH+
        log_k   10.8
        delta_h 0       kcal

H+ + Four_methylpyridine = Four_methylpyridineH+
        log_k   6
        delta_h 0       kcal

H+ + Three_methylpyridine = Three_methylpyridineH+
        log_k   5.7
        delta_h 0       kcal

H+ + Two_methylpyridine = Two_methylpyridineH+
        log_k   5.95
        delta_h 0       kcal

H+ + Citrate-3 = CitrateH-2
        log_k   6.33
        delta_h 0       kcal

H+ + Valerate- = ValerateH
        log_k   4.843
        delta_h 0       kcal

H+ + Ethylenediamine = HEthylenediamine+
        log_k   9.96
        delta_h 0       kcal

H+ + Methylamine = MethylamineH+
        log_k   10.72
        delta_h 0       kcal

H+ + Hexylamine = HexylamineH+
        log_k   10.63
        delta_h 0       kcal

H+ + Propanoate- = PropanoateH
        log_k   4.874
        delta_h 0       kcal

2H+ + Butanoate- + Cr(OH)2+ = CrButanoate+2 + 2H2O
        log_k   12.74
        delta_h 0       kcal

2H+ + Isobutyrate- + Cr(OH)2+ = CrIsobutyrate+2 +
2H2O
        log_k   12.73
        delta_h 0       kcal

2H+ + Nta-3 = NtaH2-
        log_k   13.27
        delta_h 0       kcal

2H+ + Isovalerate- + Hg(OH)2 = HgIsovalerate+ + 2H2O
        log_k   10.717
        delta_h 0       kcal

2H+ + Isovalerate- + Cr(OH)2+ = CrIsovalerate+2 +
2H2O
        log_k   12.76
        delta_h 0       kcal

2H+ + Valerate- + Cr(OH)2+ = CrValerate+2 + 2H2O
        log_k   12.75
        delta_h 0       kcal

2H+ + Edta-4 = EdtaH2-2
        log_k   16.21
        delta_h 0       kcal

2H+ + Isobutyrate- + Hg(OH)2 = HgIsobutyrate+ + 2H2O
        log_k   10.687
        delta_h 0       kcal

2H+ + Ethylenediamine = H2Ethylenediamine+2
        log_k   16.85
        delta_h 0       kcal

2H+ + Citrate-3 = CitrateH2-
        log_k   11.05
        delta_h 0       kcal

2H+ + Phthalate-2 + Hg(OH)2 = HgPhthalate + 2H2O
        log_k   10.997
        delta_h 0       kcal

2H+ + Valerate- + Hg(OH)2 = HgValerate+ + 2H2O
        log_k   10.727
        delta_h 0       kcal

2H+ + Butanoate- + Hg(OH)2 = HgButanoate+ + 2H2O
        log_k   10.097
        delta_h 0       kcal

3H+ + Glutamate-2 = GlutamateH3+
        log_k   16.6
        delta_h 0       kcal

3H+ + Citrate-3 = CitrateH3
        log_k   14.18
        delta_h 0       kcal

3H+ + Nta-3 = NtaH3
        log_k   14.12
        delta_h 0       kcal

3H+ + Edta-4 = EdtaH3-
        log_k   18.86
        delta_h 0       kcal

4H+ + Nta-3 = NtaH4+
        log_k   16.224
        delta_h 0       kcal

4H+ + Edta-4 = EdtaH4
        log_k   20.93
        delta_h 0       kcal

5H+ + Edta-4 = EdtaH5+
        log_k   23.464
        delta_h 0       kcal

Hg(OH)2 + 3Acetate- + 2H+ = HgAcetate3- + 2H2O
        log_k   19.38
        delta_h 0       kcal

Hg(OH)2 + Acetate- + 2H+ = HgAcetate+ + 2H2O
        log_k   9.417
        delta_h 0       kcal

Hg(OH)2 + 4Acetate- + 2H+ = HgAcetate4-2 + 2H2O
        log_k   23.16
        delta_h 0       kcal

Hg(OH)2 + 2Propanoate- + 2H+ = HgPropanoate2 + 2H2O
        log_k   13.107
        delta_h 0       kcal

Hg(OH)2 + 2Acetate- + 2H+ = HgAcetate2 + 2H2O
        log_k   13.11
        delta_h 0       kcal

Hg(OH)2 + Propanoate- + 2H+ = HgPropanoate+ + 2H2O
        log_k   9.417
        delta_h 0       kcal

Hg2+2 + Glycine- = Hg2Glycine+
        log_k   10.8
        delta_h 0       kcal

Hg2+2 + 2Glycine- = Hg2Glycine2
        log_k   20
        delta_h 0       kcal

0.5Hg2+2 + 2Acetate- = HgAcetate2-
        log_k   13.26
        delta_h 0       kcal

0.5Hg2+2 + Acetate- = HgAcetate
        log_k   7.14
        delta_h 0       kcal

0.5Hg2+2 + Propanoate- = HgPropanoate
        log_k   3.72
        delta_h 0       kcal

0.5Hg2+2 + 2Formate- = HgFormate2-
        log_k   5.45
        delta_h 0       kcal

0.5Hg2+2 + Formate- = HgFormate
        log_k   2.94
        delta_h 0       kcal

0.5Hg2+2 + 2Propanoate- = HgPropanoate2-
        log_k   6.99
        delta_h 0       kcal

Isobutyrate- + Ni+2 = NiIsobutyrate+
        log_k   1.23
        delta_h 0       kcal

Isobutyrate- + Pb+2 = PbIsobutyrate+
        log_k   2.67
        delta_h 0       kcal

Isobutyrate- + Fe+3 = FeIsobutyrate+2
        log_k   3.6
        delta_h 0       kcal

Isobutyrate- + Cd+2 = CdIsobutyrate+
        log_k   1.17
        delta_h 0       kcal

Isobutyrate- + Ba+2 = BaIsobutyrate+
        log_k   0.64
        delta_h 0       kcal

Isophthalate-2 + Pb+2 = PbIsophthalate
        log_k   2.17
        delta_h 0       kcal

Isophthalate-2 + Pb+2 + H+ = PbIsophthalateH+
        log_k   6.28
        delta_h 0       kcal

Isophthalate-2 + H+ = HIsophthalate-
        log_k   3.5
        delta_h 0       kcal

Isophthalate-2 + 2H+ = H2Isophthalate
        log_k   8
        delta_h 0       kcal

Isophthalate-2 + Cd+2 = CdIsophthalate
        log_k   1.33
        delta_h 0       kcal

Isophthalate-2 + Ba+2 = BaIsophthalate
        log_k   1.55
        delta_h 0       kcal

2Isophthalate-2 + Cd+2 = CdIsophthalate2-2
        log_k   2.17
        delta_h 0       kcal

2Isophthalate-2 + Pb+2 = PbIsophthalate2-2
        log_k   3.36
        delta_h 0       kcal

2Isophthalate-2 + Cd+2 + H+ = CdIsophthalate2H-
        log_k   5.32
        delta_h 0       kcal

Isovalerate- + Fe+3 = FeIsovalerate+2
        log_k   5.58
        delta_h 0       kcal

Isovalerate- + Pb+2 = PbIsovalerate+
        log_k   2.05
        delta_h 0       kcal

Isovalerate- + Ni+2 = NiIsovalerate+
        log_k   1.27
        delta_h 0       kcal

Isovalerate- + Ba+2 = BaIsovalerate+
        log_k   0.68
        delta_h 0       kcal

K+ + Edta-4 = KEdta-3
        log_k   1.7
        delta_h 0       kcal

K+ + H+ + Fe+2 + 6Cyanide- = KHFe(Cyanide)6-2
        log_k   51.4702
        delta_h -78.1   kcal

K+ + Fe+2 + 6Cyanide- = KFe(Cyanide)6-3
        log_k   48.1204
        delta_h -84     kcal

2K+ + Fe+2 + 6Cyanide- = K2Fe(Cyanide)6-2
        log_k   48.978
        delta_h -77.3   kcal

Li+ + H+ + Fe+2 + 6Cyanide- = LiHFe(Cyanide)6-2
        log_k   51.2188
        delta_h -80.999 kcal

2Li+ + Fe+2 + 6Cyanide- = Li2Fe(Cyanide)6-2
        log_k   48.5338
        delta_h -83.498 kcal

Mg+2 + Acetate- = MgAcetate+
        log_k   1.27
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        delta_h 0       kcal

Mg+2 + Ethylenediamine = MgEthylenediamine+2
        log_k   0.37
        delta_h 0       kcal

Mg+2 + Edta-4 + H+ = MgHEdta-
        log_k   15.1
        delta_h 0       kcal

Mg+2 + Butanoate- = MgButanoate+
        log_k   0.53
        delta_h 0       kcal

Mg+2 + Citrate-3 + 2H+ = MgCitrateH2+
        log_k   11.59
        delta_h 0       kcal

Mg+2 + Propanoate- = MgPropanoate+
        log_k   0.54
        delta_h 0       kcal

Mg+2 + Citrate-3 = MgCitrate-
        log_k   3.37
        delta_h 0       kcal

Mg+2 + Citrate-3 + H+ = MgCitrateH
        log_k   8.17
        delta_h 0       kcal

Mg+2 + Edta-4 = MgEdta-2
        log_k   10.6
        delta_h 0       kcal

Mn+2 + Citrate-3 + H+ = MnCitrateH
        log_k   3.02
        delta_h 0       kcal

Mn+2 + Ethylenediamine = MnEthylenediamine+2
        log_k   2.67
        delta_h 0       kcal

Mn+2 + Acetate- = MnAcetate+
        log_k   1.4
        delta_h 0       kcal

Mn+2 + Citrate-3 = MnCitrate-
        log_k   5.28
        delta_h 0       kcal

Mn+2 + 2Ethylenediamine = MnEthylenediamine2+2
        log_k   4.2
        delta_h 0       kcal

Na+ + Edta-4 = NaEdta-3
        log_k   2.5
        delta_h 0       kcal

Na+ + Fe+2 + 6Cyanide- = NaFe(Cyanide)6-3
        log_k   47.9885
        delta_h -84.9   kcal

Na+ + H+ + Fe+2 + 6Cyanide- = NaHFe(Cyanide)6-2
        log_k   51.4335
        delta_h -85.6   kcal

Na+ + Acetate- = NaAcetate
        log_k   -0.18
        delta_h 0       kcal

Na+ + Phthalate-2 = NaPhthalate-
        log_k   0.7
        delta_h 0       kcal

2Na+ + Fe+2 + 6Cyanide- = Na2Fe(Cyanide)6-2
        log_k   48.7435
        delta_h -85     kcal

NH4+ + Fe+2 + 6Cyanide- = NH4Fe(Cyanide)6-3
        log_k   48.0684
        delta_h -84.5   kcal

NH4+ + H+ + Fe+2 + 6Cyanide- = NH5Fe(Cyanide)6-2
        log_k   51.4035
        delta_h -83.9   kcal

2NH4+ + Fe+2 + 6Cyanide- = (NH4)2FeCyanide6-2
        log_k   48.8666
        delta_h -83     kcal

Ni+2 + 4Four_methylpyridine =
NiFour_methylpyridine4+2
        log_k   4.7
        delta_h 0       kcal
        -gamma  0       0.04

Ni+2 + 3Four_methylpyridine =
NiFour_methylpyridine3+2
        log_k   4.34
        delta_h 0       kcal

Ni+2 + 2Four_methylpyridine =
NiFour_methylpyridine2+2
        log_k   3.59
        delta_h 0       kcal

Ni+2 + Diethylamine = NiDiethylamine1+2
        log_k   2.78
        delta_h 0       kcal

Ni+2 + 4Diethylamine = NiDiethylamine4+2
        log_k   7.93
        delta_h 0       kcal

Ni+2 + 3Diethylamine = NiDiethylamine3+2
        log_k   6.72
        delta_h 0       kcal

Ni+2 + 2Diethylamine = NiDiethylamine2+2
        log_k   4.97
        delta_h 0       kcal

Ni+2 + 4Three_methylpyridine =
NiThree_methylpyridine4+2
        log_k   4.6
        delta_h 0       kcal

Ni+2 + 3Three_methylpyridine =
NiThree_methylpyridine3+2
        log_k   4.1
        delta_h 0       kcal

Ni+2 + 2Three_methylpyridine =
NiThree_methylpyridine2+2
        log_k   3.3
        delta_h 0       kcal

Ni+2 + Three_methylpyridine =
NiThree_methylpyridine+2
        log_k   2.02
        delta_h 0       kcal

Ni+2 + Two_methylpyridine = NiTwo_methylpyridine+2
        log_k   0.4
        delta_h 0       kcal

Ni+2 + 5Diethylamine = NiDiethylamine5+2
        log_k   8.87
        delta_h 0       kcal

Ni+2 + Four_methylpyridine = NiFour_methylpyridine+2
        log_k   2.11
        delta_h 0       kcal

Ni+2 + Edta-4 + H+ = NiHEdta-
        log_k   11.56
        delta_h 0       kcal
Ni+2 + Npropylamine = NiNpropylamine+2
        log_k   2.81
        delta_h 0       kcal

Ni+2 + 3Ethylenediamine = NiEthylenediamine3+2
        log_k   17.54
        delta_h 0       kcal

Ni+2 + 2Ethylenediamine = NiEthylenediamine2+2
        log_k   13.36
        delta_h 0       kcal

Ni+2 + 5Isopropylamine = NiIsopropylamine5+2
        log_k   8.43
        delta_h 0       kcal

Ni+2 + 4Isopropylamine = NiIsopropylamine4+2
        log_k   7.83
        delta_h 0       kcal

Ni+2 + 3Isopropylamine = NiIsopropylamine3+2
        log_k   6.57
        delta_h 0       kcal

Ni+2 + 2Isopropylamine = NiIsopropylamine2+2
        log_k   4.86
        delta_h 0       kcal

Ni+2 + Isopropylamine = NiIsopropylamine+2
        log_k   2.71
        delta_h 0       kcal

Ni+2 + 4Npropylamine = NiNpropylamine4+2
        log_k   8.31
        delta_h 0       kcal

Ni+2 + 3Npropylamine = NiNpropylamine3+2
        log_k   6.79
        delta_h 0       kcal

Ni+2 + 2Npropylamine = NiNpropylamine2+2
        log_k   5.02
        delta_h 0       kcal

Ni+2 + Ethylenediamine = NiEthylenediamine+2
        log_k   7.24
        delta_h 0       kcal

Ni+2 + 3Butanoate- = NiButanoate3-
        log_k   1.34
        delta_h 0       kcal

Ni+2 + 2Butanoate- = NiButanoate2
        log_k   0.85
        delta_h 0       kcal

Ni+2 + Butanoate- = NiButanoate+
        log_k   0.77
        delta_h 0       kcal

Ni+2 + 3Propanoate- = NiPropanoate3-
        log_k   0.97
        delta_h 0       kcal

Ni+2 + 2Propanoate- = NiPropanoate2
        log_k   0.8
        delta_h 0       kcal

Ni+2 + Propanoate- = NiPropanoate+
        log_k   0.73
        delta_h 0       kcal

Ni+2 + 3Glycine- = NiGlycine3-
        log_k   14.2
        delta_h 0       kcal

Ni+2 + Edta-4 = NiEdta-2
        log_k   20.33
        delta_h 0       kcal

Ni+2 + Citrate-3 + 2H+ = NiCitrateH2+
        log_k   2.13
        delta_h 0       kcal

Ni+2 + Citrate-3 + H+ = NiCitrateH
        log_k   4.09
        delta_h 0       kcal

Ni+2 + Citrate-3 = NiCitrate-
        log_k   6.62
        delta_h 0       kcal

Para_acetate- + 2H+ = H2Para_acetate+
        log_k   4.31
        delta_h 0       kcal

Para_acetate- + Zn+2 = ZnPara_acetate+
        log_k   1.67
        delta_h 0       kcal

Para_acetate- + Cd+2 = CdPara_acetate+
        log_k   1.15
        delta_h 0       kcal

Para_acetate- + Cu+2 = CuPara_acetate+
        log_k   1.97
        delta_h 0       kcal

Para_acetate- + Ni+2 = NiPara_acetate+
        log_k   0.65
        delta_h 0       kcal

2Para_acetate- + Ni+2 = NiPara_acetate2
        log_k   0.99
        delta_h 0       kcal

2Para_acetate- + Cd+2 = CdPara_acetate2
        log_k   1.92
        delta_h 0       kcal

Pb+2 + 2Propanoate- = PbPropanoate2
        log_k   4.15
        delta_h 0       kcal

Pb+2 + Edta-4 = PbEdta-2
        log_k   17.88
        delta_h 0       kcal

Pb+2 + Butanoate- = PbButanoate+
        log_k   2.125
        delta_h 0       kcal

Pb+2 + 2Butanoate- = PbButanoate2
        log_k   3.735
        delta_h 0       kcal

Pb+2 + Propanoate- = PbPropanoate+
        log_k   2.64
        delta_h 0       kcal

Pb+2 + Acetate- = PbAcetate+
        log_k   2.87
        delta_h 0       kcal

Pb+2 + Edta-4 + 2H+ = PbH2Edta
        log_k   6.22
        delta_h 0       kcal

Pb+2 + Edta-4 + H+ = PbHEdta-
        log_k   9.68
        delta_h 0       kcal

Pb+2 + Nta-3 + H+ = PbHNta
        log_k   3.795
        delta_h 0       kcal

Pb+2 + 3Acetate- = PbAcetate3-
        log_k   3.59
        delta_h 0       kcal

Pb+2 + 2Acetate- = PbAcetate2
        log_k   4.08
        delta_h 0       kcal

Pb+2 + 3Butanoate- = PbButanoate3-
        log_k   4.125
        delta_h 0       kcal

Pb+2 + Citrate-3 = PbCitrate-
        log_k   4.34
        delta_h 0       kcal

Pb+2 + Nta-3 = PbNta-
        log_k   11.6233
        delta_h 0       kcal

Pb+2 + 4Butanoate- = PbButanoate4-2
        log_k   4.43
        delta_h 0       kcal

Pb+2 + Glutamate-2 = PbGlutamate
        log_k   4.7
        delta_h 0       kcal

Pb+2 + 2Glutamate-2 = PbGlutamate2-2
        log_k   7.55
        delta_h 0       kcal

Pb+2 + Ethylenediamine = PbEthylenediamine+2
        log_k   7
        delta_h 0       kcal

Pb+2 + 2Ethylenediamine = PbEthylenediamine2+2
        log_k   8.45
        delta_h 0       kcal

Pb+2 + Phthalate-2 = PbPhthalate
        log_k   2.78
        delta_h 0       kcal

Pb+2 + Phthalate-2 + H+ = PbPhthalateH+
        log_k   6.56
        delta_h 0       kcal

Pb+2 + Tartrate-2 = PbTartrate
        log_k   3.78
        delta_h 0       kcal

Pb+2 + Glycine- = PbGlycine+
        log_k   5.47
        delta_h 0       kcal

Pb+2 + 3Citrate-3 = PbCitrate3-7
        log_k   6.97
        delta_h 0       kcal

Pb+2 + 2Citrate-3 = PbCitrate2-4
        log_k   6.08
        delta_h 0       kcal

Pb+2 + 2Glycine- = PbGlycine2
        log_k   8.32
        delta_h 0       kcal

Pb+2 + 4Propanoate- = PbPropanoate4-2
        log_k   4.18
        delta_h 0       kcal

Pb+2 + 3Propanoate- = PbPropanoate3-
        log_k   2.99
        delta_h 0       kcal

Pb+2 + 4Acetate- = PbAcetate4-2
        log_k   3.4
        delta_h 0       kcal

Pb+2 + 2Phthalate-2 = PbPhthalate2-2
        log_k   4.01
        delta_h 0       kcal

Phthalate-2 + H+ = HPhthalate-
        log_k   5.4
        delta_h 0       kcal
        -gamma  0       0.01

Phthalate-2 + 2H+ = H2Phthalate
        log_k   8.35
        delta_h 0       kcal
        -gamma  0       0.01

Phthalate-2 + Ni+2 + H+ = NiPhthalateH+
        log_k   6.1
        delta_h 0       kcal

Propanoate- + Fe+3 = FePropanoate-2
        log_k   3.4
        delta_h 0       kcal

Salicylate-2 + 2H+ = H2Salicylate
        log_k   16.4
        delta_h 0       kcal
        -gamma  0       0.01

Salicylate-2 + H+ = HSalicylate-
        log_k   13.4
        delta_h 0       kcal
        -gamma  0       0.01

Sr+2 + Fe+3 + 6Cyanide- = SrFe(Cyanide)6-
        log_k   55.6181
        delta_h -69.83  kcal

Tartrate-2 + H+ = HTartrate-
        log_k   4.16
        delta_h 0       kcal
        -gamma  0       0.01

Tartrate-2 + 2H+ = H2Tartrate
        log_k   6.67
        delta_h 0       kcal
        -gamma  0       0.01

Tl+ + Citrate-3 = TlCitrate-2
        log_k   1.61
        delta_h 0       kcal

Tl+ + Tartrate-2 = TlTartrate-
        log_k   1.39
        delta_h 0       kcal

Tl+ + Nta-3 = TlNta-2
        log_k   4.71
        delta_h 0       kcal

Tl+ + Edta-4 = TlEdta-3
        log_k   6.41
        delta_h 0       kcal

Tl+ + Acetate- = TlAcetate
        log_k   -0.11
        delta_h 0       kcal

Valerate- + Fe+3 = FeValerate+2
        log_k   5.58
        delta_h 0       kcal

Valerate- + Ba+2 = BaValerate+
        log_k   0.66
        delta_h 0       kcal

Valerate- + Ni+2 = NiValerate+
        log_k   1.26
        delta_h 0       kcal

Valerate- + Pb+2 = PbValerate+
        log_k   2.06
        delta_h 0       kcal

Valerate- + Cd+2 = CdValerate+
        log_k   1.19
        delta_h 0       kcal

Zn+2 + 3Diethylamine = ZnDiethylamine3+2
        log_k   7.49
        delta_h 0       kcal

Zn+2 + 2Diethylamine = ZnDiethylamine2+2
        log_k   4.96
        delta_h 20      kcal

Zn+2 + 4Diethylamine = ZnDiethylamine4+2
        log_k   9.83
        delta_h 0       kcal

Zn+2 + Diethylamine = ZnDiethylamine+2
        log_k   2.51
        delta_h 0       kcal

Zn+2 + 4Acetate- = ZnAcetate4-2
        log_k   1.36
        delta_h 0       kcal

Zn+2 + 3Acetate- = ZnAcetate3-
        log_k   1.57
        delta_h 0       kcal

Zn+2 + 2Acetate- = ZnAcetate2
        log_k   1.9
        delta_h 0       kcal

Zn+2 + Acetate- = ZnAcetate+
        log_k   1.57
        delta_h 0       kcal

Zn+2 + Edta-4 + H+ = ZnHEdta-
        log_k   9
        delta_h 0       kcal

Zn+2 + Edta-4 = ZnEdta-2
        log_k   16.44
        delta_h 0       kcal

Zn+2 + Butanoate- = ZnButanoate+
        log_k   0.983
        delta_h 0       kcal

Zn+2 + 2Butanoate- = ZnButanoate2
        log_k   1.65
        delta_h 0       kcal

Zn+2 + 3Butanoate- = ZnButanoate3-
        log_k   1.69
        delta_h 0       kcal

Zn+2 + 3Ethylenediamine = ZnEthylenediamine3+2
        log_k   13.83
        delta_h 0       kcal

Zn+2 + 2Npropylamine = ZnNpropylamine2+2
        log_k   4.85
        delta_h 0       kcal

Zn+2 + 3Npropylamine = ZnNpropylamine3+2
        log_k   7.38
        delta_h 0       kcal

Zn+2 + 3Propanoate- = ZnPropanoate3-
        log_k   1.82
        delta_h 0       kcal

Zn+2 + Propanoate- = ZnPropanoate+
        log_k   0.72
        delta_h 0       kcal

Zn+2 + 2Propanoate- = ZnPropanoate2
        log_k   1.23
        delta_h 0       kcal

Zn+2 + Phthalate-2 = ZnPhthalate
        log_k   2.91
        delta_h 0       kcal

Zn+2 + Citrate-3 + 2H+ = ZnCitrateH2+
        log_k   1.68
        delta_h 0       kcal

Zn+2 + Citrate-3 + H+ = ZnCitrateH
        log_k   3.78
        delta_h 0       kcal

Zn+2 + 2Citrate-3 = ZnCitrate2-4
        log_k   6.7
        delta_h 0       kcal

Zn+2 + Citrate-3 = ZnCitrate-
        log_k   6.1
        delta_h 0       kcal

Zn+2 + 3Glycine- = ZnGlycine3-
        log_k   12.3
        delta_h 0       kcal

Zn+2 + 2Glycine- = ZnGlycine2
        log_k   9.81
        delta_h 0       kcal

Zn+2 + Glycine- = ZnGlycine+
        log_k   5.38
        delta_h 0       kcal

Zn+2 + 4Three_methylpyridine =
ZnThree_methylpyridine4+2
        log_k   3.7
        delta_h 0       kcal
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Zn+2 + 3Three_methylpyridine =
ZnThree_methylpyridine3+2
        log_k   2.6
        delta_h 0       kcal

Zn+2 + 2Three_methylpyridine =
ZnThree_methylpyridine2+2
        log_k   2.1
        delta_h 0       kcal

Zn+2 + Three_methylpyridine =
ZnThree_methylpyridine+2
        log_k   1
        delta_h 0       kcal

Zn+2 + 3Glutamate-2 = ZnGlutamate3-4
        log_k   9.8
        delta_h 0       kcal

Zn+2 + 2Glutamate-2 = ZnGlutamate2-2
        log_k   8.25
        delta_h 0       kcal

Zn+2 + Glutamate-2 = ZnGlutamate
        log_k   3.79
        delta_h 0       kcal

Zn+2 + 2Isopropylamine = ZnIsopropylamine2+2
        log_k   4.67
        delta_h 0       kcal

Zn+2 + 3Isopropylamine = ZnIsopropylamine3+2
        log_k   7.14
        delta_h 0       kcal

Zn+2 + 4Butanoate- = ZnButanoate4-2
        log_k   2.05
        delta_h 0       kcal

Zn+2 + 4Isopropylamine = ZnIsopropylamine4+2
        log_k   9.44
        delta_h 0       kcal

Zn+2 + Ethylenediamine = ZnEthylenediamine+2
        log_k   5.65
        delta_h 0       kcal

Zn+2 + 4Propanoate- = ZnPropanoate4-2
        log_k   1.36
        delta_h 0       kcal

Zn+2 + Npropylamine = ZnNpropylamine+2
        log_k   2.42
        delta_h 0       kcal

Zn+2 + 4Npropylamine = ZnNpropylamine4+2
        log_k   9.49
        delta_h 0       kcal

Zn+2 + Isopropylamine = ZnIsopropylamine1+2
        log_k   2.37
        delta_h 0       kcal

Zn+2 + 2Ethylenediamine = ZnEthylenediamine2+2
        log_k   10.62
        delta_h 0       kcal

Zn+2 + 2Phthalate-2 = ZnPhthalate2-2
        log_k   4.2
        delta_h 0       kcal

PHASES
Acanthite
        Ag2S + H+ = 2Ag+ + HS-
        log_k   -36.05
        delta_h  53.3     kcal

Ag_Vanadate
        AgVO3 + 2H+ = Ag+ + VO2+ + H2O
        log_k     0.77
        delta_h   0       kcal

Ag2CO3
        Ag2CO3 = 2Ag+ + CO3-2
        log_k   -11.07
        delta_h   9.53    kcal

Ag2CrO4
        Ag2CrO4 = CrO4-2 + 2Ag+
        log_k   -11.5548
        delta_h  14.04    kcal

Ag2HVO4
        Ag2HVO4 + 3H+ = 2Ag+ + VO2+ + 2H2O
        log_k     1.48
        delta_h   0       kcal

Ag2O
        Ag2O + 2H+ = 2Ag+ + H2O
        log_k    12.58
        delta_h -10.43    kcal

Ag2Se
        Ag2Se + H+ = HSe- + 2Ag+
        log_k   -63.6448
        delta_h  64.95    kcal

Ag2SeO3
        Ag2SeO3 + H+ = HSeO3- + 2Ag+
        log_k    -7.07
        delta_h   9.47    kcal

Ag2SeO4
        Ag2SeO4 = SeO4-2 + 2Ag+
        log_k    -8.9014
        delta_h  10.45    kcal

Ag2SO4
        Ag2SO4 = 2Ag+ + SO4-2
        log_k    -4.92
        delta_h   4.25    kcal

Ag3H2VO5
        Ag3H2VO5 + 4H+ = 3Ag+ + VO2+ + 3H2O
        log_k     5.18
        delta_h   0       kcal

Ag3PO4
        Ag3PO4 = 3Ag+ + PO4-3
        log_k   -17.55
        delta_h   0       kcal

Ag3Sb
        Ag3Sb + 3H2O = Sb(OH)3 + 6e- + 3Ag+ + 3H+
        log_k   -56.1818
        delta_h   0       kcal

AgF:4H2O
        AgF:4H2O = Ag+ + F- + 4H2O
        log_k     0.55
        delta_h   4.27    kcal

AgMetal
        Ag = Ag+ + e-
        log_k   -13.51
        delta_h  25.234   kcal

Akerminite
        Ca2MgSi2O7 + H2O + 6H+ = 2H4SiO4 + 2Ca+2 +
Mg+2
        log_k    47.472
        delta_h -76.445   kcal

Al2O3
        Al2O3 + 6H+ = 2Al+3 + 3H2O
        log_k    22.98
        delta_h   0       kcal

AlAsO4:2H2O
        AlAsO4:2H2O + 3H+ = Al+3 + H3AsO4 + 2H2O
        log_k     4.8
        delta_h   0       kcal

Albite(low)
        NaAlSi3O8 + 4H+ + 4H2O = Na+ + Al+3 +
3H4SiO4
        log_k     2.592
        delta_h -17.4     kcal

Al(OH)3(a)
        Al(OH)3 + 3H+ = Al+3 + 3H2O
        log_k    10.38
        delta_h -27.045   kcal

AlOHSO4
        AlOHSO4 + H+ = Al+3 + SO4-2 + H2O
        log_k    -3.23
        delta_h   0       kcal

Al4(OH)10SO4
        Al4(OH)10SO4 + 10H+ = 4Al+3 + SO4-2 + 10H2O
        log_k    22.7
        delta_h   0       kcal

AlSb
        AlSb + 3H2O = Sb(OH)3 + 6e- + Al+3 + 3H+
        log_k    65.6241
        delta_h   0       kcal

AlumK
        KAl(SO4)2:12H2O = K+ + Al+3 + 2SO4-2 + 12H2O
        log_k    -5.17
        delta_h   7.22    kcal

Alunite
        KAl3(SO4)2(OH)6 + 6H+ = K+ + 3Al+3 + 2SO4-2
+ 6H2O
        log_k    -1.346
        delta_h   3.918   kcal

Am(metal)
        Am = Am+3 + 3e-
        log_k    104.8932
        delta_h -147.395  kcal

Am(OH)3(am)
        Am(OH)3 + 3H+ = Am+3 + 3H2O
        log_k    17.0009
        delta_h   0       kcal

Am(OH)3(c)
        Am(OH)3 + 3H+ = Am+3 + 3H2O
        log_k    15.2009
        delta_h -48.325   kcal

Am2O3(c)
        Am2O3 + 6H+ = 2Am+3 + 3H2O
        log_k    51.7715
        delta_h -95.719   kcal

AmBr3(c)
        AmBr3 = Am+3 + 3Br-
        log_k    21.6755
        delta_h -40.853   kcal

AmOBr(c)
        AmOBr + 2H+ = Am+3 + H2O + Br-
        log_k    13.7211
        delta_h -31.295   kcal

AmCl3(c)
        AmCl3 = Am+3 + 3Cl-
        log_k    14.3138
        delta_h -33.494   kcal

AmOCl(c)
        AmOCl + 2H+ = Am+3 + H2O + Cl-
        log_k    11.3035
        delta_h -28.635   kcal

AmF3(c)
        AmF3 = Am+3 + 3F-
        log_k    -13.2393
        delta_h   -8.305  kcal

AmI3(c)
        AmI3 = Am+3 + 3I-
        log_k    24.6266
        delta_h -41.836   kcal

AmOHCO3(c)
        AmOHCO3 + H+ = Am+3 + CO3-2 + H2O
        log_k    -7.0992
        delta_h -10.220   kcal

Am2(CO3)3(c)
        Am2(CO3)3 = 2Am+3 + 3CO3-2
        log_k    -33.4023
        delta_h   -9.104  kcal

AmO2(c)
        AmO2 + 4H+ = Am+4 + 2H2O
        log_k     -9.4353
        delta_h  -10.865  kcal

AmF4(c)
        AmF4 = Am+4 + 4F-
        log_k    -25.2962
        delta_h   -8.839  kcal

Analbite
        NaAlSi3O8 + 4H+ + 4H2O = Na+ + Al+3 +
3H4SiO4
        log_k     3.506
        delta_h  -20.0    kcal

Analcime
        NaAlSi2O6:H2O + H2O + 4H+ = Na+ + Al+3 +
2H4SiO4
        log_k     6.719
        delta_h  -22.84   kcal

Anglesite
        PbSO4 = Pb+2 + SO4-2
        log_k    -7.79
        delta_h   2.15    kcal

Anhydrite
        CaSO4 = Ca+2 + SO4-2
        log_k    -4.637
        delta_h  -3.769   kcal

Anilite
        Cu0.25Cu1.5S + H+ = 0.25Cu+2 + 1.5Cu+ + HS-
        log_k   -31.878
        delta_h  43.535   kcal

Annite
        KFe3AlSi3O10(OH)2 + 10H+ = K+ + 3Fe+2 + Al+3
+ 3H4SiO4
        log_k    23.29
        delta_h -65.72    kcal

Anorthite
        CaAl2Si2O8 + 8H+ = Ca+2 + 2Al+3 + 2H4SiO4
        log_k    25.43
        delta_h -70.66    kcal

Antlerite
        Cu3(OH)4SO4 + 4H+ = 3Cu+2 + 4H2O + SO4-2
        log_k     8.29
        delta_h   0       kcal

FCO3Apatite
        Ca9.316Na0.36Mg0.144(PO4)4.8(CO3)1.2F2.48 =
9.316Ca+2 + 0.36Na+ + 0.144Mg+2 + 4.8PO4-3 +
1.2CO3-2 + 2.48F-
        log_k   -114.4
        delta_h  39.39    kcal

Aragonite
        CaCO3 = Ca+2 + CO3-2
        log_k    -8.36
        delta_h  -2.615   kcal
        -analytical      -171.9773     -0.077993
2903.293      71.595      0.0

Arsenolite
        As4O6 + 6H2O = 4H3AsO3
        log_k    -2.801
        delta_h  14.33    kcal

Artinite
        MgCO3:Mg(OH)2:3H2O + 2H+ = 2Mg+2 + CO3-2 +
5H2O
        log_k     9.6
        delta_h  -28.742  kcal

As2O5
        As2O5 + 3H2O = 2H3AsO4
        log_k     6.699
        delta_h  -5.405   kcal

AsI3
        AsI3 + 3H2O = H3AsO3 + 3I- + 3H+
        log_k     4.155
        delta_h   1.875   kcal

Atacamite
        Cu2(OH)3Cl + 3H+ = 2Cu+2 + 3H2O + Cl-
        log_k     7.34
        delta_h  -18.69   kcal

Ca-Autunite
        Ca(UO2)2(PO4)2 = Ca+2 + 2UO2+2 + 2PO4-3
        log_k    -43.927
        delta_h  -14.340  kcal

H-Autunite
        H2(UO2)2(PO4)2 = 2H+ + 2UO2+2 + 2PO4-3
        log_k    -49.9789
        delta_h   -0.597  kcal

K-Autunite
        K2(UO2)2(PO4)2 = 2K+ + 2UO2+2 + 2PO4-3
        log_k    -48.244
        delta_h    5.76   kcal

Na-Autunite
        Na2(UO2)2(PO4)2 = 2Na+ + 2UO2+2 + 2PO4-3
        log_k    -47.409
        delta_h   -0.566  kcal

Sr-Autunite
        Sr(UO2)2(PO4)2 = Sr+2 + 2UO2+2 + 2PO4-3
        log_k    -44.457
        delta_h  -14.37   kcal

Avicennite
        Tl2O3 + 3H2O = 2Tl(OH)3
        log_k    -16.3236
        delta_h   0       kcal

Azurite
        Cu3(OH)2(CO3)2 + 2H+ = 3Cu+2 + 2H2O + 2CO3-2
        log_k    -16.92
        delta_h  -23.77   kcal

Ba3(AsO4)2
        Ba3(AsO4)2 + 6H+ = 3Ba+2 + 2H3AsO4
        log_k     -8.91
        delta_h    2.64   kcal

BaCrO4
        BaCrO4 = CrO4-2 + Ba+2
        log_k     -9.6681
        delta_h    6.39   kcal

BaF2
        BaF2 = Ba+2 + 2F-
        log_k     -5.76
        delta_h    1.0    kcal

Barite
        BaSO4 = Ba+2 + SO4-2
        log_k     -9.976
        delta_h    6.28   kcal

BaSeO3
        BaSeO3 + H+ = HSeO3- + Ba+2
        log_k      4.1634
        delta_h   -6.28   kcal

BaSeO4
        BaSeO4 = SeO4-2 + Ba+2
        log_k     -5.1895
        delta_h    2.0    kcal

BaUO4(c)
        BaUO4 + 4H+ = Ba+2 + UO2+2 + 2H2O
        log_k     17.6220
        delta_h  -31.264  kcal

Bassetite
        Fe(UO2)2(PO4)2 = Fe+2 + 2UO2+2 + 2PO4-3
        log_k    -42.462
        delta_h  -20.43   kcal

Bianchite
        ZnSO4:6H2O = Zn+2 + SO4-2 + 6H2O
        log_k     -1.765
        delta_h   -0.16   kcal

Birnessite
        MnO2 + 4H+ + e- = Mn+3 + 2H2O
        log_k     18.091
        delta_h    0      kcal

Bixbyite
        Mn2O3 + 6H+ = 2Mn+3 + 3H2O
        log_k     -0.611
        delta_h  -15.245  kcal

Blaubleii
        Cu0.9Cu0.2S + H+ = 0.9Cu+2 + 0.2Cu+ + HS-
        log_k    -24.162
        delta_h    0      kcal

BlaubleiII
        Cu0.6Cu0.8S + H+ = 0.6Cu+2 + 0.8Cu+ + HS-
        log_k    -27.279
        delta_h    0      kcal

Boehmite
        AlOOH + 3H+ = Al+3 + 2H2O
        log_k      8.578
        delta_h  -28.13   kcal

K-Boltwoodite
        KH3UO2SiO4 + 3H+ = UO2+2 + H2O + H4SiO4 +
K+
        log_k     15.0050
        delta_h    0      kcal

Brochantite
        Cu4(OH)6SO4 + 6H+ = 4Cu+2 + 6H2O + SO4-2
        log_k     15.34
        delta_h    0      kcal

Bromyrite
        AgBr = Ag+ + Br-
        log_k    -12.27
        delta_h   20.17   kcal

Brucite
        Mg(OH)2 + 2H+ = Mg+2 + 2H2O
        log_k     16.792
        delta_h  -25.84   kcal

Bunsenite
        NiO + 2H+ = Ni+2 + H2O
        log_k     12.45
        delta_h  -23.92   kcal

Ca2V2O7
        CaVO3.5 + 3H+ = Ca+2 + VO2+ + 1.5H2O
        log_k      8.75
        delta_h  -19.06   kcal

Ca3(AsO4)2:6H2O
        Ca3(AsO4)2:6H2O + 6H+ = 3Ca+2 + 2H3AsO4 +
6H2O
        log_k     22.3
        delta_h    0      kcal

Ca3(VO4)2
        Ca1.5VO4 + 4H+ = 1.5Ca+2 + VO2+ + 2H2O
        log_k     19.48
        delta_h  -35.07   kcal

Ca3Sb2
        Ca3Sb2 + 6H2O = 3Ca+2 + 2Sb(OH)3 + 6H+ +
12e-
        log_k    142.974
        delta_h -175.13   kcal

Ca3Si2O5
        Ca3Si2O5 + 6H+ = H4SiO4 + 3Ca+2 + H2O
        log_k     73.867
        delta_h -106.335  kcal

CaCrO4
        CaCrO4 = Ca+2 + CrO4-2
        log_k     -2.2657
        delta_h   -6.44   kcal

Calcite
        CaCO3 = Ca+2 + CO3-2
        log_k     -8.475
        delta_h   -2.585  kcal
        -analytical_expression 13.543     -0.0401
-3000.0
Carnotite
        K(UO2)(VO4) + 4H+ = K+ + UO2+2 + VO2+ + 2H2O
        log_k      0.5158
        delta_h   -8.806  kcal

Cassiterite
        SnO2 + 4H+ + 2e- = Sn+2 + 2H2O
        log_k     -3.1111
        delta_h    0.066  kcal

CaUO4(c)
        CaUO4 + 4H+ = Ca+2 + UO2+2 + 2H2O
        log_k     16.0465
        delta_h  -31.464  kcal

Celestite
        SrSO4 = Sr+2 + SO4-2
        log_k     -6.465
        delta_h   -0.47   kcal

Calomel
        Hg2Cl2 = Hg2+2 + 2Cl-
        log_k    -17.8427
        delta_h   23.444  kcal

CaSeO3:2H2O
        CaSeO3:2H2O + H+ = HSeO3- + Ca+2 + 2H2O
        log_k      2.8139
        delta_h   -4.65   kcal

CaSeO4:2H2O
        CaSeO4:2H2O = SeO4-2 + Ca+2 + 2H2O
        log_k     -2.9473
        delta_h    0.88   kcal

Cd(BO2)2
        Cd(BO2)2 + 2H2O + 2H+ = Cd+2 + 2H3BO3
        log_k      9.84
        delta_h    0      kcal

Cd(Gamma)
        Cd = Cd+2 + 2e-
        log_k     13.59
        delta_h  -18.14   kcal

Cd(OH)2(A)
        Cd(OH)2 + 2H+ = Cd+2 + 2H2O
        log_k     13.73
        delta_h  -20.77   kcal

Cd(OH)2(C)
        Cd(OH)2 + 2H+ = Cd+2 + 2H2O
        log_k     13.65
        delta_h    0      kcal

Cd3(OH)2(SO4)2
        Cd3(OH)2(SO4)2 + 2H+ = 3Cd+2 + 2H2O + 2SO4-2
        log_k      6.71
        delta_h    0      kcal

Cd3(OH)4SO4
        Cd3(OH)4SO4 + 4H+ = 3Cd+2 + 4H2O + SO4-2
        log_k     22.56
        delta_h    0      kcal

Cd3(PO4)2
        Cd3(PO4)2 = 3Cd+2 + 2PO4-3
        log_k    -32.6
```

```
        delta_h    0       kcal

Cd4(OH)6SO4
        Cd4(OH)6SO4 + 6H+ = 4Cd+2 + 6H2O + SO4-2
        log_k     28.4
        delta_h    0       kcal

CdBr2:4H2O
        CdBr2:4H2O = Cd+2 + 2Br- + 4H2O
        log_k     -2.42
        delta_h    7.23    kcal

CdCl2
        CdCl2 = Cd+2 + 2Cl-
        log_k     -0.68
        delta_h   -4.47    kcal

CdCl2:H2O
        CdCl2:H2O = Cd+2 + 2Cl- + H2O
        log_k     -1.71
        delta_h   -1.82    kcal

CdCl2:2.5H2O
        CdCl2:2.5H2O = Cd+2 + 2Cl- + 2.5H2O
        log_k     -1.94
        delta_h    1.71    kcal

CdF2
        CdF2 = Cd+2 + 2F-
        log_k     -2.98
        delta_h   -9.72    kcal

CdI2
        CdI2 = Cd+2 + 2I-
        log_k     -3.61
        delta_h    4.08    kcal

CdMetal
        Cd = Cd+2 + 2e-
        log_k     13.49
        delta_h  -18.0     kcal

CdOHCl
        CdOHCl + H+ = Cd+2 + H2O + Cl-
        log_k      3.52
        delta_h   -7.407   kcal

CdSb
        CdSb + 3H2O = Sb(OH)3 + 5e- + 3H+ + Cd+2
        log_k     -0.3943
        delta_h    5.345   kcal

CdSe
        CdSe + H+ = HSe- + Cd+2
        log_k    -18.0739
        delta_h   18.16    kcal

CdSiO3
        CdSiO3 + H2O + 2H+ = Cd+2 + H4SiO4
        log_k      9.06
        delta_h  -16.63    kcal

CdSO4
        CdSO4 = Cd+2 + SO4-2
        log_k     -0.1
        delta_h  -14.74    kcal

CdSO4:H2O
        CdSO4:H2O = Cd+2 + SO4-2 + H2O
        log_k     -1.657
        delta_h   -7.52    kcal

CdSO4:2.67H2O
        CdSO4:2.67H2O = Cd+2 + SO4-2 + 2.67H2O
        log_k     -1.873
        delta_h   -4.3     kcal

Cerargyrite
        AgCl = Ag+ + Cl-
        log_k     -9.75
        delta_h   15.652   kcal

Cerrusite
        PbCO3 = Pb+2 + CO3-2
        log_k    -13.13
        delta_h    4.86    kcal

Chalcanthite
        CuSO4:5H2O = Cu+2 + SO4-2 + 5H2O
        log_k     -2.64
        delta_h    1.44    kcal

Chalcedony
        SiO2 + 2H2O = H4SiO4
        log_k     -3.523
        delta_h    4.615   kcal

Chalcocite
        Cu2S + H+ = 2Cu+ + HS-
        log_k    -34.619
        delta_h   49.35    kcal

Chalcopyrite
        CuFeS2 + 2H+ = Cu+2 + Fe+2 + 2HS-
        log_k    -35.27
        delta_h   35.48    kcal

Chrysotile
        Mg3Si2O5(OH)4 + 6H+ = 3Mg+2 + 2H4SiO4 + H2O
        log_k     32.188
        delta_h  -52.485   kcal

Cinnabar
        HgS + 2H2O = Hg(OH)2 + HS- + H+
        log_k    -45.1885
        delta_h   60.43    kcal

Claudetite
        As4O6 + 6H2O = 4H3AsO3
        log_k     -3.065
        delta_h   13.29    kcal

Clausthalite
        PbSe + H+ = HSe- + Pb+2
        log_k    -21.2162
        delta_h   28.0     kcal

Clinoenstatite
        MgSiO3 + H2O + 2H+ = Mg+2 + H4SiO4
        log_k     11.338
        delta_h  -20.015   kcal

ClPyromorphite
        Pb5(PO4)3Cl = 5Pb+2 + 3PO4-3 + Cl-
        log_k    -84.43
        delta_h    0       kcal

Co(metal)
        Co = Co+2 + 2e-
        log_k      9.5216
        delta_h  -13.9     kcal

CoS(c)
        CoS + H+ = Co+2 + HS-
        log_k     -7.3740
        delta_h    2.432   kcal

Co(OH)2(c)
        Co(OH)2 + 2H+ = Co+2 + 2H2O
        log_k     12.3000
        delta_h    0       kcal

CoFe2O4(c)
        CoFe2O4 + 8H+ = Co+2 + 2Fe+3 + 4H2O
        log_k      0.8729
        delta_h  -38.404   kcal

CoO(c)
        CoO + 2H+ = Co+2 + H2O
        log_k     13.5553
        delta_h  -25.347   kcal

CoCl2(c)
        CoCl2 = Co+2 + 2Cl-
        log_k      8.2641
        delta_h  -19.032   kcal

CoCl2:2H2O(c)
        CoCl2:2H2O = Co+2 + 2Cl- + 2H2O
        log_k      4.6661
        delta_h   -9.757   kcal

CoCl2:6H2O(c)
        CoCl2:6H2O = Co+2 + 2Cl- + 6H2O
        log_k      2.6033
        delta_h    1.981   kcal

CoF2(c)
        CoF2 = Co+2 + 2F-
        log_k     -5.1343
        delta_h   -8.772   kcal

CoCO3(c)
        CoCO3 = Co+2 + CO3-2
        log_k    -10.5619
        delta_h    0       kcal

Co(NO3)2(c)
        Co(NO3)2 = Co+2 + 2NO3-
        log_k      8.0000
        delta_h    0       kcal

CoSO4(c)
        CoSO4 = Co+2 + SO4-2
        log_k      2.8996
        delta_h  -19.074   kcal

CoSO4:(Co(OH)2)3(c)
        CoSO4:(Co(OH)2)3 + 6H+ = 4Co+2 + SO4-2 +
6H2O
        log_k     33.2193
        delta_h  -90.686   kcal

CoSO4:H2O(c)
        CoSO4:H2O = Co+2 + SO4-2 + H2O
        log_k     -1.2111
        delta_h  -12.587   kcal

CoSO4:6H2O(c)
        CoSO4:6H2O = Co+2 + SO4-2 + 6H2O
        log_k     -2.3512
        delta_h    0.255   kcal

CoSe(c)
        CoSe + H+ = Co+2 + HSe-
        log_k    -16.2723
        delta_h    0       kcal

CoSeO3(c)
        CoSeO3 + H+ = Co+2 + HSeO3-
        log_k      0.2061
        delta_h   -8.956   kcal

Co3(PO4)2(c)
        Co3(PO4)2 = 3Co+2 + 2PO4-3
        log_k    -34.6559
        delta_h    0       kcal

CoHPO4(c)
        CoHPO4 = Co+2 + PO4-3 + H+
        log_k    -19.0441
        delta_h    0       kcal

Co3(AsO4)2(c)
        Co3(AsO4)2 + 6H+ = 3Co+2 + 2H3AsO4
        log_k     13.0302
        delta_h    0       kcal

Co2SiO4(c)
        Co2SiO4 + 4H+ = 2Co+2 + H4SiO4
        log_k      6.5609
        delta_h    0       kcal

CoF3(c)
        CoF3 = Co+3 + 3F-
        log_k     -4.9644
        delta_h  -24.65    kcal

Coccinite
        HgI2 + 2H2O = Hg(OH)2 + 2I- + 2H+
        log_k    -34.6599
        delta_h   49.732   kcal

Coffinite
        USiO4 + 4H+ = U+4 + H4SiO4
        log_k     -7.929
        delta_h  -12.29    kcal

Cotunnite
        PbCl2 = Pb+2 + 2Cl-
        log_k     -4.77
        delta_h    5.6     kcal

Covellite
        CuS + H+ = Cu+2 + HS-
        log_k    -23.038
        delta_h   24.01    kcal

CrMetal
        Cr = Cr+2 + 2e-
        log_k     32.244
        delta_h  -34.3     kcal

Cr(OH)2
        Cr(OH)2 + 2H+ = Cr+2 + 2H2O
        log_k     10.8189
        delta_h   -8.51    kcal

Cr(OH)3(A)
        Cr(OH)3 + H+ = Cr(OH)2+ + H2O
        log_k     -0.75
        delta_h    0       kcal

Cr(OH)3(C)
        Cr(OH)3 + H+ = Cr(OH)2+ + H2O
        log_k      1.7005
        delta_h   -7.115   kcal

Cr2O3
        Cr2O3 + 2H+ + H2O = 2Cr(OH)2+
        log_k     -3.3937
        delta_h  -12.125   kcal

CrBr3
        CrBr3 + 2H2O = Cr(OH)2+ + 3Br- + 2H+
        log_k     19.9086
        delta_h  -33.777   kcal

CrCl2
        CrCl2 = Cr+2 + 2Cl-
        log_k     15.8676
        delta_h  -19.666   kcal

CrCl3
        CrCl3 + 2H2O = Cr(OH)2+ + 3Cl- + 2H+
        log_k     13.5067
        delta_h  -27.509   kcal

CrF3
        CrF3 + 2H2O = Cr(OH)2+ + 3F- + 2H+
        log_k    -13.2597
        delta_h   -4.363   kcal

CrI3
        CrI3 + 2H2O = Cr(OH)2+ + 3I- + 2H+
        log_k     20.4767
        delta_h  -32.127   kcal

CrO3
        CrO3 + H2O = CrO4-2 + 2H+
        log_k     -3.2105
        delta_h   -1.245   kcal

Cristobalite
        SiO2 + 2H2O = H4SiO4
        log_k     -3.587
        delta_h    5.5     kcal

Cryolite
        Na3AlF6 = Al+3 + 3Na+ + 6F-
        log_k    -31.49
        delta_h   10.904   kcal

Cs(metal)
        Cs = Cs+ + e-
        log_k     51.0941
        delta_h  -61.67    kcal

Cs2CrO4(c)
        Cs2CrO4 = 2Cs+ + CrO4-2
        log_k     -0.5541
        delta_h    7.5040  kcal

Cs2Cr2O7(c)
        Cs2Cr2O7 + H2O = 2Cs+ + 2CrO4-2 + 2H+
        log_k    -17.7793
        delta_h   22.8990  kcal

Cs2U2O7(c)
        Cs2U2O7 + 6H+ = 2Cs+ + 2UO2+2 + 3H2O
        log_k     29.8692
        delta_h  -44.215   kcal

Cs2U4O12(c)
        Cs2U4O12 + 8H+ = 2Cs+ + 4UO2+2 + 4H2O + 2e-
        log_k     15.6018
        delta_h  -38.614   kcal

Cu(OH)2
        Cu(OH)2 + 2H+ = Cu+2 + 2H2O
        log_k      8.64
        delta_h  -15.25    kcal

Cu(SbO3)2
        Cu(SbO3)2 + 6H+ + 4e- = 2Sb(OH)3 + Cu+2
        log_k     45.2105
        delta_h    0       kcal

Cu2(OH)3NO3
        Cu2(OH)3NO3 + 3H+ = 2Cu+2 + 3H2O + NO3-
        log_k      9.24
        delta_h  -17.35    kcal

Cu2Sb
        Cu2Sb + 3H2O = Sb(OH)3 + 6e- + 3H+ + Cu+ +
Cu+2
        log_k    -34.8827
        delta_h   55.745   kcal

Cu2Se(alpha)
        Cu2Se + H+ = HSe- + 2Cu+
        log_k    -36.0922
        delta_h   51.21    kcal

Cu2SO4
        Cu2SO4 = 2Cu+ + SO4-2
        log_k     -1.95
        delta_h   -4.56    kcal

Cu3(AsO4)2:6H2O
        Cu3(AsO4)2:6H2O + 6H+ = 3Cu+2 + 2H3AsO4 +
6H2O
        log_k      6.1
        delta_h    0       kcal

Cu3(PO4)2
        Cu3(PO4)2 = 3Cu+2 + 2PO4-3
        log_k    -36.85
        delta_h    0       kcal

Cu3(PO4)2:3H2O
        Cu3(PO4)2:3H2O = 3Cu+2 + 2PO4-3 + 3H2O
        log_k    -35.12
        delta_h    0       kcal

Cu3Sb
        Cu3Sb + 3H2O = Sb(OH)3 + 6e- + 3H+ + 3Cu+
        log_k    -42.5937
        delta_h   73.645   kcal

Cu3Se2
        Cu3Se2 + 2H+ = 2HSe- + 2Cu+ + Cu+2
        log_k    -63.4911
        delta_h   81.34    kcal

CuBr
        CuBr = Cu+ + Br-
        log_k     -8.21
        delta_h   13.08    kcal

CuCO3
        CuCO3 = Cu+2 + CO3-2
        log_k     -9.63
        delta_h    0       kcal

CuCrO4
        CuCrO4 = CrO4-2 + Cu+2
        log_k     -5.4754
        delta_h    0       kcal

CuF
        CuF = Cu+ + F-
        log_k      7.08
        delta_h  -12.37    kcal

CuF2:2H2O
        CuF2:2H2O = Cu+2 + 2F- + 2H2O
        log_k     -4.55
        delta_h   -3.65    kcal

CuF2
        CuF2 = Cu+2 + 2F-
        log_k     -0.62
        delta_h  -13.32    kcal

CuI
        CuI = Cu+ + I-
        log_k    -11.89
        delta_h   20.14    kcal

CuMetal
        Cu = Cu+ + e-
        log_k     -8.76
        delta_h   17.13    kcal

CuOCuSO4
        CuO:CuSO4 + 2H+ = 2Cu+2 + H2O + SO4-2
        log_k     11.53
        delta_h  -35.575   kcal

CupricFerrite
        CuFe2O4 + 8H+ = Cu+2 + 2Fe+3 + 4H2O
        log_k      5.88
        delta_h  -38.69    kcal

Cuprite
        Cu2O + 2H+ = 2Cu+ + H2O
        log_k     -1.55
        delta_h    6.245   kcal

CuprousFerrite
        CuFeO2 + 4H+ = Cu+ + Fe+3 + 2H2O
        log_k     -8.92
        delta_h   -3.8     kcal

CuSe
        CuSe + H+ = HSe- + Cu+2
        log_k    -26.5121
        delta_h   28.95    kcal

CuSe2
        CuSe2 + 2H+ + 2e- = 2HSe- + Cu+2
        log_k    -33.3655
        delta_h   33.6     kcal

CuSeO3:2H2O
        CuSeO3:2H2O + H+ = HSeO3- + Cu+2 + 2H2O
        log_k      0.4838
        delta_h   -8.81    kcal

CuSO4
        CuSO4 = Cu+2 + SO4-2
        log_k      3.01
        delta_h  -18.14    kcal

Diaspore
        AlOOH + 3H+ = Al+3 + 2H2O
        log_k      6.873
        delta_h  -24.63    kcal

Diopside
        CaMgSi2O6 + 2H2O + 4H+ = Ca+2 + Mg+2 +
2H4SiO4
        log_k     19.886
        delta_h  -32.28    kcal

Dioptase
        CuSiO3:H2O + 2H+ = Cu+2 + H4SiO4
        log_k      6.5
        delta_h   -8.96    kcal

Djurleite
        Cu0.066Cu1.868S5 + H+ = 0.066Cu+2 + 1.868Cu+
+ HS-
        log_k    -33.92
        delta_h   47.881   kcal

Dolomite
        CaMg(CO3)2 = Ca+2 + Mg+2 + 2CO3-2
        log_k     -17
        delta_h   -8.29    kcal

Epsomite
        MgSO4:7H2O = Mg+2 + SO4-2 + 7H2O
        log_k     -2.14
        delta_h    2.82    kcal

Eu(metal)
        Eu = Eu+3 + 3e-
        log_k    100.6305
        delta_h -144.7     kcal

EuS(c)
        EuS + H+ = Eu+3 + HS- + e-
        log_k     20.9137
        delta_h  -41.642   kcal

Eu(OH)3(c)
        Eu(OH)3 + 3H+ = Eu+3 + 3H2O
        log_k     15.3482
        delta_h  -30.33    kcal

EuCl(OH)2(c)
        EuCl(OH)2 + 2H+ = Eu+3 + 2H2O + Cl-
        log_k      8.7974
        delta_h    0       kcal

Eu2O3(cubic)
        Eu2O3 + 6H+ = 2Eu+3 + 3H2O
        log_k     51.7818
        delta_h  -97.134   kcal

Eu2O3(monoclinic)
        Eu2O3 + 6H+ = 2Eu+3 + 3H2O
        log_k     53.3936
        delta_h  -99.782   kcal

Eu3O4(c)
        Eu3O4 + 8H+ = 3Eu+3 + 4H2O + e-
        log_k     93.0438
        delta_h -164.694   kcal

EuO(c)
        EuO + 2H+ = Eu+3 + H2O + e-
        log_k     43.4869
        delta_h  -71.468   kcal

EuBr3(c)
        EuBr3 = Eu+3 + 3Br-
        log_k     29.8934
        delta_h  -51.904   kcal

EuCl2(c)
        EuCl2 = Eu+3 + 2Cl- + e-
        log_k     11.9242
        delta_h  -27.984   kcal

EuCl3(c)
        EuCl3 = Eu+3 + 3Cl-
        log_k     19.7149
        delta_h  -40.848   kcal

EuCl3:6H2O(c)
        EuCl3:6H2O = Eu+3 + 3Cl- + 6H2O
        log_k      4.9090
        delta_h   -9.581   kcal

EuOCl(c)
        EuOCl + 2H+ = Eu+3 + H2O + Cl-
        log_k     15.6683
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        delta_h  -35.179   kcal

EuF3:0.5H2O(c)
        EuF3:0.5H2O = Eu+3 + 3F- + 0.5H2O
        log_k    -16.4847
        delta_h    0        kcal

Eu2(CO3)3:3H2O(c)
        Eu2(CO3)3:3H2O = 2Eu+3 + 3CO3-2 + 3H2O
        log_k    -36.8571
        delta_h   -2.333   kcal

Eu(NO3)3:6H2O(c)
        Eu(NO3)3:6H2O = Eu+3 + 3NO3- + 6H2O
        log_k     1.3082
        delta_h   3.633   kcal

EuSO4(c)
        EuSO4 = Eu+3 + SO4-2 + e-
        log_k    -2.8380
        delta_h  -10.506   kcal

Eu2(SO4)3:8H2O(c)
        Eu2(SO4)3:8H2O = 2Eu+3 + 3SO4-2 + 8H2O
        log_k    -10.8524
        delta_h   -0.704   kcal

Fe(OH)2.7Cl0.3
        Fe(OH)2.7Cl0.3 + 2.7H+ = Fe+3 + 2.7H2O +
0.3Cl-
        log_k     -3.04
        delta_h    0        kcal

Fe2(OH)4SeO3
        Fe2(OH)4SeO3 + 5H+ = HSeO3- + 2Fe+3 + 4H2O
        log_k      1.5539
        delta_h    0        kcal

Fe2(SeO3)3:2H2O
        Fe2(SeO3)3:2H2O + 3H+ = 3HSeO3- + 2Fe+3 +
2H2O
        log_k    -20.6262
        delta_h    0        kcal

Fe2(SO4)3
        Fe2(SO4)3 = 2Fe+3 + 3SO4-2
        log_k      3.58
        delta_h  -59.12    kcal

Fe3(OH)8
        Fe3(OH)8 + 8H+ = 2Fe+3 + Fe+2 + 8H2O
        log_k     20.222
        delta_h    0        kcal

FeAsO4:2H2O
        FeAsO4:2H2O + 3H+ = Fe+3 + H3AsO4 + 2H2O
        log_k      0.4
        delta_h    0        kcal

FeCr2O4
        FeCr2O4 + 4H+ = 2Cr(OH)2+ + Fe+2
        log_k     -0.9016
        delta_h  -24.86    kcal

Ferrihydrite
        Fe(OH)3 + 3H+ = Fe+3 + 3H2O
        log_k      4.891
        delta_h    0        kcal

Ferroselite
        FeSe2 + 2H+ + 2e- = 2HSe- + Fe+2
        log_k    -18.5959
        delta_h   11.3     kcal

FeS(ppt)
        FeS + H+ = Fe+2 + HS-
        log_k     -3.915
        delta_h    0        kcal

FeSe
        FeSe + H+ = HSe- + Fe+2
        log_k     -7.1466
        delta_h    0.5     kcal

Fluorite
        CaF2 = Ca+2 + 2F-
        log_k    -10.96
        delta_h    4.71    kcal
        -analytical     66.348   0.0      -4298.2
  -25.271          0.0
Forsterite
        Mg2SiO4 + 4H+ = 2Mg+2 + H4SiO4
        log_k     28.298
        delta_h  -48.51    kcal

Galena
        PbS + H+ = Pb+2 + HS-
        log_k     -15.132
        delta_h    19.4    kcal

Gehlenite
        Ca2Al2SiO7 + 10H+ = 2Al+3 + H4SiO4 + 2Ca+2 +
3H2O
        log_k      56.822
        delta_h  -116.125   kcal

Gibbsite(C)
        Al(OH)3 + 3H+ = Al+3 + 3H2O
        log_k      8.77
        delta_h  -22.8     kcal

Goethite
        FeOOH + 3H+ = Fe+3 + 2H2O
        log_k      0.5
        delta_h  -14.48    kcal

Goslarite
        ZnSO4:7H2O = Zn+2 + SO4-2 + 7H2O
        log_k     -1.96
        delta_h    3.3     kcal

Greenalite
        Fe3Si2O5(OH)4 + 6H+ = 3Fe+2 + 2H4SiO4 + H2O
        log_k     20.81
        delta_h    0        kcal

Greenockite
        CdS + H+ = Cd+2 + HS-
        log_k    -15.93
        delta_h   16.36    kcal

Greigite
        Fe3S4 + 4H+ = 2Fe+3 + Fe+2 + 4HS-
        log_k    -45.035
        delta_h    0        kcal

Gypsum
        CaSO4:2H2O = Ca+2 + SO4-2 + 2H2O
        log_k     -4.848
        delta_h    0.261   kcal

Haiweeite
        Ca(UO2)2(Si2O5)3:5H2O + 6H+ + 4H2O = Ca+2 +
2UO2+2 + 6H4SiO4
        log_k     -6.3291
        delta_h    0        kcal

Halite
        NaCl = Na+ + Cl-
        log_k      1.582
        delta_h    0.918   kcal

Halloysite
        Al2Si2O5(OH)4 + 6H+ = 2Al+3 + 2H4SiO4 + H2O
        log_k      8.994
        delta_h  -39.73    kcal

Hausmannite
        Mn3O4 + 8H+ + 2e- = 3Mn+2 + 4H2O
        log_k     61.54
        delta_h  -80.14    kcal

Hematite
        Fe2O3 + 6H+ = 2Fe+3 + 3H2O
        log_k     -4.008
        delta_h  -30.845   kcal

Hercynite
        FeAl2O4 + 8H+ = Fe+2 + 2Al+3 + 4H2O
        log_k     27.162
        delta_h  -78.36    kcal

Hg(OH)2
        Hg(OH)2 = Hg(OH)2
        log_k     -3.4963
        delta_h    0        kcal

Hg2(OH)2
        Hg2(OH)2 + 2H+ = Hg2+2 + 2H2O
        log_k      5.2603
        delta_h    0        kcal

Hg2Br2
        Hg2Br2 = Hg2+2 + 2Br-
        log_k    -22.2091
        delta_h   31.252   kcal

Hg2CO3
        Hg2CO3 = Hg2+2 + CO3-2
        log_k    -13.9586
        delta_h    0        kcal

Hg2CrO4
        Hg2CrO4 = Hg2+2 + CrO4-2
        log_k     -8.7031
        delta_h    0        kcal

Hg2F2
        Hg2F2 = Hg2+2 + 2F-
        log_k     -3.0811
        delta_h   -4.432   kcal

Hg2HPO4
        Hg2HPO4 = Hg2+2 + H+ + PO4-3
        log_k    -25.9795
        delta_h    0        kcal

Hg2I2
        Hg2I2 = Hg2+2 + 2I-
        log_k    -28.2782
        delta_h    0        kcal

Hg2S
        Hg2S + H+ = Hg2+2 + HS-
        log_k    -11.6765
        delta_h   16.67    kcal

Hg2SeO3
        Hg2SeO3 + H+ = Hg2+2 + HSeO3-
        log_k     -4.657
        delta_h    0        kcal

Hg2SO4
        Hg2SO4 = Hg2+2 + SO4-2
        log_k     -6.1593
        delta_h    0.23    kcal

HgBr2
        HgBr2 + 2H2O = Hg(OH)2 + 2Br- + 2H+
        log_k    -25.373
        delta_h   34.452   kcal

HgCl2
        HgCl2 + 2H2O = Hg(OH)2 + 2Cl- + 2H+
        log_k    -21.7858
        delta_h   27.264   kcal

HgCO3
        HgCO3 + 2H2O = Hg(OH)2 + CO3-2 + 2H+
        log_k    -28.6817
        delta_h   22.13    kcal

HgI2:6NH3
        HgI2:6NH3 + 2H2O + 4H+ = Hg(OH)2 + 2I- +
6NH4+
        log_k     33.8566
        delta_h  -20.568   kcal

HgI2:2NH3
        HgI2:2NH3 + 2H2O = Hg(OH)2 + 2I- + 2NH4+
        log_k    -16.1066
        delta_h   32.632   kcal

HgMetal
        Hg = 0.5Hg2+2 + e-
        log_k    -13.4552
        delta_h   19.935   kcal

HgSeO3
        HgSeO3 + 2H2O = Hg(OH)2 + HSeO3- + H+
        log_k    -12.6953
        delta_h    0        kcal

HgSO4
        HgSO4 + 2H2O = Hg(OH)2 + SO4-2 + 2H+
        log_k     -9.4189
        delta_h    3.51    kcal

Hinsdalite
        PbAl3PO4SO4(OH)6 + 6H+ = Pb+2 + 3Al+3 +
PO4-3 + SO4-2 + 6H2O
        log_k     -2.5
        delta_h    0        kcal

Huntite
        CaMg3(CO3)4 = 3Mg+2 + Ca+2 + 4CO3-2
        log_k    -29.968
        delta_h  -25.76    kcal

Hxypyromorphite
        Pb5(PO4)3OH + H+ = 5Pb+2 + 3PO4-3 + H2O
        log_k    -62.79
        delta_h    0        kcal

Hydcerrusite
        Pb(OH)2:2PbCO3 + 2H+ = 3Pb+2 + 2CO3-2 + 2H2O
        log_k    -17.46
        delta_h    0        kcal

Hydromagnesite
        Mg5(CO3)4(OH)2:4H2O + 2H+ = 5Mg+2 + 4CO3-2 +
6H2O
        log_k     -8.766
        delta_h  -52.21    kcal

Hydroxyapatite
        Ca5(PO4)3OH + H+ = 5Ca+2 + 3PO4-3 + H2O
        log_k    -44.199
        delta_h    0        kcal

Iodyrite
        AgI = Ag+ + I-
        log_k    -16.07
        delta_h   26.82    kcal

Jarosite-Na
        NaFe3(SO4)2(OH)6 + 6H+ = Na+ + 3Fe+3 +
2SO4-2 + 6H2O
        log_k    -11.2
        delta_h  -36.18    kcal

Jarosite-K
        KFe3(SO4)2(OH)6 + 6H+ = K+ + 3Fe+3 + 2SO4-2
+ 6H2O
        log_k    -14.8
        delta_h  -31.28    kcal

Jarosite-H
        (H3O)Fe3(SO4)2(OH)6 + 5H+ = 3Fe+3 + 2SO4-2 +
7H2O
        log_k    -12.1
        delta_h  -55.15    kcal

K2Cr2O7
        K2Cr2O7 + H2O = 2CrO4-2 + 2K+ + 2H+
        log_k    -15.6712
        delta_h   18.125   kcal

K2CrO4
        K2CrO4 = CrO4-2 + 2K+
        log_k      0.0073
        delta_h    4.25    kcal

KTcO4(c)
        KTcO4 = K+ + TcO4-
        log_k     -2.2667
        delta_h    0        kcal

K2UO4(c)
        K2UO4 + 4H+ = 2K+ + UO2+2 + 2H2O
        log_k     35.5176
        delta_h  -43.814   kcal

K(UO2)(AsO4)(c)
        K(UO2)(AsO4) + 3H+ = K+ + UO2+2 + H3AsO4
        log_k     -1.924
        delta_h    0        kcal

Kalsilite
        KAlSiO4 + 4H+ = H4SiO4 + Al+3 + K+
        log_k     12.838
        delta_h  -28.919   kcal

Kaolinite
        Al2Si2O5(OH)4 + 6H+ = 2Al+3 + 2H4SiO4 + H2O
        log_k      5.726
        delta_h  -35.28    kcal

Kasolite
        Pb(UO2)SiO4:H2O + 4H+ = Pb+2 + UO2+2 +
H4SiO4 + H2O
        log_k      7.3717
        delta_h    0        kcal

Langite
        Cu4(OH)6SO4:H2O + 6H+ = 4Cu+2 + 7H2O + SO4-2
        log_k     16.79
        delta_h  -39.61    kcal

Larnakite
        PbO:PbSO4 + 2H+ = 2Pb+2 + SO4-2 + H2O
        log_k     -0.28
        delta_h   -6.44    kcal

Larnite
        Ca2SiO4 + 4H+ = H4SiO4 + 2Ca+2
        log_k     39.141
        delta_h  -57.238   kcal

Laumontite
        CaAl2Si4O12:4H2O + 8H+ = Ca+2 + 2Al+3 +
4H4SiO4
        log_k     14.46
        delta_h  -50.45    kcal

Laurionite
        PbOHCl + H+ = Pb+2 + Cl- + H2O
        log_k      0.623
        delta_h    0        kcal

Leonhardite
        Ca2Al4Si8O24:7H2O + H2O + 16H+ = 2Ca+2 +
8H4SiO4 + 4Al+3
        log_k     16.49
        delta_h  -85.36    kcal

Lepidocrocite
        FeOOH + 3H+ = Fe+3 + 2H2O
        log_k      1.371
        delta_h    0        kcal

Leucite
        KAlSi2O6 + 2H2O + 4H+ = 2H4SiO4 + Al+3 + K+
        log_k      6.423
        delta_h  -22.085   kcal

Li2CrO4
        Li2CrO4 = CrO4-2 + 2Li+
        log_k      4.8568
        delta_h  -10.822   kcal

Li2UO4(c)
        Li2UO4 + 4H+ = 2Li+ + UO2+2 + 2H2O
        log_k     29.0152
        delta_h  -44.378   kcal

Lime
        CaO + 2H+ = Ca+2 + H2O
        log_k     32.797
        delta_h  -46.265   kcal

Litharge
        PbO + 2H+ = Pb+2 + H2O
        log_k     12.72
        delta_h  -16.38    kcal

Mackinawite
        FeS + H+ = Fe+2 + HS-
        log_k     -4.648
        delta_h    0        kcal

Magadiite
        NaSi7O13(OH)3:3H2O + H+ + 9H2O = Na+ +
7H4SiO4
        log_k     -14.3
        delta_h    0        kcal

Maghemite
        Fe2O3 + 6H+ = 2Fe+3 + 3H2O
        log_k      6.386
        delta_h    0        kcal

Magnesite
        MgCO3 = Mg+2 + CO3-2
        log_k     -8.029
        delta_h   -6.169   kcal

Magnetite
        Fe3O4 + 8H+ = 2Fe+3 + Fe+2 + 4H2O
        log_k      3.737
        delta_h  -50.46    kcal

Malachite
        Cu2(OH)2CO3 + 2H+ = 2Cu+2 + 2H2O + CO3-2
        log_k     -5.18
        delta_h  -15.61    kcal

Manganite
        MnOOH + 3H+ = Mn+3 + 2H2O
        log_k     -0.238
        delta_h    0        kcal

Massicot
        PbO + 2H+ = Pb+2 + H2O
        log_k     12.91
        delta_h  -16.78    kcal

Matlockite
        PbClF = Pb+2 + Cl- + F-
        log_k     -9.43
        delta_h    7.95    kcal

Melanothallite
        CuCl2 = Cu+2 + 2Cl-
        log_k      3.73
        delta_h  -12.32    kcal

Melanterite
        FeSO4:7H2O = Fe+2 + SO4-2 + 7H2O
        log_k     -2.47
        delta_h    2.86    kcal

Merwinite
        Ca3MgSi2O8 + 8H+ = 2H4SiO4 + Mg+2 + 3Ca+2
        log_k     68.543
        delta_h -107.111   kcal

Metacinnabar
        HgS + 2H2O = Hg(OH)2 + HS- + H+
        log_k    -44.822
        delta_h   59.53    kcal

Mg-Montronite
        Fe2Al.33Si3.67O10(OH)2Mg0.165 + 7.32H+ +
2.68H2O = 0.33Al+3 + 2Fe+3 + 0.165Mg+2 + 3.67H4SiO4
        log_k    -20.589
        delta_h    0        kcal

Mg-Ferrite
        MgFe2O4 + 8H+ = Mg+2 + 2Fe+3 + 4H2O
        log_k     16.765
        delta_h  -66.639   kcal

Mg_Vanadate
        MgO.5VO3 + 2H+ = 0.5Mg+2 + VO2+ + H2O
        log_k      5.64
        delta_h  -16.33    kcal

Mg2Sb3
        Mg2Sb3 + 9H2O = 2Mg+2 + 3Sb(OH)3 + 9H+ +
13e-
        log_k     74.6838
        delta_h    0        kcal

Mg2V2O7
        MgVO3.5 + 3H+ = Mg+2 + VO2+ + 1.5H2O
        log_k     13.18
        delta_h  -30.5     kcal

MgCr2O4
        MgCr2O4 + 4H+ = 2Cr(OH)2+ + Mg+2
        log_k     12.0796
        delta_h  -39.86    kcal

MgCrO4
        MgCrO4 = CrO4-2 + Mg+2
        log_k      5.3801
        delta_h  -21.26    kcal
(NH4)2CrO4
        (NH4)2CrO4 = CrO4-2 + 2NH4+
        log_k      0.4046
        delta_h    2.19    kcal

MgSeO3:6H2O
        MgSeO3:6H2O + H+ = HSeO3- + Mg+2 + 6H2O
        log_k      4.0314
        delta_h    1.25    kcal

MgUO4(c)
        MgUO4 + 4H+ = Mg+2 + UO2+2 + 2H2O
        log_k     23.0543
        delta_h  -47.621   kcal

Microcline
        KAlSi3O8 + 4H2O + 4H+ = 3H4SiO4 + Al+3 + K+
        log_k      0.616
        delta_h  -12.309   kcal

Millerite
        NiS + H+ = Ni+2 + HS-
        log_k     -8.042
        delta_h    2.5     kcal

Minium
        Pb3O4 + 8H+ + 2e- = 3Pb+2 + 4H2O
        log_k     73.69
        delta_h -102.76    kcal

Mirabilite
        Na2SO4:10H2O = 2Na+ + SO4-2 + 10H2O
        log_k     -1.114
        delta_h   18.987   kcal

Mn2(SO4)3
        Mn2(SO4)3 = 2Mn+3 + 3SO4-2
        log_k     -5.711
        delta_h  -39.06    kcal

Mn2Sb
        Mn2Sb + 3H2O = 2Mn+2 + Sb(OH)3 + 7e- + 3H+
        log_k     61.0796
        delta_h    0        kcal

Mn3(AsO4)2:8H2O
        Mn3(AsO4)2:8H2O + 6H+ = 3Mn+2 + 2H3AsO4 +
8H2O
        log_k     12.5
        delta_h    0        kcal

Mn3(PO4)2
        Mn3(PO4)2 = 3Mn+2 + 2PO4-3
        log_k    -23.827
        delta_h    2.12    kcal

MnCl2:4H2O
        MnCl2:4H2O = Mn+2 + 2Cl- + 4H2O
        log_k      2.71
        delta_h   17.38    kcal

MnHPO4(C)
        MnHPO4 = Mn+2 + PO4-3 + H+
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        log_k     -25.4
        delta_h    0        kcal

MnS(Green)
        MnS + H+ = Mn+2 + HS-
        log_k     3.8
        delta_h   -5.79     kcal

MnSb
        MnSb + 3H2O = Mn+3 + Sb(OH)3 + 6e- + 3H+
        log_k     -2.9099
        delta_h    5.045    kcal

MnSe
        MnSe + H+ = HSe- + Mn+2
        log_k     5.3508
        delta_h  -13.46     kcal

MnSeO3:2H2O
        MnSeO3:2H2O + H+ = HSeO3- + Mn+2 + 2H2O
        log_k     0.9822
        delta_h    2.03     kcal

MnSeO3
        MnSeO3 + H+ = HSeO3- + Mn+2
        log_k     1.21
        delta_h    0        kcal

MnSO4
        MnSO4 = Mn+2 + SO4-2
        log_k     2.669
        delta_h  -15.48     kcal

Monteponite
        CdO + 2H+ = Cd+2 + H2O
        log_k     15.12
        delta_h  -24.76     kcal

Monticellite
        CaMgSiO4 + 4H+ = H4SiO4 + Ca+2 + Mg+2
        log_k     30.272
        delta_h  -49.421    kcal

Montmorillonite
        Mg0.485Fe.22Al1.71Si3.81O10(OH)2 + 6.76H+ +
3.24H2O = 3.81H4SiO4 + 0.485Mg+2 + 0.22Fe+3 +
1.71Al+3
        log_k     2.67
        delta_h    0        kcal

Montroydite
        HgO + H2O = Hg(OH)2
        log_k    -3.6503
        delta_h   5.115     kcal

Morenosite
        NiSO4:7H2O = Ni+2 + SO4-2 + 7H2O
        log_k    -2.36
        delta_h   2.94      kcal

Muscovite
        KAl3Si3O10(OH)2 + 10H+ = K+ + 3Al+3 +
3H4SiO4
        log_k     12.99
        delta_h  -59.34     kcal

Na2Cr2O7
        Na2Cr2O7 + H2O = 2CrO4-2 + 2Na+ + 2H+
        log_k    -9.8953
        delta_h   5.305     kcal

Na2CrO4
        Na2CrO4 = CrO4-2 + 2Na+
        log_k     3.2618
        delta_h  -4.61      kcal

Na3Sb
        Na3Sb + 3H2O = 3Na+ + Sb(OH)3 + 3H+ + 6e-
        log_k    -94.4084
        delta_h -103.245    kcal

Na3VO4
        Na3VO4 + 4H+ = 3Na+ + VO2+ + 2H2O
        log_k     36.94
        delta_h  -44.42     kcal

Na4V2O7
        Na2VO3.5 + 3H+ = 2Na+ + VO2+ + 1.5H2O
        log_k     18.7
        delta_h  -24.03     kcal

NaTcO4(c)
        NaTcO4 = Na+ + TcO4-
        log_k     1.5208
        delta_h    0        kcal

NaUO3(c)
        NaUO3 + 2H+ = Na+ + UO2+2 + H2O + e-
        log_k     6.8688
        delta_h    0        kcal

Na2UO4(alpha)
        Na2UO4 + 4H+ = 2Na+ + UO2+2 + 2H2O
        log_k     30.0224
        delta_h  -41.39     kcal

Na3UO4(c)
        Na3UO4 + 4H+ = 3Na+ + UO2+ + 2H2O
        log_k     56.2575
        delta_h  -70.063    kcal

Na2U2O7(c)
        Na2U2O7 + 6H+ = 2Na+ + 2UO2+2 + 3H2O
        log_k     22.5908
        delta_h  -41.027    kcal

Na4UO2(CO3)3(c)
        Na4UO2(CO3)3 = 4Na+ + UO2+2 + 3CO3-2
        log_k    -26.9765
        delta_h    0        kcal

NaSb
        NaSb + 3H2O = Na+ + Sb(OH)3 + 3H+ + 4e-
        log_k     23.177
        delta_h  -22.385    kcal

Nantokite
        CuCl = Cu+ + Cl-
        log_k    -6.76
        delta_h   9.98      kcal

Natron
        Na2CO3:10H2O = 2Na+ + CO3-2 + 10H2O
        log_k    -1.311
        delta_h  15.745     kcal

Nepheline
        NaAlSiO4 + 4H+ = H4SiO4 + Al+3 + Na+
        log_k     14.218
        delta_h  -33.204    kcal

Nesquehonite
        MgCO3:3H2O = Mg+2 + CO3-2 + 3H2O
        log_k     -5.621
        delta_h   -5.789    kcal

NH4VO3
        NH4VO3 + 2H+ = NH4+ + VO2+ + H2O
        log_k      2.69
        delta_h   -3.77     kcal

Ni(OH)2
        Ni(OH)2 + 2H+ = Ni+2 + 2H2O
        log_k     10.8
        delta_h   30.45     kcal

Ni2SiO4
        Ni2SiO4 + 4H+ = 2Ni+2 + H4SiO4
        log_k     14.54
        delta_h  -33.36     kcal

Ni3(AsO4)2:8H2O
        Ni3(AsO4)2:8H2O + 6H+ = 3Ni+2 + 2H3AsO4 +
8H2O
        log_k     15.7
        delta_h    0        kcal

Ni3(PO4)2
        Ni3(PO4)2 = 3Ni+2 + 2PO4-3
        log_k    -31.3
        delta_h    0        kcal

Ni4(OH)6SO4
        Ni4(OH)6SO4 + 6H+ = 4Ni+2 + SO4-2 + 6H2O
        log_k     32
        delta_h    0        kcal

NiCO3
        NiCO3 = Ni+2 + CO3-2
        log_k     -6.84
        delta_h   -9.94     kcal

NiSb
        NiSb + 3H2O = Sb(OH)3 + 5e- + 3H+ + Ni+2
        log_k    -18.5225
        delta_h   22.945    kcal

NiSe
        NiSe + H+ = HSe- + Ni+2
        log_k    -17.7382
        delta_h    0        kcal

NiSeO3:2H2O
        NiSeO3:2H2O + H+ = HSeO3- + Ni+2 + 2H2O
        log_k      2.8147
        delta_h   -7.41     kcal

Ningyoite
        CaUP2O8:2H2O = Ca+2 + U+4 + 2PO4-3 + 2H2O
        log_k    -54.4314
        delta_h   -1.693    kcal

Ca-Nontronite
        Fe2Al.33Si3.67O10(OH)2Ca0.165 + 7.32H+ +
2.68H2O = 0.33Al+3 + 2Fe+3 + 0.165Ca+2 + 3.67H4SiO4
        log_k    -20.889
        delta_h    0        kcal

K-Nontronite
        Fe2Al.33Si3.67O10(OH)2K0.33 + 7.32H+ +
2.68H2O = 0.33Al+3 + 2Fe+3 + 0.33K+ + 3.67H4SiO4
        log_k    -15.549
        delta_h    0        kcal

Na-Nontronite
        Fe2Al.33Si3.67O10(OH)2Na0.33 + 7.32H+ +
2.68H2O = 0.33Al+3 + 2Fe+3 + 0.33Na+ + 3.67H4SiO4
        log_k    -14.504
        delta_h    0        kcal

Np(metal)
        Np = Np+4 + 4e-
        log_k     88.0894
        delta_h -132.887    kcal

Np(OH)4(c)
        Np(OH)4 + 4H+ = Np+4 + 4H2O
        log_k      0.8103
        delta_h   -18.762   kcal

NpO2(c)
        NpO2 + 4H+ = Np+4 + 2H2O
        log_k     -7.8026
        delta_h   -12.813   kcal

Np(HPO4)2(c)
        Np(HPO4)2 = Np+4 + 2H+ + 2PO4-3
        log_k    -55.6222
        delta_h    2.573    kcal

NpO2OH(am)
        NpO2OH + H+ = NpO2+ + H2O
        log_k      4.2364
        delta_h   -9.481    kcal

Np2O5(c)
        Np2O5 + 2H+ = 2NpO2+ + H2O
        log_k      9.5000
        delta_h   22.576    kcal

NpO2(OH)2(c)
        NpO2(OH)2 + 2H+ = NpO2+2 + 2H2O
        log_k      5.9851
        delta_h  -13.145    kcal

Neutite
        MnO2 + 4H+ + e- = Mn+3 + 2H2O
        log_k     17.504
        delta_h    0        kcal

Ca-Olivine
        Ca2SiO4 + 4H+ = H4SiO4 + 2Ca+2
        log_k     37.649
        delta_h  -54.695    kcal

Orpiment
        As2S3 + 6H2O = 2H3AsO3 + 3HS- + 3H+
        log_k    -60.971
        delta_h   82.89     kcal

Otavite
        CdCO3 = Cd+2 + CO3-2
        log_k    -13.74
        delta_h   -0.58     kcal

Ottemannite
        Sn2S3 + 3H+ + 2e- = 2Sn+2 + 3HS-
        log_k    -40.957
        delta_h    0        kcal

Parsonsite
        Pb2UO2(PO4)2:2H2O = 2Pb+2 + UO2+2 + 2PO4-3 +
2H2O
        log_k    -52.4332
        delta_h    0        kcal

Pb(BO2)2
        Pb(BO2)2 + 2H2O + 2H+ = Pb+2 + 2H3BO3
        log_k      7.61
        delta_h   -5.8      kcal

Pb(OH)2(C)
        Pb(OH)2 + 2H+ = Pb+2 + 2H2O
        log_k      8.15
        delta_h  -13.99     kcal

Pb2(OH)3Cl
        Pb2(OH)3Cl + 3H+ = 2Pb+2 + 3H2O + Cl-
        log_k      8.793
        delta_h    0        kcal

Pb2O(OH)2
        Pb2O(OH)2 + 4H+ = 2Pb+2 + 3H2O
        log_k     26.2
        delta_h    0        kcal

Pb2O3
        Pb2O3 + 6H+ + 2e- = 2Pb+2 + 3H2O
        log_k     61.04
        delta_h    0        kcal

Pb2OCO3
        Pb2OCO3 + 2H+ = 2Pb+2 + H2O + CO3-2
        log_k     -0.5
        delta_h  -11.46     kcal

Pb2SiO4
        Pb2SiO4 + 4H+ = 2Pb+2 + H4SiO4
        log_k     19.76
        delta_h  -26.0      kcal

Pb2V2O7
        PbVO3.5 + 3H+ = Pb+2 + VO2+ + 1.5H2O
        log_k     -0.95
        delta_h   -3.22     kcal

Pb3(AsO4)2
        Pb3(AsO4)2 + 6H+ = 3Pb+2 + 2H3AsO4
        log_k      5.8
        delta_h    0        kcal

Pb3(PO4)2
        Pb3(PO4)2 = 3Pb+2 + 2PO4-3
        log_k    -44.5
        delta_h    0        kcal

Pb3(VO4)2
        Pb1.5VO4 + 4H+ = 1.5Pb+2 + VO2+ + 2H2O
        log_k      3.07
        delta_h   -8.68     kcal

Pb3O2CO3
        Pb3O2CO3 + 4H+ = 3Pb+2 + CO3-2 + 2H2O
        log_k     11.02
        delta_h  -26.43     kcal

Pb3O2SO4
        Pb3O2SO4 + 4H+ = 3Pb+2 + SO4-2 + 2H2O
        log_k     10.4
        delta_h  -20.75     kcal

Pb4(OH)6SO4
        Pb4(OH)6SO4 + 6H+ = 4Pb+2 + SO4-2 + 6H2O
        log_k     21.1
        delta_h    0        kcal

Pb4O3SO4
        Pb4O3SO4 + 6H+ = 4Pb+2 + SO4-2 + 3H2O
        log_k     22.1
        delta_h  -35.07     kcal

PbBr2
        PbBr2 = Pb+2 + 2Br-
        log_k     -5.18
        delta_h    8.1      kcal

PbBrF
        PbBrF = Pb+2 + Br- + F-
        log_k     -8.49
        delta_h    0        kcal

PbCrO4
        PbCrO4 = CrO4-2 + Pb+2
        log_k    -13.6848
        delta_h   10.23     kcal

PbF2
        PbF2 = Pb+2 + 2F-
        log_k     -7.44
        delta_h   -0.7      kcal

PbHPO4
        PbHPO4 = Pb+2 + PO4-3 + H+
        log_k    -23.9
        delta_h    0        kcal

PbI2
        PbI2 = Pb+2 + 2I-
        log_k     -8.07
        delta_h   15.16     kcal

PbMetal
        Pb = Pb+2 + 2e-
        log_k      4.27
        delta_h    0.4      kcal

PbO:0.3H2O
        PbO:0.33H2O + 2H+ = Pb+2 + 1.33H2O
        log_k     12.98
        delta_h    0        kcal

PbSeO4
        PbSeO4 = SeO4-2 + Pb+2
        log_k     -6.8387
        delta_h    3.8      kcal

PbSiO3
        PbSiO3 + H2O + 2H+ = Pb+2 + H4SiO4
        log_k      7.32
        delta_h   -9.26     kcal

Periclase
        MgO + 2H+ = Mg+2 + H2O
        log_k     21.51
        delta_h  -36.135    kcal

Phlogopite
        KMg3AlSi3O10(OH)2 + 10H+ = K+ + 3Mg+2 + Al+3
+ 3H4SiO4
        log_k     66.3
        delta_h  -86.36     kcal

Phosgenite
        PbCl2:PbCO3 = 2Pb+2 + 2Cl- + CO3-2
        log_k    -19.81
        delta_h    0        kcal

Plattnerite
        PbO2 + 4H+ + 2e- = Pb+2 + 2H2O
        log_k     49.3
        delta_h  -70.73     kcal

Plumbogummite
        PbAl3(PO4)2(OH)5:H2O + 5H+ = Pb+2 + 3Al+3 +
2PO4-3 + 6H2O
        log_k    -32.79
        delta_h    0        kcal

Portlandite
        Ca(OH)2 + 2H+ = Ca+2 + 2H2O
        log_k     22.675
        delta_h  -30.69     kcal

Przhevalskite
        Pb(UO2)2(PO4)2 = Pb+2 + 2UO2+2 + 2PO4-3
        log_k    -44.682
        delta_h   -9.977    kcal

Pu(metal)
        Pu = Pu+4 + 4e-
        log_k     84.3578
        delta_h -128.081    kcal

Pu(OH)3(c)
        Pu(OH)3 + 3H+ = Pu+3 + 3H2O
        log_k     22.4499
        delta_h  -35.39     kcal

Pu2O3(beta)
        Pu2O3 + 6H+ = 2Pu+3 + 3H2O
        log_k     48.1332
        delta_h  -86.112    kcal

PuF3(c)
        PuF3 = Pu+3 + 3F-
        log_k    -10.1872
        delta_h  -11.068    kcal

Pu(OH)4(c)
        Pu(OH)4 + 4H+ = Pu+4 + 4H2O
        log_k      0.7578
        delta_h  -16.41     kcal

PuO2(c)
        PuO2 + 4H+ = Pu+4 + 2H2O
        log_k     -7.3646
        delta_h  -12.401    kcal

PuF4(c)
        PuF4 = Pu+4 + 4F-
        log_k    -13.2091
        delta_h  -23.925    kcal

Pu(HPO4)2(c)
        Pu(HPO4)2 = Pu+4 + 2H+ + 2PO4-3
        log_k    -52.3461
        delta_h   -0.967    kcal

PuO2OH(am)
        PuO2OH + H+ = PuO2+ + H2O
        log_k      5.4277
        delta_h  -10.101    kcal

PuO2(OH)2(c)
        PuO2(OH)2 + 2H+ = PuO2+2 + 2H2O
        log_k      3.5499
        delta_h   -8.541    kcal

PuO2(HPO4)(c)
        PuO2(HPO4) = PuO2+2 + H+ + PO4-3
        log_k    -24.9292
        delta_h    1.097    kcal

Pyrite
        FeS2 + 2H+ + 2e- = Fe+2 + 2HS-
        log_k    -18.479
        delta_h   11.3      kcal

Pyrocroite
        Mn(OH)2 + 2H+ = Mn+2 + 2H2O
        log_k     15.088
        delta_h  -22.59     kcal

Pyrolusite
        MnO2 + 4H+ + e- = Mn+3 + 2H2O
        log_k     15.861
        delta_h  -29.18     kcal

Pyrophyllite
        Al2Si4O10(OH)2 + 4H2O + 6H+ = 2Al+3 +
4H4SiO4
        log_k     -1.598
        delta_h    0        kcal

Quartz
        SiO2 + 2H2O = H4SiO4
        log_k     -4.006
        delta_h    6.22     kcal

Ra(metal)
        Ra = Ra+2 + 2e-
        log_k     98.362
        delta_h -126.1      kcal

Ra(NO3)2(c)
        Ra(NO3)2 = Ra+2 + 2NO3-
        log_k     -2.2419
        delta_h   12.062    kcal

Ra(Cl)2:2H2O(c)
        Ra(Cl)2:2H2O = Ra+2 + 2Cl- + 2H2O
        log_k     -0.7647
        delta_h    7.304    kcal

RaSO4(c)
        RaSO4 = Ra+2 + SO4-2
        log_k    -10.4499
        delta_h    9.632    kcal

Rb2CrO4
        Rb2CrO4 = CrO4-2 + 2Rb+
        log_k     -0.0968
        delta_h    5.892    kcal

Realgar
        AsS + 3H2O = H3AsO3 + HS- + 2H+ + e-
        log_k    -19.747
        delta_h   30.545    kcal

Retgersite
        NiSO4:6H2O = Ni+2 + SO4-2 + 6H2O
        log_k     -2.04
        delta_h    1.1      kcal

Rhodochrosite
        MnCO3 = Mn+2 + CO3-2
        log_k    -10.41
        delta_h   -2.079    kcal

Romarchite
        SnO + 2H+ = Sn+2 + H2O
        log_k     1.3625
        delta_h   -2.077    kcal

Ru(metal)
        Ru + 4H2O = RuO4-2 + 8H+ + 6e-
        log_k   -112.5104
        delta_h 164.026     kcal

Ru(OH)3:H2O(c)
        Ru(OH)3:H2O + 3H+ = Ru+3 + 4H2O
        log_k     1.6338
        delta_h    0        kcal

RuO2:2H2O(am)
        RuO2:2H2O + 2H+ = Ru(OH)2+2 + 2H2O
        log_k      0.9045
        delta_h    0        kcal

RuO2(c)
        RuO2 + 2H2O = RuO4-2 + 4H+ + 2e-
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        log_k     -73.7397
        delta_h  100.824    kcal

RuBr3(c)
        RuBr3 + 4H2O = RuO4-2 + 3Br- + 8H+ + 3e-
        log_k     -78.9807
        delta_h  112.238    kcal

RuCl3(c)
        RuCl3 + 4H2O = RuO4-2 + 3Cl- + 8H+ + 3e-
        log_k     -71.3071
        delta_h   97.109    kcal

RuI3(c)
        RuI3 + 4H2O = RuO4-2 + 3I- + 8H+ + 3e-
        log_k     -94.5901
        delta_h  137.198    kcal

Rutherfordine
        UO2CO3 = UO2+2 + CO3-2
        log_k     -14.4900
        delta_h    -1.13    kcal

Saleeite
        Mg(UO2)2(PO4)2 = Mg+2 + 2UO2+2 + 2PO4-3
        log_k     -44.0993
        delta_h   -19.469    kcal

Sanidine(H)
        KAlSi3O8 + 4H2O + 4H+ = 3H4SiO4 + Al+3 + K+
        log_k       1.062
        delta_h   -14.252    kcal

Sb
        Sb + 3H2O = Sb(OH)3 + 3H+ + 3e-
        log_k     -11.7058
        delta_h    20.045    kcal

Sb(OH)3(s)
        Sb(OH)3 = Sb(OH)3
        log_k      -7.1099
        delta_h     7.2      kcal

Sb2O3
        Sb2O3 + 3H2O = 2Sb(OH)3
        log_k      -8.4806
        delta_h     4.545    kcal

Sb2O3
        Sb2O3 + 3H2O = 2Sb(OH)3
        log_k     -12.3654
        delta_h     7.325    kcal

Sb2O4
        Sb2O4 + 2H2O + 2H+ + 2e- = 2Sb(OH)3
        log_k       3.4597
        delta_h   -16.27     kcal

Sb2O5
        Sb2O5 + 7H2O = 2Sb(OH)6- + 2H+
        log_k     -12.4827
        delta_h     0        kcal

Sb2Se3
        Sb2Se3 + 6H2O = 2Sb(OH)3 + 3HSe- + 3H+
        log_k     -67.7571
        delta_h    81.99     kcal

Sb4O6I
        Sb4O6 + 6H2O = 4Sb(OH)3
        log_k     -17.0346
        delta_h     8.99     kcal

Sb4O6II
        Sb4O6 + 6H2O = 4Sb(OH)3
        log_k     -19.6586
        delta_h    14.6      kcal

SbBr3
        SbBr3 + 3H2O = Sb(OH)3 + 3Br- + 3H+
        log_k       1.0562
        delta_h    -5.072    kcal

SbCl3
        SbCl3 + 3H2O = Sb(OH)3 + 3Cl- + 3H+
        log_k       0.5915
        delta_h    -8.414    kcal

SbF3
        SbF3 + 3H2O = Sb(OH)3 + 3H+ + 3F-
        log_k     -10.2251
        delta_h    -1.608    kcal

SbI3
        SbI3 + 3H2O = Sb(OH)3 + 3H+ + 3I-
        log_k      -0.538
        delta_h     3.248    kcal

SbO2
        SbO2 + 4H2O = Sb(OH)6- + e- + 2H+
        log_k     -27.8241
        delta_h     0        kcal

Schoepite
        UO3:2H2O + 2H+ = UO2+2 + 3H2O
        log_k       4.8326
        delta_h   -11.961    kcal

Schoepite-Dehyd(0.393)
        UO3:0.393H2O + 2H+ = UO2+2 + 1.393H2O
        log_k       6.7240
        delta_h   -16.4956   kcal

Schoepite-Dehyd(0.648)
        UO3:0.648H2O + 2H+ = UO2+2 + 1.648H2O
        log_k       6.2059
        delta_h   -15.5764   kcal

Schoepite-Dehyd(0.850)
        UO3:0.850H2O + 2H+ = UO2+2 + 1.850H2O
        log_k       5.0966
        delta_h   -13.4065   kcal

Schoepite-Dehyd(0.900)
        UO3:0.900H2O + 2H+ = UO2+2 + 1.900H2O
        log_k       5.0163
        delta_h   -13.2623   kcal

Schoepite-Dehyd(1.00)
        UO3:1.00H2O + 2H+ = UO2+2 + 2H2O
        log_k       5.1026
        delta_h   -13.664    kcal

Se(A)
        Se + H+ + 2e- = HSe-
        log_k      -7.1099
        delta_h     2.6      kcal

Se(hex)
        Se + H+ + 2e- = HSe-
        log_k      -7.6963
        delta_h     3.8      kcal

SeO2
        SeO2 + H2O = HSeO3- + H+
        log_k      -0.1246
        delta_h     0.335    kcal

SeO3
        SeO3 + H2O = SeO4-2 + 2H+
        log_k      21.044
        delta_h   -34.985    kcal

Sepiolite(s)
        Mg2Si3O7.5OH:3H2O + 0.5H2O + 4H+ = 2Mg+2 +
3H4SiO4
        log_k      18.78
        delta_h     0        kcal

Sepiolite(c)
        Mg2Si3O7.5OH:3H2O + 0.5H2O + 4H+ = 2Mg+2 +
3H4SiO4
        log_k      15.913
        delta_h   -27.268    kcal

Siderite
        FeCO3 = Fe+2 + CO3-2
        log_k     -10.55
        delta_h    -5.328    kcal

SiO2(a)
        SiO2 + 2H2O = H4SiO4
        log_k      -3.018
        delta_h     4.44     kcal

SiO2(am)
        SiO2 + 2H2O = H4SiO4
        log_k      -2.71
        delta_h     3.91     kcal

Sklodowskite
        Mg(H3O)2(UO2)2(SiO4)2:4H2O + 6H+ = Mg+2 +
2UO2+2 + 2H4SiO4 + 6H2O
        log_k      14.0302
        delta_h     0        kcal

Smithsonite
        ZnCO3 = Zn+2 + CO3-2
        log_k     -10.0
        delta_h    -4.36     kcal

Sn(metal)
        Sn = Sn+2 + 2e-
        log_k       4.8523
        delta_h    -2.1      kcal

SnBr2(c)
        SnBr2 = Sn+2 + 2Br-
        log_k      -1.4352
        delta_h     1.97     kcal

SnCl2(c)
        SnCl2 = Sn+2 + 2Cl-
        log_k       0.3185
        delta_h    -2.866    kcal

Sn(OH)2(c)
        Sn(OH)2 + 2H+ = Sn+2 + 2H2O
        log_k       1.8400
        delta_h    -4.704    kcal

Sn3S4
        Sn3S4 + 4H+ + 2e- = 3Sn+2 + 4HS-
        log_k     -56.6668
        delta_h    66.8      kcal

SnSO4
        SnSO4 = Sn+2 + SO4-2
        log_k     -23.9292
        delta_h    23.0      kcal

SnSe
        SnSe + 4H2O = Sn+2 + SeO4-2 + 8H+ + 8e-
        log_k     -99.2068
        delta_h     0        kcal

SnSe2
        SnSe2 + 8H2O = Sn+2 + 2SeO4-2 + 16H+ + 14e-
        log_k   -193.8640
        delta_h     0        kcal

SnBr4(c)
        SnBr4 = Sn+4 + 4Br-
        log_k      11.1272
        delta_h   -18.732    kcal

Sn(SO4)2
        Sn(SO4)2 = Sn+4 + 2SO4-2
        log_k      16.0352
        delta_h   -38.173    kcal

Soddyite
        (UO2)2SiO4:2H2O + 4H+ = 2UO2+2 + H4SiO4 +
2H2O
        log_k       0.5123
        delta_h     0        kcal

Sphalerite
        ZnS + H+ = Zn+2 + HS-
        log_k     -11.618
        delta_h     8.25     kcal

Spinel
        MgAl2O4 + 8H+ = Mg+2 + 2Al+3 + 4H2O
        log_k      36.333
        delta_h   -89.089    kcal

Sr(metal)
        Sr = Sr+2 + 2e-
        log_k      98.7725
        delta_h     0        kcal

SrBr2(c)
        SrBr2 = Sr+2 + 2Br-
        log_k      13.1128
        delta_h     0        kcal

SrBr2:H2O(c)
        SrBr2:H2O = Sr+2 + 2Br- + H2O
        log_k       9.6057
        delta_h     0        kcal

SrBr2:6H2O(c)
        SrBr2:6H2O = Sr+2 + 2Br- + 6H2O
        log_k       3.6678
        delta_h     0        kcal

SrCl2(c)
        SrCl2 = Sr+2 + 2Cl-
        log_k       7.9389
        delta_h     0        kcal

SrCl2:H2O(c)
        SrCl2:H2O = Sr+2 + 2Cl- + H2O
        log_k       4.7822
        delta_h     0        kcal

SrCl2:2H2O(c)
        SrCl2:2H2O = Sr+2 + 2Cl- + 2H2O
        log_k       3.3248
        delta_h     0        kcal

SrCl2:6H2O(c)
        SrCl2:6H2O = Sr+2 + 2Cl- + 6H2O
        log_k       1.5038
        delta_h     0        kcal

SrCrO4(c)
        SrCrO4 = Sr+2 + CrO4-2
        log_k      -4.8443
        delta_h    -2.42     kcal

SrF2(c)
        SrF2 = Sr+2 + 2F-
        log_k      -8.540
        delta_h     0        kcal

SrI2(c)
        SrI2 = Sr+2 + 2I-
        log_k      19.2678
        delta_h     0        kcal

Sr(NO3)2(c)
        Sr(NO3)2 = Sr+2 + 2NO3-
        log_k       1.1493
        delta_h     0        kcal

Sr(NO3)2:4H2O(c)
        Sr(NO3)2:4H2O = Sr+2 + 2NO3- + 4H2O
        log_k       0.6976
        delta_h     0        kcal

SrO(c)
        SrO + 2H+ = Sr+2 + H2O
        log_k      41.8916
        delta_h     0        kcal

Sr(OH)2(c)
        Sr(OH)2 + 2H+ = Sr+2 + 2H2O
        log_k      27.5229
        delta_h     0        kcal

SrHPO4(c)
        SrHPO4 = Sr+2 + PO4-3 + H+
        log_k     -18.5634
        delta_h     0        kcal

SrS(c)
        SrS + H+ = Sr+2 + HS-
        log_k      14.7284
        delta_h     0        kcal

SrSeO3(c)
        SrSeO3 + H+ = Sr+2 + HSeO3-
        log_k       0.1034
        delta_h     0        kcal

SrSeO4(c)
        SrSeO4 = Sr+2 + SeO4-2
        log_k      -4.40
        delta_h     2.69     kcal

Sr2SiO4(c)
        Sr2SiO4 + 4H+ = 2Sr+2 + H4SiO4
        log_k      42.926
        delta_h     0        kcal

SrSiO3(c)
        SrSiO3 + 2H+ + H2O = Sr+2 + H4SiO4
        log_k      14.7254
        delta_h     0        kcal

SrUO4(alpha)
        SrUO4 + 4H+ = Sr+2 + UO2+2 + 2H2O
        log_k      19.1497
        delta_h     0        kcal

SrZrO3(c)
        SrZrO3 + 6H+ = Sr+2 + Zr+4 + 3H2O
        log_k     131.228
        delta_h     0        kcal

Stibnite
        Sb2S3 + 6H2O = 2Sb(OH)3 + 3HS- + 3H+
        log_k     -60.156
        delta_h    69.29     kcal

Strengite
        FePO4:2H2O = Fe+3 + PO4-3 + 2H2O
        log_k     -26.4
        delta_h    -2.03     kcal

Strontianite
        SrCO3 = Sr+2 + CO3-2
        log_k     -10.6425
        delta_h    -0.69     kcal

SULFUR
        S + H+ + 2e- = HS-
        log_k      -2.11
        delta_h    -4.2      kcal

Talc
        Mg3Si4O10(OH)2 + 4H2O + 6H+ = 3Mg+2 +
4H4SiO4
        log_k      23.055
        delta_h   -35.005    kcal

Tc(metal)
        Tc + 4H2O = TcO4- + 7e- + 8H+
        log_k     -56.9510
        delta_h   102.068    kcal

TcOH(c)
        TcOH = TcO+2 + H+ + 3e-
        log_k     -23.5047
        delta_h     0        kcal

Tc(OH)2(c)
        Tc(OH)2 + 2H+ = Tc+3 + 2H2O + e-
        log_k     -16.2332
        delta_h     0        kcal

Tc(OH)3(c)
        Tc(OH)3 + 3H+ = Tc+3 + 3H2O
        log_k      -9.2425
        delta_h     0        kcal

TcO2:2H2O(am)
        TcO2:2H2O + 2H+ = TcO+2 + 3H2O
        log_k      -4.2319
        delta_h     0        kcal

TcO3(c)
        TcO3 + H2O = TcO4-2 + 2H+
        log_k     -23.1494
        delta_h     0        kcal

Tc3O4(c)
        Tc3O4 + 8H+ = 3Tc+3 + 4H2O + e-
        log_k     -40.7316
        delta_h     0        kcal

Tc4O7(c)
        Tc4O7 + 10H+ = 2Tc+3 + 2TcO+2 + 5H2O
        log_k     -26.0149
        delta_h     0        kcal

TcS2(c)
        TcS2 + H2O = TcO+2 + 2HS-
        log_k     -65.9742
        delta_h     0        kcal

TcS3(c)
        TcS3 + 4H2O = TcO4-2 + 3HS- + 5H+
        log_k    -119.5008
        delta_h     0        kcal

Tc2S7(c)
        Tc2S7 + 8H2O = 2TcO4- + 7HS- + 9H+
        log_k    -230.2410
        delta_h   324.176    kcal

Tenorite
        CuO + 2H+ = Cu+2 + H2O
        log_k       7.62
        delta_h   -15.24     kcal

Th(metal)
        Th = Th+4 + 4e-
        log_k     123.5848
        delta_h  -183.80     kcal

ThBr4(c)
        ThBr4 = Th+4 + 4Br-
        log_k      34.0806
        delta_h   -69.367    kcal

ThCl4(c)
        ThCl4 = Th+4 + 4Cl-
        log_k      23.8494
        delta_h   -60.029    kcal

ThF4(c)
        ThF4 = Th+4 + 4F-
        log_k     -29.9943
        delta_h    -3.045    kcal

ThF4:2.5H2O(c)
        ThF4:2.5H2O = Th+4 + 4F- + 2.5H2O
        log_k     -31.8564
        delta_h     5.402    kcal

ThI4(c)
        ThI4 = Th+4 + 4I-
        log_k      45.200
        delta_h   -79.545    kcal

Th(NO3)4:5H2O(c)
        Th(NO3)4:5H2O = Th+4 + 4NO3- + 5H2O
        log_k       1.7792
        delta_h    -4.335    kcal

Th(OH)4(c)
        Th(OH)4 + 4H+ = Th+4 + 4H2O
        log_k       9.6546
        delta_h   -33.542    kcal

ThO2(c)
        ThO2 + 4H+ = Th+4 + 2H2O
        log_k       1.8620
        delta_h   -27.317    kcal

Th(SO4)2(c)
        Th(SO4)2 = Th+4 + 2SO4-2
        log_k     -20.3003
        delta_h   -11.024    kcal

ThS2(c)
        ThS2 + 2H+ = Th+4 + 2HS-
        log_k      10.7876
        delta_h   -41.914    kcal

Th2S3(c)
        Th2S3 + 3H+ = 2Th+4 + 3HS- + 2e-
        log_k      52.2204
        delta_h  -120.333    kcal

Th7S12(c)
        Th7S12 + 12H+ = 7Th+4 + 12HS- + 4e-
        log_k     118.0579
        delta_h  -344.134    kcal

Th2Se3(c)
        Th2Se3 + 9H2O = 2Th+4 + 3HSeO3- + 15H+ +
20e-
        log_k     -73.6817
        delta_h   102.232    kcal

Thenardite
        Na2SO4 = 2Na+ + SO4-2
        log_k      -0.179
        delta_h    -0.572    kcal

Thermonatrite
        Na2CO3:H2O = 2Na+ + CO3-2 + H2O
        log_k       0.125
        delta_h    -2.802    kcal

Tl(OH)3
        Tl(OH)3 = Tl(OH)3
        log_k      -6.4503
        delta_h     0        kcal

Tl2CO3
        Tl2CO3 = 2Tl+ + CO3-2
        log_k      -3.8482
        delta_h     8.02     kcal

Tl2CrO4
        Tl2CrO4 = 2Tl+ + CrO4-2
        log_k     -12.0136
        delta_h    25.31     kcal

Tl2O
        Tl2O + 2H+ = 2Tl+ + H2O
        log_k      27.0984
        delta_h   -23.055    kcal

Tl2S
        Tl2S + H+ = 2Tl+ + HS-
        log_k      -7.1832
        delta_h    21.56     kcal

Tl2Se
        Tl2Se + H+ = 2Tl+ + HSe-
        log_k      -6.6848
        delta_h    20.36     kcal

Tl2SeO4
        Tl2SeO4 = 2Tl+ + SeO4-2
        log_k      -4.0168
        delta_h     9.76     kcal

Tl2SO4
        Tl2SO4 = 2Tl+ + SO4-2
        log_k      -3.6942
        delta_h     7.94     kcal

TlBr
        TlBr = Tl+ + Br-
        log_k      -5.419
        delta_h    13.641    kcal

TlCl
        TlCl = Tl+ + Cl-
        log_k      -3.7243
        delta_h    10.137    kcal

TlI
        TlI = Tl+ + I-
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        log_k     -7.1964
        delta_h   17.281   kcal

Tlmetal
        Tl = Tl+ + e-
        log_k     5.6733
        delta_h   1.28    kcal

TlNO3
        TlNO3 = Tl+ + NO3-
        log_k     -1.5319
        delta_h   10.02    kcal

TlOH
        TlOH + H+ = Tl+ + H2O
        log_k     12.9225
        delta_h   -9.935   kcal

Torbernite
        Cu(UO2)2(PO4)2 = Cu+2 + 2UO2+2 + 2PO4-3
        log_k     -44.9642
        delta_h   -16.262   kcal

Tremolite
        Ca2Mg5Si8O22(OH)2 + 8H2O + 14H+ = 2Ca+2 +
5Mg+2 + 8H4SiO4
        log_k     56.546
        delta_h   -96.615   kcal

Tsumebite
        Pb2CuPO4(OH)3:3H2O + 3H+ = 2Pb+2 + Cu+2 +
PO4-3 + 6H2O
        log_k     -9.79
        delta_h   0         kcal

Tyuyamunite
        Ca(UO2)2(VO4)2 + 8H+ = Ca+2 + 2UO2+2 + 2VO2+
+ 4H2O
        log_k     3.5211
        delta_h   -36.251   kcal

USb2(c)
        USb2 + 8H2O = UO2+2 + 2Sb(OH)3 + 10H+ + 12e-
        log_k     29.5246
        delta_h   -24.68    kcal

U3Sb4(c)
        U3Sb4 + 12H2O = 3U+4 + 4Sb(OH)3 + 12H+ +
24e-
        log_k     152.3288
        delta_h   -235.72   kcal

UBr2Cl(c)
        UBr2Cl = U+3 + 2Br- + Cl-
        log_k     17.5351
        delta_h   -35.473   kcal

UBr3(c)
        UBr3 = U+3 + 3Br-
        log_k     20.0084
        delta_h   -36.99    kcal

UCl3(c)
        UCl3 = U+3 + 3Cl-
        log_k     12.2886
        delta_h   -29.649   kcal

UBrCl2(c)
        UBrCl2 = U+3 + Br- + 2Cl-
        log_k     14.2575
        delta_h   -31.666   kcal

UOCl(c)
        UOCl + 2H+ = U+3 + H2O + Cl-
        log_k     10.1424
        delta_h   -25.8     kcal

UF3(c)
        UF3 = U+3 + 3F-
        log_k     -19.7853
        delta_h   1.74    kcal


UI3(c)
        UI3 = U+3 + 3I-
        log_k     28.7741
        delta_h   -45.97    kcal

UO2(am)
        UO2 + 4H+ = U+4 + 2H2O
        log_k     0.1144
        delta_h   -26.23    kcal

U4O9(c)
        U4O9 + 18H+ + 2e- = 4U+4 + 9H2O
        log_k     -3.384
        delta_h   -102.133  kcal

U3O8(c)
        U3O8 + 16H+ + 4e- = 3U+4 + 8H2O
        log_k     21.107
        delta_h   -116.036  kcal

UBr4(c)
        UBr4 = U+4 + 4Br-
        log_k     31.2956
        delta_h   -65.71    kcal

UOBr2(c)
        UOBr2 + 2H+ = U+4 + H2O + 2Br-
        log_k     7.9771
        delta_h   -34.947   kcal

UBrCl3(c)
        UBrCl3 = U+4 + Br- + 3Cl-
        log_k     23.5225
        delta_h   -58.899   kcal

UBr3Cl(c)
        UBr3Cl = U+4 + 3Br- + Cl-
        log_k     29.1202
        delta_h   -64.603   kcal

UCl4(c)
        UCl4 = U+4 + 4Cl-
        log_k     21.9707
        delta_h   -57.482   kcal

UBr2Cl2(c)
        UBr2Cl2 = U+4 + 2Br- + 2Cl-
        log_k     26.2181
        delta_h   -62.206   kcal

UOCl2(c)
        UOCl2 + 2H+ = U+4 + H2O + 2Cl-
        log_k     5.8756
        delta_h   -34.433   kcal

U2O2Cl5(c)
        U2O2Cl5 = U+4 + UO2+ + 5Cl-
        log_k     19.2670
        delta_h   -60.645   kcal

UF4(c)
        UF4 = U+4 + 4F-
        log_k     -29.2065
        delta_h   -4.3      kcal

UF4:2.5H2O(c)
        UF4:2.5H2O = U+4 + 4F- + 2.5H2O
        log_k     -33.3796
        delta_h   5.9475  kcal

U2F9(c)
        U2F9 + 2H2O = U+4 + UO2+ + 9F- + 4H+
        log_k     -45.4954
        delta_h   -11.203   kcal

U4F17(c)
        U4F17 + 2H2O = 3U+4 + UO2+ + 17F- + 4H+
        log_k     -104.7483
        delta_h   -18.747   kcal

UClF3(c)
        UClF3 = U+4 + Cl- + 3F-
        log_k     -17.5183
        delta_h   -17.673   kcal

UCl2F2(c)
        UCl2F2 = U+4 + 2Cl- + 2F-
        log_k     -3.5146
        delta_h   -31.006   kcal

UCl3F(c)
        UCl3F = U+4 + 3Cl- + F-
        log_k     10.3139
        delta_h   -44.099   kcal

UOF2(c)
        UOF2 + 2H+ = U+4 + H2O + 2F-
        log_k     -18.1481
        delta_h   -10.227   kcal

UOF2:H2O(c)
        UOF2:H2O + 2H+ = U+4 + 2H2O + 2F-
        log_k     -18.7030
        delta_h   -7.454    kcal

UOFOH(c)
        UOFOH + 3H+ = U+4 + 2H2O + F-
        log_k     -8.9257
        delta_h   -17.024   kcal

UI4(c)
        UI4 = U+4 + 4I-
        log_k     39.3155
        delta_h   -71.68    kcal

UClI3(c)
        UClI3 = U+4 + Cl- + 3I-
        log_k     35.2392
        delta_h   -68.133   kcal

UCl2I2(c)
        UCl2I2 = U+4 + 2Cl- + 2I-
        log_k     30.2957
        delta_h   -64.576   kcal

UCl3I(c)
        UCl3I = U+4 + 3Cl- + I-
        log_k     25.5355
        delta_h   -59.959   kcal

U(CO3)2(c)
        U(CO3)2 = U+4 + 2CO3-2
        log_k     -13.1296
        delta_h   -33.773   kcal

USO4(OH)2(c)
        USO4(OH)2 + 2H+ = U+4 + SO4-2 + 2H2O
        log_k     -3.0743
        delta_h   0         kcal

U(SO4)2(c)
        U(SO4)2 = U+4 + 2SO4-2
        log_k     -11.5156
        delta_h   -23.97    kcal

U(SO4)2:4H2O(c)
        U(SO4)2:4H2O = U+4 + 2SO4-2 + 4H2O
        log_k     -11.5274
        delta_h   -16.688   kcal

U(SO4)2:8H2O(c)
        U(SO4)2:8H2O = U+4 + 2SO4-2 + 8H2O
        log_k     -12.5553
        delta_h   -8.246    kcal

U(HPO4)2:4H2O(c)
        U(HPO4)2:4H2O = U+4 + 2PO4-3 + 2H+ + 4H2O
        log_k     -57.5099
        delta_h   10.882    kcal

UBr5(c)
        UBr5 + 2H2O = UO2+ + 5Br- + 4H+
        log_k     41.6328
        delta_h   -59.816   kcal

UOBr3(c)
        UOBr3 + H2O = UO2+ + 3Br- + 2H+
        log_k     23.5663
        delta_h   -35.723   kcal

UCl5(c)
        UCl5 + 2H2O = UO2+ + 5Cl- + 4H+
        log_k     33.8682
        delta_h   -54.941   kcal

UOCl3(c)
        UOCl3 + H2O = UO2+ + 3Cl- + 2H+
        log_k     8.5585
        delta_h   -18.442   kcal

U5O12Cl(c)
        U5O12Cl + 4H+ = 5UO2+ + Cl- + 2H2O
        log_k     -18.7793
        delta_h   -1.927    kcal

UF5(alpha)
        UF5 + 2H2O = UO2+ + 5F- + 4H+
        log_k     -12.8503
        delta_h   -12.986   kcal

UF5(beta)
        UF5 + 2H2O = UO2+ + 5F- + 4H+
        log_k     -13.1844
        delta_h   -11.096   kcal

UPO5(c)
        UPO5 + H2O = UO2+ + PO4-3 + 2H+
        log_k     -31.8976
        delta_h   11.447    kcal

UO2(OH)2(beta)
        UO2(OH)2 + 2H+ = UO2+2 + 2H2O
        log_k     4.9453
        delta_h   -13.514   kcal

UO3(alpha)
        UO3 + 2H+ = UO2+2 + H2O
        log_k     8.6389
        delta_h   -20.817   kcal

UO3(beta)
        UO3 + 2H+ = UO2+2 + H2O
        log_k     8.3103
        delta_h   -20.147   kcal

UO3(gamma)
        UO3 + 2H+ = UO2+2 + H2O
        log_k     7.7076
        delta_h   -19.307   kcal

Gummite
        UO3 + 2H+ = UO2+2 + H2O
        log_k     10.403
        delta_h   -23.077   kcal

UO2Br2(c)
        UO2Br2 = UO2+2 + 2Br-
        log_k     16.5105
        delta_h   -29.73    kcal

UO2Br2:H2O(c)
        UO2Br2:H2O = UO2+2 + 2Br- + H2O
        log_k     12.1233
        delta_h   -21.907   kcal

UO2Br2:3H2O(c)
        UO2Br2:3H2O = UO2+2 + 2Br- + 3H2O
        log_k     9.4108
        delta_h   -14.601   kcal

UO2BrOH:2H2O(c)
        UO2BrOH:2H2O + H+ = UO2+2 + Br- + 3H2O
        log_k     4.2020
        delta_h   -9.421    kcal

UCl6(c)
        UCl6 + 2H2O = UO2+2 + 6Cl- + 4H+
        log_k     53.1053
        delta_h   -85.464   kcal

UO2Cl2(c)
        UO2Cl2 = UO2+2 + 2Cl-
        log_k     12.1338
        delta_h   -26.126   kcal

UO2Cl2:H2O(c)
        UO2Cl2:H2O = UO2+2 + 2Cl- + H2O
        log_k     8.2822
        delta_h   -18.853   kcal

UO2Cl2:3H2O(c)
        UO2Cl2:3H2O = UO2+2 + 2Cl- + 3H2O
        log_k     5.6101
        delta_h   -10.857   kcal

UO2ClOH:2H2O(c)
        UO2ClOH:2H2O + H+ = UO2+2 + Cl- + 3H2O
        log_k     2.3029
        delta_h   -7.834    kcal
(UO2)2Cl3(c)
        (UO2)2Cl3 = UO2+2 + UO2+ + 3Cl-
        log_k     12.7264
        delta_h   -33.639   kcal

UF6(c)
        UF6 + 2H2O = UO2+2 + 6F- + 4H+
        log_k     17.5357
        delta_h   -62.606   kcal

UO2FOH(c)
        UO2FOH + H+ = UO2+2 + F- + H2O
        log_k     -1.8416
        delta_h   -9.977    kcal

UO2FOH:H2O(c)
        UO2FOH:H2O + H+ = UO2+2 + F- + 2H2O
        log_k     -2.2829
        delta_h   -7.54     kcal

UO2FOH:2H2O(c)
        UO2FOH:2H2O + H+ = UO2+2 + F- + 3H2O
        log_k     -2.6593
        delta_h   -5.233    kcal

UO2F2(c)
        UO2F2 = UO2+2 + 2F-
        log_k     -7.2357
        delta_h   -8.57     kcal

UO2F2:3H2O(c)
        UO2F2:3H2O = UO2+2 + 2F- + 3H2O
        log_k     -7.3772
        delta_h   -2.931    kcal

U2O3F6(c)
        U2O3F6 + H2O = 2UO2+2 + 6F- + 2H+
        log_k     -2.7332
        delta_h   -43.763   kcal

U3O5F8(c)
        U3O5F8 + H2O = 3UO2+2 + 8F- + 2H+
        log_k     -2.6604
        delta_h   -62.253   kcal

UOF4(c)
        UOF4 + H2O = UO2+2 + 4F- + 2H+
        log_k     4.5629
        delta_h   -35.743   kcal

UO2(NO3)2(c)
        UO2(NO3)2 = UO2+2 + 2NO3-
        log_k     11.9578
        delta_h   -19.438   kcal

UO2(NO3)2:H2O(c)
        UO2(NO3)2:H2O = UO2+2 + 2NO3- + H2O
        log_k     8.5080
        delta_h   -12.935   kcal

UO2(NO3)2:2H2O(c)
        UO2(NO3)2:2H2O = UO2+2 + 2NO3- + 2H2O
        log_k     4.9456
        delta_h   -6.125    kcal

UO2(NO3)2:3H2O(c)
        UO2(NO3)2:3H2O = UO2+2 + 2NO3- + 3H2O
        log_k     3.7133
        delta_h   -2.209    kcal

UO2(NO3)2:6H2O(c)
        UO2(NO3)2:6H2O = UO2+2 + 2NO3- + 6H2O
        log_k     2.3155
        delta_h   4.9       kcal

UO2SO4(c)
        UO2SO4 = UO2+2 + SO4-2
        log_k     1.9667
        delta_h   -19.86    kcal

UO2SO4:H2O(c)
        UO2SO4:H2O = UO2+2 + SO4-2 + H2O
        log_k     -6.0223
        delta_h   -9.367    kcal

UO2SO4:2.5H2O(c)
        UO2SO4:2.5H2O = UO2+2 + SO4-2 + 2.5H2O
        log_k     -1.4912
        delta_h   -8.5385   kcal

UO2SO4:3H2O(c)
        UO2SO4:3H2O = UO2+2 + SO4-2 + 3H2O
        log_k     -1.4017
        delta_h   -7.231    kcal

UO2SO4:3.5H2O(c)
        UO2SO4:3.5H2O = UO2+2 + SO4-2 + 3.5H2O
        log_k     -1.4804
        delta_h   -6.5635   kcal

(UO2)3(PO4)2(c)
        (UO2)3(PO4)2 = 3UO2+2 + 2PO4-3
        log_k     -38.6703
        delta_h   -28.8     kcal

(UO2)3(PO4)2:4H2O(c)
        (UO2)3(PO4)2:4H2O = 3UO2+2 + 2PO4-3 + 4H2O
        log_k     -51.6764
        delta_h   -3.841    kcal

(UO2)2P2O7(c)
        (UO2)2P2O7 + H2O = 2UO2+2 + 2PO4-3 + 2H+
        log_k     -39.3286
        delta_h   50.554    kcal

UO2(PO3)2(c)
        UO2(PO3)2 + 2H2O = UO2+2 + 2PO4-3 + 4H+
        log_k     -40.9262
        delta_h   -6.796    kcal

UO2HPO4(c)
        UO2HPO4 = UO2+2 + PO4-3 + H+
        log_k     -25.0000
        delta_h   0         kcal

UO2HPO4:4H2O(c)
        UO2HPO4:4H2O = UO2+2 + PO4-3 + H+ + 4H2O
        log_k     -25.3442
        delta_h   7.22      kcal

UP2O7:2OH2O(c)
        UP2O7:2OH2O = U+4 + 2PO4-3 + 2H+ + 19H2O
        log_k     -53.2684
        delta_h   0         kcal

UO2(AsO3)2(c)
        UO2(AsO3)2 + 2H2O + 2H+ = UO2+2 + 2H3AsO4
        log_k     11.4956
        delta_h   -22.864   kcal

(UO2)2As2O7(c)
        (UO2)2As2O7 + H2O + 4H+ = 2UO2+2 + 2H3AsO4
        log_k     12.2643
        delta_h   -31.447   kcal

(UO2)3(AsO4)2(c)
        (UO2)3(AsO4)2 + 6H+ = 3UO2+2 + 2H3AsO4
        log_k     13.8752
        delta_h   -41.355   kcal

Uramphite
        (UO2)2(NH4)2(PO4)2 = 2UO2+2 + 2NH4+ + 2PO4-3
        log_k     -51.749
        delta_h   9.70      kcal

Uraninite
        UO2 = UO2+2 + 2e-
        log_k     -13.8955
        delta_h   15.83     kcal

Uranocircite
        Ba(UO2)2(PO4)2 = Ba+2 + 2UO2+2 + 2PO4-3
        log_k     -44.4475
        delta_h   -89.2     kcal

Uranophane
        Ca(UO2)2(SiO3)2(OH)2 + 6H+ = Ca+2 + 2UO2+2 +
2H4SiO4
        log_k     17.5237
        delta_h   0         kcal

V(OH)3
        V(OH)3 + 3H+ = V+3 + 3H2O
        log_k     7.65
        delta_h   0         kcal

V2O3
        VO1.5 + 3H+ = V+3 + 1.5H2O
        log_k     4.9
        delta_h   -19.72    kcal

V2O4
        VO2 + 2H+ = VO+2 + H2O
        log_k     4.27
        delta_h   -14.07    kcal

V2O5
        VO2.5 + H+ = VO2+ + 0.5H2O
        log_k     -0.72
        delta_h   -4.16     kcal

V3O5
        V3O5 + 4H+ = 3VO+2 + 2H2O + 2e-
        log_k     1.87
        delta_h   -23.53    kcal

V4O7
        V4O7 + 6H+ = 4VO+2 + 3H2O + 2e-
        log_k     7.14
        delta_h   -39.15    kcal

V6O13
        V6O13 + 2H+ = 6VO2+ + H2O + 4e-
        log_k     -60.86
        delta_h   64.89     kcal

VCl2
        VCl2 = V+3 + 2Cl- + e-
        log_k     17.97
        delta_h   -35.8     kcal

VCl3
        VCl3 = V+3 + 3Cl-
        log_k     21.73
        delta_h   -43.96    kcal

VF4
        VF4 + H2O = VO+2 + 4F- + 2H+
        log_k     14.93
        delta_h   -47.59    kcal

Vivianite
        Fe3(PO4)2:8H2O = 3Fe+2 + 2PO4-3 + 8H2O
        log_k     -36.0
        delta_h   0         kcal

VMetal
        V = V+3 + 3e-
        log_k     42.35
        delta_h   -62.9     kcal

VO
        VO + 2H+ = V+3 + H2O + e-
        log_k     13.08
        delta_h   -28.02    kcal

VO(OH)2
        VO(OH)2 + 2H+ = VO+2 + 2H2O
```

```
        log_k     5.85
        delta_h   0        kcal

VO2Cl
        VO2Cl = VO2+ + Cl-
        log_k     2.81
        delta_h   -9.65    kcal

VOCl
        VOCl + 2H+ = V+3 + Cl- + H2O
        log_k     9.41
        delta_h   -26.17   kcal

VOCl2
        VOCl2 = VO+2 + 2Cl-
        log_k     12.79
        delta_h   -28.2    kcal

VOSO4(C)
        VOSO4 = VO+2 + SO4-2
        log_k     3.57
        delta_h   -20.72   kcal

Ca_Vanadate
        Ca0.5VO3 + 2H+ = 0.5Ca+2 + VO2+ + H2O
        log_k     2.83
        delta_h   -10.13   kcal

Fe_Vanadate
        Fe0.5VO3 + 2H+ = 0.5Fe+2 + VO2+ + H2O
        log_k     -1.86
        delta_h   -7.37    kcal

Mn_Vanadate
        Mn0.5VO3 + 2H+ = 0.5Mn+2 + VO2+ + H2O
        log_k     2.45
        delta_h   -11.05   kcal

Na_Vanadate
        NaVO3 + 2H+ = Na+ + VO2+ + H2O
        log_k     3.71
        delta_h   -7.01    kcal

Wairakite
        CaAl2Si4O12:2H2O + 8H+ + 2H2O = Ca+2 + 2Al+3
+ 4H4SiO4
        log_k     18.87
        delta_h   -63.15   kcal

Weeksite
        K2(UO2)2Si6O15:4H2O + 5H2O + 6H+ = 2K+ +
2UO2+2 + 6H4SiO4
        log_k     16.0872
        delta_h   0        kcal

Willemite
        Zn2SiO4 + 4H+ = 2Zn+2 + H4SiO4
        log_k     15.33
        delta_h   -33.37   kcal

Witherite
        BaCO3 = Ba+2 + CO3-2
        log_k     -8.585
        delta_h   0.36     kcal

P-Wollstanite
        CaSiO3 + H2O + 2H+ = H4SiO4 + Ca+2
        log_k     13.846
        delta_h   -21.068  kcal

Wollastonite
        CaSiO3 + H2O + 2H+ = H4SiO4 + Ca+2
        log_k     12.996
        delta_h   -19.498  kcal

Wurtzite
        ZnS + H+ = Zn+2 + HS-
        log_k     -9.682
        delta_h   5.06     kcal

Zincite
        ZnO + 2H+ = Zn+2 + H2O
        log_k     11.14
        delta_h   -21.86   kcal

Zincosite
        ZnSO4 = Zn+2 + SO4-2
        log_k     3.01
        delta_h   -19.2    kcal

Zircon
        ZrSiO4 + 4H+ = Zr+4 + H4SiO4
        log_k     -15.5394
        delta_h   0        kcal

Zn(BO2)2
        Zn(BO2)2 + 2H2O + 2H+ = Zn+2 + 2H3BO3
        log_k     8.29
        delta_h   0        kcal

Zn(NO3)2:6H2O
        Zn(NO3)2:6H2O = Zn+2 + 2NO3- + 6H2O
        log_k     3.44
        delta_h   5.51     kcal

Zn(OH)2(A)
        Zn(OH)2 + 2H+ = Zn+2 + 2H2O
        log_k     12.45
        delta_h   0        kcal

Zn(OH)2(B)
        Zn(OH)2 + 2H+ = Zn+2 + 2H2O
        log_k     11.75
        delta_h   0        kcal

Zn(OH)2(C)
        Zn(OH)2 + 2H+ = Zn+2 + 2H2O
        log_k     12.2
        delta_h   0        kcal

Zn(OH)2(E)
        Zn(OH)2 + 2H+ = Zn+2 + 2H2O
        log_k     11.5
        delta_h   0        kcal

Zn(OH)2(G)
        Zn(OH)2 + 2H+ = Zn+2 + 2H2O
        log_k     11.71
        delta_h   0        kcal

Zn2(OH)2SO4
        Zn2(OH)2SO4 + 2H+ = 2Zn+2 + 2H2O + SO4-2
        log_k     7.5
        delta_h   0        kcal

Zn2(OH)3Cl
        Zn2(OH)3Cl + 3H+ = 2Zn+2 + 3H2O + Cl-
        log_k     15.2
        delta_h   0        kcal

Zn3(AsO4)2:2.5H2O
        Zn3(AsO4)2:2.5H2O + 6H+ = 3Zn+2 + 2H3AsO4 +
2.5H2O
        log_k     13.65
        delta_h   0        kcal

Zn3(PO4)2:4H2O
        Zn3(PO4)2:4H2O = 3Zn+2 + 2PO4-3 + 4H2O
        log_k     -32.04
        delta_h   0        kcal

Zn3O(SO4)2
        Zn3O(SO4)2 + 2H+ = 3Zn+2 + 2SO4-2 + H2O
        log_k     19.02
        delta_h   -62.0    kcal

Zn4(OH)6SO4
        Zn4(OH)6SO4 + 6H+ = 4Zn+2 + 6H2O + SO4-2
        log_k     28.4
        delta_h   0        kcal

Zn5(OH)8Cl2
        Zn5(OH)8Cl2 + 8H+ = 5Zn+2 + 8H2O + 2Cl-
        log_k     38.5
        delta_h   0        kcal

ZnBr2:2H2O
        ZnBr2:2H2O = Zn+2 + 2Br- + 2H2O
        log_k     5.21
        delta_h   -7.51    kcal

ZnCl2
        ZnCl2 = Zn+2 + 2Cl-
        log_k     7.03
        delta_h   -17.48   kcal

ZnCO3:H2O
        ZnCO3:H2O = Zn+2 + CO3-2 + H2O
        log_k     -10.26
        delta_h   0        kcal

ZnF2
        ZnF2 = Zn+2 + 2F-
        log_k     -1.52
        delta_h   -13.08   kcal

ZnI2
        ZnI2 = Zn+2 + 2I-
        log_k     7.23
        delta_h   -13.44   kcal

ZnMetal
        Zn = Zn+2 + 2e-
        log_k     25.757
        delta_h   -36.78   kcal

ZnO(Active)
        ZnO + 2H+ = Zn+2 + H2O
        log_k     11.31
        delta_h   0        kcal

ZnS(A)
        ZnS + H+ = Zn+2 + HS-
        log_k     -9.052
        delta_h   3.67     kcal

ZnSb
        ZnSb + 3H2O = Sb(OH)3 + 5e- + Zn+2 + 3H+
        log_k     11.0138
        delta_h   -13.116  kcal

ZnSe
        ZnSe + H+ = HSe- + Zn+2
        log_k     -11.3642
        delta_h   6.439    kcal

ZnSiO3
        ZnSiO3 + 2H+ + H2O = Zn+2 + H4SiO4
        log_k     2.93
        delta_h   -18.27   kcal

ZnSO4:H2O
        ZnSO4:H2O = Zn+2 + SO4-2 + H2O
        log_k     -0.57
        delta_h   -10.64   kcal

Zr(metal)
        Zr = Zr+4 + 4e-
        log_k     91.3903
        delta_h   0        kcal

Ag4Fe(Cyanide)6
        Ag4Fe(Cyanide)6 = 6Cyanide- + 4Ag+ + Fe+2
        log_k     -193.914
        delta_h   260.91   kcal

Ag4FeCyanide6:H2O
        Ag4FeCyanide6:H2O = 6Cyanide- + 4Ag+ + Fe+2
+ H2O
        log_k     -89.6909
        delta_h   0        kcal

AgCyanate
        AgCyanate = Cyanate- + Ag+
        log_k     -6.6159
        delta_h   13.175   kcal

AgCyanide
        AgCyanide = Cyanide- + Ag+
        log_k     -16.218
        delta_h   26.385   kcal

Cd2Fe(Cyanide)6
        Cd2Fe(Cyanide)6 = 6Cyanide- + 2Cd+2 + Fe+2
        log_k     -28.2243
        delta_h   0        kcal

Cd2FeCyanide6:7H2O
        Cd2FeCyanide6:7H2O = 6Cyanide- + 2Cd+2 +
Fe+2 + 7H2O
        log_k     -62.9824
        delta_h   0        kcal

Cr2Cyanide
        Cr2Cyanide = Cyanide- + 2Cr+2 + 3e-
        log_k     56.645
        delta_h   0        kcal

CrCyanide
        CrCyanide = Cyanide- + Cr+2 + e-
        log_k     23.888
        delta_h   0        kcal

Cu2FeCyanide6
        Cu2FeCyanide6 = 6Cyanide- + 2Cu+2 + Fe+2
        log_k     -61.4168
        delta_h   0        kcal

CuCyanide
        CuCyanide = Cyanide- + Cu+
        log_k     -19.4974
        delta_h   30.2     kcal

CyanideI
        CyanideI + 2e- = Cyanide- + I-
        log_k     11.3114
        delta_h   -17.309  kcal

Hg(Cyanide)2
        Hg(Cyanide)2 + 2H2O = Hg(OH)2 + 2Cyanide- +
2H+
        log_k     -45.3791
        delta_h   60.73    kcal

K12Cd8(FeCyanide6)7
        K12Cd8(FeCyanide6)7 = 42Cyanide- + 12K+ +
8Cd+2 + 7Fe+2
        log_k     -441.985
        delta_h   0        kcal

K12Ni8(FeCyanide6)7
        K12Ni8(FeCyanide6)7 = 42Cyanide- + 12K+ +
8Ni+2 + 7Fe+2
        log_k     -431.09
        delta_h   0        kcal

K2CdFeCyanide6
        K2CdFeCyanide6 = 6Cyanide- + 2K+ + Cd+2 +
Fe+2
        log_k     -63.0279
        delta_h   0        kcal

K2Cu2FeCyanide6
        K2Cu2FeCyanide6 = 6Cyanide- + 2K+ + 2Cu+ +
Fe+2
        log_k     -72.5142
        delta_h   0        kcal

K2Mn3(FeCyanide6)2
        K2Mn3(FeCyanide6)2 = 12Cyanide- + 2K+ +
3Mn+2 + 2Fe+2
        log_k     -121.001
        delta_h   0        kcal

K2Ni3(FeCyanide6)2
        K2Ni3(FeCyanide6)2 = 12Cyanide- + 2K+ +
3Ni+2 + 2Fe+2
        log_k     -123.127
        delta_h   0        kcal

K3FeCyanide6
        K3FeCyanide6 = 6Cyanide- + 3K+ + Fe+3
        log_k     -54.644
        delta_h   83.29    kcal

K4FeCyanide6
        K4FeCyanide6 = 6Cyanide- + 4K+ + Fe+2
        log_k     -48.8241
        delta_h   95.62    kcal

K4FeCyanide6:3H2O
        K4FeCyanide6:3H2O = 6Cyanide- + 4K+ + Fe+2 +
3H2O
        log_k     -49.5424
        delta_h   99.175   kcal

K4Ni4(FeCyanide6)3
        K4Ni4(FeCyanide6)3 = 18Cyanide- + 4K+ +
4Ni+2 + 3Fe+2
        log_k     -183.547
        delta_h   0        kcal

K8Mn6(FeCyanide6)5
        K8Mn6(FeCyanide6)5 = 30Cyanide- + 8K+ +
6Mn+2 + 5Fe+2
        log_k     -293.685
        delta_h   0        kcal

KCyanide(I)
        KCyanide = Cyanide- + K+
        log_k     1.4403
        delta_h   2.74     kcal

KZn1.5FeCyanide6
        KZn1.5FeCyanide6 = 6Cyanide- + K+ + 1.5Zn+2
+ Fe+2
        log_k     -66.8086
        delta_h   0        kcal

Mn2FeCyanide6
        Mn2FeCyanide6 = 6Cyanide- + 2Mn+2 + Fe+2
        log_k     -59.0272
        delta_h   0        kcal

NaCyanide
        NaCyanide = Cyanide- + Na+
        log_k     2.2869
        delta_h   -0.52    kcal

Pb2Fe(Cyanide)6
        Pb2Fe(Cyanide)6 = 6Cyanide- + 2Pb+2 + Fe+2
        log_k     -27.5895
        delta_h   0        kcal

Pb2FeCyanide6:3H2O
        Pb2FeCyanide6:3H2O = 6Cyanide- + 2Pb+2 +
Fe+2 + 3H2O
        log_k     -63.6011
        delta_h   0        kcal

T14FeCyanide6:2H2O
        T14FeCyanide6:2H2O = 6Cyanide- + 4Tl+ + Fe+2
+ 2H2O
        log_k     -56.9162
        delta_h   0        kcal

Zn2Fe(Cyanide)6
        Zn2Fe(Cyanide)6 = 6Cyanide- + 2Zn+2 + Fe+2
        log_k     -29.9263
        delta_h   0        kcal

Zn2FeCyanide6:2H2O
        Zn2FeCyanide6:2H2O = 6Cyanide- + 2Zn+2 +
Fe+2 + 2H2O
        log_k     -61.2321
        delta_h   0        kcal

CH4(g)
        CH4 + 3H2O = CO3-2 + 8e- + 10H+
        log_k     -40.1
        delta_h 61         kcal
CO2(g)
        CO2 + H2O = CO3-2 + 2H+
        log_k     -18.16
        delta_h 0.53       kcal
O2(g)
        O2 + 4H+ + 4e- = 2H2O
        log_k     83.12
        delta_h -133.83 kcal
Hg(g)
        Hg = 0.5Hg2+2 + e-
        log_k     -7.8708
        delta_h 5.265      kcal
Hg2(g)
        Hg2 = Hg2+2 + 2e-
        log_k     -14.963
        delta_h 13.87      kcal
Hg(CH3)2(g)
        Hg(CH3)2 + 8H2O = Hg(OH)2 + 2CO3-2 + 16e- +
20H+
        log_k     -73.724
        delta_h 115.4      kcal
HgBr(g)
        HgBr = 0.5Hg2+2 + Br-
        log_k     16.79
        delta_h -34.004 kcal
HgCl(g)
        HgCl = 0.5Hg2+2 + Cl-
        log_k     20.9
        delta_h -40.098 kcal
HgF(g)
        HgF = 0.5Hg2+2 + F-
        log_k     32.72
        delta_h -60.916 kcal
HgI(g)
        HgI = 0.5Hg2+2 + I-
        log_k     11.15
        delta_h -25.264 kcal
HgBr2(g)
        HgBr2 + 2H2O = Hg(OH)2 + 2Br- + 2H+
        log_k     -18.47
        delta_h 14.35      kcal
HgF2(g)
        HgF2 + 2H2O = Hg(OH)2 + 2F- + 2H+
        log_k     0.38
        delta_h -0         kcal
HgI2(g)
        HgI2 + 2H2O = Hg(OH)2 + 2I- + 2H+
        log_k     -27.28
        delta_h 28.63      kcal
SURFACE_MASTER_SPECIES
        Hfo_s   Hfo_sOH
        Hfo_w   Hfo_wOH
SURFACE_SPECIES
Hfo_wOH = Hfo_wOH
        log_k 0.0
Hfo_sOH = Hfo_sOH
        log_k 0.0
Hfo_wOH = Hfo_wO- + H+
        log_k     -8.93
Hfo_wOH + H+  = Hfo_wOH2+
        log_k     7.29
Hfo_sOH = Hfo_sO- + H+
        log_k     -8.93
Hfo_sOH + H+  = Hfo_sOH2+
        log_k     7.29
Hfo_wOH  + Zn+2 = Hfo_wOZn+ + H+
        log_k     -1.99
Hfo_sOH  + Zn+2 = Hfo_sOZn+ + H+
        log_k     0.97
Hfo_wOH  + Cd+2 = Hfo_wOCd+ + H+
        log_k     -2.9
Hfo_sOH  + Cd+2 = Hfo_sOCd+ + H+
        log_k     0.43
Hfo_sOH  + Cu+2 = Hfo_sOCu+ + H+
        log_k     2.85
Hfo_wOH  + Cu+2 = Hfo_wOCu+ + H+
        log_k     0.6
Hfo_sOH  + Be+2 = Hfo_sOBe+ + H+
        log_k     1.898
Hfo_wOH  + Be+2 = Hfo_wOBe+ + H+
        log_k     -0.8626
Hfo_sOH  + Ni+2 = Hfo_sONi+ + H+
        log_k     0.15
Hfo_wOH  + Ni+2 = Hfo_wONi+ + H+
        log_k     -2.5
Hfo_sOH  + Pb+2 = Hfo_sOPb+ + H+
        log_k     4.71
Hfo_wOH  + Pb+2 = Hfo_wOPb+ + H+
        log_k     0.3
Hfo_wOH  + Ca+2 = Hfo_wOCa+ + H+
        log_k     -5.85
Hfo_sOH + Ca+2 = Hfo_sOHCa+2
        log_k     4.97
Hfo_sOH + Ba+2 = Hfo_sOHBa+2
        log_k     5.46
Hfo_wOH + Ba+2 = Hfo_wOBa+ + H+
        log_k     -7.2
Hfo_sOH + H+ + SO4-2 = Hfo_sSO4-  + H2O
        log_k     7.78
Hfo_wOH + H+ + SO4-2 = Hfo_wSO4-  + H2O
        log_k     7.78
Hfo_sOH + SO4-2 = Hfo_sOHSO4-2
        log_k     0.79
Hfo_wOH + SO4-2 = Hfo_wOHSO4-2
        log_k     0.79
Hfo_sOH + PO4-3 + 3H+ = Hfo_sH2PO4 + H2O
        log_k     31.29
Hfo_wOH + PO4-3 + 3H+ = Hfo_wH2PO4 + H2O
        log_k     31.29
Hfo_sOH + PO4-3 + 2H+ = Hfo_sHPO4-  + H2O
        log_k     25.39
Hfo_wOH + PO4-3 + 2H+ = Hfo_wHPO4-  + H2O
        log_k     25.39
Hfo_sOH + PO4-3 + H+ = Hfo_sPO4-2 + H2O
        log_k     17.72
Hfo_wOH + PO4-3 + H+ = Hfo_wPO4-2 + H2O
        log_k     17.72
Hfo_sOH + H3AsO3 = Hfo_sH2AsO3 + H2O
        log_k     5.41
Hfo_wOH + H3AsO3 = Hfo_wH2AsO3 + H2O
        log_k     5.41
Hfo_sOH + H3AsO4 = Hfo_sH2AsO4 + H2O
        log_k     8.67
Hfo_wOH + H3AsO4 = Hfo_wH2AsO4 + H2O
        log_k     8.67
Hfo_sOH + H3AsO4 = Hfo_sHAsO4- + H2O + H+
        log_k     2.99
Hfo_wOH + H3AsO4 = Hfo_wHAsO4- + H2O + H+
        log_k     2.99
Hfo_sOH + H3AsO4 = Hfo_sAsO4-2 + H2O + 2H+
        log_k     -4.7
Hfo_wOH + H3AsO4 = Hfo_wAsO4-2 + H2O + 2H+
        log_k     -4.7
Hfo_sOH + H3AsO4 = Hfo_sOHAsO4-3 + 3H+
        log_k     -10.15
Hfo_wOH + H3AsO4 = Hfo_wOHAsO4-3 + 3H+
        log_k     -10.15
Hfo_sOH + H3BO3 = Hfo_sH2BO3 + H2O
        log_k     0.62
Hfo_wOH + H3BO3 = Hfo_wH2BO3 + H2O
        log_k     0.62
END
```

1/31/00 DRT

## TPA 3.2 Sensitivity Analyses to Determine the Effects of Correlation of $K_d$ Values on Performance

As part of the development of TPA 3.2, RT KTI staff provided correlation coefficients for sorption coefficient (Kd) values for Am(III), Np(V), Pu(V), Th(IV), and U(VI) (See pages 60-85 of this Scientific Notebook, No. 252). Due to computational requirements, these correlations were only implemented for the Saturated Zone Alluvium unit (SAV in tpa.inp). These values were converted to retardation factors (RD) by the TSPAI KTI staff using the relationship:

$$R_D = 1 + \frac{\rho_b K_D}{\theta} \quad [1]$$

DRTurner

Sensitivity analyses were conducted to examine (i) whether the correlation coefficients were correctly implemented in the TPA 3.2 input file; (ii) the effects of correlated $K_d$s (or $R_D$) on dose as compared to the non-correlated $K_d$s of previous versions of the TPA code.

For the sensitivity analyses, the following conditions were used:

t = 50,000 y
no. realizations = 250
Location of critical group = 20 km downgradient from repository
All base case parameters as reported in Mohanty and McCartin (1998). Five parameters were varied parameters included RD_AmSAV, RD_NpSAV, RD_PuSAV, RD_ThSAV, RD_USAV. The pdfs for these RD values remained constant, and runs were made either with or without correlation coefficients.

Correct Implementation of Correlation Coefficients:

To check the output from TPA 3.2 for correct implementation of correlation coefficients, I wrote a short FORTRAN program to read the parameter sampling file sample.par.res. This file contains the values for each sampled parameters (including RD_AmSAV, RD_NpSAV, RD_PuSAV, RD_ThSAV, RD_USAV) used for each of the 250 realizations. The source code for the program is included here. Additional explanatory notes are included in the comment blocks:

```
      PROGRAM TPARD
c
C  4567890123456789012345678901234567890123456789012345678901234567890123456789012
c  The following program was written to read the output file
c  sample.par.res from TPA Version 3.2, and write selected parameters
c  to comma-delimited ASCII files for subsequent analysis. The program
c  was written in FORTRAN77 by D.R. Turner for Center For Nuclear Waste
c  Regulatory Analyses in San Antonio, TX for the Radionuclide
c  Transport KTI 20-1402-871. Many of the necessary parameters/flags
c  are hard-wired and cannot currently be modified by the user during
c  the run session. (12/10/98)
c
c
      IMPLICIT NONE
      CHARACTER  Line*76,Filin*12,Filout*12,AmTsW*13,NpTsW*13,
     + UTsW*13,PuTsW*13,ThTsW*13,AmSAV*13,NpSAV*13,USAV*13,
     + PuSAV*13,ThSAV*13,Count*5
      INTEGER  I,Flag
c
c  Prompt the user for the names of the input file containing the
c  TPA parameter values and the output file to be created.
c
      PRINT*, 'Enter the name of the TPA parameter output file?'
      READ(*,11) Filin
```



```
11    FORMAT(A12)
      PRINT*, 'Enter the name of output file to be created (8.3)?'
      READ(*,12) Filout
12    FORMAT(A12)
c
c  Open the input and output files
c
       OPEN(Unit=8, File=Filin, Status='Old', Access='Sequential',
     +Form='Formatted', Action='Read')
       OPEN(Unit=9, File=Filout, Status='Unknown', Access='Append',
     +Form='Formatted', Position='Append')
c
C  4567890123456789012345678901234567890123456789012345678901234567890123456789012
c  Reading the data out of samplpar.res. The order of the variables
c  is established in samplpar.hdr.This program will read the
c  output file line-by-line, checking for the phrase " 244 ". Then a
c  line-by-line search is initiated for the correct number of blanks
c  and the values are read into the output file. The process
c  is then repeated for the next realization.
c
c  Write headers
c
      WRITE(9,20)
20    FORMAT('Iteration,','KD_AmTsW,','KD_NpTsW,','KD_UTsW,',
     + 'KD_PuTsW,','KD_ThTsW,','RD_AmSAV,','RD_NpSAV,','RD_USAV,',
     + 'RD_PuSAV,','RD_ThSAV')
c
c  Set Flag and start reading TPA 3.2 Samplpar.res output file
c
      Flag=0
      Count='    1'
30    READ(8,40,end=31)Line
40    FORMAT (A76)
c
c  Look for start of file
c
      IF(Line(29:31).eq.'244')THEN
c
c  Write AmTsW,NpTsW,UTsW,PuTsW,ThTsW,AmSAV,NpSAV,USAV,PuSAV,
c  ThSAV to the output file
c
          IF(Line(29:31).eq.'244'.and.Flag.gt.0)THEN
             WRITE(9,42)Count,AmTsW,NpTsW,UTsW,PuTsW,ThTsW,AmSAV,
     +       NpSAV,USAV,PuSAV,ThSAV
42           FORMAT(A5,',',A13,',',A13,',',A13,',',A13,',',A13,',',A13,
     +       ',',A13,',',A13,',',A13,',',A13)
             Count=Line(12:16)
          ENDIF
c
c  Set Initial Values for AmTsW,NpTsW,UTsW,PuTsW,ThTsW,AmSAV,NpSAV,
c  USAV,PuSAV,ThSAV,Count
c
      AmTsW='n.c.'
      NpTsW='n.c.'
      UTsW='n.c.'
      PuTsW='n.c.'
      ThTsW='n.c.'
      AmSAV='n.c.'
      NpSAV='n.c.'
      USAV='n.c.'
      PuSAV='n.c.'
      ThSAV='n.c.'
c
c
c  Skip Lines to find first parameter (KD_AmTsW)
c
          do 50 I=1,23
            read(8,45,end=31)Line
45          FORMAT (A76)
50        continue
c
c  Read file and assign variable 'KD_AmTsW'
```

1/31/00 DRT

Includes $K_D$ values for Topopah Spring Welded (TSW)

DRTurner

```
c
      READ(8,55,end=31)Line
55    FORMAT (A76)
      AmTsW=Line(4:16)
      Flag=1
c
c  Read file and assign variable 'KD_NpTsW'
c
      READ(8,60,end=31)Line
60    FORMAT (A76)
      NpTsW=Line(34:46)
c
c  Read file and assign variable 'KD_UTsW'
c
      READ(8,65,end=31)Line
65    FORMAT (A76)
      UTsW=Line(64:76)
c
c  Skip Lines to find KD_PuTsW
c
      do 70 I=1,1
        read(8,66,end=31)Line
66      FORMAT (A76)
70    continue
c
c  Read file and assign variable 'KD_PuTsW'
c
      READ(8,72,end=31)Line
72    FORMAT (A76)
      PuTsW=Line(19:31)
c
c  Read file and assign variable 'KD_ThTsW'
c
      READ(8,75,end=31)Line
75    FORMAT (A76)
      ThTsW=Line(49:61)
c
c
c  Skip Lines to find first parameter (KD_AmTsW)
c
      do 85 I=1,12
        read(8,80,end=31)Line
80      FORMAT (A76)
85    continue
c
c  Read file and assign variables 'RD_AmSAV' and RD_NpSAV'
c
      READ(8,90,end=31)Line
90    FORMAT (A76)
      AmSAV=Line(19:31)
      NpSAV=Line(34:46)
c
c  Read file and assign variables 'RD_USAV', RD_PuSAV', and
c  RD_ThSAV'
c
      READ(8,95,end=31)Line
95    FORMAT (A76)
      USAV=Line(4:16)
      PuSAV=Line(19:31)
      ThSAV=Line(34:46)
    ENDIF
   GOTO 30
31 CONTINUE
c
      WRITE(9,92)Count,AmTsW,NpTsW,UTsW,PuTsW,ThTsW,AmSAV,NpSAV,
     +  USAV,PuSAV,ThSAV
92    FORMAT(A5,',',A13,',',A13,',',A13,',',A13,',',A13,',',A13,
     +  ',',A13,',',A13,',',A13,',',A13)
c 4567890123456789012345678901234567890123456789012345678901234567890123456789012
      STOP
      END
```



EXAMPLE OUTPUT FROM TPA 3.2 OUTPUT FILE SAMPLPAR.HDR

```
Input file tpa.inp as supplied with TPA Version 3.2 Code.
Base case data set Rev 3.2   7/16/98
TPA 3.2, Job started: Mon Oct 19 14:59:49 1998
Names for Sampled Parameters (Nonconstant)

Specified in "tpa.inp" - Values for Each Vector

    1  AAMAI@S    ArealAverageMeanAnnualInfiltrationAtStart[mm/yr]
    2  MAPM@GM    MeanAveragePrecipitationMultiplierAtGlacialMaximum
    3  MATI@GM    MeanAverageTemperatureIncreaseAtGlacialMaximum[degC]
    4  FOC-R      FractionOfCondensateRemoved[1/yr]
    5  FOCTR      FractionOfCondensateTowardRepository[1/yr]
    6  FOCTR-R    FractionOfCondensateTowardRepositoryRemoved[1/yr]
    7  TempGrBI   TemperatureGradientInVicinityOfBoilingIsotherm[K/m]
    8  YMR-TC     ThermalConductivityofYMRock[W/(m-K)]
    9  CritRHAC   CriticalRelativeHumidityAqueousCorrosion
   10  H2O-FThk   ThicknessOfWaterFilm[m]
   11  InnOvrEI   InnerOverpackErpIntercept
   12  AA_2_1     AA_2_1[C/m2/yr]
   13  OO-CofLC   CoefForLocCorrOfOuterOverpack
   14  *Chlorid   ChlorideMultFactor
   15  SSMO-RE    RockModulusOfElasticityforSEISMO[Pa]
   16  SSMO-RPR   RockPoissonRatioforSEISMO[]
   17  SSMO-JS1   SEISMOJointSpacing1[m]
   18  SSMO-JS2   SEISMOJointSpacing2[m]
   19  SSMO-JS3   SEISMOJointSpacing3[m]
   20  SSMO-JS4   SEISMOJointSpacing4[m]
   21  SSMO-JS5   SEISMOJointSpacing5[m]
   22  SSMOV201   VerticalExtentOfRockFall2_1[m]
   23  SSMOV202   VerticalExtentOfRockFall2_2[m]
   24  SSMOV203   VerticalExtentOfRockFall2_3[m]
   25  SSMOV204   VerticalExtentOfRockFall2_4[m]
   26  SSMOV205   VerticalExtentOfRockFall2_5[m]
   27  SSMOV206   VerticalExtentOfRockFall2_6[m]
   28  SSMOV207   VerticalExtentOfRockFall2_7[m]
   29  SSMOV208   VerticalExtentOfRockFall2_8[m]
   30  SSMOV209   VerticalExtentOfRockFall2_9[m]
   31  SSMOV210   VerticalExtentOfRockFall2_10[m]
   32  SSMOV301   VerticalExtentOfRockFall3_1[m]
   33  SSMOV302   VerticalExtentOfRockFall3_2[m]
   34  SSMOV303   VerticalExtentOfRockFall3_3[m]
   35  SSMOV304   VerticalExtentOfRockFall3_4[m]
   36  SSMOV305   VerticalExtentOfRockFall3_5[m]
   37  SSMOV306   VerticalExtentOfRockFall3_6[m]
   38  SSMOV307   VerticalExtentOfRockFall3_7[m]
   39  SSMOV308   VerticalExtentOfRockFall3_8[m]
   40  SSMOV309   VerticalExtentOfRockFall3_9[m]
   41  SSMOV310   VerticalExtentOfRockFall3_10[m]
   42  SSMOV401   VerticalExtentOfRockFall4_1[m]
   43  SSMOV402   VerticalExtentOfRockFall4_2[m]
   44  SSMOV403   VerticalExtentOfRockFall4_3[m]
   45  SSMOV404   VerticalExtentOfRockFall4_4[m]
   46  SSMOV405   VerticalExtentOfRockFall4_5[m]
   47  SSMOV406   VerticalExtentOfRockFall4_6[m]
   48  SSMOV407   VerticalExtentOfRockFall4_7[m]
   49  SSMOV408   VerticalExtentOfRockFall4_8[m]
   50  SSMOV409   VerticalExtentOfRockFall4_9[m]
   51  SSMOV410   VerticalExtentOfRockFall4_10[m]
   52  SSMOV501   VerticalExtentOfRockFall5_1[m]
   53  SSMOV502   VerticalExtentOfRockFall5_2[m]
   54  SSMOV503   VerticalExtentOfRockFall5_3[m]
   55  SSMOV504   VerticalExtentOfRockFall5_4[m]
   56  SSMOV505   VerticalExtentOfRockFall5_5[m]
   57  SSMOV506   VerticalExtentOfRockFall5_6[m]
   58  SSMOV507   VerticalExtentOfRockFall5_7[m]
   59  SSMOV508   VerticalExtentOfRockFall5_8[m]
   60  SSMOV509   VerticalExtentOfRockFall5_9[m]
   61  SSMOV510   VerticalExtentOfRockFall5_10[m]
   62  Fow*       FowFactor
   63  Fmult*     FmultFactor
```

| | | |
|---|---|---|
| 64 | SbArWt% | SubAreaWetFraction |
| 65 | WP-Def% | DefectiveFractionOfWPs/cell |
| 66 | InitRSFP | InitialRadiusOfSFParticle[m] |
| 67 | SbGFRATF | SubGrainFragmentRadiusAfterTransFrac[m] |
| 68 | Solbl-Am | SolubilityAm[kg/m3] |
| 69 | Solbl-Np | SolubilityNp[kg/m3] |
| 70 | Solbl-Pu | SolubilityPu[kg/m3] |
| 71 | SFWt%I1 | SFWettedFraction_Initial_1 |
| 72 | SFWt%I2 | SFWettedFraction_Initial_2 |
| 73 | SFWt%I3 | SFWettedFraction_Initial_3 |
| 74 | SFWt%I4 | SFWettedFraction_Initial_4 |
| 75 | SFWt%I5 | SFWettedFraction_Initial_5 |
| 76 | SFWt%I6 | SFWettedFraction_Initial_6 |
| 77 | SFWt%I7 | SFWettedFraction_Initial_7 |
| 78 | SFWt%F0 | SFWettedFraction_FAULTO |
| 79 | SFWt%V0 | SFWettedFraction_VOLCANO |
| 80 | SFWt%S11 | SFWettedFraction_SEISMO1_1 |
| 81 | SFWt%S12 | SFWettedFraction_SEISMO1_2 |
| 82 | SFWt%S13 | SFWettedFraction_SEISMO1_3 |
| 83 | SFWt%S14 | SFWettedFraction_SEISMO1_4 |
| 84 | SFWt%S15 | SFWettedFraction_SEISMO1_5 |
| 85 | SFWt%S16 | SFWettedFraction_SEISMO1_6 |
| 86 | SFWt%S17 | SFWettedFraction_SEISMO1_7 |
| 87 | SFWt%S21 | SFWettedFraction_SEISMO2_1 |
| 88 | SFWt%S22 | SFWettedFraction_SEISMO2_2 |
| 89 | SFWt%S23 | SFWettedFraction_SEISMO2_3 |
| 90 | SFWt%S24 | SFWettedFraction_SEISMO2_4 |
| 91 | SFWt%S25 | SFWettedFraction_SEISMO2_5 |
| 92 | SFWt%S26 | SFWettedFraction_SEISMO2_6 |
| 93 | SFWt%S27 | SFWettedFraction_SEISMO2_7 |
| 94 | SFWt%S31 | SFWettedFraction_SEISMO3_1 |
| 95 | SFWt%S32 | SFWettedFraction_SEISMO3_2 |
| 96 | SFWt%S33 | SFWettedFraction_SEISMO3_3 |
| 97 | SFWt%S34 | SFWettedFraction_SEISMO3_4 |
| 98 | SFWt%S35 | SFWettedFraction_SEISMO3_5 |
| 99 | SFWt%S36 | SFWettedFraction_SEISMO3_6 |
| 100 | SFWt%S37 | SFWettedFraction_SEISMO3_7 |
| 101 | SFWt%S41 | SFWettedFraction_SEISMO4_1 |
| 102 | SFWt%S42 | SFWettedFraction_SEISMO4_2 |
| 103 | SFWt%S43 | SFWettedFraction_SEISMO4_3 |
| 104 | SFWt%S44 | SFWettedFraction_SEISMO4_4 |
| 105 | SFWt%S45 | SFWettedFraction_SEISMO4_5 |
| 106 | SFWt%S46 | SFWettedFraction_SEISMO4_6 |
| 107 | SFWt%S47 | SFWettedFraction_SEISMO4_7 |
| 108 | SFWt%C1 | SFWettedFraction_Corrosion_1 |
| 109 | SFWt%C2 | SFWettedFraction_Corrosion_2 |
| 110 | SFWt%C3 | SFWettedFraction_Corrosion_3 |
| 111 | SFWt%C4 | SFWettedFraction_Corrosion_4 |
| 112 | SFWt%C5 | SFWettedFraction_Corrosion_5 |
| 113 | SFWt%C6 | SFWettedFraction_Corrosion_6 |
| 114 | SFWt%C7 | SFWettedFraction_Corrosion_7 |
| 115 | InvMPerm | InvertMatrixPermeability[m^2] |
| 116 | MKDTSwAm | MatrixKD_TSw_Am[m3/kg] |
| 117 | MKDCHvAm | MatrixKD_CHnvAm[m3/kg] |
| 118 | MKDCHzAm | MatrixKD_CHnzAm[m3/kg] |
| 119 | MKDPPwAm | MatrixKD_PPw_Am[m3/kg] |
| 120 | MKDUCFAm | MatrixKD_UCF_Am[m3/kg] |
| 121 | MKDBFwAm | MatrixKD_BFw_Am[m3/kg] |
| 122 | MKDUFZAm | MatrixKD_UFZ_Am[m3/kg] |
| 123 | MKDTSwNp | MatrixKD_TSw_Np[m3/kg] |
| 124 | MKDCHvNp | MatrixKD_CHnvNp[m3/kg] |
| 125 | MKDCHzNp | MatrixKD_CHnzNp[m3/kg] |
| 126 | MKDPPwNp | MatrixKD_PPw_Np[m3/kg] |
| 127 | MKDUCFNp | MatrixKD_UCF_Np[m3/kg] |
| 128 | MKDBFwNp | MatrixKD_BFw_Np[m3/kg] |
| 129 | MKDUFZNp | MatrixKD_UFZ_Np[m3/kg] |
| 130 | MKD_TSwU | MatrixKD_TSw_U[m3/kg] |
| 131 | MKD_CHvU | MatrixKD_CHnvU[m3/kg] |
| 132 | MKD_CHzU | MatrixKD_CHnzU[m3/kg] |
| 133 | MKD_PPwU | MatrixKD_PPw_U[m3/kg] |
| 134 | MKD_UCFU | MatrixKD_UCF_U[m3/kg] |
| 135 | MKD_BFwU | MatrixKD_BFw_U[m3/kg] |



| | | |
|---|---|---|
| 136 | MKDUFZ_U | MatrixKD_UFZ_U[m3/kg] |
| 137 | MKDTSwPu | MatrixKD_TSw_Pu[m3/kg] |
| 138 | MKDCHvPu | MatrixKD_CHnvPu[m3/kg] |
| 139 | MKDCHzPu | MatrixKD_CHnzPu[m3/kg] |
| 140 | MKDPPwPu | MatrixKD_PPw_Pu[m3/kg] |
| 141 | MKDUCFPu | MatrixKD_UCF_Pu[m3/kg] |
| 142 | MKDBFwPu | MatrixKD_BFw_Pu[m3/kg] |
| 143 | MKDUFZPu | MatrixKD_UFZ_Pu[m3/kg] |
| 144 | MKDTSwTh | MatrixKD_TSw_Th[m3/kg] |
| 145 | MKDCHvTh | MatrixKD_CHnvTh[m3/kg] |
| 146 | MKDCHzTh | MatrixKD_CHnzTh[m3/kg] |
| 147 | MKDPPwTh | MatrixKD_PPw_Th[m3/kg] |
| 148 | MKDUCFTh | MatrixKD_UCF_Th[m3/kg] |
| 149 | MKDBFwTh | MatrixKD_BFw_Th[m3/kg] |
| 150 | MKDUFZTh | MatrixKD_UFZ_Th[m3/kg] |
| 151 | MKDTSwRa | MatrixKD_TSw_Ra[m3/kg] |
| 152 | MKDCHvRa | MatrixKD_CHnvRa[m3/kg] |
| 153 | MKDCHzRa | MatrixKD_CHnzRa[m3/kg] |
| 154 | MKDPPwRa | MatrixKD_PPw_Ra[m3/kg] |
| 155 | MKDUCFRa | MatrixKD_UCF_Ra[m3/kg] |
| 156 | MKDBFwRa | MatrixKD_BFw_Ra[m3/kg] |
| 157 | MKDUFZRa | MatrixKD_UFZ_Ra[m3/kg] |
| 158 | MKDTSwPb | MatrixKD_TSw_Pb[m3/kg] |
| 159 | MKDCHvPb | MatrixKD_CHnvPb[m3/kg] |
| 160 | MKDCHzPb | MatrixKD_CHnzPb[m3/kg] |
| 161 | MKDPPwPb | MatrixKD_PPw_Pb[m3/kg] |
| 162 | MKDUCFPb | MatrixKD_UCF_Pb[m3/kg] |
| 163 | MKDBFwPb | MatrixKD_BFw_Pb[m3/kg] |
| 164 | MKDUFZPb | MatrixKD_UFZ_Pb[m3/kg] |
| 165 | MKDTSwCs | MatrixKD_TSw_Cs[m3/kg] |
| 166 | MKDCHvCs | MatrixKD_CHnvCs[m3/kg] |
| 167 | MKDCHzCs | MatrixKD_CHnzCs[m3/kg] |
| 168 | MKDPPwCs | MatrixKD_PPw_Cs[m3/kg] |
| 169 | MKDUCFCs | MatrixKD_UCF_Cs[m3/kg] |
| 170 | MKDBFwCs | MatrixKD_BFw_Cs[m3/kg] |
| 171 | MKDUFZCs | MatrixKD_UFZ_Cs[m3/kg] |
| 172 | MKDTSwNi | MatrixKD_TSw_Ni[m3/kg] |
| 173 | MKDCHvNi | MatrixKD_CHnvNi[m3/kg] |
| 174 | MKDCHzNi | MatrixKD_CHnzNi[m3/kg] |
| 175 | MKDPPwNi | MatrixKD_PPw_Ni[m3/kg] |
| 176 | MKDUCFNi | MatrixKD_UCF_Ni[m3/kg] |
| 177 | MKDBFwNi | MatrixKD_BFw_Ni[m3/kg] |
| 178 | MKDUFZNi | MatrixKD_UFZ_Ni[m3/kg] |
| 179 | MKDTSwSe | MatrixKD_TSw_Se[m3/kg] |
| 180 | MKDCHvSe | MatrixKD_CHnvSe[m3/kg] |
| 181 | MKDCHzSe | MatrixKD_CHnzSe[m3/kg] |
| 182 | MKDPPwSe | MatrixKD_PPw_Se[m3/kg] |
| 183 | MKDUCFSe | MatrixKD_UCF_Se[m3/kg] |
| 184 | MKDBFwSe | MatrixKD_BFw_Se[m3/kg] |
| 185 | MKDUFZSe | MatrixKD_UFZ_Se[m3/kg] |
| 186 | MPrm_TSw | MatrixPermeability_TSw_[m2] |
| 187 | MPrm_CHv | MatrixPermeability_CHnv[m2] |
| 188 | MPrm_CHz | MatrixPermeability_CHnz[m2] |
| 189 | MPrm_PPw | MatrixPermeability_PPw_[m2] |
| 190 | MPrm_UCF | MatrixPermeability_UCF_[m2] |
| 191 | MPrm_BFw | MatrixPermeability_BFw_[m2] |
| 192 | MPrm_UFZ | MatrixPermeability_UFZ_[m2] |
| 193 | FPrm_TSw | FracturePermeability_TSw_[m2] |
| 194 | FPrm_CHv | FracturePermeability_CHnv[m2] |
| 195 | FPrm_CHz | FracturePermeability_CHnz[m2] |
| 196 | FPrm_PPw | FracturePermeability_PPw_[m2] |
| 197 | FPrm_UCF | FracturePermeability_UCF_[m2] |
| 198 | FPrm_BFw | FracturePermeability_BFw_[m2] |
| 199 | FPrm_UFZ | FracturePermeability_UFZ_[m2] |
| 200 | FPrs_TSw | FracturePorosity_TSw_ |
| 201 | FPrs_CHv | FracturePorosity_CHnv |
| 202 | FPrs_CHz | FracturePorosity_CHnz |
| 203 | FPrs_PPw | FracturePorosity_PPw_ |
| 204 | FPrs_UCF | FracturePorosity_UCF_ |
| 205 | FPrs_BFw | FracturePorosity_BFw_ |
| 206 | FPrs_UFZ | FracturePorosity_UFZ_ |
| 207 | ARDSAVAm | AlluviumMatrixRD_SAV_Am |

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