```
#-----------------------------------------------------------------------
---------------
#   Thermodynamic database: SKB-09
#-----------------------------------------------------------------------
---------------
#
# This is the NAGRA-PSI 01/01 thermodynamic database (Hummel et al. 2003),
but without Am, As, B,
# Ba, Cs, Eu, Mn, Mo, Nb, Ni, Np, Pd, Pu, Ra, Se, Sn, Sr, Tc, Th, U, Zr and
Tn(=Sn4).
#
# Update March 2009
# Arcos & PiquÈ (2009) to correct data where unselected thermodynamic data
for Fe and Fe+2 has used.
#
# Update August 2008
# Review from (Grive et al., 2008) for the S-TDB project for S bearing
species
#
# Update August 2006
# Review by (Duro et al., 2006a) and Duro et al. (2006b)
# Elements reviewed for SKB-TDB: Ag, Am, Cs, Ho, Nb, Ni, Np, Pa, Pu, Se,
Sm, Sn, Tc, Th and U
#
# Nagra/PSI Chemical Thermodynamic Data Base Version 01/01 (Nagra/PSI TDB
01/01)
# NAPSI_290502.DAT
LAST MOD. 26-AUG-2002
#
#######################################################################
#########################
#
# This file contains the Nagra/PSI TDB 01/01 formatted for PHREEQC. It was
developed by
#
#      W. Hummel, U. Berner, E. Curti, and T. Thoenen from the
#                                                      Waste Management
Laboratory
#                                                      Paul Scherrer
Institut
#                                                      CH-5232 Villigen PSI
#                                                      Switzerland
#
#                                 and by F.J. Pearson from
#                                                      Ground-Water
Geochemistry
#                                                      411 East Front St.
#                                                      New Bern, NC, 28560
#                                                      U.S.A.
#
```

# The Nagra/PSI Chemical Thermodynamic Data Base has been updated from version 05/92 to 01/01in order
# to support the ongoing safety assessment of a planned Swiss repository for high-level radioactive
# waste. This update is thoroughly documented in  Hummel et al. (2002).
# Data base version 05/92 distinguished between "core data" (Pearson & Berner 1991) and "supplemental
# data" (Pearson, Berner & Hummel 1992). Core data are for elements commonly found as major solutes in
# natural waters. These data are well established and have not been changed to any significant degree.
# Supplemental data comprise actinides and fission products, as well as Fe, Si and Al. The update
# from version 05/92 to 01/01 involved major revisions for most of the supplemental data. Altogether,
# more than 70% of the data base contents have been updated.
# Thermodynamic data for Al, and solubility and metal complexation of sulfides and
# silicates were extensively reviewed.
#
#                                WARNING: TEMPERATURE EXTRAPOLATIONS
#
# The Nagra/PSI Chemical Thermodynamic Data Base 01/01 provides thermodynamic data for use at 25 C.
# PHREEQC allows the calculation of equilibria at temperatures other than 25 C. The temperature de-
# pendence of an equilibrium constant is taken care of by either an analytical expression of the form
#                                logK(T) = A + B T + C/T + D logT + E/T^2
# or by the integrated van't Hoff equation
#                          logK(T) = logK(T0) - (1/T - 1/T0) (deltaH[reaction]/(R ln10))
# if only the reaction enthalpy is known.
# Both types of data are available for some but not all of the species and phases contained in the
# data base.
# If a temperature differing from 25 C is used in a PHREEQC calculation, but reaction enthalpies or
# analytical expressions are known only for some of the species, PHREEQC will use the data valid at
# 25 C for all the other species. This may lead to inconsistencies, and it is therefore essential that
# users examine outputs carefully to determine whether species with insufficient data for temperature
# extrapolations have had a significant effect on the calculation results.
# Users are advised to restrict their calculations at temperatures other than 25 C to subsets of the
# data base that contain all necessary data.
# In the light of these caveats, all lines containing data for temperature extrapolations (delta_h for

# the integrated van't Hoff equation and -a_ for the analytical expression) have been commented out.
# In order to use these data, the #-signs at the beginning of the corresponding lines have to be
# deleted.
#
#  NOTE: ACTIVITY COEFFICIENTS OF UNCHARGED SPECIES
#
# With the Nagra/PSI TDB 01/01 activity coefficients of uncharged species are calculated by PHREEQC
# according to the Setchenow equation:
#  ln(gamma) = b*I,
# where I is the ionic strength, and b = 0.1 (default value, because the Nagra/PSI TDB 01/01 does not
# provide any values of b for uncharged species). In order to use an activity coefficient of one for
# uncharged species,the #-signs at the beginning of the lines with "-gamma 0.00    0.00" have to
# be deleted.
#
#  REFERENCES:
#

# Arcos, D., PiquÈ, A. (2009): Update of the thermodynamic database used in SKB TR-06-32 and SKB TR-06-17.
#       Amphos technical note to SKB.
# Duro, L., GrivÈ, M., Cera, E., DomËnech, C., Bruno, J. (2006a): Update of a thermodynamic database for
#       radionuclides to assist solubility limits calculation for performance assessment. SKB TR-06-17.
# Duro, L., GrivÈ, M., Cera, E., Gaona, X., DomËnech, C., Bruno, J. (2006b): Determination and assessment
#       of the concentration limits to be used in SR-Can. SKB TR-06-32.
# GrivÈ, M., DomËnech, C., Motoya, V., Duro, L. (2008): Update of the Thermodynamic Database of sulphur
#       aqueous species and solids phases. Project S-TDB Final Report. Amphos report.
# Hummel W., Berner U. (2001): Application of the Nagra/PSI Thermochemical Data Base 01/01: Solubility
#      and sorption of Th, U, Np and Pu. PSI Internal Report TM-44-01-04, Paul Scherrer Institut,
#      Villigen, Switzerland.
# Hummel W., Berner U. (submitted): Solubility of actinides in a planned underground repository:
#      Application of chemical thermodynamics for estimation of limiting values. Submitted to Applied
#      Geochemistry.
# Hummel W., Berner U., Curti E., Pearson F.J. & Thoenen T. (2002): Nagra/PSI Chemical Thermodynamic
#      Data Base 01/01. Universal Publishers/uPUBLISH.com USA, available from:

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#      http://www.upublish.com/books/hummel.htm. Also issued as Nagra
Technical Report NTB 02-16,
#      Nagra, Wettingen, Switzerland.
# Pearson F.J. & Berner U. (1991): Nagra Thermochemical Data Base I. Core
Data. Nagra Technical Report
#      NTB 91-17, Nagra, Wettingen, Switzerland.
# Pearson F.J., Berner U. & Hummel W. (1992): Nagra Thermochemical Data
Base II. Supplemental Data
#      05/92. Nagra Technical Report NTB 91-18, Nagra, Wettingen,
Switzerland.


SOLUTION_MASTER_SPECIES
#        ATOMIC WEIGHTS
#        Naturally occuring elements: IUPAC 1993 Table 1 rounded to 0.001
#        Radioelements: Mass number of longest-lived isotope
#
#       elemen          species         alk     gfw_formula     element_gfw
atomic number
#
        H               H+              -1.0    H               1.008   #
        1
        H(0)            H2              0.0     H                       #
        H(1)            H+              -1.0    H                       #
        E               e-              0.0     0.0             0.0     #
        O               H2O             0.0     O               15.999  #
        8
        O(0)            O2              0.0     O                       #
        O(-2)           H2O             0.0     O                       #
        Ag              Ag+             0.0     Ag              107.8682
        Ag(1)           Ag+             0.0     Ag
        Am              Am+3            0.0     Am              243.0000
        Am(+3)          Am+3            0.0     Am
        Al              Al+3            0.0     Al              26.982  #
        13
        Ba              Ba+2            0.0     Ba              137.3270
        Br              Br-             0.0     Br              79.904  #
        35
        C               HCO3-           1.0     C               12.011  #
        6
        C(+4)           HCO3-           1.0     HCO3-                   #
        C(-4)           CH4             0.0     CH4                     #
        Alkalinity      HCO3-           1.0     HCO3-           61.016  #
        Ca              Ca+2            0.0     Ca              40.078  #
        20
        Cd              Cd+2            0.0     Cd              112.400
        Cl              Cl-             0.0     Cl              35.453  #
        17
        Cs              Cs+             0.0     Cs              132.9054
        Cu              Cu+2            0.0     Cu              63.546
```

```
Cu(+1)          Cu+             0.0     Cu
Cu(+2)          Cu+2            0.0     Cu
F               F-              0.0     F               18.998  #
9
Fe              Fe+2            0.0     Fe              55.845  #
26
Fe(2)           Fe+2            0.0     Fe                      #
Fe(3)           Fe+3            0.0     Fe                      #
Hg              Hg+2            0.0     Hg              200.59
Hg(+1)          Hg2+2           0.0     Hg
Hg(+2)          Hg+2            0.0     Hg
Ho              Ho+3            0.0     Ho              164.9303
Ho(+3)          Ho+3            0.0     Ho
I               I-              0.0     I               126.904 #
53
I(-1)           I-              0.0     I                       #
I(0)            I2              0.0     I                       #
K               K+              0.0     K               39.098  #
19
Li              Li+             0.0     Li              6.941   #
6
Mg              Mg+2            0.0     Mg              24.305  #
12
Mn              Mn+2            0.0     Mn              54.938
Mn(+2)          Mn+2            0.0     Mn
N               NO3-            1.0     N               14.007  #
7
N(0)            N2              0.0     N2                      #
N(-3)           NH4+            0.0     NH4                     #
N(5)            NO3-            0.0     NO3                     #
Na              Na+             0.0     Na              22.99   #
11
Nb              NbO3-           0.0     Nb              92.906
Ni              Ni+2            0.0     Ni              58.69
Np              NpO2+2          0.0     Np              237.048
Np(+3)          Np+3            0.0     Np
Np(+4)          Np+4            0.0     Np
Np(+5)          NpO2+           0.0     Np
Np(+6)          NpO2+2          0.0     Np
P               HPO4-2          1.0     P               30.974  #
15
Pa              Pa+4            0.0     Pa              231.00
Pa(+4)          Pa+4            0.0     Pa
Pa(+5)          PaO2+           0.0     Pa
Pb              Pb+2            0.0     Pb              207.20
Pb(+2)          Pb+2            0.0     Pb
Pd              Pd+2            0.0     Pd              106.42
Pu              PuO2+2          0.0     Pu              244.00
Pu(+3)          Pu+3            0.0     Pu
Pu(+4)          Pu+4            0.0     Pu
```

```
        Pu(+5)          PuO2+           0.0     Pu
        Pu(+6)          PuO2+2          0.0     Pu
        Ra              Ra+2            0.0     Ra              226
        S               SO4-2           0.0     S               32.067  #
        16
        S(-2)           HS-             1.0     HS                      #
        S(2)            S2O3-2          0.0     S2O3                    #
        S(4)            SO3-2           0.0     SO3                     #
        S(6)            SO4-2           0.0     SO4                     #
        Se              SeO4-2          0.0     Se              78.96
        Se(-2)          HSe-            0.0     Se
        Se(+4)          SeO3-2          0.0     Se
        Se(+6)          SeO4-2          0.0     Se
        Si              Si(OH)4         0.0     Si(OH)4         28.0855
        Sm              Sm+3            0.0     Sm              150.36
        Sm(+3)          Sm+3            0.0     Sm
        Sn              Sn+2            0.0     Sn              118.71
        Sn(+2)          Sn+2            0.0     Sn
        Sn(+4)          Sn+4            0.0     Sn
        Sr              Sr+2            0.0     Sr              87.621
        Tc              TcO(OH)2        0.0     Tc              98      #
        43
        Tc(7)           TcO4-           0.0     TcO4                    #
        Tc(4)           TcO(OH)2       -1.0     TcO(OH)2                #
        Th              Th+4            0.0     Th              232.0381
        U               UO2+2           0.0     U               238.0289
        U(+4)           U+4             0.0     U
        U(+5)           UO2+            0.0     U
        U(+6)           UO2+2           0.0     U
        Zn              Zn+2            0.0     Zn              65.39
        Zr              Zr+4            0.0     Zr              91.22

SOLUTION_SPECIES

# PMATCH MASTER SPECIES

H+                      = H+
    log_k      0.0
    -gamma     9.00    0.00

e-                      = e-
    log_k      0.0

H2O                     = H2O
    log_k      0.0

Ag+ =  Ag+
        log_k 0
        -delta_H        0       kJ/mol  # Calculated enthalpy of reaction
        Ag+
```

```
#       Enthalpy of formation:  105.790 kJ/mol

Al+3                 = Al+3
    log_k      0.0
    -gamma     6.65    0.19

Am+3 =  Am+3
        log_k 0
        -delta_H        0       kJ/mol
#       Enthalpy of formation:  -616.7 kJ/mol

Ba+2 =  Ba+2
        log_k 0
        -delta_H        0       kJ/mol  # Calculated enthalpy of reaction
        Ba+2
#       Enthalpy of formation:  -534.800 kJ/mol

Br-                  = Br-
    log_k      0.0
    -gamma     3.00    0.00

HCO3-                = HCO3-
    log_k      0.0
    -gamma     5.40    0.00

Ca+2                 = Ca+2
    log_k      0.0
    -gamma     4.86    0.15

Cd+2 =  Cd+2
        log_k 0
        -delta_H        0       kJ/mol
#       Enthalpy of formation:  -75.920 kJ/mol

Cs+ =  Cs+
        log_k 0
        -delta_H        0       kJ/mol
#       Enthalpy of formation:  -258.000 kJ/mol

Cu+2 =  Cu+2
        log_k 0
        -delta_H        0       kJ/mol
#       Enthalpy of formation:  64.900 kJ/mol

Cl-                  = Cl-
    log_k      0.0
    -gamma     3.71    0.01

F-                   = F-
    log_k      0.0
```

```
    -gamma     3.46    0.08

Fe+2                 = Fe+2
    log_k      0.0
    -gamma     5.08    0.16

Hg+2 =  Hg+2
        log_k 0
        -delta_H        0       kJ/mol
#       Enthalpy of formation:  170.21 kJ/mol

Ho+3 =  Ho+3
        log_k 0
        -delta_H        0       kJ/mol
#       Enthalpy of formation:  -707.042 kJ/mol

I-                   = I-
    log_k      0.0
    -gamma     3.00    0.00

K+                   = K+
    log_k      0.0
    -gamma     3.71    0.01

Li+                  = Li+
    log_k      0.0
    -gamma     4.76    0.20

Mg+2                 = Mg+2
    log_k      0.0
    -gamma     5.46    0.22

Mn+2 =  Mn+2
        log_k 0
        -delta_H        0       kJ/mol  # Calculated enthalpy of reaction
        Mn+2
#       Enthalpy of formation:  -52.724 kcal/mol #from LLNL.dat

NO3-                 = NO3-
    log_k      0.0
    -gamma     3.00    0.00

Na+                  = Na+
    log_k      0.0
    -gamma     4.32    0.06

NbO3-                = NbO3-
    log_k      0.0
    -gamma     3.00    0.00
```

```
Ni+2 =  Ni+2
        log_k 0
        -delta_H        0       kJ/mol  # Calculated enthalpy of reaction
        Ni+2
#       Enthalpy of formation:  -54.1 kJ/mol

NpO2+2 =  NpO2+2
        log_k 0
        -delta_H        0       kJ/mol  # Calculated enthalpy of reaction
        NpO2+2
#       Enthalpy of formation:  -860.733 kJ/mol #01LEM/FUG

HPO4-2               = HPO4-2
    log_k      0.0
    -gamma     4.00    0.00

Pa+4 = Pa+4
        log_k   0
        -delta_H        0       kJ/mol
#       Enthalpy of formation:  -620.000 kJ/mol #85BAR/PAR

Pb+2 =  Pb+2
        log_k 0
        -delta_H        0       kJ/mol  # Calculated enthalpy of reaction
        Pb+2
#       Enthalpy of formation:  0.920 kJ/mol

Pd+2 =  Pd+2
        log_k 0                                 # Basic species
        -delta_H        0       kJ/mol          # Basic species
#       Enthalpy of formation:  161.416 kJ/mol  # calculated internally, Sf
82WAG/EVA, DGf 99LOT/OCH

PuO2+2 =  PuO2+2
        log_k 0
        -delta_H        0       kJ/mol  # Calculated enthalpy of reaction
        PuO2+2
#       Enthalpy of formation:  -822.036 kJ/mol #01LEM/FUG

Ra+2                 = Ra+2
    log_k      0.0
    -delta_H    0       kJ/mol  # Calculated enthalpy of reaction       Ra
+2
#       Enthalpy of formation:  -527.600 kJ/mol

SO4-2                = SO4-2
    log_k      0.0
    -gamma     5.31   -0.07

SeO4-2 =  SeO4-2
```

```
        log_k 0
        -delta_H        0       kJ/mol  # Calculated enthalpy of reaction
        SeO4-2
#       Enthalpy of formation:  -599.149 kJ/mol

Si(OH)4 = Si(OH)4
        log_k 0
        -delta_H        0       kJ/mol  # Calculated enthalpy of reaction
        Si(OH)4
#       Enthalpy of formation:  -1456.960 kJ/mol

Sm+3 =  Sm+3
        log_k 0
        -delta_H        0       kJ/mol
#       Enthalpy of formation:  -691.199 kJ/mol

Sn+2 =  Sn+2
        log_k 0
        -delta_H        0       kJ/mol  # Calculated enthalpy of reaction
        Sn+2
#       Enthalpy of formation:  -8.9 kJ/mol

Sr+2                 = Sr+2
    log_k      0.0
    -delta_H    0       kJ/mol  # Calculated enthalpy of reaction       Sr
+2
#       Enthalpy of formation:  -550.900 kJ/mol

TcO(OH)2          = TcO(OH)2
    log_k      0.0
    -gamma     3.50    0.00

Th+4 =  Th+4
        log_k 0
        -delta_H        0       kJ/mol  # Calculated enthalpy of reaction
        Th+4
#       Enthalpy of formation:  -769.020 kJ/mol

UO2+2 =  UO2+2
        log_k 0
        -delta_H        0       kJ/mol  # Calculated enthalpy of reaction
        UO2+2
#       Enthalpy of formation:  -1019 kJ/mol

Zn+2 =  Zn+2
        log_k 0
        -delta_H        0       kJ/mol  # Calculated enthalpy of reaction
        Zn+2
#       Enthalpy of formation:  -153.390 kJ/mol
```

```
Zr+4 =  Zr+4
        log_k 0
        -delta_H        0       kJ/mol  # Calculated enthalpy of reaction
        Zr+4
#       Enthalpy of formation:  -560.194 kJ/mol
```

```
# PMATCH SECONDARY MASTER SPECIES

 +2.000H+                   +2.000e-                   = H2
    log_k      -3.1055
    delta_h    -4.0390
#    -a_e   -7.645285E+01 -6.533210E-03  3.037267E+03  2.631234E+01
-0.000000E+00
#    -gamma      0.00    0.00

 +2.000H2O                  -4.000H+                   -4.000e-
= O2
    log_k     -85.9862
    delta_h   559.6010
#    -a_e   -2.163762E+01  4.101330E-03 -2.747501E+04  1.074196E+01
-0.000000E+00
#    -gamma      0.00    0.00

 +1.000HCO3-                +9.000H+                   +8.000e-
-3.000H2O                  = CH4
    log_k      27.8493
    delta_h  -255.8820
#    -a_e    1.366894E+02  4.100659E-02  2.778061E+03 -5.730937E+01
1.015550E+06
#    -gamma      0.00    0.00

 +2.000NO3-                +12.000H+                  +10.000e-
-6.000H2O                  = N2
    log_k     207.2676
    delta_h -1311.7170
#    -a_e   -2.637226E+02  0.000000E+00  7.925347E+04  8.291702E+01
-0.000000E+00
#    -gamma      0.00    0.00


 +1.000NO3-                +10.000H+                   +8.000e-
-3.000H2O                  = NH4+
```

```
    log_k     119.1372
    delta_h  -783.9000
#    -a_e   -1.151682E+02  0.000000E+00  4.526337E+04  3.333745E+01
-0.000000E+00
    -gamma      2.50    0.00

 +1.000SO4-2                +2.000H+                   +2.000e-
-1.000H2O                  = SO3-2
    log_k      -3.40            #Grenthe et al. (1992)
#    delta_h
#    -a_e   -1.576202E+02  0.000000E+00  7.398158E+03  5.229849E+01
-0.000000E+00
#    -gamma      4.50    0.00


 +2.000SO4-2               +10.000H+                   +8.000e-
-5.000H2O                  = S2O3-2
    log_k      38.01    #Grenthe et al. (1992)
#    delta_h            #Not reviewed
#    -a_e   -3.450029E+02  0.000000E+00  2.855787E+04  1.160806E+02
-0.000000E+00
#    -gamma      4.00    0.00

 +1.000SO4-2                +9.000H+                   +8.000e-
-4.000H2O                  = HS-
    log_k      33.6900             #Grenthe et al. (1992)
#    delta_h  -250.2800               # Not reviewed
#    -a_e   -1.956803E+02  0.000000E+00  2.133208E+04  6.378207E+01
-0.000000E+00
#    -gamma      3.50    0.00

 +1.000H2O                  -1.000H+                   = OH-
    log_k     -13.9995
    delta_h    55.9043
#    -a_e   -2.839710E+02 -5.069842E-02  1.332300E+04  1.022445E+02
-1.119669E+06
    -gamma     10.65    0.00

 +1.000H+                   -1.000H2O                  +1.000HCO3-
= CO2
    log_k       6.3519
    delta_h    -9.1092
#    -a_e    3.563094E+02  6.091964E-02 -2.183437E+04 -1.268339E+02
1.684915E+06
#    -gamma      0.00    0.00

 -1.000H+                   +1.000HCO3-                = CO3-2
    log_k     -10.3289
#    delta_h    14.9007
#    -a_e   -1.078871E+02 -3.252849E-02  5.151790E+03  3.892561E+01
```

```
-5.637139E+05
    -gamma      5.40    0.00

 +1.000HPO4-2               +2.000H+                   = H3PO4
    log_k       9.3520
    delta_h     4.8800
#    -a_e    1.020695E+01  0.000000E+00 -2.549047E+02  0.000000E+00
-0.000000E+00
#    -gamma      0.00    0.00

 +1.000HPO4-2               +1.000H+                   = H2PO4-
    log_k       7.2120
    delta_h    -3.6000
#    -a_e    6.581296E+00  0.000000E+00  1.880444E+02  0.000000E+00
-0.000000E+00
    -gamma      4.50    0.00

 +1.000HPO4-2               -1.000H+                   = PO4-3
    log_k     -12.3500
    delta_h    14.6000
#    -a_e   -9.792144E+00  0.000000E+00 -7.626247E+02  0.000000E+00
-0.000000E+00
    -gamma      4.00    0.00

 +1.000NH4+                 -1.000H+                   = NH3
    log_k      -9.2370
    delta_h    52.0900
#    -a_e   -1.110615E-01  0.000000E+00 -2.720899E+03  0.000000E+00
-0.000000E+00
#    -gamma      0.00    0.00

 +1.000Fe+2                 -1.000e-                   = Fe+3
    log_k     -13.0200
    delta_h    40.5000
#    -a_e   -5.924578E+00  0.000000E+00 -2.115500E+03  0.000000E+00
-0.000000E+00
    -gamma      9.00    0.00

 +1.000Si(OH)4              -1.000H+                   = SiO(OH)3-
    log_k      -9.8100
    delta_h    25.6000
#    -a_e   -5.324993E+00  0.000000E+00 -1.337205E+03  0.000000E+00
-0.000000E+00
    -gamma      4.00    0.00

 +1.000Si(OH)4              -2.000H+                   = SiO2(OH)2-2
    log_k     -23.1400
    delta_h    75.0000
#    -a_e   -1.000033E+01  0.000000E+00 -3.917592E+03  0.000000E+00
-0.000000E+00
```

```
    -gamma      4.00    0.00

 +2.000Si(OH)4              -2.000H+         -1.000H2O                  =
Si2O3(OH)4-2
    log_k     -19.000

 +2.000Si(OH)4              -1.000H+         -1.000H2O                  =
Si2O2(OH)5-
    log_k     -8.100

 +3.000Si(OH)4              -3.000H+         -3.000H2O                  =
Si3O6(OH)3-3
    log_k     -28.600

 +3.000Si(OH)4              -3.000H+         -2.000H2O                  =
Si3O5(OH)5-3
    log_k     -27.500

 +4.000Si(OH)4              -4.000H+         -4.000H2O                  =
Si4O8(OH)4-4
    log_k     -36.300

 +4.000Si(OH)4              -3.000H+         -4.000H2O                  =
Si4O7(OH)5-3
    log_k     -25.500

 +1.000Al+3                 +4.000H2O                  -4.000H+
= Al(OH)4-
    log_k     -22.8797
    delta_h   180.8990
#    -a_e    2.886657E+01  0.000000E+00 -1.034188E+04 -6.894257E+00
-0.000000E+00
    -gamma      4.00    0.00


 +2.000I-                   -2.000e-                   = I2
    log_k      20.9500
#    -a_e    2.095000E+01  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00
    -gamma      0.00    0.00


# PMATCH PRODUCT SPECIES

 +1.000Al+3                 +1.000F-                   = AlF+2
    log_k       7.0800
    delta_h     4.8000
#    -a_e    7.920939E+00  0.000000E+00 -2.507259E+02  0.000000E+00
-0.000000E+00
    -gamma      4.00    0.00
```

```
 +1.000Al+3                 +2.000F-                   = AlF2+
    log_k      12.7300
    delta_h     8.1000
#    -a_e    1.414908E+01  0.000000E+00 -4.231000E+02  0.000000E+00
-0.000000E+00
    -gamma      4.00    0.00

 +1.000Al+3                 +3.000F-                   = AlF3
    log_k      16.7800
    delta_h     8.9000
#    -a_e    1.833924E+01  0.000000E+00 -4.648876E+02  0.000000E+00
-0.000000E+00
#    -gamma      0.00    0.00

 +1.000Al+3                 +4.000F-                   = AlF4-
    log_k      19.2900
    delta_h    10.1000
#    -a_e    2.105948E+01  0.000000E+00 -5.275691E+02  0.000000E+00
-0.000000E+00
    -gamma      4.00    0.00

 +1.000Al+3                 +5.000F-                   = AlF5-2
    log_k      20.3000
    delta_h     7.0000
#    -a_e    2.152637E+01  0.000000E+00 -3.656420E+02  0.000000E+00
-0.000000E+00
    -gamma      4.00    0.00

 +1.000Al+3                 +6.000F-                   = AlF6-3
    log_k      20.3000
    delta_h     0.5000
#    -a_e    2.038760E+01  0.000000E+00 -2.611728E+01  0.000000E+00
-0.000000E+00
    -gamma      4.00    0.00

 +1.000Al+3                 +2.000H2O                  -2.000H+
= Al(OH)2+
    log_k     -10.5943
    delta_h    98.2820
#    -a_e   -4.036210E+01  0.000000E+00 -3.042071E+03  1.615359E+01
0.000000E+00
    -gamma      4.00    0.00

 +1.000Al+3                 +3.000H2O                  -3.000H+
= Al(OH)3
    log_k     -16.4328
    delta_h   144.7040
#    -a_e   -4.553311E+01  0.000000E+00 -5.134577E+03  1.872013E+01
0.000000E+00
```

```
#    -gamma      0.00    0.00

 +1.000Al+3                  +1.000SO4-2                = AlSO4+
    log_k       3.9000
#    -a_e    3.900000E+00  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00
    -gamma      4.00    0.00

 +1.000Ba+2                                       +1.000S2O3-2
= BaS2O3
    log_k      2.27             # Martell et al. 2004
#    delta_h                           # not reviewed
#       Enthalpy of formation:   kJ/mol

 +1.000Ca+2                  -1.000H+                   +1.000HCO3-
= CaCO3
    log_k      -7.1048
    delta_h    29.7327
#    -a_e   -1.336619E+03 -3.319725E-01  4.066454E+04  5.247436E+02
-5.637139E+05
#    -gamma      0.00    0.00

 +1.000Ca+2                  +1.000F-                   = CaF+
    log_k       0.9400
    delta_h    17.2381
#    -a_e    3.960036E+00  0.000000E+00 -9.004236E+02  0.000000E+00
-0.000000E+00
    -gamma      4.00    0.00

 +1.000Ca+2                  +1.000HCO3-                = CaHCO3+
    log_k       1.1057
    delta_h    11.2630
#    -a_e    1.209120E+03  3.129400E-01 -3.476505E+04 -4.787820E+02
0.000000E+00
    -gamma      4.00    0.00

 +1.000Ca+2                  +1.000H2O                  -1.000H+
= CaOH+
    log_k     -12.7800
#    -a_e   -1.278000E+01  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00
    -gamma      4.00    0.00

 +1.000Ca+2                  +1.000SO4-2                = CaSO4
    log_k       2.3000
    delta_h     6.9036
#    -a_e    3.509480E+00  0.000000E+00 -3.606066E+02  0.000000E+00
-0.000000E+00
#    -gamma      0.00    0.00
```

```
 +1.000Ca+2                  +1.000S2O3-2                = CaS2O3
    log_k       1.9800                   #Martell et al. (2004)
#    delta_h                                   #not reviewed
#       Enthalpy of formation:   kJ/mol


 +2.000H2O                   -2.000H+                   +1.000Fe+3
= Fe(OH)2+
    log_k      -5.6700
    delta_h    71.5475
#    -a_e    6.864807E+00  0.000000E+00 -3.737253E+03  0.000000E+00
-0.000000E+00
    -gamma      4.00    0.00

 +3.000H2O                   -3.000H+                   +1.000Fe+3
= Fe(OH)3
    log_k     -12.5600
    delta_h   103.7643
#    -a_e    5.619048E+00  0.000000E+00 -5.420083E+03  0.000000E+00
-0.000000E+00
#    -gamma      0.00    0.00

 +4.000H2O                   -4.000H+                   +1.000Fe+3
= Fe(OH)4-
    log_k     -21.6000
    delta_h   133.4707
#    -a_e    1.783479E+00  0.000000E+00 -6.971784E+03  0.000000E+00
-0.000000E+00
    -gamma      4.00    0.00


 +2.000H2O                   -2.000H+                   +2.000Fe+3
= Fe2(OH)2+4
    log_k      -2.9500
    delta_h    56.4862
#    -a_e    6.946133E+00  0.000000E+00 -2.950532E+03  0.000000E+00
-0.000000E+00
    -gamma      4.00    0.00

 +4.000H2O                   -4.000H+                   +3.000Fe+3
= Fe3(OH)4+5
    log_k      -6.3000
    delta_h    59.8345
#    -a_e    4.182741E+00  0.000000E+00 -3.125429E+03  0.000000E+00
-0.000000E+00
    -gamma      9.00    0.00

 +1.000Fe+2                  +1.000Cl-                  = FeCl+
    log_k       0.1400
#    -a_e    1.400000E-01  0.000000E+00  0.000000E+00  0.000000E+00
```

```
0.000000E+00
    -gamma      4.00    0.00

 +1.000Cl-                  +1.000Fe+3                 = FeCl+2
    log_k       1.4800
    delta_h    23.4315
#    -a_e    5.585096E+00  0.000000E+00 -1.223934E+03  0.000000E+00
-0.000000E+00
    -gamma      4.00    0.00

 +2.000Cl-                  +1.000Fe+3                 = FeCl2+
    log_k       2.1300
#    -a_e    2.130000E+00  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00
    -gamma      4.00    0.00

 +3.000Cl-                  +1.000Fe+3                 = FeCl3
    log_k       1.1300
#    -a_e    1.130000E+00  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00
#    -gamma      0.00    0.00

 +1.000Fe+2                 +1.000HCO3-                -1.000H+
= FeCO3
    log_k      -5.4671
#    -a_e   -5.949000E+00  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00
#    -gamma      0.00    0.00

 +1.000Fe+2                 +1.000F-                   = FeF+
    log_k       1.0000
#    -a_e    1.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00
    -gamma      4.00    0.00

 +1.000F-                   +1.000Fe+3                 = FeF+2
    log_k       6.2000
    delta_h    11.2970
#    -a_e    8.179185E+00  0.000000E+00 -5.900939E+02  0.000000E+00
-0.000000E+00
    -gamma      4.00    0.00

 +2.000F-                   +1.000Fe+3                 = FeF2+
    log_k      10.8000
    delta_h    20.0840
#    -a_e    1.431863E+01  0.000000E+00 -1.049079E+03  0.000000E+00
-0.000000E+00
    -gamma      4.00    0.00

 +3.000F-                   +1.000Fe+3                 = FeF3
```

```
    log_k      14.0000
    delta_h    22.5950
#    -a_e    1.795854E+01  0.000000E+00 -1.180240E+03  0.000000E+00
-0.000000E+00
#    -gamma      0.00    0.00

 +1.000Fe+2                 +1.000HCO3-                = FeHCO3+
    log_k       2.1700
#    -a_e    2.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00
    -gamma      4.00    0.00

 +1.000Fe+2                 +1.000H+                   +1.000SO4-2
= FeHSO4+
    log_k       3.0680
#    -a_e    3.068000E+00  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00
    -gamma      4.00    0.00

 +1.000H+                   +1.000SO4-2                +1.000Fe+3
= FeHSO4+2
    log_k       4.4680
#    -a_e    4.468000E+00  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00
    -gamma      4.00    0.00

 +1.000Fe+2                 +1.000H2O                  -1.000H+
= FeOH+
    log_k      -9.5000
    delta_h    55.2288
#    -a_e    1.758424E-01  0.000000E+00 -2.884852E+03  0.000000E+00
-0.000000E+00
    -gamma      4.00    0.00

 +1.000H2O                  -1.000H+                   +1.000Fe+3
= FeOH+2
    log_k      -2.1900
    delta_h    43.5147
#    -a_e    5.433584E+00  0.000000E+00 -2.272971E+03  0.000000E+00
-0.000000E+00
    -gamma      4.00    0.00


 +1.000SO4-2                +1.000Fe+3                 = FeSO4+
    log_k       4.0400
    delta_h    16.3605
#    -a_e    6.906288E+00  0.000000E+00 -8.545836E+02  0.000000E+00
-0.000000E+00
    -gamma      4.00    0.00
```

```
 +1.000Fe+2                 +1.000SO4-2                = FeSO4
    log_k       2.2500
    delta_h    13.5143
#    -a_e    4.617649E+00  0.000000E+00 -7.059146E+02  0.000000E+00
-0.000000E+00
#    -gamma      0.00    0.00

 +2.000SO4-2                +1.000Fe+3                 = Fe(SO4)2-
    log_k       5.3800
    delta_h    19.2475
#    -a_e    8.752077E+00  0.000000E+00 -1.005385E+03  0.000000E+00
-0.000000E+00
    -gamma      4.00    0.00


 +1.000Fe+3                 +1.000S2O3-2                = FeS2O3+
    log_k       3.3500          #Martell et al. (2004)
#    delta_h                    #Not reviewed
#       Enthalpy of formation:   kJ/mol

 +1.000Fe+3                 +2.000S2O3-2                = Fe(S2O3)2-
    log_k       4.7500          #Martell et al. (2004)
#    delta_h                    # Not reviewed
#       Enthalpy of formation:   kJ/mol

 +1.000Fe+2                 +1.000HS-                = Fe(HS)+
    log_k       3.3000
#    delta_h                           #Not reviewed
#       Enthalpy of formation:   kJ/mol

 +1.000Fe+2                 +2.000HS-                = Fe(HS)2
    log_k       7.0000
#    delta_h            #Not reviewed
#       Enthalpy of formation:   kJ/mol

 +1.000Fe+2                 +1.000HS-                = FeS
1.000H+
    log_k       -2.2000
#    delta_h            #Not reviewed
#       Enthalpy of formation:   kJ/mol


 +1.000H+                   +1.000F-                   = HF
    log_k       3.1760
    delta_h    13.3063
#    -a_e   -2.033000E+00  1.264500E-02  4.290100E+02  0.000000E+00
0.000000E+00
#    -gamma      0.00    0.00

 +1.000H+                   +2.000F-                   = HF2-
```

```
    log_k       3.6201
    delta_h    15.2000
#    -a_e   -8.943484E+01  0.000000E+00  3.467009E+03  3.290711E+01
-0.000000E+00
    -gamma      4.00    0.00

 +1.000H+                   +1.000SO3-2                = HSO3-
    log_k       7.2200
#    delta_h   120.9500                 #Not reviewed
#    -a_e    2.841007E+01  0.000000E+00 -6.317771E+03  0.000000E+00
-0.000000E+00
#    -gamma      4.00    0.00

 +2.000H+                   +1.000SO3-2                = H2SO3
    log_k       9.06
#    delta_h            #not reviewed
#       Enthalpy of formation:   kJ/mol


 +1.000H+                   +1.000SO4-2                = HSO4-
    log_k       1.98
#    delta_h            #Not reviewed
#    -a_e   -5.688900E+01  6.473000E-03  2.307900E+03  1.988580E+01
0.000000E+00
#    -gamma      4.00    0.00

 +1.000K+                   +1.000H2O                  -1.000H+
= KOH
    log_k     -14.4600
#    -a_e   -1.446000E+01  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00
#    -gamma      0.00    0.00

 +1.000K+                   +1.000SO4-2                = KSO4-
    log_k       0.8500
    delta_h     9.4140
#    -a_e    2.499291E+00  0.000000E+00 -4.917362E+02  0.000000E+00
-0.000000E+00
    -gamma      4.00    0.00

 +1.000K+                   +1.000S2O3-2                = KS2O3-
    log_k       0.9600                 #Martell et al. (2004)
#    delta_h                           #not reviewed
#       Enthalpy of formation:   kJ/mol


 +1.000Li+                  +1.000H2O                  -1.000H+
= LiOH
    log_k     -13.6400
#    -a_e   -1.364000E+01  0.000000E+00  0.000000E+00  0.000000E+00
```

```
0.000000E+00
#    -gamma      0.00    0.00

 +1.000Li+                  +1.000SO4-2                = LiSO4-
    log_k       0.6400
#    -a_e    6.400000E-01  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00
    -gamma      4.00    0.00

 +1.000Mg+2                 -1.000H+                   +1.000HCO3-
= MgCO3
    log_k      -7.3492
    delta_h    26.2518
#    -a_e   -1.068961E+02 -2.585849E-02  5.151790E+03  3.892561E+01
-5.637139E+05
#    -gamma      0.00    0.00

 +1.000Mg+2                 +1.000F-                   = MgF+
    log_k       1.8200
    delta_h    13.3888
#    -a_e    4.165659E+00  0.000000E+00 -6.993582E+02  0.000000E+00
-0.000000E+00
    -gamma      4.00    0.00

 +1.000Mg+2                 +1.000HCO3-                = MgHCO3+
    log_k       1.0682
    delta_h     3.2881
#    -a_e   -5.921500E+01  0.000000E+00  2.537455E+03  2.092298E+01
0.000000E+00
    -gamma      4.00    0.00

 +1.000Mg+2                 +1.000H2O                  -1.000H+
= MgOH+
    log_k     -11.4400
#    -a_e   -1.144000E+01  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00
    -gamma      4.00    0.00

 +1.000Mg+2                 +1.000SO4-2                = MgSO4
    log_k       2.3700
    delta_h    19.0372
#    -a_e    5.705234E+00  0.000000E+00 -9.943999E+02  0.000000E+00
-0.000000E+00
#    -gamma      0.00    0.00

 +1.000Mg+2                 +1.000S2O3-2                = MgS2O3
    log_k       1.8200                          #Martell et al. (2004)
#    delta_h                                             #not reviewed
#       Enthalpy of formation:   kJ/mol
```

```
 +1.000Na+                  -1.000H+                  +1.000HCO3-
= NaCO3-
    log_k      -9.0590
    delta_h    52.1800
#    -a_e    8.270610E-02  0.000000E+00 -2.725600E+03  0.000000E+00
-0.000000E+00
    -gamma      4.00    0.00

 +1.000Na+                  +1.000F-                  = NaF
    log_k      -0.2400
#    -a_e   -2.400000E-01  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00
#    -gamma      0.00    0.00

 +1.000Na+                  +1.000HCO3-               = NaHCO3
    log_k      -0.2500
#    -a_e   -2.500000E-01  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00
#    -gamma      0.00    0.00

 +1.000Na+                  +1.000H2O                 -1.000H+
= NaOH
    log_k     -14.1800
#    -a_e   -1.418000E+01  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00
#    -gamma      0.00    0.00

 +1.000Na+                  +1.000SO4-2               = NaSO4-
    log_k       0.7000
    delta_h     4.6861
#    -a_e    1.520981E+00  0.000000E+00 -2.447754E+02  0.000000E+00
-0.000000E+00
    -gamma      4.00    0.00

 +1.000Na+                  +1.000S2O3-2                  = NaS2O3-
    log_k       0.63                   #Martell et al. (2004)
#    delta_h                           #not reviewed
#       Enthalpy of formation:   kJ/mol

 +1.000HS-                  -1.000H+                  = S-2
    log_k     -19.0000                 #Grenthe et al. (1992)
#    delta_h                           #not reviewed
#    -a_e   -1.900000E+01  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00
#    -gamma      5.00    0.00

 +1.000HS-                  +1.000H+                  = H2S
    log_k       6.99                   #Grenthe et al. (1992)
#    delta_h   -22.3000                #Not reviewed
```

```
#    -a_e    3.083138E+00  0.000000E+00  1.164831E+03  0.000000E+00
-0.000000E+00
#    -gamma      0.00    0.00


 +2.000HS-                  -2.000H+    -2.000e-                   = S2-2
    log_k     -9.32                      #Kamyshny et al. (2004)
#       -delta_H                kJ/mol   # Hf not reviewed
#       Enthalpy of formation:   kJ/mol

 +3.000HS-                  -3.000H+    -4.000e-                   = S3-2
    log_k     -6.16                      #Kamyshny et al. (2004)
#       -delta_H                kJ/mol   # Hf not reviewed
#       Enthalpy of formation:   kJ/mol

 +4.000HS-                  -4.000H+    -6.000e-                   = S4-2
    log_k     -3.28                      #Kamyshny et al. (2004)
#       -delta_H                kJ/mol   # Hf not reviewed
#       Enthalpy of formation:   kJ/mol

 +5.000HS-                  -5.000H+    -8.000e-                   = S5-2
    log_k     -0.91                      #Kamyshny et al. (2004)
#       -delta_H                kJ/mol   # Hf not reviewed
#       Enthalpy of formation:   kJ/mol

 +6.000HS-                  -6.000H+    -10.000e-                   = S6-2
    log_k     1.10                       #Kamyshny et al. (2004)
#       -delta_H                kJ/mol   # Hf not reviewed
#       Enthalpy of formation:   kJ/mol

 +1.000S2-2                  +1.000H+                      = HS2-
    log_k     10.03                      #Kamyshny et al. (2004)
#       -delta_H                kJ/mol   # Hf not reviewed
#       Enthalpy of formation:   kJ/mol

 +1.000S3-2                  +1.000H+                      = HS3-
    log_k     7.83                       #Kamyshny et al. (2004)
#       -delta_H                kJ/mol   # Hf not reviewed
#       Enthalpy of formation:   kJ/mol

 +1.000S4-2                  +1.000H+                      = HS4-
    log_k     6.63                       #Kamyshny et al. (2004)
#       -delta_H                kJ/mol   # Hf not reviewed
#       Enthalpy of formation:   kJ/mol

 +1.000S5-2                  +1.000H+                      = HS5-
    log_k     6.03                       #Kamyshny et al. (2004)
#       -delta_H                kJ/mol   # Hf not reviewed
#       Enthalpy of formation:   kJ/mol
```

```
 +1.000S6-2                  +1.000H+                      = HS6-
    log_k     5.51                        #Kamyshny et al. (2004)
#       -delta_H                kJ/mol   # Hf not reviewed
#       Enthalpy of formation:   kJ/mol

 +1.000S2O3-2                  +1.000H+                    = HS2O3-
    log_k       1.59                    #Grenthe et al. (1992)
#    delta_h                            # Not reviewed
#       Enthalpy of formation:   kJ/mol

 +3.000SO4-2                  +12.000H+                  +8.000e-
= S3O6-2                +6.000H2O
    log_k       25.96                   #Latimer (1952)
#    delta_h                            #not reviewed
#       Enthalpy of formation:   kJ/mol

 +4.000SO4-2                  +20.000H+                  +14.000e-
= S4O6-2                +10.000H2O
    log_k       73.16                   #Latimer (1952)
#    delta_h                            #not reviewed
#       Enthalpy of formation:   kJ/mol

 +5.000SO4-2                  +28.000H+                  +20.000e-
= S5O6-2                +14.000H2O
    log_k       97.28                   #Latimer (1952)
#    delta_h                            #not reviewed
#       Enthalpy of formation:   kJ/mol


 +1.000Al+3                  +2.000SO4-2                = Al(SO4)2-
    log_k       5.9000
#    -a_e    5.900000E+00  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00
    -gamma      4.00    0.00

 +1.000Ca+2                  +1.000SiO(OH)3-            = CaSiO(OH)3+
    log_k       1.2000
#    -a_e    1.200000E+00  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00
    -gamma      4.00    0.00

 +1.000Ca+2                  +1.000SiO2(OH)2-2          = CaSiO2(OH)2
    log_k       4.6000
#    -a_e    4.600000E+00  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00
#    -gamma      0.00    0.00

 +1.000Mg+2                  +1.000SiO(OH)3-            = MgSiO(OH)3+
    log_k       1.5000
```

```
#    -a_e    1.500000E+00  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00
    -gamma      4.00    0.00

 +1.000Mg+2                 +1.000SiO2(OH)2-2          = MgSiO2(OH)2
    log_k       5.7000
#    -a_e    5.700000E+00  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00
#    -gamma      0.00    0.00

 +1.000Al+3                 +1.000SiO(OH)3-            = AlSiO(OH)3+2
    log_k       7.4000
#    -a_e    7.400000E+00  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00
    -gamma      4.00    0.00

 +1.000Fe+3                 +1.000SiO(OH)3-            = FeSiO(OH)3+2
    log_k       9.5695
#    -a_e    9.700000E+00  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00
    -gamma      4.00    0.00

 +1.000Al+3                 +1.000H2O                  -1.000H+
= AlOH+2
    log_k      -4.9573
    delta_h    49.7980
#    -a_e   -4.073126E+01  0.000000E+00 -6.202912E+02  1.529820E+01
-0.000000E+00
    -gamma      4.00    0.00

 +1.000Al(OH)4-             +1.000Si(OH)4              -1.000H2O
= Al(OH)6SiO-
    log_k       3.6000
#    -a_e    3.600000E+00  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00
    -gamma      4.00    0.00

 +1.000I-                   +1.000I2                   = I3-
    log_k       2.8700
#    -a_e    2.870000E+00  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00
    -gamma      4.00    0.00

1.0000 Cu+2 + 1.0000 e-  = Cu+
        log_k           2.64
        -delta_H        71.670  kJ/mol

2.0000 Hg+2 + 2.0000 e-  = Hg2+2
        log_k           30.79
        -delta_H        166.870 kJ/mol
```

```
1.0000 H2O + 1.0000 Ag+  =  AgOH + 1.0000 H+
        log_k           -12.00          #76BAE/MES
        -delta_H        47.178  kJ/mol  #DSr estimated 97SHO/SAS, H calc
#       Enthalpy of formation:  -132.862 kJ/mol

2.0000 H2O + 1.0000 Ag+  =  Ag(OH)2- + 2.0000 H+
        log_k           -24.00          #76BAE/MES
        -delta_H        111.634 kJ/mol  #DSr estimated 97SHO/SAS, H calc
#       Enthalpy of formation:  -354.236 kJ/mol

1.0000 CO3-2 + 1.0000 Ag+  =  AgCO3-
        log_k           2.69                    #DGf 97SVE/SHO, logK calc
        -delta_H        -22.832 kJ/mol  #Sf 97SVE/SHO, H calc
#       Enthalpy of formation:  -592.272 kJ/mol

2.0000 CO3-2 + 1.0000 Ag+  =  Ag(CO3)2-3
        log_k           2.16                    #DGf 97SVE/SHO, logK calc
        -delta_H        -28.044 kJ/mol  #Sf 97SVE/SHO, H calc
#       Enthalpy of formation:  -1272.714 kJ/mol

1.0000 NO3- + 1.0000 Ag+  =  AgNO3
        log_k           -0.29                   #DGf 82WAG/EVA, logK calc
        -delta_H        -0.74   kJ/mol          #Sf 82WAG/EVA, H calc
#       Enthalpy of formation:  -101.8 kJ/mol

2.0000 NO3- + 1.0000 Ag+ + 4.0000 e- + 4.0000 H+   =  Ag(NO2)2- + 2.0000
H2O
        log_k           57.78                   #DGf 82WAG/EVA, logK calc
        -delta_H        -0      kJ/mol          # Not possible to calculate

# 1.0000 HS- + 1.0000 Ag+  =  AgHS
#        log_k           +14.05          #74NAU/RYZ
#       -delta_H        -78.826 kJ/mol  #DSr estimated 97SVE/SHO, H calc
#       Enthalpy of formation:  10.664 kJ/mol

# 2.0000 HS- + 1.0000 Ag+  =  Ag(HS)2-
#        log_k           +18.45          #74NAU/RYZ
#       -delta_H        -105.805        kJ/mol  #Sf 97SVE/SHO, H calc
#       Enthalpy of formation:  -32.615 kJ/mol

#1.0000 S2O3-2 + 1.0000 Ag+  =  AgS2O3-
#        log_k           +9.23                   #DGf 82WAG/EVA, logK calc
#       -delta_H        -58.994 kJ/mol  #Sf 82WAG/EVA, H calc
#       Enthalpy of formation:  -601.724 kJ/mol

#2.0000 S2O3-2 + 1.0000 Ag+  =  Ag(S2O3)2-3
#        log_k           +13.64          #DGf 82WAG/EVA, logK calc
#       -delta_H        -94.450 kJ/mol  #Sf 82WAG/EVA, H calc
#       Enthalpy of formation:  -1285.700 kJ/mol
```

```
1.0000 SO3-2 + 1.0000 Ag+  =  AgSO3-
        log_k           +5.21                   #DGf 82WAG/EVA, logK calc
        -delta_H        -0      kJ/mol          #Sf 82WAG/EVA, H calc

1.0000 SO4-2 + 1.0000 Ag+  =  AgSO4-
        log_k           +1.38                   #76SMI/MAR
        -delta_H        4.646   kJ/mol          #Sf 82WAG/EVA, H calc
#       Enthalpy of formation:  -798.904 kJ/mol

1.0000 Cl- + 1.0000 Ag+  =  AgCl
        log_k           +3.27                   #91BAL/NOR
        -delta_H        -17.105 kJ/mol  #Sf estimated 97SVE/SHO, H calc
#       Enthalpy of formation:  -78.395 kJ/mol

2.0000 Cl- + 1.0000 Ag+  =  AgCl2-
        log_k           +5.27                   #91BAL/NOR
        -delta_H        -28.766 kJ/mol  #Sf estimated 97SVE/SHO, H calc
#       Enthalpy of formation:  -257.136 kJ/mol

3.0000 Cl- + 1.0000 Ag+  =  AgCl3-2
        log_k           +5.29                   #91BAL/NOR
        -delta_H        -29.172 kJ/mol  #Sf estimated 97SVE/SHO, H calc
#       Enthalpy of formation:  -424.622 kJ/mol

4.0000 Cl- + 1.0000 Ag+  =  AgCl4-3
        log_k           +5.51                   #91BAL/NOR0
#      -gamma           4.0
        -delta_H        -26.102 kJ/mol  #Sf estimated 97SVE/SHO, H calc
#       Enthalpy of formation:  -588.632 kJ/mol

1.0000 Br- + 1.0000 Ag+  =  AgBr
        log_k           +4.24                   #91BAL/NOR
        -delta_H        -23.153 kJ/mol  #Sf estimated 97SVE/SHO, H calc
#       Enthalpy of formation:  -38.773 kJ/mol

2.0000 Br- + 1.0000 Ag+  =  AgBr2-
        log_k           +7.28                   #91BAL/NOR
        -delta_H        -45.338 kJ/mol  #Sf estimated 97SVE/SHO, H calc
#       Enthalpy of formation:  -182.368 kJ/mol

3.0000 Br- + 1.0000 Ag+  =  AgBr3-2
        log_k           +8.71                   #91BAL/NOR
        -delta_H        -66.795 kJ/mol  #Sf estimated 97SVE/SHO, H calc
#       Enthalpy of formation:  -325.235 kJ/mol

1.0000 I- + 1.0000 Ag+  =  AgI
        log_k           +6.58                   #76SMI/MAR
        -delta_H        -36.981 kJ/mol  #DSr estimated 97SVE/SHO, H calc
#       Enthalpy of formation:  -12.187 kJ/mol
```

```
2.0000 I- + 1.0000 Ag+  =  AgI2-
        log_k           +11.70          #76SMI/MAR
        -delta_H        -76.578 kJ/mol  #DSr estimated 97SVE/SHO, H calc
#       Enthalpy of formation:  -84.348 kJ/mol

3.0000 I- + 1.0000 Ag+  =  AgI3-2
        log_k           +13.28          #DGf 82WAG/EVA, logK calc
        -delta_H        -114.911        kJ/mol  #DSr estimated 97SVE/SHO, H
calc
#       Enthalpy of formation:  -179.461 kJ/mol

1.0000 H2O + 1.0000 Am+3  =  AmOH+2 +1.0000 H+
        log_k           -7.20                   #03GUI/FAN
        -delta_H        78.411 kJ/mol           #Sf estimated 97SHO/SAS, H
calc
#       Enthalpy of formation:  -824.119 kJ/mol

2.0000 H2O + 1.0000 Am+3  =  Am(OH)2+ +2.0000 H+
        log_k           -15.10          #03GUI/FAN
        -delta_H        143.704 kJ/mol          #Sf estimated 97SHO/SAS, H
calc
#       Enthalpy of formation:  -1044.656 kJ/mol

3.0000 H2O + 1.0000 Am+3  =  Am(OH)3 +3.0000 H+
        log_k           -26.20          #03GUI/FAN
        -delta_H        230.125 kJ/mol          #Sf estimated 97 SHO/SAS, H
calc
#       Enthalpy of formation:  -1244.065 kJ/mol

1.0000 CO3-2 + 1.0000 Am+3  =  AmCO3+
        log_k           8.00                    #03GUI/FAN
        -delta_H        157.585 kJ/mol          #DSr estimated 97SVE/SHO, H
calc
#       Enthalpy of formation:  -1134.345 kJ/mol

2.0000 CO3-2 + 1.0000 Am+3  =  Am(CO3)2-
        log_k           12.90                   #03GUI/FAN
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction    Am(CO3)2-
#       Enthalpy of formation:  -0 kcal/mol

3.0000 CO3-2 + 1.0000 Am+3  =  Am(CO3)3-3
        log_k           15.00                   #03GUI/FAN
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction    Am(CO3)3-3
#       Enthalpy of formation:  -0 kcal/mol

1.0000 CO3-2 + 1.0000 Am+3 + 1.0000 H+  =  AmHCO3+2
        log_k           13.43                   #03GUI/FAN
```

```
        -delta_H        0 kJ/mol                        # Not possible to
calculate enthalpy of reaction
#       Enthalpy of formation:  -0 kJ/mol

1.0000 Si(OH)4 + 1.0000 Am+3  =  AmOSi(OH)3+2 + 1.0000 H+
        log_k           -1.68                   #03GUI/FAN
        -delta_H        0 kJ/mol                        # Not possible to
calculate enthalpy of reaction
#       Enthalpy of formation:  -0 kJ/mol

1.0000 NO3- + 1.0000 Am+3  =  AmNO3+2
        log_k           +1.33                   #95SIL/BID
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction    AmNO3+2
#       Enthalpy of formation:  -0 kcal/mol

1.0000 H2PO4- + 1.0000 Am+3  =  AmPO4 + 2.0000 H+
        log_k           -7.76                   #estimated from lanthanides
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction    AmH2PO4+2
#       Enthalpy of formation:  -0 kcal/mol

2.0000 H2PO4- + 1.0000 Am+3  =  Am(PO4)2-3 + 4.0000 H+
        log_k           -19.43          #estimated from lanthanides
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction    AmH2PO4+2
#       Enthalpy of formation:  -0 kcal/mol

1.0000 H2PO4- + 1.0000 Am+3  =  AmHPO4+ + 1.0000 H+
        log_k           -1.74                   #estimated from lanthanides
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction    AmH2PO4+2
#       Enthalpy of formation:  -0 kcal/mol

2.0000 H2PO4- + 1.0000 Am+3  =  Am(HPO4)2- + 2.0000 H+
        log_k           -5.31                   #estimated from lanthanides
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction    AmH2PO4+2
#       Enthalpy of formation:  -0 kcal/mol

1.0000 H2PO4- + 1.0000 Am+3  =  AmH2PO4+2
        log_k           +3.00                   #95SIL/BID
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction    AmH2PO4+2
#       Enthalpy of formation:  -0 kcal/mol

1.0000 SO4-2 + 1.0000 Am+3  =  AmSO4+
        log_k           +3.30                   #03GUI/FAN
        -delta_H        15.493 kJ/mol           #DHf estimated from
lanthanides, H calc
```

```
#       Enthalpy of formation:  -1510.547 kJ/mol

2.0000 SO4-2 + 1.0000 Am+3  =  Am(SO4)2-
        log_k           +3.70                   #03GUI/FAN
        -delta_H        20.927 kJ/mol           #DHf estimated from
lanthanides, H calc
#       Enthalpy of formation:  -2414.453 kJ/mol

1.0000 F- + 1.0000 Am+3  =  AmF+2
        log_k           +3.40                   #95SIL/BID
        -delta_H        27.134                  # 97SVE/SHO     AmF+2
#       Enthalpy of formation:  -924.916 kcal/mol

2.0000 F- + 1.0000 Am+3  =  AmF2+
        log_k           +5.80                   #95SIL/BID
        -delta_H        22.320                  # 97SVE/SHO     AmF2+
#       Enthalpy of formation:  -1265.080 kcal/mol

3.0000 F- + 1.0000 Am+3  =  AmF3
        log_k           +10.82          #69AZI/LYL
        -delta_H        -12.119                 # 97SVE/SHO     AmF2+
#       Enthalpy of formation:  -1634.869 kcal/mol

1.0000 Cl- + 1.0000 Am+3  =  AmCl+2
        log_k           +0.24                   #03GUI/FAN
        -delta_H        25.106                  # 97SVE/SHO     AmCl+2
#       Enthalpy of formation:  -758.674 kcal/mol

2.0000 Cl- + 1.0000 Am+3  =  AmCl2+
        log_k           -0.74                   #03GUI/FAN
        -delta_H        40.568                  # 97SVE/SHO     AmCl+2
#       Enthalpy of formation:  -910.929 kcal/mol


1.0000 Cs+ + 1.0000 H2O  =  CsOH + 1.0000 H+
        log_k           -15.64          #DGf 85BAR/PAR, logK calc
        -delta_H        65.736  kJ/mol  #Sf 85BAR/PAR, H calc
#       Enthalpy of formation:  -478.094 kJ/mol

1.0000 Cs+ + 1.0000 NO3-  =  CsNO3
          log_k          -1.71                   #DGf 85BAR/PAR, logK calc
        -delta_H        10.450  kJ/mol  #DHf 85BAR/PAR, H calc
#       Enthalpy of formation:  -454.400 kJ/mol

1.0000 Cs+ + 1.0000 F-  =  CsF
        log_k           -0.38                   #DGf 82WAG/EVA, logK calc
        -delta_H        2.446   kJ/mol          #Sf 82WAG/EVA, logK calc
#       Enthalpy of formation:  -590.904 kJ/mol

1.0000 Cs+ + 1.0000 Cl-  =  CsCl
```

```
        log_k           -0.09                   #DGf 97SVE/SHO, logK calc
        -delta_H        7.523   kJ/mol          #Sf 97SVE/SHO, logK calc
#       Enthalpy of formation:  -417.557 kJ/mol

1.0000 Cs+ + 1.0000 Br-  =  CsBr
        log_k           0.09                    #DGf 97SVE/SHO, logK calc
        -delta_H        5.922   kJ/mol          #Sf 97SVE/SHO, logK calc
#       Enthalpy of formation:  -373.488 kJ/mol

1.0000 I- + 1.0000 Cs+  =  CsI
        log_k           +1.05                   #DGf 97SVE/SHO, logK calc
        -delta_H        -0.055  kJ/mol  #Sf 97SVE/SHO, logK calc
#       Enthalpy of formation:  -314.835 kJ/mol

1.0000 Ho+3 + 1.0000 H2O  =  HoOH+2 + 1.0000 H+
        log_k           -7.90                   #95SPA/BRU
        -delta_H        79.900  kJ/mol  #Sf estimated 97SHO/SAS, H calc
#       Enthalpy of formation:  -912.972 kJ/mol

1.0000 Ho+3 + 2.0000 H2O  =  Ho(OH)2+ + 2.0000 H+
        log_k           -16.10          #95SPA/BRU
        -delta_H        146.130 kJ/mol  #Sf estimated 97SHO/SAS, H calc
#       Enthalpy of formation:  -1132.572 kJ/mol

1.0000 Ho+3 + 3.0000 H2O  =  Ho(OH)3 + 3.0000 H+
        log_k           -24.50          #95SPA/BRU
        -delta_H        216.364 kJ/mol  #Sf estimated 97SHO/SAS, H calc
#       Enthalpy of formation:  -1348.168 kJ/mol

1.0000 Ho+3 + 4.0000 H2O  =  Ho(OH)4- + 4.0000 H+
        log_k           -33.40          #81TUR/WHI
        -delta_H        254.153 kJ/mol  #Sf estimated 97SHO/SAS, H calc
#       Enthalpy of formation:  -1596.209 kJ/mol

1.0000 Ho+3 + 1.0000 CO3-2  =  HoCO3+
        log_k           8.00                    #95SPA/BRU
        -delta_H        168.562 kJ/mol  #DSr estimated 97SVE/SHO, H calc
#       Enthalpy of formation:  -1213.710 kJ/mol

2.0000 CO3-2 + 1.0000 Ho+3  =  Ho(CO3)2-
        log_k           13.30                   #95SPA/BRU
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction    Ho(CO3)2-
#       Enthalpy of formation:  -0 kcal/mol

1.0000 Ho+3 + 1.0000 CO3-2 + 1.0000 H+  =  HoHCO3+2
        log_k           +12.50          #95SPA/BRU
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction
```

```
1.0000 NO3- + 1.0000 Ho+3  =  HoNO3+2
        log_k           +0.50                   #95SPA/BRU
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction

1.0000 Ho+3 + 1.0000 H2PO4-  =  HoH2PO4+2
        log_k           +2.30                   #95SPA/BRU
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction

1.0000 Ho+3 + 1.0000 H2PO4-  =  HoHPO4+ +1.0000 H+
        log_k           -1.41                   #95SPA/BRU
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction    HoHPO4+
#       Enthalpy of formation:  -0 kcal/mol

2.0000 H2PO4- + 1.0000 Ho+3  =  Ho(HPO4)2- +2.0000 H+
        log_k           -4.52                   #95SPA/BRU
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction    Ho(HPO4)2-
#       Enthalpy of formation:  -0 kcal/mol

1.0000 Ho+3 + 1.0000 H2PO4-  =  HoPO4 +2.0000 H+
        log_k           -6.96                   #95SPA/BRU
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction    HoPO4
#       Enthalpy of formation:  -0 kcal/mol

2.0000 H2PO4- + 1.0000 Ho+3  =  Ho(PO4)2-3 +4.0000 H+
        log_k           -17.82          #95SPA/BRU
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction    Ho(PO4)2-3
#       Enthalpy of formation:  -0 kcal/mol

1.0000 SO4-2 + 1.0000 Ho+3  =  HoSO4+
        log_k           +3.40                   #95SPA/BRU
        -delta_H        15.387  kJ/mol  #Sf 82WAG/EVA, H calc
#       Enthalpy of formation:  -1600.995 kJ/mol

2.0000 SO4-2 + 1.0000 Ho+3  =  Ho(SO4)2-
        log_k           +4.90                   #95SPA/BRU
        -delta_H        23.670 kJ/mol           #Sf 82WAG/EVA, H calc
#       Enthalpy of formation:  -2502.052 kJ/mol

1.0000 Ho+3 + 1.0000 F-  =  HoF+2
        log_k           +4.30                   #95SPA/BRU
        -delta_H        25.932  kJ/mol  #Sf 97SVE/SHO, H calc
#       Enthalpy of formation:  -1016.46 kJ/mol

1.0000 Ho+3 + 1.0000 Cl-  =  HoCl+2
```

```
        log_k           +0.30                   #95SPA/BRU
        -delta_H        24.525  kJ/mol  #Sf 97SVE/SHO, H calc
#       Enthalpy of formation:  -849.597 kJ/mol

2.0000 Cl- + 1.0000 Ho+3  =  HoCl2+
        log_k           -0.29                   #81TUR/WHI
        -delta_H        36.300  kJ/mol  #Sf 97SVE/SHO, H calc
#       Enthalpy of formation:  -1004.902 kJ/mol

 +1.000NbO3-                +2.000H+                  +1.000H2O
= Nb(OH)4+
    log_k       6.896                           #01HUM/BER
# log_k entered manually, -a_e changed accordingly
#    -a_e    6.896000E+00  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00
    -gamma      4.00    0.00

 +1.000NbO3-                +1.000H+                  +2.000H2O
= Nb(OH)5
    log_k       7.344                           #01HUM/BER
# log_k entered manually, -a_e changed accordingly
#    -a_e    7.344000E+00  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00
#    -gamma      0.00    0.00

1.0000 H2O + 1.0000 Ni+2  =  NiOH+ + 1.0000 H+
        log_k           -9.50                   #98PLY/ZHA
        -delta_H        50.000 kJ/mol           #98PLY/ZHA
#       Enthalpy of formation:  -289.93 kJ/mol

2.0000 H2O + 1.0000 Ni+2  =  Ni(OH)2 +2.0000 H+
        log_k           -18.00          #98PLY/ZHA
        -delta_H        85.760 kJ/mol           #DHf 98PLY/ZHA, H calc
#       Enthalpy of formation:  -540.000 kJ/mol

3.0000 H2O + 1.0000 Ni+2  =  Ni(OH)3- +3.0000 H+
        log_k           -29.70          #98PLY/ZHA
        -delta_H        120.590 kJ/mol          #DHf 98PLY/ZHA, H calc
#       Enthalpy of formation:  -791.0 kJ/mol

4.0000 H2O + 1.0000 Ni+2  =  Ni(OH)4-2 +4.0000 H+
        log_k           -44.90          #98PLY/ZHA
        -delta_H        136.391 kJ/mol          #98PLY/ZHA
#       Enthalpy of formation:  -1066.838 kJ/mol

2.0000 Ni+2 + 1.0000 H2O  =  Ni2OH+3 +1.0000 H+
        log_k           -9.80                   #98PLY/ZHA
        -delta_H        35.000 kJ/mol           #98PLY/ZHA
#       Enthalpy of formation:  -359.030 kJ/mol
```

```
4.0000 Ni+2 + 4.0000 H2O  =  Ni4(OH)4+4 +4.0000 H+
        log_k           -27.90          #98PLY/ZHA
        -delta_H        170.000 kJ/mol          #98PLY/ZHA
#       Enthalpy of formation:  -1189.720 kJ/mol

1.0000 Ni+2 + 1.0000 CO3-2  =  NiCO3
        log_k           4.0                     #01HUM/BER
        -delta_H        0                               # Not possible to
calculate it
#       Enthalpy of formation:  -734.803 kJ/mol

2.0000 CO3-2 + 1.0000 Ni+2  =  Ni(CO3)2-2
        log_k           6.0                     #01HUM/BER
        -delta_H        0                               # Not possible to
calculate it
#       Enthalpy of formation:  -0 kJ/mol

1.0000 Ni+2 + 1.0000 CO3-2 + 1.0000 H+  =  NiHCO3+
        log_k           11.33                   #01HUM/BER
        -delta_H        0 kJ/mol                #Not possible to calculate
it
#       Enthalpy of formation:  -0 kJ/mol

1.0000 Ni+2 + 1.0000 NO3-  =  NiNO3+
        log_k           0.40                    #01HUM/BER
        -delta_H        0                       #Not possible to calculate
it
#       Enthalpy of formation:  -0 kcal/mol

2.0000 NO3- + 1.0000 Ni+2  =  Ni(NO3)2
        log_k           -0.60                   #01HUM/BER
        -delta_H        0                               #Not possible to
calculate it
#       Enthalpy of formation:  -0 kJ/mol

1.0000 NH3 + 1.0000 Ni+2  =  NiNH3+2
        log_k           2.70                    #01HUM/BER
        -delta_H        0                               #Not possible to
calculate it
#       Enthalpy of formation:  -0 kJ/mol

2.0000 NH3 + 1.0000 Ni+2  =  Ni(NH3)2+2
        log_k           4.90                    #01HUM/BER
        -delta_H        0                               #Not possible to
calculate it
#       Enthalpy of formation:  -0 kJ/mol

3.0000 NH3 + 1.0000 Ni+2  =  Ni(NH3)3+2
        log_k           6.50                    #01HUM/BER
        -delta_H        0                               #Not possible to
```

```
calculate it
#       Enthalpy of formation:  -0 kJ/mol

4.0000 NH3 + 1.0000 Ni+2  =  Ni(NH3)4+2
        log_k           7.60                    #01HUM/BER
        -delta_H        0                               #Not possible to
calculate it
#       Enthalpy of formation:  -0 kJ/mol

5.0000 NH3 + 1.0000 Ni+2  =  Ni(NH3)5+2
        log_k           8.30                    #01HUM/BER
        -delta_H        0                               #Not possible to
calculate it
#       Enthalpy of formation:  -0 kJ/mol

6.0000 NH3 + 1.0000 Ni+2  =  Ni(NH3)6+2
        log_k           8.20                    #01HUM/BER
        -delta_H        0                               #Not possible to
calculate it

1.0000 H2PO4- + 1.0000 Ni+2  =  NiH2PO4+
        log_k           1.54                    #92PEA/BER
        -delta_H        0                       #Not possible to calculate
it
#       Enthalpy of formation:  -0 kcal/mol

1.0000 H2PO4- + 1.0000 Ni+2  =  NiHPO4 + 1.0000 H+
        log_k           -4.28                   #92PEA/BER
        -delta_H        0                       #Not possible to calculate
it
#       Enthalpy of formation:  -0 kcal/mol

1.0000 H2PO4- + 1.0000 Ni+2  =  NiPO4- + 2.0000 H+
        log_k           -11.19          #92PEA/BER
        -delta_H        0                       #Not possible to calculate
it
#       Enthalpy of formation:  -0 kcal/mol

1.0000 H2PO4- + 1.0000 Ni+2 + 2.0000 H2O  =  Ni(OH)2HPO4-2 + 3.0000 H+
        log_k           -22.59          #89ZIE/JON
        -delta_H        64.698 kJ/mol           #89ZIE/JON
#       Enthalpy of formation:  -1863.662 kJ/mol

1.0000 H2PO4- + 1.0000 Ni+2 + 3.0000 H2O  =  Ni(OH)3H2PO4-2 + 3.0000 H+
        log_k           -25.24          #89ZIE/JON
        -delta_H        85.727 kJ/mol           #89ZIE/JON
#       Enthalpy of formation:  -2128.463 kJ/mol

2.0000 H2PO4- + 1.0000 Ni+2  =  NiHP2O7- +1.0000 H2O +1.0000 H+
        log_k           -7.54                   #DGf 89BAE/McK, logK calc
```

```
        -delta_H        0                       #Not possible to calculate
it
#       Enthalpy of formation:  -0 kcal/mol

2.0000 H2PO4- + 1.0000 Ni+2  =  NiP2O7-2 +1.0000 H2O +2.0000 H+
        log_k           -13.71          #DGf 89BAE/McK, logK calc
        -delta_H        30.870 kJ/mol           #Not possible to calculate
it
#       Enthalpy of formation:  -0 kJ/mol

#1.0000 S2O3-2 + 1.0000 Ni+2  =  NiS2O3
#        log_k           +2.06                   #64SIL/MAR
#       -delta_H        0       kJ/mol          #Not possible to calculate
it
#       Enthalpy of formation:  -0 kJ/mol

1.0000 SO4-2 + 1.0000 Ni+2  =  NiSO4
        log_k           +2.35                   #Gamsjager et al. (2005)
#       -delta_H                kJ/mol          #Not reviewed
#       Enthalpy of formation:   kJ/mol


 1.0000 Ni+2 + 1.0000 HS-  =  NiHS+
        log_k           5.18                    #Gamsjager et al. (2005)
#       -delta_H        0       kJ/mol          #Not reviewed
#       Enthalpy of formation:


1.0000 Ni+2 + 1.0000 F-  =  NiF+
        log_k           1.00                    #extrapolation to I=0 by
SIT (64SILMAR, 64GRI/LIB, 70HAL/VAN, 72BON/HEF, 74BLO/RAZ, 74ARU, 76KUL/BLO
and 83SOL/BON)
        -delta_H        0       kJ/mol          #Not possible to calculate
it
#       Enthalpy of formation:  -381.330 kJ/mol

1.0000 Ni+2 + 1.0000 Cl-  =  NiCl+
        log_k           1.00                    #extrapolation to I=0 by
SIT (64SILMAR, 64GRI/LIB, 70HAL/VAN, 72BON/HEF, 74BLO/RAZ, 74ARU, 76KUL/BLO
and 83SOL/BON)
        -delta_H        0       kJ/mol          #Not possible to calculate
it
#       Enthalpy of formation:  -211.555 kJ/mol

1.0000 Ni+2 + 2.0000 Cl-  =  NiCl2
        log_k           0.90                    #extrapolation to I=0 by
SIT (64SILMAR, 64GRI/LIB, 70HAL/VAN, 72BON/HEF, 74BLO/RAZ, 74ARU, 76KUL/BLO
and 83SOL/BON)
        -delta_H        0       kJ/mol          #Not possible to calculate
it
```

```
#       Enthalpy of formation:  -383.081 kJ/mol

1.0000 Np+4 + 1.0000 e-  =  Np+3
        log_k           3.70                    #DHf and Sf 01LEM/FUG, logK
calc
        -delta_H        28.838  kJ/mol  #DHf 01LEM/FUG, H calc
#       Enthalpy of formation:  -527.184 kJ/mol

1.0000 Np+3 + 1.0000 H2O  =  NpOH+2 +1.0000 H+
        log_k           -6.80                   #01LEM/FUG
        -delta_H        77.089  kJ/mol  #Sf estimated 97SHO/SAS, H calc
#       Enthalpy of formation:  -735.925 kJ/mol

1.0000 Np+3 + 2.0000 H2O  =  Np(OH)2+ +2.0000 H+
        log_k           -17.00          #80ALL/KIP
        -delta_H        155.529 kJ/mol  #Sf estimated 97 SHO/SAS, H calc
#       Enthalpy of formation:  -943.315 kJ/mol

1.0000 Np+3 + 3.0000 H2O  =  Np(OH)3 +3.0000 H+
        log_k           -27.00          #80ALL/KIP
        -delta_H        235.824 kJ/mol  #Sf estimated 97 SHO/SAS, H calc
#       Enthalpy of formation:  -1148.850 kJ/mol

1.0000 Np+3 + 1.0000 CO3-2  =  NpCO3+
        log_k           7.67                    #estimated from
actinides(III)
        -delta_H        156.374 kJ/mol  #DSr estimated 97SVE/SHO, H calc
#       Enthalpy of formation:  -1046.04 kJ/mol

1.0000 Np+3 + 2.0000 CO3-2  =  Np(CO3)2-
        log_k           12.60                   #estimated from
actinides(III)
        -delta_H        0       kJ/mol          #Not possible to calculate
#       Enthalpy of formation:  -0 kJ/mol

1.0000 Np+3 + 3.0000 CO3-2  =  Np(CO3)3-3
        log_k           15.66                   #01LEM/FUG
        -delta_H        0       kJ/mol          #Not possible to calculate
#       Enthalpy of formation:  -0 kJ/mol

1.0000 Np+3 + 1.0000 H2PO4-  =  NpPO4 + 2.0000 H+
        log_k          -7.83                    #estimated from
actinides(III)
        -delta_H        0       kJ/mol  #Not possible to calculate
#       Enthalpy of formation:  -0 kJ/mol

1.0000 Np+3 + 2.0000 H2PO4-  =  Np(PO4)2-3 + 4.0000 H+
        log_k          -19.57                   #estimated from
actinides(III)
        -delta_H        0       kJ/mol          #Not possible to calculate
```

```
#       Enthalpy of formation:  -0 kJ/mol

1.0000 Np+3 + 1.0000 H2PO4-  =  NpHPO4+ + 1.0000 H+
        log_k          -1.78                    #estimated from
actinides(III)
        -delta_H        0       kJ/mol          #Not possible to calculate
#       Enthalpy of formation:  -0 kJ/mol

1.0000 Np+3 + 2.0000 H2PO4-  =  Np(HPO4)2- + 2.0000 H+
        log_k          -5.38                    #estimated from
actinides(III)
        -delta_H        0       kJ/mol          #Not possible to calculate
#       Enthalpy of formation:  -0 kJ/mol

1.0000 Np+3 + 1.0000 SO4-2  =  NpSO4+
        log_k           3.86                    #estimated from
actinides(III)
        -delta_H        17.891  kJ/mol  #DSr estimated 97SVE/SHO, H calc
#       Enthalpy of formation:  -1418.633 kJ/mol

1.0000 Np+3 + 2.0000 SO4-2  =  Np(SO4)2-
        log_k           5.56                    #estimated from
actinides(III)
        -delta_H        0       kJ/mol          #Not possible to calculate
#       Enthalpy of formation:  -0 kJ/mol

1.0000 NpO2+ +4.0000 H+ + 1.0000 e-  =  Np+4 + 2.0000 H2O
        log_k           +10.21          #DHf and Sf 01LEM/FUG, logK calc
        -delta_H        -149.501        kJ/mol  #DHf 01LEM/FUG, H calc
#       Enthalpy of formation:  -566.022 kJ/mol

1.0000 Np+4 + 1.0000 H2O  =  NpOH+3 +1.0000 H+
        log_k           0.55                    #03GUI/FAN
        -delta_H        38.192  kJ/mol  #Sf estimated 78LAN, H calc
#       Enthalpy of formation:  -803.660 kJ/mol

2.0000 H2O + 1.0000 Np+4  =  Np(OH)2+2 +2.0000 H+
        log_k           0.35                    #03GUI/FAN
        -delta_H        54.530  kJ/mol  #Sf estimated 78LAN, H calc
#       Enthalpy of formation:  -1073.152 kJ/mol

3.0000 H2O + 1.0000 Np+4  =  Np(OH)3+ +3.0000 H+
        log_k           -2.8                    #03GUI/FAN
        -delta_H        74.932  kJ/mol  #Sf estimated 78LAN, H calc
#       Enthalpy of formation:  -1338.580 kJ/mol

4.0000 H2O + 1.0000 Np+4  =  Np(OH)4 +4.0000 H+
        log_k           -8.3                    #03GUI/FAN
        -delta_H        101.442 kJ/mol  #Sf estimated 78LAN, H calc
#       Enthalpy of formation:  -1597.900 kJ/mol
```

```
4.0000 CO3-2 + 1.0000 Np+4  =  Np(CO3)4-4
        log_k           36.68                   #01LEM/FUG
        -delta_H        -0      kJ/mol          # Not possible to calculate
#       Enthalpy of formation:  -0 kJ/mol

5.0000 CO3-2 + 1.0000 Np+4  =  Np(CO3)5-6
        log_k           35.61                   #01LEM/FUG
        -delta_H        -1.612  kJ/mol  #80LEM/TRE
#       Enthalpy of formation:  -3933.784 kJ/mol

1.0000 CO3-2 + 1.0000 Np+4 + 3.0000 H2O  =  NpCO3(OH)3- + 3.0000 H+
        log_k           3.82                    #93ERI/NDA
        -delta_H        -0      kJ/mol          # Not possible to calculate
#       Enthalpy of formation:  -0 kJ/mol

1.0000 CO3-2 + 1.0000 Np+4 + 4.0000 H2O  =  NpCO3(OH)4-2 + 4.0000 H+
        log_k           -6.83                   #93ERI/NDA
        -delta_H        -0      kJ/mol          # Not possible to calculate
#       Enthalpy of formation:  -0 kJ/mol

2.0000 CO3-2 + 1.0000 Np+4 + 2.0000 H2O  =  Np(OH)2(CO3)2-2 + 2.0000 H+
        log_k           15.17                   #99RAI/HES
        -delta_H        -0      kJ/mol          # Not possible to calculate
#       Enthalpy of formation:  -0 kJ/mol

1.0000 NO3- + 1.0000 Np+4  =  NpNO3+3
        log_k           1.90                    #01LEM/FUG
        -delta_H        -0      kJ/mol          # Not possible to calculate
#       Enthalpy of formation:  -0 kJ/mol

1.0000 SO4-2 + 1.0000 Np+4  =  NpSO4+2
        log_k           +6.85                   #DGf 01LEM/FUG, logK calc
        -delta_H        29.840  kJ/mol  #Sf 01LEM/FUG, H calc
#       Enthalpy of formation:  -1435.522 kJ/mol

2.0000 SO4-2 + 1.0000 Np+4  =  Np(SO4)2
        log_k           +11.05          #DGf 01LEM/FUG, logK calc
        -delta_H        55.380  kJ/mol  #Sf 01LEM/FUG, H calc
#       Enthalpy of formation:  -2319.322 kJ/mol

1.0000 Np+4 + 1.0000 F-  =  NpF+3
        log_k           +8.9600         #01LEM/FUG
        -delta_H        1.500   kJ/mol          #01LEM/FUG
#       Enthalpy of formation:  -889.872 kJ/mol

2.0000 F- + 1.0000 Np+4  =  NpF2+2
        log_k           +15.7000                #01LEM/FUG
        -delta_H        15.930  kJ/mol  #84LEM
#       Enthalpy of formation:  -1210.792 kJ/mol
```

```
1.0000 Np+4 + 1.0000 Cl-  =  NpCl+3
        log_k           +1.50                   #01LEM/FUG
        -delta_H        24.173  kJ/mol  #84LEM
#       Enthalpy of formation:  -698.929 kJ/mol

1.0000 Np+4 + 1.0000 Br-  =  NpBr+3
        log_k           +1.55                   #estimated from
actinides(IV)
        -delta_H        -0      kJ/mol          # Not possible to calculate
#       Enthalpy of formation:  -0 kJ/mol

1.0000 Np+4 + 1.0000 I-  =  NpI+3
        log_k           +1.50                   #01LEM/FUG
        -delta_H        -0      kJ/mol          # Not possible to calculate
#       Enthalpy of formation:  -0 kJ/mol

1.0000 NpO2+2 + 1.0000 e-  =  NpO2+
        log_k           +19.59          #DHf and Sf 01LEM/FUG, logK calc
        -delta_H        -117.448        kJ/mol  #DHf 01LEM/FUG, H calc
#       Enthalpy of formation:  -978.181 kJ/mol

1.0000 NpO2+ + 1.0000 H2O  =  NpO2OH +1.0000 H+
        log_k           -11.30          #01LEM/FUG
        -delta_H        64.785  kJ/mol  #Sf 01LEM/FUG, H calc
#       Enthalpy of formation:  -1199.226 kJ/mol

1.0000 NpO2+ + 2.0000 H2O  =  NpO2(OH)2- +2.0000 H+
        log_k           -23.60          #01LEM/FUG
        -delta_H        118.610 kJ/mol  #Sf 01LEM/FUG, H calc
#       Enthalpy of formation:  -1431.230 kJ/mol

1.0000 NpO2+ + 1.0000 CO3-2  =  NpO2CO3-
        log_k           4.96                    #01LEM/FUG
        -delta_H        59.904  kJ/mol  #Sf 84LEM, H calc
#       Enthalpy of formation:  -1593.507 kJ/mol

2.0000 CO3-2 + 1.0000 NpO2+  =  NpO2(CO3)2-3
        log_k           6.53                    #01LEM/FUG
        -delta_H        39.027  kJ/mol  #Sf 84LEM, H calc
#       Enthalpy of formation:  -2289.614 kJ/mol

3.0000 CO3-2 + 1.0000 NpO2+  =  NpO2(CO3)3-5
        log_k           5.50                    #DHf and Sf 01LEM/FUG, logK
calc
        -delta_H        -13.249 kJ/mol  #DHf 01LEM/FUG, H calc
#       Enthalpy of formation:  -3017.120 kJ/mol

2.0000 CO3-2 + 1.0000 NpO2+ + 1.0000 H2O  =  NpO2(CO3)2OH-4 + 1.0000 H+
        log_k           -5.31                   #01LEM/FUG
```

```
        -delta_H        0       kJ/mol          # Not possible to calculate
#       Enthalpy of formation:  -0 kJ/mol

1.0000 NpO2+ + 1.0000 HPO4-2  =  NpO2HPO4-
        log_k           2.95                    #01LEM/FUG
        -delta_H        0       kJ/mol          # Not possible to calculate
#       Enthalpy of formation:  -0 kJ/mol

1.0000 SO4-2 + 1.0000 NpO2+  =  NpO2SO4-
        log_k           +0.4400         #01LEM/FUG
        -delta_H        23.200  kJ/mol  #01LEM/FUG
#       Enthalpy of formation:  -1864.321 kJ/mol

1.0000 NpO2+ + 1.0000 F-  =  NpO2F
        log_k           +1.2000         #01LEM/FUG
        -delta_H        40.768  kJ/mol  #Sf 84LEM, H calc
#       Enthalpy of formation:  -1272.763 kJ/mol

1.0000 NpO2+2 + 1.0000 H2O  =  NpO2OH+ +1.0000 H+
        log_k           -5.1                    #01LEM/FUG
        -delta_H        42.957  kJ/mol  #Sf 84LEM, H calc
#       Enthalpy of formation:  -1103.606 kJ/mol

1.0000 NpO2+2 + 2.0000 H2O  =  NpO2(OH)2 +2.0000 H+
        log_k           -12.21          #estimated from actinides(VI)
        -delta_H        0       kJ/mol          #Not possible to calculate
#       Enthalpy of formation:  -0 kJ/mol

1.0000 NpO2+2 + 3.0000 H2O  =  NpO2(OH)3- +3.0000 H+
        log_k           -19.00          #01HUM/BER
        -delta_H        0       kJ/mol          # Not possible to calculate
#       Enthalpy of formation:  -0 kJ/mol

1.0000 NpO2+2 + 4.0000 H2O  =  NpO2(OH)4-2 +4.0000 H+
        log_k           -33.00          #01HUM/BER
        -delta_H        0       kJ/mol          # Not possible to calculate
#       Enthalpy of formation:  -0 kJ/mol

2.0000 NpO2+2 + 2.0000 H2O  =  (NpO2)2(OH)2+2 +2.0000 H+
        log_k           -6.27                   #01LEM/FUG
        -delta_H        44.996  kJ/mol  #Sf 84LEM, H calc
#       Enthalpy of formation:  -2248.130 kJ/mol

5.0000 H2O + 3.0000 NpO2+2  =  (NpO2)3(OH)5+ +5.0000 H+
        log_k           -17.12          #01LEM/FUG
        -delta_H        110.667 kJ/mol  #Sf 84LEM, H calc
#       Enthalpy of formation:  -3900.682 kJ/mol

1.0000 CO3-2 + 1.0000 NpO2+2  =  NpO2CO3
        log_k           9.32                    #01LEM/FUG
```

```
        -delta_H        0       kJ/mol          # Not possible to calculate
#       Enthalpy of formation:  -0 kJ/mol

2.0000 CO3-2 + 1.0000 NpO2+2  =  NpO2(CO3)2-2
        log_k           16.52                   #01LEM/FUG
        -delta_H        13.776  kJ/mol  #Sf 84LEM, H calc
#       Enthalpy of formation:  -2197.417 kJ/mol

3.0000 CO3-2 + 1.0000 NpO2+2  =  NpO2(CO3)3-4
        log_k           19.37                   #DHf and Sf 01LEM/FUG
        -delta_H        -41.900 kJ/mol  #DHf 01LEM/FUG, H calc
#       Enthalpy of formation:  -2928.323 kJ/mol

6.0000 CO3-2 + 3.0000 NpO2+2  =  (NpO2)3(CO3)6-6
        log_k           49.84                   #01LEM/FUG
        -delta_H        0       kJ/mol          # Not possible to calculate
#       Enthalpy of formation:  -0 kJ/mol

1.0000 CO3-2 + 2.0000 NpO2+2 + 3.0000 H2O  =  (NpO2)2CO3(OH)3- + 3.0000 H+
        log_k           -2.87                   #01LEM/FUG
        -delta_H        0       kJ/mol          # Not possible to calculate
#       Enthalpy of formation:  -0 kJ/mol

6.0000 CO3-2 + 1.0000 NpO2+2 + 2.0000 UO2+2  =  (UO2)2NpO2(CO3)6-6
        log_k           53.59                   #01LEM/FUG
        -delta_H        0       kJ/mol          # Not possible to calculate
#       Enthalpy of formation:  -0 kJ/mol

1.0000 NO3- + 1.0000 NpO2+2  =  NpO2NO3+
        log_k           0.30                    #in analogy to UO2NO3+
        -delta_H        0       kJ/mol          # Not possible to calculate
#       Enthalpy of formation:  -0 kJ/mol

1.0000 NpO2+2 + 1.0000 H2PO4-  =  NpO2H2PO4+
        log_k           3.32                    #01LEM/FUG
        -delta_H        0       kJ/mol          # Not possible to calculate
#       Enthalpy of formation:  -0 kJ/mol

1.0000 NpO2+2 + 1.0000 H2PO4-  =  NpO2HPO4 +1.0000 H+
        log_k           -1.01                   #01LEM/FUG
        -delta_H        92.209  kJ/mol  #Sf 89LEM/GAR, H calc
#       Enthalpy of formation:  -2071.124 kJ/mol

1.0000 NpO2+2 + 2.0000 H2PO4-  =  NpO2(HPO4)2-2 +2.0000 H+
        log_k           -4.92                   #01LEM/FUG
        -delta_H        0       kJ/mol          #Not possible to calculate
#       Enthalpy of formation:  -0 kJ/mol

1.0000 SO4-2 + 1.0000 NpO2+2  =  NpO2SO4
        log_k           +3.2800         #01LEM/FUG
```

```
        -delta_H        16.700  kJ/mol  #01LEM/FUG
#       Enthalpy of formation:  -1753.373 kJ/mol

2.0000 SO4-2 + 1.0000 NpO2+2  =  NpO2(SO4)2-2
        log_k           +4.70                   #01LEM/FUG
        -delta_H        26.000  kJ/mol  #01LEM/FUG
#       Enthalpy of formation:  -2653.413 kJ/mol

1.0000 NpO2+2 + 1.0000 Cl-  =  NpO2Cl+
        log_k           0.40                    #01LEM/FUG
        -delta_H        8.387   kJ/mol          #Sf 84LEM, H calc
#       Enthalpy of formation:  -1019.426 kJ/mol

1.0000 NpO2+2 + 1.0000 F-  =  NpO2F+
        log_k           +4.5700         #01LEM/FUG
        -delta_H        1.4000  kJ/mol  #Sf 84LEM, H calc
#       Enthalpy of formation:  -1194.683 kJ/mol

2.0000 F- + 1.0000 NpO2+2  =  NpO2F2
        log_k           +7.6000         #01LEM/FUG
        -delta_H        4.321   kJ/mol          #Sf 84LEM, H calc
#       Enthalpy of formation:  -1527.112 kJ/mol

1.0000 Pa+4 + 1.0000 H2O  =  PaOH+3 + 1.0000 H+
        log_k           0.84                            #76BAE/MES
        -delta_H        0 kJ/mol                        #Not possible to
calculate
#       Enthalpy of formation:  -0 kJ/mol

1.0000 Pa+4 + 2.0000 H2O  =  Pa(OH)2+2 + 2.0000 H+
        log_k           -0.02                           #76BAE/MES
        -delta_H        0 kJ/mol                        #Not possible to
calculate
#       Enthalpy of formation:  -0 kJ/mol

1.0000 Pa+4 + 3.0000 H2O  =  Pa(OH)3+ + 3.0000 H+
        log_k           -1.50                           #76BAE/MES
        -delta_H        0 kJ/mol                        #Not possible to
calculate
#       Enthalpy of formation:  -0 kJ/mol

1.0000 Pa+4 + 2.0000 H2O  =  PaO2+ + 4.0000 H+ + 1.0000 e-
        log_k           4.22                            #85BAR/PAR, 76BAE/
MES
        -delta_H        0 kJ/mol                        #Not possible to
calculate
#       Enthalpy of formation:  -0 kJ/mol

1.0000 PaO2+ + 1.0000 H+  =  PaOOH+2
        log_k           -0.50                           #76BAE/MES
```

```
        -delta_H        0 kJ/mol                        #Not possible to
calculate
#       Enthalpy of formation:  -0 kJ/mol

1.0000 PaOOH+2  +1.000SO4-2             +1.000H+  =  PaOSO4+
+1.000H2O
        log_k           3.89                            #Giandomenico et
al. (2007)
#       -delta_H        0 kJ/mol                        #Not reviewed
#       Enthalpy of formation:  -0 kJ/mol

1.0000 PaOOH+2  +2.000SO4-2             +1.000H+  =  PaO(SO4)2-
+1.000H2O
        log_k           7.00                            #Giandomenico et
al. (2007)
#       -delta_H        0 kJ/mol                        #Not reviewed
#       Enthalpy of formation:  -0 kJ/mol

1.0000 PaOOH+2  +3.000SO4-2             +1.000H+  =  PaO(SO4)3-3
        +1.000H2O
        log_k           8.59                            #Giandomenico et
al. (2007)
#       -delta_H        0 kJ/mol                        #Not reviewed
#       Enthalpy of formation:  -0 kJ/mol


1.0000 PaO2+ + 1.0000 H2O  =  PaO2OH + 1.0000 H+
        log_k           -4.50                           #76BAE/MES
        -delta_H        0 kJ/mol                        #Not possible to
calculate
#       Enthalpy of formation:  -0 kJ/mol

1.0000 Pd+2 + 1.0000 H2O  =  PdOH+ +1.0000 H+
        log_k           -1.86                   # 92PEA/BER
        -delta_H        11.9    kJ/mol          # Calculated internally, Sf
97SHO/SAS
#       Enthalpy of formation:  -84.047 kJ/mol # Calculated internally, Sf
97SHO/SAS

1.0000 Pd+2 + 2.0000 H2O  =  Pd(OH)2 +2.0000 H+
        log_k           -3.79                   # 92PEA/BER
        -delta_H        15.293  kJ/mol          # Calculated internally, Sf
97SHO/SAS
#       Enthalpy of formation:  -366.483 kJ/mol # Calculated internally, Sf
97SHO/SAS

1.0000 Pd+2 + 3.0000 H2O  =  Pd(OH)3- +3.0000 H+
        log_k           -15.93                  # 92PEA/BER
        -delta_H        54.863  kJ/mol          # Calculated internally, Sf
97SHO/SAS
```

```
#       Enthalpy of formation:  -612.744 kJ/mol # Calculated internally, Sf
97SHO/SAS

1.0000 Pd+2 + 4.0000 H2O  =  Pd(OH)4-2 +4.0000 H+
        log_k           -29.36                  # 92PEA/BER
        -delta_H        118.563 kJ/mol          # Calculated internally, Sf
97SHO/SAS
#       Enthalpy of formation:  -834.874 kJ/mol # Calculated internally, Sf
97SHO/SAS

1.0000 Pd+2 + 1.0000 CO3-2  =  PdCO3
        log_k           +6.83                   # 87BRO/WAN
        -delta_H        -8.829  kJ/mol          # Calculated internally, Sr
97SVE/SHO
#       Enthalpy of formation:  -494.175 kJ/mol # Calculated internally, Sr
97SVE/SHO

1.0000 Pd+2 + 2.0000 CO3-2  =  Pd(CO3)2-2
        log_k           +12.53                  # 87BRO/WAN
        -delta_H        -0      kJ/mol          # no data available
#       Enthalpy of formation:  -0 kJ/mol       # no data available

1.0000 NH3 + 1.0000 Pd+2  =  PdNH3+2
        log_k           +9.60                   # 68RAS/JOR
        -delta_H        0                       # no data available
#       Enthalpy of formation:  -0 kJ/mol       # no data available

2.0000 NH3 + 1.0000 Pd+2  =  Pd(NH3)2+2
        log_k           +18.50                  # 68RAS/JOR
        -delta_H        0                       # no data available
#       Enthalpy of formation:  -0 kJ/mol       # no data available

3.0000 NH3 + 1.0000 Pd+2  =  Pd(NH3)3+2
        log_k           +26.00                  # 68RAS/JOR
        -delta_H        0                       # No data available
#       Enthalpy of formation:  -0 kJ/mol       # No data available

4.0000 NH3 + 1.0000 Pd+2  =  Pd(NH3)4+2
        log_k           +32.80                  # 68RAS/JOR
        -delta_H        0                       # No data available
#       Enthalpy of formation:  -0 kJ/mol       # No data available

1.0000 Pd+2 + 1.0000 SO4-2  =  PdSO4
        log_k           +2.91                   # 87BRO/WAN
        -delta_H        4.596   kJ/mol          # Calculated internally, Sr
estimated by 97SVE/SHO
#       Enthalpy of formation:  -714.86 kJ/mol # Calculated internally, Sr
estimated by 97SVE/SHO

1.0000 Pd+2 + 2.0000 SO4-2  =  Pd(SO4)2-2
```

```
        log_k           +4.17                   # 82H÷G
        -delta_H        0                       # no data available
#       Enthalpy of formation:  -0 kJ/mol       # no data available

1.0000 Pd+2 + 1.0000 Cl-  =  PdCl+
        log_k           +5.10                   # 72ELD
        -delta_H        -24.542 kJ/mol          # Calculated internally, Sf
estimated by 97SVE/SHO
#       Enthalpy of formation:  -1.739 kJ/mol  # Calculated internally, Sf
estimated by 97SVE/SHO

2.0000 Cl- + 1.0000 Pd+2  =  PdCl2
        log_k           +8.30                   # 72ELD
        -delta_H        -47.297 kJ/mol          # Calculated internally, Sf
estimated by 97SVE/SHO
#       Enthalpy of formation:  -191.573 kJ/mol # Calculated internally, Sf
estimated by 97SVE/SHO

3.0000 Cl- + 1.0000 Pd+2  =  PdCl3-
        log_k           +10.90                  # 72ELD
        -delta_H        -77.344 kJ/mol          # Calculated internally, Sf
estimated by 97SVE/SHO
#       Enthalpy of formation:  -388.7 kJ/mol   # Calculated internally, Sf
estimated by 97SVE/SHO

4.0000 Cl- + 1.0000 Pd+2  =  PdCl4-2
        log_k           +11.70                  # 72ELD
        -delta_H        -112.469        kJ/mol          # Calculated
internally, Sf estimated by 97SVE/SHO
#       Enthalpy of formation:  -590.906 kJ/mol # Calculated internally, Sf
estimated by 97SVE/SHO

3.0000 Cl- + 1.0000 Pd+2 + 1.000 H2O  =  PdCl3OH-2 + 1.0000 H+
        log_k           +2.31                   # 00BYR/YAO
        -delta_H        0                       # No data available
#       Enthalpy of formation:  -0 kJ/mol       # No data available

1.0000 Pd+2 + 1.0000 Br-  =  PdBr+
        log_k           +5.77                   # 72ELD
        -delta_H        -30.140 kJ/mol          # Calculated internally, Sf
estimated by 97SVE/SHO
#       Enthalpy of formation:  38.334 kJ/mol   # Calculated internally, Sf
estimated by 97SVE/SHO

2.0000 Br- + 1.0000 Pd+2  =  PdBr2
        log_k           +10.06                  # 72ELD
        -delta_H        -57.708 kJ/mol          # Calculated internally, Sf
estimated by 97SVE/SHO
#       Enthalpy of formation:  -110.645 kJ/mol # Calculated internally, Sf
estimated by 97SVE/SHO
```

```
3.0000 Br- + 1.0000 Pd+2  =  PdBr3-
        log_k           +13.75                  # 72ELD
        -delta_H        -92.385 kJ/mol          # Calculated internally, Sf
estimated by 97SVE/SHO
#       Enthalpy of formation:  -266.731 kJ/mol # Calculated internally, Sf
estimated by 97SVE/SHO

4.0000 Br- + 1.0000 Pd+2  =  PdBr4-2
        log_k           +15.11                  # 72ELD
        -delta_H        -126.683        kJ/mol          # Calculated
internally, Sf estimated by 97SVE/SHO
#       Enthalpy of formation:  -422.439 kJ/mol # Calculated internally, Sf
estimated by 97SVE/SHO

1.0000 Pd+2 + 1.0000 I-  =  PdI+
        log_k           +10.40                  # 89BAe/MCK
        -delta_H        -58.201 kJ/mol          # Calculated internally, Sf
estimated by 97SVE/SHO
#       Enthalpy of formation:  74.902 kJ/mol  # Calculated internally, Sf
estimated by 97SVE/SHO

4.0000 I- + 1.0000 Pd+2  =  PdI4-2
        log_k           +24.64                  # Calculated internally, Sf
estimated by 97SVE/SHO, DGF 82WAG/EVA
        -delta_H        -190.052 kJ/mol # Calculated internally, Sf
estimated by 97SVE/SHO, DGF 82WAG/EVA
#       Enthalpy of formation:  -227.288 kJ/mol # Calculated internally, Sf
estimated by 97SVE/SHO, DGF 82WAG/EVA

1.0000 Pu+4 + 1.0000 e-  =  Pu+3
        log_k           17.69                   #DGf 01LEM/FUG, logk calc
        -delta_H        -51.895 kJ/mol  #DHf 01LEM/FUG, H calc
#       Enthalpy of formation:  -591.790 kJ/mol

1.0000 Pu+3 + 1.0000 H2O  =  PuOH+2 +1.0000 H+
        log_k           -6.90                   #01LEM/FUG
        -delta_H        78.274  kJ/mol  #Sf estimated 97SHO/SAS, H calc
#       Enthalpy of formation:  -799.346 kJ/mol

1.0000 Pu+3 + 2.0000 H2O  =  Pu(OH)2+ +2.0000 H+
        log_k           -15.90          #80ALL/KIP
        -delta_H        150.342 kJ/mol  #Sf estimated 97SHO/SAS, H calc
#       Enthalpy of formation:  -1013.108 kJ/mol

1.0000 Pu+3 + 3.0000 H2O  =  Pu(OH)3 +3.0000 H+
        log_k           -25.30          #80ALL/KIP
        -delta_H        227.540 kJ/mol  #Sf estimated 97SHO/SAS, H calc
#       Enthalpy of formation:  -1221.740 kJ/mol
```

```
1.0000 CO3-2 + 1.0000 Pu+3  =  PuCO3+
        log_k           +7.64                   #estimated from
actinides(III) and lanthanides
        -delta_H        152.754kJ/mol           #DSr estimated 97SVE/SHO, H
calc
#       Enthalpy of formation:  -1114.261 kJ/mol

2.0000 CO3-2 + 1.0000 Pu+3  =  Pu(CO3)2-
        log_k           +12.54          #estimated from actinides(III) and
lanthanides
        -delta_H        0       kJ/mol          #Not possible to calculate
#       Enthalpy of formation:  -0 kJ/mol

3.0000 CO3-2 + 1.0000 Pu+3  =  Pu(CO3)3-3
        log_k           +16.40          #estimated from actinides(III) and
lanthanides
        -delta_H        0       kJ/mol          # Not possible to calculate
#       Enthalpy of formation:  -0 kJ/mol

1.0000 NO3- + 1.0000 Pu+3  =  PuNO3+2
        log_k           +1.33                   #in analogy to Am 95SIL/BID
        -delta_H        0       kJ/mol          #Not possible to calculate
#       Enthalpy of formation:  -0 kJ/mol

1.0000 H2PO4- + 1.0000 Pu+3  =  PuPO4 + 2.0000 H+
        log_k           -7.92                   #estimated from
actinides(III) and lanthanides
        -delta_H        0       kJ/mol          # Not possible to calculate
#       Enthalpy of formation:  -0 kJ/mol

2.0000 H2PO4- + 1.0000 Pu+3  =  Pu(PO4)2-3 + 4.0000 H+
        log_k           -19.73          #estimated from actinides(III) and
lanthanides
        -delta_H        0       kJ/mol          # Not possible to calculate
#       Enthalpy of formation:  -0 kJ/mol

1.0000 H2PO4- + 1.0000 Pu+3  =  PuHPO4+ + 1.0000 H+
        log_k           -1.82                   #estimated from
actinides(III) and lanthanides
        -delta_H        0       kJ/mol          # Not possible to calculate
#       Enthalpy of formation:  -0 kJ/mol

2.0000 H2PO4- + 1.0000 Pu+3  =  Pu(HPO4)2- + 2.0000 H+
        log_k           -5.46                   #estimated from
actinides(III) and lanthanides
        -delta_H        0       kJ/mol          # Not possible to calculate
#       Enthalpy of formation:  -0 kJ/mol

1.0000 SO4-2 + 1.0000 Pu+3  =  PuSO4+
        log_k           +3.91                   #01LEM/FUG
```

```
        -delta_H        17.240  kJ/mol  #01LEM/FUG
#       Enthalpy of formation:  -1483.890 kJ/mol

2.0000 SO4-2 + 1.0000 Pu+3  =  Pu(SO4)2-
        log_k           +5.70                   #01LEM/FUG
        -delta_H        11.880 kJ/mol           #DHf 01LEM/FUG, H calc
#       Enthalpy of formation:  -2398.590 kJ/mol

1.0000 I- + 1.0000 Pu+3  =  PuI+2
        log_k           +1.10                   #01LEM/FUG
        -delta_H        0       kJ/mol          # Not possible to calculate
#       Enthalpy of formation:  -0 kJ/mol

#Especies de Plutoni(IV)  Pu(IV)

1.0000 PuO2+ + 4.0000 H+ + 1.0000 e-   =   Pu+4 + 2.0000 H2O
        log_k           17.45                   #DGf 01LEM/FUG, logk calc
        -delta_H        -201.428        kJ/mol  #DHf 01LEM/FUG, H calc
#       Enthalpy of formation:  -539.895 kJ/mol

1.0000 Pu+4 + 1.0000 H2O  =  PuOH+3 +1.0000 H+
        log_k           0.60                    #03GUI/FAN
        -delta_H        36.000  kJ/mol  #01LEM/FUG
#       Enthalpy of formation:  -789.725 kJ/mol

2.0000 H2O + 1.0000 Pu+4  =  Pu(OH)2+2 +2.0000 H+
        log_k           0.60                    #03GUI/FAN
        -delta_H        49.569  kJ/mol  #Sf estimated 78LAN, H calc
#       Enthalpy of formation:  -1061.986 kJ/mol

3.0000 H2O + 1.0000 Pu+4  =  Pu(OH)3+ +3.0000 H+
        log_k           -2.30                   #03GUI/FAN
        -delta_H        68.543  kJ/mol  #Sf estimated 78LAN, H calc
#       Enthalpy of formation:  -1328.842 kJ/mol

4.0000 H2O + 1.0000 Pu+4  =  Pu(OH)4 +4.0000 H+
        log_k           -8.50                   #03GUI/FAN
        -delta_H        99.049  kJ/mol  #Sf estimated 78LAN, H calc
#       Enthalpy of formation:  -1584.166 kJ/mol

4.0000 CO3-2 + 1.0000 Pu+4  =  Pu(CO3)4-4
        log_k           +37.00          #03GUI/FAN
        -delta_H        0       kJ/mol          #Not possible to calculate
#       Enthalpy of formation:  -0 kJ/mol

5.0000 CO3-2 + 1.0000 Pu+4  =  Pu(CO3)5-6
        log_k           +35.65          #03GUI/FAN
        -delta_H        0       kJ/mol          # Not possible to calculate
#       Enthalpy of formation:  -0 kJ/mol
```

```
1.0000 NO3- + 1.0000 Pu+4  =  PuNO3+3
        log_k           +1.95                   #01LEM/FUG
        -delta_H        0       kJ/mol          #Not possible to calculate
#       Enthalpy of formation:  -0 kJ/mol

1.0000 H2PO4- + 1.0000 Pu+4 + 1.0000 H+  =  PuH3PO4+4
        log_k           +4.54                   #01LEM/FUG
        -delta_H        0       kJ/mol          #Not possible to calculate
#       Enthalpy of formation:  -0 kJ/mol

1.0000 SO4-2 + 1.0000 Pu+4  =  PuSO4+2
        log_k           +6.89                   #01LEM/FUG
        -delta_H        13.753  kJ/mol  #Sf 80LEM/TRE, H calc
#       Enthalpy of formation:  -1435.482 kJ/mol

2.0000 SO4-2 + 1.0000 Pu+4  =  Pu(SO4)2
        log_k           +11.14          #01LEM/FUG
        -delta_H        43.906  kJ/mol  #Sf 80LEM/TRE, H calc
#       Enthalpy of formation:  -2314.669 kJ/mol

1.0000 Pu+4 + 1.0000 F-  =  PuF+3
        log_k           +8.84                   #01LEM/FUG
        -delta_H        9.100 kJ/mol            #01LEM/FUG
#       Enthalpy of formation:  -866.145 kJ/mol

2.0000 F- + 1.0000 Pu+4  =  PuF2+2
        log_k           +15.70          #01LEM/FUG
        -delta_H        11.000                  #01LEM/FUG
#       Enthalpy of formation:  -1199.595 kJ/mol

1.0000 Pu+4 + 1.0000 Cl-  =  PuCl+3
        log_k           +1.80                   #01LEM/FUG
        -delta_H        19.820 kJ/mol           #Sf 80LEM/TRE, H calc
#       Enthalpy of formation:  -687.155 kJ/mol

1.0000 Pu+4 + 1.0000 Br-  =  PuBr+3
        log_k           +1.60                   #01LEM/FUG
        -delta_H        0                       # Not possible to calculate
#       Enthalpy of formation:  -0 kcal/mol

1.0000 Pu+4 + 1.0000 I-  =  PuI+3
        log_k           +1.62                   #estimated from
actinides(IV)
        -delta_H        0                       # Not possible to calculate
#       Enthalpy of formation:  -0 kcal/mol

1.0000 PuO2+2 + 1.0000 e-  =  PuO2+
        log_k           15.82                   #DGr 01LEM/FUG, logK calc
        -delta_H        -88.091 kJ/mol  #DHr 01LEM/FUG
#       Enthalpy of formation:  -910.127 kJ/mol
```

```
1.0000 PuO2+ + 1.0000 H2O  =  PuO2OH +1.0000 H+
        log_k           -11.30          #01LEM/FUG
        -delta_H        71.826  kJ/mol  #Sf 80LEM/TRE, H calc
#       Enthalpy of formation:  -1124.131 kJ/mol

1.0000 PuO2+ + 1.0000 CO3-2  =  PuO2CO3-
        log_k           5.12                    #01LEM/FUG
        -delta_H        44.874  kJ/mol  #Sf 89LEM/GAR, H calc
#       Enthalpy of formation:  -1540.483 kJ/mol

1.0000 PuO2+ + 3.0000 CO3-2  =  PuO2(CO3)3-5
        log_k           5.03                    #DGr 01LEM/FUG, logK calc
        -delta_H        -19.110 kJ/mol  #01LEM/FUG
#       Enthalpy of formation:  -2954.927 kJ/mol

1.0000 PuO2+ + 1.0000 H2PO4-  =  PuO2HPO4- + 1.0000 H+
        log_k           -4.86                   #01LEM/FUG
        -delta_H        0                       # Not possible to calculate
#       Enthalpy of formation:  -0 kcal/mol

1.0000 PuO2+ + 1.0000 F-  =  PuO2F
        log_k           1.20                    #in  analogy to NpO2F
        -delta_H        0                       # Not possible to calculate
#       Enthalpy of formation:  -0 kcal/mol

1.0000 PuO2+2 + 1.0000 H2O  =  PuO2OH+ +1.0000 H+
        log_k           -5.50                   #01LEM/FUG
        -delta_H        28.000  kJ/mol  #01LEM/FUG
#       Enthalpy of formation:  -1079.866 kJ/mol

1.0000 PuO2+2 + 2.0000 H2O  =  PuO2(OH)2 +2.0000 H+
        log_k           -13.20          #01LEM/FUG
        -delta_H        0                       # Not possible to calculate
#       Enthalpy of formation:  -0 kcal/mol

2.0000 PuO2+2 + 2.0000 H2O  =  (PuO2)2(OH)2+2 +2.0000 H+
        log_k           -7.50                   #01LEM/FUG
        -delta_H        43.583  kJ/mol  #Sf 80LEM/TRE, H calc
#       Enthalpy of formation:  -2172.149 kJ/mol

1.0000 CO3-2 + 1.0000 PuO2+2  =  PuO2CO3
        log_k           9.50                    #03GUI/FAN
        -delta_H        0                       # Not possible to calculate
#       Enthalpy of formation:  -0 kcal/mol

2.0000 CO3-2 + 1.0000 PuO2+2  =  PuO2(CO3)2-2
        log_k           14.70                   #03GUI/FAN
        -delta_H        -27.000 kJ/mol  #03GUI/FAN
#       Enthalpy of formation:  -2199.496 kJ/mol
```

```
3.0000 CO3-2 + 1.0000 PuO2+2  =  PuO2(CO3)3-4
        log_k           18.00                   #03GUI/FAN
        -delta_H        -38.600 kJ/mol  #03GUI/FAN
#       Enthalpy of formation:  -2886.326 kJ/mol

6.0000 CO3-2 + 1.0000 PuO2+2 + 2.0000 UO2+2  =  PuO2(CO3)6(UO2)2-6
        log_k           53.48                   #03GUI/FAN
        -delta_H        0                       # Not possible to calculate
#       Enthalpy of formation:  -0 kcal/mol

6.0000 CO3-2 + 3.0000 PuO2+2  =  (PuO2)3(CO3)6-6
        log_k           46.02                   #01LEM/FUG
        -delta_H        0                       # Not possible to calculate
#       Enthalpy of formation:  -0 kcal/mol

1.0000 NO3- + 1.0000 PuO2+2  =  PuO2NO3+
        log_k           0.30                    #in analogy to UO2NO3 +
        -delta_H        0                       # Not possible to calculate
#       Enthalpy of formation:  -0 kcal/mol

1.0000 SO4-2 + 1.0000 PuO2+2  =  PuO2SO4
        log_k           +3.38                   #01LEM/FUG
        -delta_H        16.100  kJ/mol  #01LEM/FUG
#       Enthalpy of formation:  -1715.276 kJ/mol

2.0000 SO4-2 + 1.0000 PuO2+2  =  PuO2(SO4)2-2
        log_k           +4.40                   #01LEM/FUG
        -delta_H        43.000  kJ/mol  #01LEM/FUG
#       Enthalpy of formation:  -2597.716 kJ/mol

1.0000 PuO2+2 + 1.0000 Cl-  =  PuO2Cl+
        log_k           0.23                    #03GUI/FAN
        -delta_H        4.187   kJ/mol          #Sf 80LEM/TRE, H calc
#       Enthalpy of formation:  -984.929 kJ/mol

1.0000 PuO2+2 + 2.0000 Cl-  =  PuO2Cl2
        log_k           -1.15                   #03GUI/FAN
        -delta_H        0       kJ/mol          # Not possible to calculate
#       Enthalpy of formation:  -0 kJ/mol

1.0000 PuO2+2 + 1.0000 F-  =  PuO2F+
        log_k           +4.56                   #01LEM/FUG
        -delta_H        -3.653  kJ/mol  #Sf 80LEM/TRE, H calc
#       Enthalpy of formation:  -1161.039 kJ/mol

2.0000 F- + 1.0000 PuO2+2  =  PuO2F2
        log_k           +7.25                   #01LEM/FUG
        -delta_H        1.208   kJ/mol          #Sf 80LEM/TRE, H calc
#       Enthalpy of formation:  -1491.528 kJ/mol
```

```
 +1.000Ra+2                 +1.000OH-                  = RaOH+
    log_k       -13.49                          #01HUM/BER
    -delta_h     4.6000         kJ/mol          #01HUM/BER
#    -a_e    1.305900E+00  0.000000E+00 -2.402790E+02  0.000000E+00
-0.000000E+00
#    -gamma      4.00    0.00

 +1.000Ra+2                 +1.000Cl-                  = RaCl+
    log_k      -0.1000                          #01HUM/BER
    -delta_h     2.1000         kJ/mol          #01HUM/BER
#    -a_e    2.679107E-01  0.000000E+00 -1.096926E+02  0.000000E+00
-0.000000E+00
#    -gamma      4.00    0.00

 +1.000Ra+2                 +1.000CO3-2                = RaCO3
    log_k       2.5000                          #01HUM/BER
    -delta_h     4.4800  kJ/mol                 #01HUM/BER
#    -a_e    3.284876E+00  0.000000E+00 -2.340109E+02  0.000000E+00
-0.000000E+00
#    -gamma      0.00    0.00

 +1.000Ra+2                 +1.000SO4-2                = RaSO4
    log_k       2.7500                          #01HUM/BER
    -delta_h     5.4000  kJ/mol                 #01HUM/BER
#    -a_e    3.696056E+00  0.000000E+00 -2.820667E+02  0.000000E+00
-0.000000E+00
#    -gamma      0.00    0.00

1.0000 SeO4-2 + 9.0000 H+ + 8.0000 e-  =  HSe- + 4.0000 H2O
        log_k           81.13                   #01SEB/POT
        -delta_H        -528.272        kJ/mol  #DHf 88SHO/HEL, H calc
#       Enthalpy of formation:  15.899 kJ/mol

1.0000 H+ + 1.0000 HSe-  =  H2Se
        log_k           +3.80                   #01SEB/POT
        -delta_H        3.301 kJ/mol            #DHf 82WAG/EVA, H calc
#       Enthalpy of formation:  19.200 kJ/mol

#4.0000 HSe- =  Se4-2 + 4.0000 H+ + 6.0000 e-
#        log_k           9.20                   #01IID/YAM
#       -delta_H        0     kJ/mol            #Not possible to calculate
#       Enthalpy of formation:  -0 kJ/mol

2.0000 Na+ + 1.0000 HSe- =  Na2Se + 1.0000 H+
        log_k           -14.96          #DGf 82WAG/EVA, logK calc
        -delta_H        0     kJ/mol            #Not possible to calculate
#       Enthalpy of formation:  -0 kJ/mol

1.0000 K+ + 1.0000 HSe- =  KHSe
```

```
        log_k           0.12                    #DGf 82WAG/EVA, logK calc
        -delta_H        -0.159     kJ/mol               #DHf 82WAG/EVA, H
calc
#       Enthalpy of formation:  -236.400 kJ/mol

2.0000 K+ + 1.0000 HSe- =  K2Se + 1.0000 H+
        log_k           -14.70          #DGf 82WAG/EVA, logK calc
        -delta_H        56.777     kJ/mol               #Sf in analogy to
K2S, H calc
#       Enthalpy of formation:  -431.604 kJ/mol

1.0000 NH3 + 1.0000 H+ + 1.0000 HSe- =  NH4HSe
        log_k           9.24                    #DGf 82WAG/EVA, logK calc
        -delta_H        -23.549     kJ/mol      #DHf 82WAG/EVA, H calc
#       Enthalpy of formation:  -118.000 kJ/mol

2.0000 NH3 + 1.0000 H+ + 1.0000 HSe- =  (NH4)2Se
        log_k           3.44                    #DGf 82WAG/EVA, logK calc
        -delta_H        -45.002     kJ/mol      #Sf in analogy to (NH4)2S,
H calc
#       Enthalpy of formation:  -191.442 kJ/mol

1.0000 SeO4-2 + 2.0000 H+ + 2.0000 e-  =  SeO3-2 + 1.0000 H2O
        log_k           27.49                   #01SEB/POT
        -delta_H        -195.874        kJ/mol  #DHf 88SHO/HEL, H calc
#       Enthalpy of formation:  -509.193 kJ/mol

1.0000 SeO3-2 + 1.0000 H+  =  HSeO3-
        log_k           +8.54                   #01SEB/POT
        -delta_H        5.020   kJ/mol          #92GRE/FUG
#       Enthalpy of formation:  -504.173 kJ/mol

2.0000 H+ + 1.0000 SeO3-2  =  H2SeO3
        log_k           +11.24          #01SEB/POT
        -delta_H        12.090  kJ/mol  #92GRE/FUG
#       Enthalpy of formation:  -497.103 kJ/mol

1.0000 Na+ + 1.0000 H+ + 1.0000 SeO3-2  =  NaHSeO3
        log_k           +8.77                   #DGf 82WAG/EVA, logK calc
        -delta_H        -5.137  kJ/mol  #DHf 82WAG/EVA, H calc
#       Enthalpy of formation:  -754.670 kJ/mol

2.0000 Na+ + 1.0000 SeO3-2  =  Na2SeO3
        log_k           1.48                    #DGf 82WAG/EVA, logK calc
        -delta_H        0.373   kJ/mol          #DHf 82WAG/EVA, H calc
#       Enthalpy of formation:  -989.500 kJ/mol

2.0000 K+ + 1.0000 SeO3-2  =  K2SeO3
        log_k           1.74                    #DGf 82WAG/EVA, logK calc
        -delta_H        -0.327 kJ/mol                   #DHf 82WAG/EVA, H
```

```
calc
#       Enthalpy of formation:  -1013.800 kJ/mol

1.0000 NH3 + 2.0000 H+ + 1.0000 SeO3-2  =  NH4HSeO3
        log_k           +18.00          #DGf 82WAG/EVA, logK calc
        -delta_H        -56.697 kJ/mol  #DHf 82WAG/EVA, H calc
#       Enthalpy of formation:  -647.060 kJ/mol

2.0000 NH3 + 2.0000 H+ + 1.0000 SeO3-2  =  (NH4)2SeO3
        log_k           +19.89          #DGf 82WAG/EVA, logK calc
        -delta_H        -102.467        kJ/mol  #DHf 82WAG/EVA, H calc
#       Enthalpy of formation:  -774.000 kJ/mol

1.0000 Mg+2 + 1.0000 SeO3-2  =  MgSeO3
        log_k           2.87                    #01SEB/POT
        -delta_H        0 kJ/mol                #Not possible to calculate

1.0000 Ca+2 + 1.0000 SeO3-2  =  CaSeO3
        log_k           3.17                    #01SEB/POT
        -delta_H        0 kJ/mol                #Not possible to calculate

1.0000 Fe+3 + 1.0000 H+ + 1.0000 SeO3-2  =  FeHSeO3+2
        log_k           11.57                   #01SEB/POT
        -delta_H        0 kJ/mol                #Not possible to calculate

1.0000 Fe+3 + 1.0000 SeO3-2  =  FeSeO3+
        log_k           11.15                   #01SEB/POT
        -delta_H        0 kJ/mol                #Not possible to calculate

1.0000 Cu+2 + 1.0000 SeO3-2  =  CuSeO3
        log_k           1.37                    #DGf 82WAG/EVA, logK calc
        -delta_H        0 kJ/mol                #Not possible to calculate

1.0000 Ag+ + 1.0000 SeO3-2  =  AgSeO3-
        log_k           3.23                    #01SEB/POT
        -delta_H        0 kJ/mol                #Not possible to calculate

1.0000 Ag+ + 2.0000 SeO3-2  =  Ag(SeO3)2-3
        log_k           3.76                    #01SEB/POT
        -delta_H        0 kJ/mol                #Not possible to calculate

2.0000 Ag+ + 1.0000 SeO3-2  =  Ag2SeO3
        log_k           1.45                    #DGf 82WAG/EVA, logK calc
        -delta_H        -0.287 kJ/mol           #DHf 82WAG/EVA, H calc
#       Enthalpy of formation:  -297.900 kJ/mol

1.0000 Zn+2 + 1.0000 SeO3-2  =  ZnSeO3
        log_k           1.43                    #DGf 82WAG/EVA, logK calc
        -delta_H        -0.617 kJ/mol           #DHf 82WAG/EVA, H calc
#       Enthalpy of formation:  -663.200 kJ/mol
```

```
1.0000 Cd+2 + 1.0000 SeO3-2  =  CdSeO3
        log_k           1.42                    #DGf 82WAG/EVA, logK calc
        -delta_H        0.213 kJ/mol            #DHf 82WAG/EVA, H calc
#       Enthalpy of formation:  -584.900 kJ/mol

1.0000 Cd+2 + 2.0000 SeO3-2  =  Cd(SeO3)2-2
        log_k           6.78                    #01SEB/POT
        -delta_H        0 kJ/mol                #Not possible to calculate
#       Enthalpy of formation:  -0 kJ/mol

1.0000 Hg+2 + 2.0000 SeO3-2  =  Hg(SeO3)2-2
        log_k           14.11                   #01SEB/POT
        -delta_H        0 kJ/mol                #Not possible to calculate
#       Enthalpy of formation:  -0 kJ/mol

1.0000 Pb+2 + 1.0000 SeO3-2  =  PbSeO3
        log_k           5.41                    #01SEB/POT
        -delta_H        0 kJ/mol                #Not possible to calculate
#       Enthalpy of formation:  -0 kJ/mol

1.0000 SeO4-2 + 1.0000 H+  =  HSeO4-
        log_k           +1.80                   #01SEB/POT
        -delta_H        23.800  kJ/mol  #92GRE/FUG
#       Enthalpy of formation:  -575.349 kJ/mol

1.0000 SeO4-2 + 2.0000 H+  =  H2SeO4
        log_k           -0.21                   #01SEB/POT
        -delta_H        12.149  kJ/mol  #DHf 82WAG/EVA, H calc
#       Enthalpy of formation:  -587.000 kJ/mol

1.0000 Na+ + 1.0000 SeO4-2 + 1.0000 H+  =  NaHSeO4
        log_k           +1.85                   #DGf 82WAG/EVA, logK calc
        -delta_H        17.789  kJ/mol  #DHf 82WAG/EVA, H calc
#       Enthalpy of formation:  -821.700 kJ/mol

1.0000 SeO4-2 + 2.0000 Na+  =  Na2SeO4
        log_k           -0.05                   #DGf 82WAG/EVA, logK calc
        -delta_H        0.329   kJ/mol          #DHf 82WAG/EVA, H calc
#       Enthalpy of formation:  -1079.500 kJ/mol

1.0000 K+ + 1.0000 SeO4-2 + 1.0000 H+  =  KHSeO4
        log_k           +2.00                   #DGf 82WAG/EVA, logK calc
        -delta_H        17.389  kJ/mol  #DHf 82WAG/EVA, H calc
#       Enthalpy of formation:  -833.900 kJ/mol

1.0000 SeO4-2 + 2.0000 K+  =  K2SeO4
        log_k           0.23                    #DGf 82WAG/EVA, logK calc
        -delta_H        -0.271  kJ/mol  #DHf 82WAG/EVA, H calc
#       Enthalpy of formation:  -1103.700 kJ/mol
```

```
1.0000 NH3 + 1.0000 SeO4-2 + 2.0000 H+  =  NH4HSeO4
        log_k           11.10                   #DGf 82WAG/EVA, logK calc
        -delta_H        -33.832 kJ/mol  #Sf in analogy to NH4HSO4, H calc
#       Enthalpy of formation:  -714.151 kJ/mol

2.0000 NH3 + 1.0000 SeO4-2 + 2.0000 H+  =  (NH4)2SeO4
        log_k           18.38                   #DGf 82WAG/EVA, logK calc
        -delta_H        -102.533        kJ/mol  #Sf in analogy to
NH4(SO4)2, H calc
#       Enthalpy of formation:  -864.021 kJ/mol

1.0000 SeO4-2 + 1.0000 Mg+2  =  MgSeO4
        log_k           +2.20                   #01SEB/POT
        -delta_H        -19.692 kJ/mol          #Sf in analogy to MgSO4, H
calc
#       Enthalpy of formation:  -1085.841 kJ/mol

1.0000 SeO4-2 + 1.0000 Ca+2  =  CaSeO4
        log_k           2.00                    #01SEB/POT
        -delta_H        -16.314 kJ/mol          #Sf in analogy to CaSO4, H
calc
#       Enthalpy of formation:  -1158.463 kJ/mol

1.0000 SeO4-2 + 1.0000 Fe+2  =  FeSeO4
        log_k           2.71                    #01SEB/POT
        -delta_H        4.762 kJ/mol            #Sf in analogy to FeSO4, H
calc
#       Enthalpy of formation:  -684.387 kJ/mol

1.0000 SeO4-2 + 1.0000 Ni+2  =  NiSeO4
        log_k           +2.6700         #01SEB/POT
        -delta_H        -21.624 kJ/mol          #Sf in analogy to FeSO4, H
calc
#       Enthalpy of formation:  -674.984 kJ/mol

1.0000 SeO4-2 + 1.0000 Mn+2  =  MnSeO4
        log_k           +2.4300         #01SEB/POT
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction    MnSeO4

1.0000 SeO4-2 + 2.0000 Ag+  =  Ag2SeO4
        log_k           -0.07                   #DGf 82WAG/EVA, logK calc
        -delta_H        -0.331 kJ/mol           #DHf 82WAG/EVA, H calc
#       Enthalpy of formation:  -387.900 kJ/mol

1.0000 Zn+2 + 1.0000 SeO4-2  =  ZnSeO4
        log_k           +2.3900         #01SEB/POT
        -delta_H        -0.561 kJ/mol           #DHf 82WAG/EVA, H calc
#       Enthalpy of formation:  -753.100 kJ/mol
```

```
1.0000 Zn+2 + 2.0000 SeO4-2  =  Zn(SeO4)2-2
        log_k           +3.01                   #01SEB/POT
        -delta_H        -0 kJ/mol               #Not possible to calculate

1.0000 SeO4-2 + 1.0000 Cd+2  =  CdSeO4
        log_k           -0.09                   #DGf 82WAG/EVA, logK calc
        -delta_H        0.169 kJ/mol            #DHf 82WAG/EVA, H calc
#       Enthalpy of formation:  -674.9 kJ/mol

1.0000 SeO4-2 + 1.0000 UO2+2  =  UO2SeO4
        log_k           2.64                    #01SEB/POT
        -delta_H        19.949 kJ/mol           #DHf 82WAG/EVA, H calc
#       Enthalpy of formation:  -1598.200 kJ/mol

1.0000 Sm+3 + 1.0000 H2O  =  SmOH+2 +1.0000 H+
        log_k           -7.90                   #95SPA/BRU
        -delta_H        81.304  kJ/mol  # Sf estimated 97SHO/SAS, H calc
#       Enthalpy of formation:  -895.725 kJ/mol

1.0000 Sm+3 + 2.0000 H2O  =  Sm(OH)2+ +2.0000 H+
        log_k           -16.50          #95SPA/BRU
        -delta_H        150.264                 # Sf estimated 97SHO/SAS, H
calc
#       Enthalpy of formation:  -1112.595 kJ/mol

1.0000 Sm+3 + 3.0000 H2O  =  Sm(OH)3 +3.0000 H+
        log_k           -25.90          #95SPA/BRU
        -delta_H        226.683 kJ/mol  # Sf estimated 97SHO/SAS, H calc
#       Enthalpy of formation:  -1322.006 kJ/mol

4.0000 H2O + 1.0000 Sm+3  =  Sm(OH)4- +4.0000 H+
        log_k           -36.90          #95SPA/BRU
        -delta_H        276.904 kJ/mol          # Sf estimated 97SHO/SAS, H
calc
#       Enthalpy of formation:  -1557.615 kJ/mol

1.0000 Sm+3 + 1.0000 CO3-2  =  SmCO3+
        log_k           7.80                    #95SPA/BRU
        -delta_H        163.392 kJ/mol  # DSr estimated 97SVE/SHO, H calc
#       Enthalpy of formation:  -1203.037 kJ/mol

2.0000 CO3-2 + 1.0000 Sm+3  =  Sm(CO3)2-
        log_k           12.80                   #95SPA/BRU
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction    Sm(CO3)2-

1.0000 Sm+3 + 1.0000 CO3-2 + 1.0000 H+  =  SmHCO3+2
        log_k           +12.43          #95SPA/BRU
        -delta_H        0                       # Not possible to calculate
```

```
enthalpy of reaction

1.0000 Sm+3 + 1.0000 NO3-  =  SmNO3+2
        log_k           +0.90                   #95SPA/BRU
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction

1.0000 Sm+3 + 1.0000 H2PO4-  =  SmH2PO4+2
        log_k           2.35                    #95SPA/BRU
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction

1.0000 Sm+3 + 1.0000 H2PO4-  =  SmHPO4+ + 1.0000 H+
        log_k           -1.61                   #95SPA/BRU
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction    SmHPO4+
#       Enthalpy of formation:  -0 kcal/mol

2.0000 H2PO4- + 1.0000 Sm+3  =  Sm(HPO4)2- + 2.0000 H+
        log_k           -5.02                   #95SPA/BRU
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction    Sm(HPO4)2-
#       Enthalpy of formation:  -0 kcal/mol

1.0000 Sm+3 + 1.0000 H2PO4-  =  SmPO4 +2.0000 H+
        log_k           -7.46                   #95SPA/BRU
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction    SmPO4
#       Enthalpy of formation:  -0 kcal/mol

2.0000 H2PO4- + 1.0000 Sm+3  =  Sm(PO4)2-3 +4.0000 H+
        log_k           -18.72          #95SPA/BRU
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction    Sm(PO4)2-3
#       Enthalpy of formation:  -0 kcal/mol

1.0000 Sm+3 + 1.0000 SO4-2  =  SmSO4+
        log_k           +3.50                   #95SPA/BRU
        -delta_H        16.575  kJ/mol  # Sf 82WAG/EVA, H calc
#       Enthalpy of formation:  -1583.964 kJ/mol

2.0000 SO4-2 + 1.0000 Sm+3  =  Sm(SO4)2-
        log_k           +5.20                   #95SPA/BRU
        -delta_H        24.910 kJ/mol           # Sf 82WAG/EVA, H calc
#       Enthalpy of formation:  -2484.969 kJ/mol

1.0000 Sm+3 + 1.0000 F-  =  SmF+2
        log_k           +3.80                   #95SPA/BRU
        -delta_H        26.520  kJ/mol  #97SVE/SHO
#       Enthalpy of formation:  -1000.029 kJ/mol
```

```
1.0000 Sm+3 + 1.0000 Cl-  =  SmCl+2
        log_k           +0.40                   #95SPA/BRU
        -delta_H        24.103  kJ/mol  #97SVE/SHO
#       Enthalpy of formation:  -834.176 kJ/mol

1.0000 Sm+3 + 1.0000 Br-  =  SmBr+2
        log_k           +0.23                   #96FAL/REA
        -delta_H        17.023  kJ/mol  # DSr estimated 97SVE/SHO, H calc
#       Enthalpy of formation:  -795.586 kJ/mol

1.0000 Sn+2 + 1.0000 H2O  =  SnOH+ +1.0000 H+
        log_k           -3.80                   #01SEB/POT2
        -delta_H        29.765  kJ/mol  #Sf 97SHO/SAS, H calc
#       Enthalpy of formation:  -264.965 kJ/mol

2.0000 H2O + 1.0000 Sn+2  =  Sn(OH)2 +2.0000 H+
        log_k           -7.80                   #01SEB/POT2
        -delta_H        41.721  kJ/mol  #Sf estimated 69HEL, H calc
#       Enthalpy of formation:  -538.838 kJ/mol

3.0000 H2O + 1.0000 Sn+2  =  Sn(OH)3- +3.0000 H+
        log_k           -17.50          #01SEB/POT2
        -delta_H        95.570  kJ/mol  #Sf estimated 69HEL, H calc
#       Enthalpy of formation:  -770.820 kJ/mol

2.0000 H2O + 2.0000 Sn+2  =  Sn2(OH)2+2 + 2.0000 H+
        log_k           -2.40                   #01SEB/POT2
        -delta_H        0       kJ/mol          #Not possible to calculate
it

4.0000 H2O + 3.0000 Sn+2  =  Sn3(OH)4+2 + 4.0000 H+
        log_k           -5.60                   #01SEB/POT2
        -delta_H        0       kJ/mol          #Not possible to calculate
it

1.0000 Sn+2 + 1.0000 NO3-  =  SnNO3+
        log_k           1.25                    #99LOT/OCH
        -delta_H        0       kJ/mol          #Not possible to calculate
it

1.0000 Sn+2 + 2.0000 NO3-  =  Sn(NO3)2
        log_k           1.74                    #99LOT/OCH
        -delta_H        0       kJ/mol          #Not possible to calculate
it

1.0000 Sn+2 + 3.0000 NO3-  =  Sn(NO3)3-
        log_k           1.37                    #99LOT/OCH
        -delta_H        0       kJ/mol          #Not possible to calculate
it
```

```
1.0000 Sn+2 + 4.0000 NO3-  =  Sn(NO3)4-2
        log_k           0.30                    #99LOT/OCH
        -delta_H        0       kJ/mol          #Not possible to calculate
it

1.0000 Sn+2 + 1.0000 SO4-2  =  SnSO4
        log_k           2.91                    #99LOT/OCH
        -delta_H        0       kJ/mol          #Not possible to calculate
it

1.0000 Sn+2 + 1.0000 F-  =  SnF+
        log_k           +5.22                   #01SEB/POT2
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction    SnF+

2.0000 F- + 1.0000 Sn+2  =  SnF2
        log_k           +8.90                   #01SEB/POT2
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction    SnF2

3.0000 F- + 1.0000 Sn+2  =  SnF3-
        log_k           +12.90          #01SEB/POT2
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction    SnF3-
#       Enthalpy of formation:  -0 kcal/mol

1.0000 Sn+2 + 1.0000 Cl-  =  SnCl+
        log_k           +1.54                   #01SEB/POT2
        -delta_H        11.180 kJ/mol           #DHf 82WAG/EVA, H calc
#       Enthalpy of formation:  -164.800 kJ/mol

2.0000 Cl- + 1.0000 Sn+2  =  SnCl2
        log_k           +2.30                   #01SEB/POT2
        -delta_H        13.360 kJ/mol           #DHf 82WAG/EVA, H calc
#       Enthalpy of formation:  -329.700 kJ/mol

3.0000 Cl- + 1.0000 Sn+2  =  SnCl3-
        log_k           +1.9700         #01SEB/POT2
        -delta_H        23.140 kJ/mol           #DHf 82WAG/EVA, H calc
#       Enthalpy of formation:  -487.000 kJ/mol

1.0000 Sn+2 + 1.0000 Cl- + 1.0000 H2O  =  SnOHCl + 1.0000 H+
        log_k           -2.27                   #99LOT/OCH
        -delta_H        8.310 kJ/mol            #DHf 82WAG/EVA, H calc
#       Enthalpy of formation:  -453.500 kJ/mol

1.0000 Sn+2 + 1.0000 Br-  =  SnBr+
        log_k           +1.07                   #01SEB/POT2
        -delta_H        5.610 kJ/mol            #DHf 82WAG/EVA, H calc
```

```
#       Enthalpy of formation:  -124.700 kJ/mol

2.0000 Br- + 1.0000 Sn+2  =  SnBr2
        log_k           +1.88                   #01SEB/POT2
        -delta_H        5.720 kJ/mol            #DHf 82WAG/EVA, H calc
#       Enthalpy of formation:  -246.000 kJ/mol

3.0000 Br- + 1.0000 Sn+2  =  SnBr3-
        log_k           +1.500          #01SEB/POT2
        -delta_H        -1.770  kJ/mol          #DHf 82WAG/EVA, H calc
#       Enthalpy of formation:  -374.900 kJ/mol

1.0000 Sn+2 + 1.0000 I-  =  SnI+
        log_k           +1.72                   #68HAI/JOH
        -delta_H        0 kJ/mol                        #Not possible to
calculate it

2.0000 I- + 1.0000 Sn+2  =  SnI2
        log_k           +2.66                   #68HAI/JOH
        -delta_H        0 kJ/mol                        #Not possible to
calculate it

1.0000 Sn+2  =  Sn+4 +2.0000 e-
        log_k           -5.08                   #01SEB/POT2
        -delta_H        39.146  kJ/mol  #DHf 85JAC/HEL, H calc
#       Enthalpy of formation:  30.246 kJ/mol

1.0000 Sn+4 + 1.0000 H2O  =  SnOH+3 +1.0000 H+
        log_k           +1.79                   #71NAZ/ANT
        -delta_H        -62.218 kJ/mol  #Sf estimated 78LAN, H calc
#       Enthalpy of formation:  -317.802 kJ/mol

2.0000 H2O + 1.0000 Sn+4  =  Sn(OH)2++ +2.0000 H+
        log_k           2.71                    #71NAZ/ANT
        -delta_H        -52.279 kJ/mol  #Sf estimated 78LAN, H calc
#       Enthalpy of formation:  -593.692 kJ/mol

3.0000 H2O + 1.0000 Sn+4  =  Sn(OH)3+ +3.0000 H+
        log_k           +2.79                   #71NAZ/ANT
        -delta_H        -50.306 kJ/mol  #Sf estimated 78LAN, H calc
#       Enthalpy of formation:  -877.549 kJ/mol

4.0000 H2O + 1.0000 Sn+4  =  Sn(OH)4 +4.0000 H+
        log_k           -0.53                   #99LOT/OCH
        -delta_H        -36.254 kJ/mol  #Sf estimated 78LAN, H calc
#       Enthalpy of formation:  -1149.327 kJ/mol

5.0000 H2O + 1.0000 Sn+4  =  Sn(OH)5- +5.0000 H+
        log_k           -8.50                   #01HUM/BER, 00LOT/OCH
        -delta_H        -0      kJ/mol          #Not possible to calculate
```

```
it

6.0000 H2O + 1.0000 Sn+4  =  Sn(OH)6-2 +6.0000 H+
        log_k           -18.93          #01HUM/BER, 00LOT/OCH
        -delta_H        -0      kJ/mol          #Not possible to calculate
it

1.0000 Sn+4 + 1.0000 SO4-2  =  SnSO4+2
        log_k           -3.22                   #99LOT/OCH
        -delta_H        0                       #Not possible to calculate
it

2.0000 SO4-2 + 1.0000 Sn+4  =  Sn(SO4)2
        log_k           -0.85                   #01SEB/POT2
        -delta_H        0                       #Not possible to calculate
it

1.0000 Sn+4 + 1.0000 Cl-  =  SnCl+3
        log_k           5.80                    #99LOT/OCH
        -delta_H        0        kJ/mol         #Not possible to calculate
it

1.0000 Sn+4 + 2.0000 Cl-  =  SnCl2+2
        log_k           10.12                   #99LOT/OCH
        -delta_H        0        kJ/mol         #Not possible to calculate
it

1.0000 Sn+4 + 3.0000 Cl-  =  SnCl3+
        log_k           13.49                   #99LOT/OCH
        -delta_H        0        kJ/mol         #Not possible to calculate
it

1.0000 Sn+4 + 4.0000 Cl-  =  SnCl4
        log_k           12.62                   #99LOT/OCH
        -delta_H        0        kJ/mol         #Not possible to calculate
it

1.0000 Sn+4 + 5.0000 Cl-  =  SnCl5-
        log_k           16.46                   #99LOT/OCH
        -delta_H        0        kJ/mol         #Not possible to calculate
it

1.0000 Sn+4 + 6.0000 Cl-  =  SnCl6-2
        log_k           17.11                   #99LOT/OCH
        -delta_H        0        kJ/mol         #Not possible to calculate
it

 +1.000Sr+2                 -1.000H+                  +1.000HCO3-
= SrCO3
    log_k      -7.5238                          #01HUM/BER
```

```
    -delta_h    36.7281                         #01HUM/BER
#    -a_e   -1.089061E+02 -1.970249E-02  5.151790E+03  3.892561E+01
-5.637139E+05
#    -gamma      0.00    0.00

 +1.000Sr+2                 +1.000HCO3-                = SrHCO3+
    log_k       1.1846                          #01HUM/BER
    -delta_h    25.3008                         #01HUM/BER
#    -a_e   -3.248000E+00  1.486700E-02  0.000000E+00  0.000000E+00
0.000000E+00
    -gamma      4.00    0.00

 +1.000Sr+2                 +1.000H2O                  -1.000H+
= SrOH+
    log_k     -13.2900                          #01HUM/BER
#    -a_e   -1.329000E+01  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00
    -gamma      4.00    0.00

 +1.000Sr+2                 +1.000SO4-2                = SrSO4
    log_k       2.2900                          #01HUM/BER
    -delta_h     8.7027                         #01HUM/BER
#    -a_e    3.814678E+00  0.000000E+00 -4.545828E+02  0.000000E+00
-0.000000E+00
#    -gamma      0.00    0.00

 +1.000Sr+2                 +1.000S2O3-2                = SrS2O3
    log_k       2.0400                          #Denney and Monk (1951)
#    -delta_h                                            # Not reviewed
#       Enthalpy of formation:  0 kJ/mol


 +1.000TcO(OH)2                  +1.000H2O                  -4.000H+
-3.000e-                =       TcO4-
    log_k      -29.4000                         #01HUM/BER
#    -a_e    2.940000E+01  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00
#    -gamma      0.00    0.00

 +1.000TcO(OH)2             +2.000H+                   -2.000H2O
= TcO+2
    log_k       4.0000                          #01HUM/BER
#    -a_e    4.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00
    -gamma      4.50    0.00

 +1.000TcO(OH)2             +1.000H+                   -1.000H2O
= TcO(OH)+
    log_k       2.5000                          #01HUM/BER
#    -a_e    2.500000E+00  0.000000E+00  0.000000E+00  0.000000E+00
```

```
0.000000E+00
    -gamma      4.00    0.00

 +1.000TcO(OH)2             +1.000H2O                  -1.000H+
= TcO(OH)3-
    log_k     -10.9000                          #01HUM/BER
#    -a_e   -1.090000E+01  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00
    -gamma      4.00    0.00

 +1.000TcO(OH)2             +1.000CO3-2                +2.000H+
-1.000H2O                  = TcCO3(OH)2
    log_k      19.3000                          #01HUM/BER
#    -a_e    1.930000E+01  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00
#    -gamma      0.00    0.00

 +1.000TcO(OH)2             +1.000H+                   +1.000CO3-2
= TcCO3(OH)3-
    log_k      11.0000                          #01HUM/BER
#    -a_e    1.100000E+01  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00
    -gamma      4.00    0.00

1.0000 TcO4- + 1.0000 e-  =  TcO4-2
        log_k           -10.80                  # 99RAR/RAN
        -delta_H        0 kJ/mol                # Not available
#       Enthalpy of formation:  0 kJ/mol # Not available

1.0000 Th+4 + 1.0000 H2O  =  ThOH+3 +1.0000 H+
        log_k           -2.20                   #01NEC/KIM
        -delta_H        53.670  kJ/mol  #Sf estimated 78LAN, H calc
#       Enthalpy of formation:  -994.111 kJ/mol

2.0000 H2O + 1.0000 Th+4  =  Th(OH)2+2 +2.0000 H+
        log_k           -6.00                   #01NEC/KIM
        -delta_H        90.557  kJ/mol  #Sf estimated 78LAN, H calc
#       Enthalpy of formation:  -1173.509 kJ/mol

3.0000 H2O + 1.0000 Th+4  =  Th(OH)3+ +3.0000 H+
        log_k           -11.00          #01NEC/KIM
        -delta_H        121.518 kJ/mol  #Sf estimated 78LAN, H calc
#       Enthalpy of formation:  -1358.832 kJ/mol

4.0000 H2O + 1.0000 Th+4  =  Th(OH)4 +4.0000 H+
        log_k           -17.50          #01NEC/KIM
        -delta_H        153.736 kJ/mol  #Sf estimated 78LAN, H calc
#       Enthalpy of formation:  -1542.898 kJ/mol

2.0000 Th+4 + 2.0000 H2O  =  Th2(OH)2+6 +2.0000 H+
```

```
        log_k           -5.70                   #02NEC/MUL
        -delta_H        0                               # Not possible to
calculate
#       Enthalpy of formation:  -0 kcal/mol

8.0000 H2O + 4.0000 Th+4  =  Th4(OH)8+8 +8.0000 H+
        log_k           -20.40          #02NEC/MUL
        -delta_H        0                               # Not possible to
calculate
#       Enthalpy of formation:  -0 kcal/mol

#15.0000 H2O + 6.0000 Th+4  =  Th6(OH)15+9 +15.0000 H+
 #       log_k           -34.00         #02NEC/MUL
#       -delta_H        0                               # Not possible to
calculate
#       Enthalpy of formation:  -0 kcal/mol

12.0000 H2O + 4.0000 Th+4  =  Th4(OH)12+4 + 12.0000 H+
        log_k           -26.7                   #02NEC/MUL
        -delta_H        0                               # Not possible to
calculate
#       Enthalpy of formation:  -0 kcal/mol

1.0000 Th+4 + 4.0000 CO3-2  =  Th(CO3)4-4
        log_k           31.60                   #99RIG/CAP
        -delta_H        0                               # Not possible to
calculate
#       Enthalpy of formation:  -0 kcal/mol

1.0000 Th+4 + 5.0000 CO3-2  =  Th(CO3)5-6
        log_k           28.60                   #99RIG/CAP
        -delta_H        0                               # Not possible to
calculate
#       Enthalpy of formation:  -0 kcal/mol

1.0000 Th+4 + 1.0000 CO3-2 + 3.0000 H2O   =  ThCO3(OH)3- + 3.0000 H+
        log_k           -1.90                   #99RIG/CAP
        -delta_H        0                               # Not possible to
calculate
#       Enthalpy of formation:  -0 kcal/mol

1.0000 Th+4 + 3.0000 CO3-2 + 2.0000 H2O   =  Th(CO3)3(OH)2-4 + 2.0000 H+
        log_k           10.20                   #99RIG/CAP
        -delta_H        0                               # Not possible to
calculate
#       Enthalpy of formation:  -0 kcal/mol

1.0000 Th+4 + 1.0000 NO3-  =  ThNO3+3
        log_k           0.80                    #estimated from
Actinides(IV)
```

```
        -delta_H        0                               # Not possible to
calculate
#       Enthalpy of formation:  -0 kcal/mol

1.0000 Th+4 + 1.0000 H2PO4- + 4.0000 H2O  =  Th(OH)4PO4-3 + 6.0000 H+
        log_k           -34.45          #94÷ST

1.0000 Th+4 + 1.0000 SO4-2  =  ThSO4+2
        log_k           +7.86                   #92FEL/RAI, 02HUM/BER
        -delta_H        2.934   kJ/mol          #Sf 80LAN/HER, H calc

2.0000 SO4-2 + 1.0000 Th+4  =  Th(SO4)2
        log_k           +11.80          #92FEL/RAI, 02HUM/BER
        -delta_H        21.085  kJ/mol  #Sf 80LAN/HER, H calc

3.0000 SO4-2 + 1.0000 Th+4  =  Th(SO4)3-2
        log_k           +12.74          #92FEL/RAI, 01HUMBER

1.0000 Th+4 + 1.0000 F-  =  ThF+3
        log_k           +7.64                   #DGf 82WAG/EVA, logK calc
        -delta_H        -2.011  kJ/mol  #Sf 82WAG/EVA, H calc

2.0000 F- + 1.0000 Th+4  =  ThF2+2
        log_k           +13.36          #DGf 82WAG/EVA, logK calc
        -delta_H        -2.249  kJ/mol  #Sf 82WAG/EVA, H calc

3.0000 F- + 1.0000 Th+4  =  ThF3+
        log_k           +17.54          #DGf 82WAG/EVA, logK calc
        -delta_H        -3.228  kJ/mol  #Sf 82WAG/EVA, H calc

4.0000 F- + 1.0000 Th+4  =  ThF4
        log_k           +20.41          #DGf 82WAG/EVA, logK calc
        -delta_H        -4.459  kJ/mol  #Sf 82WAG/EVA, H calc

1.0000 Th+4 + 1.0000 Cl-  =  ThCl+3
        log_k           +1.21                   #DGf 82WAG/EVA, logK calc
        -delta_H        0.873   kJ/mol          #Sf 82WAG/EVA, H calc

4.0000 H+ + 1.0000 UO2+2 + 2.0000 e-  =  U+4 +2.0000 H2O
        log_k           9.04                    #92GRE/FUG
        -delta_H        -143.860        kJ/mol  #92GRE/FUG
#       Enthalpy of formation:  -591.2 kJ/mol

1.0000 H2O + 1.0000 U+4  =  UOH+3 +1.0000 H+
        log_k           -0.54                   #92GRE/FUG
        -delta_H        46.910  kJ/mol  #92GRE/FUG
#       Enthalpy of formation:  -830.120 kJ/mol

2.0000 H2O + 1.0000 U+4  =  U(OH)2+2 +2.0000 H+
        log_k           -1.10             #01NEC/KIM
```

```
        -delta_H        59.974  kJ/mol  # Sf estimated 78LAN, H calc
#       Enthalpy of formation:  -1102.886 kJ/mol

3.0000 H2O + 1.0000 U+4  =  U(OH)3+ +3.0000 H+
        log_k           -4.70          #01NEC/KIM
        -delta_H        82.944  kJ/mol  # Sf estimated 78LAN, H calc
#       Enthalpy of formation:  -1365.746 kJ/mol

4.0000 H2O + 1.0000 U+4  =  U(OH)4 +4.0000 H+
        log_k           -10.0            #01NEC/KIM
        -delta_H        109.881 kJ/mol  # Sf 92GRE/FUG
#       Enthalpy of formation:  -1624.639 kJ/mol

4.0000 CO3-2 + 1.0000 U+4  =  U(CO3)4-4
        log_k           35.12      #92GRE/FUG + 95SIL/BID
        -delta_H        0               # Not possible to calculate it
#       Enthalpy of formation:  -0 kcal/mol

5.0000 CO3-2 + 1.0000 U+4  =  U(CO3)5-6
        log_k           34.00        #03GUI/FAN
        -delta_H        -20.00  kJ/mol  # 95SIL/BID
#       Enthalpy of formation:  -3987.35 kJ/mol

1.0000 U+4 + 1.0000 NO3-  =  UNO3+3
        log_k           +1.47            #92GRE/FUG
        -delta_H        0               # Not possible to calculate it
#       Enthalpy of formation:  -0 kcal/mol

2.0000 NO3- + 1.0000 U+4  =  U(NO3)2+2
        log_k           +2.30   #92GRE/FUG
        -delta_H        0               # Not possible to calculate it
#       Enthalpy of formation:  -0 kcal/mol

1.0000 SO4-2 + 1.0000 U+4  =  USO4+2
        log_k           +6.58    #92GRE/FUG
        -delta_H        8.0000  kJ/mol  # 92GRE/FUG
#       Enthalpy of formation:  -1492.540 kJ/mol

2.0000 SO4-2 + 1.0000 U+4  =  U(SO4)2
        log_k           +10.51            #92GRE/FUG
        -delta_H        32.700  kJ/mol  # 92GRE/FUG
#       Enthalpy of formation:  -2377.18 kJ/mol

1.0000 U+4 + 1.0000 F-  =  UF+3
        log_k           +9.42          #03GUI/FAN
        -delta_H        -5.600  kJ/mol  # 92GRE/FUG
#       Enthalpy of formation:  -932.15 kJ/mol

2.0000 F- + 1.0000 U+4  =  UF2+2
        log_k           +16.56     #03GUI/FAN
```

```
        -delta_H        -3.500  kJ/mol  #92GRE/FUG
#       Enthalpy of formation:  -1265.4 kJ/mol

3.0000 F- + 1.0000 U+4  =  UF3+
        log_k           +21.89  #03GUI/FAN
        -delta_H        0.5000  kJ/mol  # #92GRE/FUG
#       Enthalpy of formation:  -1596.75 kJ/mol

4.0000 F- + 1.0000 U+4  =  UF4
        log_k           +26.34     #03GUI/FAN
        -delta_H        -8.429  kJ/mol  ##92GRE/FUG
#       Enthalpy of formation:  -1941.029 kJ/mol

5.0000 F- + 1.0000 U+4  =  UF5-
        log_k           +27.73          #03GUI/FAN
        -delta_H        -11.624 kJ/mol          #Sf estimated 78LAN, H
calc.
#       Enthalpy of formation:  -2279.574 kJ/mol

6.0000 F- + 1.0000 U+4  =  UF6-2
        log_k           +29.80          #03GUI/FAN
        -delta_H        0                       # Not possible to calculate
it
#       Enthalpy of formation:  -0 kcal/mol

1.0000 U+4 + 1.0000 Cl-  =  UCl+3
        log_k           +1.72           #92GRE/FUG
        -delta_H        -19.00  kJ/mol  #92GRE/FUG
#       Enthalpy of formation:  -777.280 kJ/mol

1.0000 U+4 + 1.0000 Br-  =  UBr+3
        log_k           +1.460            #92GRE/FUG
        -delta_H        0                       # Not possible to calculate
it
#       Enthalpy of formation:  -0 kcal/mol

1.0000 U+4 + 1.0000 I-  =  UI+3
        log_k           +1.25   #92GRE/FUG
        -delta_H        0               # Not possible to calculate
enthalpy of reaction    UI+3
#       Enthalpy of formation:  -0 kcal/mol

 1.0000 UO2+2 + 1.0000 e-  =  UO2+
        log_k           1.48     #92GRE/FUG
        -delta_H        -6.127  kJ/mol  ##92GRE/FUG Calculated enthalpy of
reaction        UO2+
#       Enthalpy of formation:  -1025.127 kJ/mol

1.0000 UO2+2 + 1.0000 H2O  =  UO2OH+ +1.0000 H+
        log_k           -5.25           #nagra/03GUI/FAN
```

```
        -delta_H        43.458  kJ/mol  # Sf 92GRE/FUGCalculated enthalpy
of reaction     UO2OH+
#       Enthalpy of formation:  -1261.372 kJ/mol

2.0000 H2O + 1.0000 UO2+2  =  UO2(OH)2 +2.0000 H+
        log_k           -12.15   #03GUI/FAN
        -delta_H        111.16  kJ/mol   #Sf LEM/TRE
#       Enthalpy of formation:  -1479.500 kJ/mol

3.0000 H2O + 1.0000 UO2+2  =  UO2(OH)3- +3.0000 H+
        log_k           -20.25    #03GUI/FAN
        -delta_H        148.06  kJ/mol  #ESTIM. LINEAR INTERP. DHf
#       Enthalpy of formation:  -1728.430 kJ/mol

4.0000 H2O + 1.0000 UO2+2  =  UO2(OH)4-2 +4.0000 H+
        log_k           -32.40           #98YAM/KIT
        -delta_H        156.138 kJ/mol  #Sf 89LEM/GRE
#       Enthalpy of formation:  -2006.182 kJ/mol

2.0000 UO2+2 + 1.0000 H2O  =  (UO2)2OH+3 +1.0000 H+
        log_k           -2.70   #92GRE/FUG
        -delta_H        14.354 KJ/mol       #Sf 89LEM/TRE
#       Enthalpy of formation:  -2309.476 kJ/mol

2.0000 UO2+2 + 2.0000 H2O  =  (UO2)2(OH)2+2 +2.0000 H+
        log_k           -5.62      #92GRE/FUG
        -delta_H        37.595  kJ/mol  # #92GRE/FUG Calculated enthalpy of
reaction        (UO2)2(OH)2+2
#       Enthalpy of formation:  -2572.065 kJ/mol

4.0000 H2O + 3.0000 UO2+2  =  (UO2)3(OH)4+2 +4.0000 H+
        log_k           -11.90 #92GRE/FUG
        -delta_H        84.264 kJ/mol         #Sf 89LEM/TRE
#       Enthalpy of formation:  -4251.906 kJ/mol

5.0000 H2O + 3.0000 UO2+2  =  (UO2)3(OH)5+ +5.0000 H+
        log_k           -15.55         #92GRE/FUG
        -delta_H        97.063  kJ/mol  # #92GRE/FUG  Calculated enthalpy
of reaction     (UO2)3(OH)5+
#       Enthalpy of formation:  -4389.086 kJ/mol

7.0000 H2O + 3.0000 UO2+2  =  (UO2)3(OH)7- +7.0000 H+
        log_k           -32.20   #92SAN/BRU
        -delta_H        227.014 kJ/mol        #Sf 89LEM/GAR
#       Enthalpy of formation:  -4830.796 kJ/mol


7.0000 H2O + 4.0000 UO2+2  =  (UO2)4(OH)7+ +7.0000 H+
        log_k           -21.90   #92GRE/FUG
        -delta_H        0               # Not possible to calculate
```

```
enthalpy of reaction    (UO2)4(OH)7+
#       Enthalpy of formation:  -0 kcal/mol

1.0000 UO2+2 + 1.0000 CO3-2  =  UO2CO3
        log_k           9.94  #03GUI/FAN
        -delta_H        5.0000  kJ/mol  # Calculated enthalpy of reaction
        UO2CO3
#       Enthalpy of formation:  -1689.23 kJ/mol

2.0000 CO3-2 + 1.0000 UO2+2  =  UO2(CO3)2-2
        log_k           16.61               #03GUI/FAN
        -delta_H        18.500  kJ/mol  # Calculated enthalpy of reaction
        UO2(CO3)2-2
#       Enthalpy of formation:  -2350.96 kJ/mol

3.0000 CO3-2 + 1.0000 UO2+2  =  UO2(CO3)3-4
        log_k           21.84     #03GUI/FAN
        -delta_H        -39.200 kJ/mol  #Calculated enthalpy of reaction
        UO2(CO3)3-4
#       Enthalpy of formation:  -3083.89 kJ/mol

6.0000 CO3-2 + 3.0000 UO2+2  =  (UO2)3(CO3)6-6
        log_k           54.00           # 92GRE/FUG
        -delta_H        -62.7   kJ/mol  # # 92GRE/FUG  Calculated enthalpy
of reaction     (UO2)3(CO3)6-6
#       Enthalpy of formation:  -7171.08 kJ/mol

3.0000 H2O + 2.0000 UO2+2 + 1.0000 CO3-2  =  (UO2)2CO3(OH)3- +3.0000 H+
        log_k           -0.86  # 92GRE/FUG
        -delta_H        0               # Not possible to calculate
enthalpy of reaction    (UO2)2CO3(OH)3-
#       Enthalpy of formation:  -0 kcal/mol

3.0000 H2O + 3.0000 UO2+2 + 1.0000 CO3-2  =  (UO2)3CO3(OH)3+ +3.0000 H+
        log_k           0.66   #92GRE/FUG
        -delta_H        81.16           # Sf LEM/GAR
#       Enthalpy of formation:  -0 kcal/mol

1.0000 Si(OH)4 + 1.0000 UO2+2  =  UO2SiO(OH)3+ +1.0000 H+
        log_k           -1.84   #03GUI/FAN
        -delta_H        0               # Not possible to calculate
enthalpy of reaction    (UO2)2CO3(OH)3-
#       Enthalpy of formation:  -0 kcal/mol

1.0000 UO2+2 + 1.0000 NO3-  =  UO2NO3+
        log_k           +0.30  #92GRE/FUG
        -delta_H        993.035 kJ/mol   #89SMI/MAR
#       Enthalpy of formation:  -232.815 kJ/mol

1.0000 UO2+2 + 1.0000 H2PO4-  =  UO2PO4- +2.0000 H+
```

```
        log_k           -6.33            #92GRE/FUG
        -delta_H        0               # Not possible to calculate
enthalpy of reaction    UO2PO4-
#       Enthalpy of formation:  -0 kcal/mol

1.0000 UO2+2 + 1.0000 H2PO4-  =  UO2HPO4 +1.0000 H+
        log_k           +0.03    #92GRE/FUG
        -delta_H        2.795 kJ/mol     #Sf 78LAN
#       Enthalpy of formation:  -4408.507 kJ/mol

1.0000 UO2+2 + 1.0000 H2PO4-  =  UO2H2PO4+
        log_k           +3.26     #92GRE/FUG
        -delta_H        -15.340 kJ/mol    #Sf 78LAN
#       Enthalpy of formation:  -2336.940 kJ/mol

2.0000 H2PO4- + 1.0000 UO2+2  =  UO2(H2PO4)2
        log_k           4.92    #92GRE/FUG
        -delta_H        -51.871 kJ/mol #Sf 78LAN
#       Enthalpy of formation:  -6902.925 kJ/mol

1.0000 H+ + 1.0000 UO2+2 + 1.0000 H2PO4-  =  UO2H3PO4+2
        log_k           +2.90    #92GRE/FUG
        -delta_H        0               # Not possible to calculate
enthalpy of reaction    UO2H3PO4+2
#       Enthalpy of formation:  -0 kcal/mol

1.0000 H+ + 2.0000 H2PO4- + 1.0000 UO2+2  =  UO2H5(PO4)2+
        log_k           +5.93   #92GRE/FUG
        -delta_H        0               # Not possible to calculate
enthalpy of reaction    UO2(H2PO4)(H3PO4)+
#       Enthalpy of formation:  -0 kcal/mol

1.0000 UO2+2 + 1.0000 SO3-2  =  UO2SO3
        log_k           +6.60        #92GRE/FUG
        -delta_H        0               # Not possible to calculate
enthalpy of reaction    UO2SO3
#       Enthalpy of formation:  -0 kcal/mol

1.0000 UO2+2 + 1.0000 SO4-2  =  UO2SO4
        log_k           +3.15    #03GUI/FAN
        -delta_H        19.500  kJ/mol  # #92GRE/FUG Calculated enthalpy of
reaction        UO2SO4
#       Enthalpy of formation:  -1908.84 kJ/mol

2.0000 SO4-2 + 1.0000 UO2+2  =  UO2(SO4)2-2
        log_k           +4.14  #03GUI/FAN
        -delta_H        35.100  kJ/mol  #92GRE/FUG # Calculated enthalpy of
reaction        UO2(SO4)2-2
#       Enthalpy of formation:  -2802.58 kJ/mol
```

```
3.0000 SO4-2 + 1.0000 UO2+2  =  UO2(SO4)3-4
        log_k           +3.02    #03GUI/FAN
        -delta_H        0       kJ/mol  # NO POSSIBLE TO CALCULATE it
#       Enthalpy of formation:

#1.0000 S2O3-2 + 1.0000 UO2+2  =  UO2S2O3
#        log_k           2.80   #92GRE/FUG
#       -delta_H        0               # Not possible to calculate
enthalpy of reaction    UO2S2O3
#       Enthalpy of formation:  -0 kcal/mol

1.0000 UO2+2 + 1.0000 F-  =  UO2F+
        log_k           +5.16  #93FER/SAL, 03GUI/FAN
        -delta_H        1.7000  kJ/mol  # 92GRE/FUG Calculated enthalpy of
reaction        UO2F+
#       Enthalpy of formation:  -1352.65 kJ/mol

2.0000 F- + 1.0000 UO2+2  =  UO2F2
        log_k           +8.83 #93FER/SAL, 03GUI/FAN
        -delta_H        2.1000  kJ/mol  # Calculated enthalpy of reaction
        UO2F2
#       Enthalpy of formation:  -1687.6 kJ/mol

3.0000 F- + 1.0000 UO2+2  =  UO2F3-
        log_k           +10.90 #03GUI/FAN
        -delta_H        2.3500  kJ/mol  # 92GRE/FUGCalculated enthalpy of
reaction        UO2F3-
#       Enthalpy of formation:  -2022.7 kJ/mol

4.0000 F- + 1.0000 UO2+2  =  UO2F4-2
        log_k           +11.84 #93FER/SAL 03GUI/FAN
        -delta_H        0.2900  kJ/mol  # 92GRE/FUG Calculated enthalpy of
reaction        UO2F4-2
#       Enthalpy of formation:  -2360.11 kJ/mol

1.0000 UO2+2 + 1.0000 Cl-  =  UO2Cl+
        log_k           +0.17  #92GRE/FUG
        -delta_H        8.0000  kJ/mol  #92GRE/FUG # Calculated enthalpy of
reaction        UO2Cl+
#       Enthalpy of formation:  -1178.08 kJ/mol

2.0000 Cl- + 1.0000 UO2+2  =  UO2Cl2
        log_k           -1.10 #92GRE/FUG
        -delta_H        15.000  kJ/mol  #92GRE/FUG  Calculated enthalpy of
reaction        UO2Cl2
#       Enthalpy of formation:  -1338.16 kJ/mol

1.0000 UO2+2 + 1.0000 Br-  =  UO2Br+
        log_k           +0.220   #92GRE/FUG
        -delta_H        0               # Not possible to calculate
```

```
enthalpy of reaction    UO2Br+
#       Enthalpy of formation:  -0 kcal/mol

1.0000 UO2+2 + 1.0000 Cl- + 3.0000 H2O  =  UO2ClO3+ +6.0000 H+ +6.0000 e-
        log_k           -145.74   #92GRE/FUG
        -delta_H        916.670 kJ/mol  #92GRE/FUG Calculated enthalpy of
reaction        UO2ClO3+
#       Enthalpy of formation:  -1126.9 kJ/mol

1.0000 Zr+4 + 1.0000 H2O  =  Zr(OH)+3 + 1.0000 H+
        log_k           0.27                    # extrapolated by SIT in
03DOM/DUR
        -delta_H        13.704  kJ/mol          # Calculated internally, Sf
estimated by 78LAN
#       Enthalpy of formation:  -832.320 kJ/mol # Calculated internally, Sf
estimated by 78LAN

1.0000 Zr+4 + 2.0000 H2O  =  Zr(OH)2+2 + 2.0000 H+
        log_k           -2.7                    # maximum value (03DOM/DUR)
        -delta_H        0       kJ/mol          # no data available
#       Enthalpy of formation:  0 kJ/mol        # no data available

1.0000 Zr+4 + 3.0000 H2O  =  Zr(OH)3+  + 3.0000 H+
        log_k           -4.5                    # maximum valuem (03DOM/
DUR)
        -delta_H        0       kJ/mol          # no data available
#       Enthalpy of formation:  0 kJ/mol        # no data available

1.0000 Zr+4 + 4.0000 H2O  =  Zr(OH)4  + 4.0000 H+
        log_k           -5.13                   # calculated in 03DOM/DUR
        -delta_H        57.257  kJ/mol          # Calculated internally, Sf
estimated by 78LAN
#       Enthalpy of formation:  -1646.257 kJ/mol # Calculated internally,
Sf estimated by 78LAN

1.0000 Zr+4 + 5.0000 H2O  =  Zr(OH)5-  + 5.0000 H+
        log_k           -17.97                  # calculated in 03DOM/DUR
        -delta_H        119.921 kJ/mol          # Calculated internally, Sf
estimated by 78LAN
#       Enthalpy of formation:  -1869.423 kJ/mol # Calculated internally,
Sf estimated by 78LAN

1.0000 Zr+4 + 6.0000 H2O  =  Zr(OH)6-2 + 6.0000 H+
        log_k           -31.96                  # calculated in 03DOM/DUR
        -delta_H        181.092 kJ/mol          # Calculated internally, Sf
estimated by 78LAN
#       Enthalpy of formation:  -2094.082 kJ/mol # Calculated internally,
Sf estimated by 78LAN

4.0000 Zr+4 + 15.0000 H2O  =  Zr4(OH)15+ + 15.0000 H+
```

```
        log_k           0.04                    # calculated in 03DOM/DUR
        -delta_H        0       kJ/mol          # no data available
#       Enthalpy of formation:  0 kJ/mol        # no data available

4.0000 Zr+4 + 16.0000 H2O  =  Zr4(OH)16 + 16.0000 H+
        log_k           -4.36                   # calculated in 03DOM/DUR
        -delta_H        -0      kJ/mol          # no data available
#       Enthalpy of formation:  -0 kJ/mol       # no data available

1.0000 NO3- + 1.0000 Zr+4  =  ZrNO3+3
        log_k           1.77                    # extrapolated by SIT in
03DOM/DUR
        -delta_H        0                       # no data available
#       Enthalpy of formation:  -0 kJ/mol       # no data available

2.0000 NO3- + 1.0000 Zr+4  =  Zr(NO3)2+2
        log_k           3.15                    # extrapolated by SIT in
03DOM/DUR
        -delta_H        0                       # no data available
#       Enthalpy of formation:  -0 kJ/mol       # no data available

1.0000 Zr+4 + 1.0000 SO4-2  =  ZrSO4+2
        log_k           7.04                    # Brown et al. (2005)
        -delta_H        0  kJ/mol               # data not reviewed
#       Enthalpy of formation:  -0 kJ/mol       # data not reviewed

1.0000 Zr+4 + 2.0000 SO4-2  =  Zr(SO4)2
        log_k           11.54           # Brown et al. (2005)
        -delta_H        0  kJ/mol               # data not reviewed
#       Enthalpy of formation:  -0 kJ/mol       # data not reviewed

1.0000 Zr+4 + 3.0000 SO4-2  =  Zr(SO4)3-2
        log_k           14.30           # Brown et al. (2005)
        -delta_H        0  kJ/mol               # data not reviewed
#       Enthalpy of formation:  -0 kJ/mol       # data not reviewed


1.0000 Zr+4 + 1.0000 Cl-  =  ZrCl+3
        log_k           1.45                    # extrapolated by SIT in
03DOM/DUR
        -delta_H        0  kJ/mol               # no data available
#       Enthalpy of formation:  0 kJ/mol        # no data available

2.0000 Cl- + 1.0000 Zr+4  =  ZrCl2+2
        log_k           1.24                    # extrapolated by SIT in
03DOM/DUR
        -delta_H        0  kJ/mol               # no data available
#       Enthalpy of formation:  0 kJ/mol        # no data available

3.0000 Cl- + 1.0000 Zr+4  =  ZrCl3+
```

```
        log_k           1.44                    # extrapolated by SIT in
03DOM/DUR
        -delta_H        0  kJ/mol               # no data available
#       Enthalpy of formation:  0 kJ/mol        # no data available

1.0000 Zr+4 + 1.0000 F-  =  ZrF+3
        log_k           9.71                    # extrapolated by SIT in
03DOM/DUR
        -delta_H        -5.300  kJ/mol          # 90AHR/HEF
#       Enthalpy of formation:  -900.844 kJ/mol # calculated internally

1.0000 Zr+4 + 2.0000 F-  =  ZrF2+2
        log_k           17.21                   # extrapolated by SIT in
03DOM/DUR
        -delta_H        -9.900  kJ/mol          # 90AHR/HEF
#       Enthalpy of formation:  -1240.794 kJ/mol# calculated internally

1.0000 Zr+4 + 3.0000 F-  =  ZrF3+
        log_k           23.40                   # extrapolated by SIT in
03DOM/DUR
        -delta_H        -8.900  kJ/mol          # 90AHR/HEF
#       Enthalpy of formation:  -1575.144 kJ/mol# calculated internally

1.0000 Zr+4 + 4.0000 F-  =  ZrF4
        log_k           28.86                   # extrapolated by SIT in
03DOM/DUR
        -delta_H        -18.700 kJ/mol          # 90AHR/HEF
#       Enthalpy of formation:  -1920.294 kJ/mol# calculated internally

1.0000 Zr+4 + 5.0000 F-  =  ZrF5-
        log_k           33.38                   # extrapolated by SIT in
03DOM/DUR
        -delta_H        0  kJ/mol               # no data available
#       Enthalpy of formation:  0 kJ/mol        # no data available


1.0000 Zr+4 + 6.0000 F-  =  ZrF6-2
        log_k           37.12                   # extrapolated by SIT in
03DOM/DUR
        -delta_H        0  kJ/mol               # no data available
#       Enthalpy of formation:  0 kJ/mol        # no data available

PHASES

# PMATCH MINERALS

Anhydrite
CaSO4                   =  +1.000Ca+2                  +1.000SO4-2
    log_k      -4.3575
    delta_h    -7.1558
```

```
#    -a_e    1.975200E+02 -0.000000E+00 -8.668800E+03 -6.983500E+01
-0.000000E+00

Aragonite
CaCO3                  =  +1.000Ca+2                 -1.000H+
+1.000HCO3-
    log_k       1.9928
   delta_h   -25.7343
#    -a_e   -6.409020E+01 -4.546451E-02 -2.248497E+03  3.266939E+01
5.637139E+05

Brucite
Mg(OH)2                =  +1.000Mg+2                 +2.000H2O
-2.000H+
    log_k      16.8400
    delta_h  -113.3864
#    -a_e   -3.024798E+00 -0.000000E+00  5.922689E+03 -0.000000E+00
0.000000E+00

Calcite
CaCO3                  =  +1.000Ca+2                 -1.000H+
+1.000HCO3-
    log_k       1.8490
    delta_h   -24.5095
#    -a_e   -6.401940E+01 -4.546451E-02 -2.312471E+03  3.266939E+01
5.637139E+05

Dolomite(dis)
CaMg(CO3)2             =  +1.000Ca+2                 +1.000Mg+2
-2.000H+                   +2.000HCO3-
    log_k       4.1180
    delta_h   -76.2020
#    -a_e   -9.232255E+00 -0.000000E+00  3.980378E+03 -0.000000E+00
0.000000E+00

Dolomite(ord)
CaMg(CO3)2             =  +1.000Ca+2                 +1.000Mg+2
-2.000H+                   +2.000HCO3-
    log_k       3.5680
    delta_h   -69.2820
#    -a_e   -8.569901E+00 -0.000000E+00  3.618915E+03 -0.000000E+00
0.000000E+00

Fe(cr)
Fe                     =  +1.000Fe+2                 +2.000e-
    log_k      15.8601
    delta_h   -90.00
#    -a_e   -1.786995E+00 -0.000000E+00  4.654100E+03 -0.000000E+00
0.000000E+00
```

```
Fluorite
CaF2                    =  +1.000Ca+2                 +2.000F-
    log_k     -10.5997
    delta_h    19.6419
#    -a_e    6.634800E+01 -0.000000E+00 -4.298200E+03 -2.527100E+01
-0.000000E+00

Goethite
FeOOH                   =  +2.000H2O                  -3.000H+
+1.000Fe+3
    log_k      -1.0000
#    -a_e   -1.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00
-0.000000E+00

Graphite
C                       =  +1.000HCO3-                +5.000H+
+4.000e-                   -3.000H2O
    log_k     -21.8197
    delta_h   167.2750
#    -a_e   -2.081775E+02 -4.106888E-02  4.606129E+03  7.863525E+01
-1.015550E+06

Gypsum
CaSO4:2H2O              =  +1.000Ca+2                 +1.000SO4-2
+2.000H2O
    log_k      -4.5809
    delta_h    -0.4543
#    -a_e    6.824010E+01 -0.000000E+00 -3.221510E+03 -2.506270E+01
-0.000000E+00

Melanterite
FeSO4:7H2O              =  +1.000Fe+2                 +1.000SO4-2
+7.000H2O
    log_k      -2.2093
    delta_h    20.5364
#    -a_e    1.447000E+00 -4.153000E-03 -0.000000E+00 -0.000000E+00
-2.149490E+05

Portlandite
Ca(OH)2                 =  +1.000Ca+2                 +2.000H2O
-2.000H+
    log_k      22.8000
    delta_h  -129.7040
#    -a_e    7.643067E-02 -0.000000E+00  6.775032E+03 -0.000000E+00
0.000000E+00

Siderite
FeCO3                   =  +1.000Fe+2                 +1.000HCO3-
-1.000H+
    log_k      -0.5585
```

```
    delta_h   -24.2807
#    -a_e    9.517921E+01  3.252849E-02 -4.609790E+03 -3.892561E+01
5.637139E+05

FeCO3(pr)
FeCO3                  =  +1.000Fe+2                +1.000HCO3-
-1.000H+
    log_k      -0.1211
    delta_h   -14.9007
#    -a_e    9.743710E+01  3.252849E-02 -5.151790E+03 -3.892561E+01
5.637139E+05

Hematite
Fe2O3                  =  +3.000H2O                 -6.000H+
+2.000Fe+3
    log_k       1.1200
#    -a_e    1.120000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00
-0.000000E+00

 Pyrite
 FeS2                   =  +1.000Fe+2                +2.000HS-
-2.000H+                   -2.000e-
    log_k     -16.5700
#    delta_h
#       Enthalpy of formation:  0 kJ/mol        # no reviewed

 Marcasite
 FeS2                   =  +1.000Fe+2                +2.000HS-
-2.000H+                   -2.000e-
    log_k     -16.1600
#    delta_h
#       Enthalpy of formation:  0 kJ/mol        # no reviewed

 Greigite
 Fe3S4                   =  +3.000Fe+2                +4.000HS-
-4.000H+                   -2.000e-
    log_k     -15.0000          #Rickard and Luther III (2007)
#    delta_h
#       Enthalpy of formation:  0 kJ/mol        # not reviewed


 Troilite
 FeS                    =  +1.000Fe+2                +1.000HS-
-1.000H+
   log_k      -5.5000
#    delta_h
#       Enthalpy of formation:  0 kJ/mol        # not reviewed

Mackinawite
 FeS                    =  +1.000Fe+2                +1.000HS-
```

```
-1.000H+
    log_k      -4.1000
#    delta_h
#       Enthalpy of formation:  0 kJ/mol        # no reviewed


Magnesite
MgCO3                  =  +1.000Mg+2                 -1.000H+
+1.000HCO3-
    log_k       2.0410
#    -a_e    2.041000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00
-0.000000E+00

 S(cr)
S                      =  +1.000HS-                  -1.000H+
-2.000e-
    log_k      -2.14                   #Grenthe et al. 1992
#    delta_h   -16.3000                    # Hf not reviewed
#    -a_e   -5.000608E+00 -0.000000E+00  8.514234E+02 -0.000000E+00
0.000000E+00

Fe(OH)3(am)
Fe(OH)3                =  +3.000H2O                  -3.000H+
+1.000Fe+3
    log_k       5.0000
#    -a_e    5.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00
-0.000000E+00

Fe(OH)3(mic)
Fe(OH)3                =  +3.000H2O                  -3.000H+
+1.000Fe+3
    log_k       3.0000
#    -a_e    3.000000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00
-0.000000E+00

Magnetite
Fe3O4                  =  +1.000Fe+2                 +4.000H2O
-8.000H+                   +2.000Fe+3
    log_k      10.0200
#    -a_e    1.002000E+01 -0.000000E+00 -0.000000E+00 -0.000000E+00
-0.000000E+00

Quartz
SiO2                   =  +1.000Si(OH)4              -2.000H2O
    log_k      -3.7460
    delta_h    20.6370
#    -a_e   -1.325045E+01 -0.000000E+00 -4.939341E+02  4.510415E+00
0.000000E+00

SiO2(am)
```

```
SiO2                    =  +1.000Si(OH)4              -2.000H2O
    log_k      -2.7140
    delta_h    14.5940
#    -a_e   -1.571955E-01 -0.000000E+00 -7.623113E+02 -0.000000E+00
0.000000E+00

Kaolinite
Al2Si2O5(OH)4           =  +2.000Al+3                 +2.000Si(OH)4
+1.000H2O                  -6.000H+
    log_k       7.4350
    delta_h  -147.7000
#    -a_e   -1.844139E+01 -0.000000E+00  7.715045E+03 -0.000000E+00
0.000000E+00

Gibbsite
Al(OH)3                 =  +1.000Al+3                 +3.000H2O
-3.000H+
    log_k       7.7561
    delta_h  -102.7840
#    -a_e   -1.069028E+01 -0.000000E+00  5.388423E+03  1.509445E-01
0.000000E+00

Ag(cr)
       Ag  =  + 1.0000 Ag+ + 1.0000 e-
        log_k           -13.51          #Sf 95SIL/BID, logK calc
        -delta_H        105.790 kJ/mol  #Sf 95SIL/BID, H calc
#       Enthalpy of formation:  0 kJ/mol

AgOH(s)
       AgOH + 1.0000 H+  =  + 1.0000 Ag+ + 1.0000 H2O
        log_k           6.30                    #76BAE/MES
        -delta_H        0       kJ/mol          # Not possible to
calculated enthalpy of reaction
#       Enthalpy of formation:  0 kJ/mol

Ag2CO3(s)
       Ag2CO3  =  + 2.0000 Ag+ + 1.0000 CO3-2
        log_k           -11.05          #DGf 82WAG/EVA, logK calc
        -delta_H        42.073  kJ/mol  #Sf 82WAG/EVA, H calc
#       Enthalpy of formation:  -505.723 kJ/mol

Ag3PO4
       Ag3PO4 +2.0000 H+  =  + 1.0000 H2PO4- + 3.0000 Ag+
        log_k           2.01                    #76SMI/MAR
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction    Ag3PO4
#       Enthalpy of formation:  0 kcal/mol

Ag2SO4(s)
        Ag2SO4  =  + 1.0000 SO4-2 + 2.0000 Ag+
```

```
        log_k           -5.01                   #76SMI/MAR
        -delta_H        18.162  kJ/mol  #Sf 82WAG/EVA, H calc
#       Enthalpy of formation:  -715.922 kJ/mol

# Ag2S(s)
#        Ag2S +1.0000 H+  =  + 1.0000 HS- + 2.0000 Ag+
#        log_k           -36.07          #76SMI/MAR
#       -delta_H        224.768 kJ/mol  #Sf 82WAG/EVA, H calc
#       Enthalpy of formation:  -29.488 kJ/mol

AgCl(cr)
        AgCl  =  + 1.0000 Ag+ + 1.0000 Cl-
        log_k           -9.75                   #DGf 92GRE/FUG, logK calc
        -delta_H        65.720  kJ/mol  #Sf 92GRE/FUG, H calc
#       Enthalpy of formation:  -127.010 kJ/mol

AgBr(s)
        AgBr  =  + 1.0000 Ag+ + 1.0000 Br-
        log_k           -12.29          #DGf 82WAG/EVA, logK calc
        -delta_H        84.725  kJ/mol  #Sf 82WAG/EVA, H calc
#       Enthalpy of formation:  -100.345 kJ/mol

AgI(s)
        AgI  =  + 1.0000 Ag+ + 1.0000 I-
        log_k           -16.04          #DGf 82WAG/EVA, logK calc
        -delta_H        110.764 kJ/mol  #Sf 82WAG/EVA, H calc
#       Enthalpy of formation:  -61.754/mol

Am(cr)
       Am  =  + 1.0000 Am+3 + 3.0000 e-
        log_k           104.89          #Sf 95SIL/BID, logK calc
        -delta_H        -616.700        kJ/mol  #Sf 95SIL/BID, H calc
#       Enthalpy of formation:  0 kJ/mol

Am(OH)3(am)
       Am(OH)3 +3.0000 H+  =  + 1.0000 Am+3 + 3.0000 H2O
        log_k           16.90                   #03GUI/FAN
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction    Am(OH)3(am)
#       Enthalpy of formation:  0 kcal/mol

Am(OH)3(cr)
       Am(OH)3 +3.0000 H+  =  + 1.0000 Am+3 + 3.0000 H2O
        log_k           15.60                   #03GUI/FAN
        -delta_H        -120.990 kJ/mol         #Sf 01K÷N, H calc
#       Enthalpy of formation:  -1353.200 kJ/mol

Am2O3(cr)
       Am2O3 +6.0000 H+  =  + 2.0000 Am+3 + 3.0000 H2O
        log_k           53.15                   #DHf 95SIL/BID, Sf 01K÷N,
```

```
logK calc
        -delta_H        -400.490        kJ/mol  #DHf 95SIL/BID, H calc
#       Enthalpy of formation:  -1690.4 kJ/mol

AmO2
       AmO2 +4.0000 H+ + 1.0000 e-  =  + 1.0000 Am+3 + 2.0000 H2O
        log_k           34.21                   #DHf 95SIL/BID, Sf 01K÷N2,
logK calc
        -delta_H        -256.160        kJ/mol  #DHf 95SIL/BID, H calc
#       Enthalpy of formation:  -932.2 kJ/mol

AmCO3OH(am)
       AmCO3OH +1.0000 H+  =  + 1.0000 Am+3 + 1.0000 H2O + 1.0000 CO3-2
        log_k           -6.20                   #03GUI/FAN
        -delta_H        0                               # Not possible to
calculate enthalpy of reaction
#       Enthalpy of formation:  0 kcal/mol

AmCO3OH:0.5H2O(cr)
       AmCO3OH +1.0000 H+  =  + 1.0000 Am+3 + 1.0000 H2O + 1.0000 CO3-2
        log_k           -8.40                   #03GUI/FAN
        -delta_H        -37.775 kJ/mol  #
#       Enthalpy of formation:  -1682.900 kJ/mol

Am2(CO3)3(s)
       Am2(CO3)3  =  + 2.0000 Am+3 + 3.0000 CO3-2
        log_k           -33.40          #03GUI/FAN
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction
#       Enthalpy of formation:  0 kcal/mol

Am(CO3)2Na:5H2O(s)
       Am(CO3)2Na:5H2O  =  + 1.0000 Am+3 + 2.0000 CO3-2 + 5.0000 H2O +
1.0000 Na+
        log_k           -21.00          #03GUI/FAN
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction
#       Enthalpy of formation:  0 kcal/mol

AmPO4:xH2O(am)
        AmPO4 +2.0000 H+  =  + 1.0000 Am+3 + 1.0000 H2PO4-
        log_k           -5.23                   #95SIL/BID
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction    AmPO4(am)
#       Enthalpy of formation:  0 kcal/mol

Cs2O(s)
       Cs2O + 2.0000 H+  =  + 1.0000 H2O + 2.0000 Cs+
        log_k           89.68                   #DGf 82WAG/EVA, logK calc
        -delta_H        -456.100        kJ/mol  #Sf 82WAG/EVA, logK calc
```

```
#       Enthalpy of formation:  -345.73 kJ/mol

Cs(s)
       Cs  =  + 1.0000 e- + 1.0000 Cs+
        log_k           51.06                   #Sf 92GRE/FUG, logK calc
        -delta_H        -258.000        kJ/mol  #Sf 92GRE/FUG, H calc
#       Enthalpy of formation:  0 kJ/mol

Cs2CO3(s)
       Cs2CO3  =  + 1.0000 CO3-2 + 2.0000 Cs+
        log_k           9.90                    #DGf 82WAG/EVA, logK calc
        -delta_H        -55.348 kJ/mol  #Sf 82WAG/EVA, logK calc
#       Enthalpy of formation:  -1135.882 kJ/mol

Cs2SO4(s)
       Cs2SO4  =  + 1.0000 SO4-2 + 2.0000 Cs+
        log_k           0.58                    #DGf 82WAG/EVA, logK calc
        -delta_H        17.756  kJ/mol  #Sf 82WAG/EVA, logK calc
#       Enthalpy of formation:  -1443.096 kJ/mol

CsCl(cr)
       CsCl  =  + 1.0000 Cl- + 1.0000 Cs+
        log_k           1.55                    #DHf and Sf 01LEM/FUG, logK
calc
        -delta_H        17.230  kJ/mol  #DHf 01LEM/FUG, H calc
#       Enthalpy of formation:  -442.310 kJ/mol

CsBr(cr)
       CsBr  =  + 1.0000 Br- + 1.0000 Cs+
        log_k           0.72                    #DHf and Sf 01LEM/FUG, logK
calc
        -delta_H        26.190  kJ/mol  #DHf 01LEM/FUG, H calc
#       Enthalpy of formation:  -405.600 kJ/mol

Ho(cr)
       Ho  =  + 1.0000 Ho+3 + 3.0000 e-
        log_k           118.31          #Sf 82WAG/EVA, logK calc
        -delta_H        -707.042        kJ/mol  #Sf 82WAG/EVA, H calc
#       Enthalpy of formation:  0 kJ/mol

Ho(OH)3(s)
       Ho(OH)3 +3.0000 H+  =  + 1.0000 Ho+3 + 3.0000 H2O
        log_k           15.40                   #95SPA/BRU
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction    Ho(OH)3
#       Enthalpy of formation:  0 kcal/mol

Ho2O3(s)
       Ho2O3 +6.0000 H+  =  + 2.0000 Ho+3 + 3.0000 H2O
        log_k           47.41                   #DGf 79ROB/HEM, logK calc
```

```
        -delta_H        -390.718 kJ/mol                 #Sf 79ROB/HEM, H
calc
#       Enthalpy of formation:  -1880.856 kJ/mol

Ho(OH)3(am)
       Ho(OH)3 +3.0000 H+  =  + 1.0000 Ho+3 + 3.0000 H2O
        log_k           17.80                   #95SPA/BRU
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction    Ho(OH)3(am)
#       Enthalpy of formation:  0 kcal/mol

Ho2(CO3)3(c)
       Ho2(CO3)3  =  + 2.0000 Ho+3 + 3.0000 CO3-2
        log_k           -33.80          #95SPA/BRU
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction    Ho2(CO3)3
#       Enthalpy of formation:  0 kcal/mol

HoPO4(s)
       HoPO4 + 2.0000 H+  =  + 1.0000 H2PO4- + 1.0000 Ho+3
        log_k           -5.56                   #97LIU/BYR
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction    HoPO4:10H2O
#       Enthalpy of formation:  0 kcal/mol

HoPO4:xH2O(s)
HoPO4 +2.0000 H+  =  + 1.0000 H2PO4- + 1.0000 Ho+3
        log_k           -4.64                   #95SPA/BRU
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction
#       Enthalpy of formation:  0 kcal/mol

HoF3:0.5H2O
       HoF3:0.5H2O  =  + 0.5000 H2O + 1.0000 Ho+3 + 3.0000 F-
        log_k           -16.4000                #95SPA/BRU
        -delta_H        -149.007 kJ/mol                 #DHf 82WAG/EVA, H
calc
#       Enthalpy of formation:  -1707.000 kJ/mol

HoCl3:6H2O
       HoCl3:6H2O  =  + 6.0000 H2O + 1.0000 Ho+3 + 3.0000 Cl-
        log_k           5.39                    #96FAL/REA
        -delta_H        -43.855 kJ/mol          #Sf 82WAG/EVA, H calc
#       Enthalpy of formation:  -2879.407 kJ/mol

Nb2O5(cr)
Nb2O5                  =  +2.000NbO3-                +2.000H+
-1.000H2O
    log_k     -24.3417                          #01HUM/BER
#    -a_e   -2.434168E+01 -0.000000E+00 -0.000000E+00 -0.000000E+00
```

```
-0.000000E+00

NbO2(cr)
NbO2                   =  +1.000NbO3-                +2.000H+
+1.000e-                   -1.000H2O
    log_k      -7.9784                          #01HUM/BER
#    -a_e   -7.978407E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00
-0.000000E+00

Ni(cr)
       Ni  =  + 2.0000 e- + 1.0000 Ni+2
        log_k           7.97                    #Sf 98PLY/ZHA, logK calc
        -delta_H        -54.100 kJ/mol  #Sf 98PLY/ZHA, H calc
#       Enthalpy of formation:  0 kJ/mol

Ni(OH)2(s)
       Ni(OH)2 + 2.0000 H+  =  + 1.0000 Ni+2 + 2.0000 H2O
        log_k           10.50                   #98PLY/ZHA
        -delta_H        -78.837 kJ/mol  #DHf 98PLY/ZHA, H calc
#       Enthalpy of formation:  -546.969 kJ/mol

NiO(s)
        NiO + 2.0000 H+  =  + 1.0000 H2O + 1.0000 Ni+2
        log_k           12.41                   #DGf 86HOL/O'NE, logK calc
        -delta_H        -100.012        kJ/mol  #Sf 79ROB/HEM, H calc
#       Enthalpy of formation:  -239.918 kJ/mol

Fe2NiO4
        Fe2NiO4 +8.0000 H+  =  + 1.0000 Ni+2 + 2.0000 Fe+3 + 4.0000 H2O
        log_k           9.40                    #DGf 69WAG/EVA, logK calc
        -delta_H        -214.413        kJ/mol  #Sf 79ROB/HEM, H calc
#       Enthalpy of formation:  -1081.007 kJ/mol

Ni2O3(s)
        Ni2O3 + 6.0000 H+ + 2.0000 e-  =  + 3.0000 H2O + 2.0000 Ni+2
        log_k           58.29                   #DGf 69WAG/EVA, logK calc
        -delta_H        -414.456        kJ/mol  #DHf 69WAG/EVA, H calc
#       Enthalpy of formation:  -550.851 kJ/mol

Ni3O4(s)
        Ni3O4 + 8.0000 H+ + 2.0000 e-  =  + 4.0000 H2O + 3.0000 Ni+2
        log_k           65.36                   #DGf 69WAG/EVA, logK calc
        -delta_H        -486.888        kJ/mol  #DHf 69WAG/EVA, H calc
#       Enthalpy of formation:  -818.732 kJ/mol

NiCO3(cr)
       NiCO3  =  + 1.0000 CO3-2 + 1.0000 Ni+2
        log_k          -11.28                   #01HUM/BER
        -delta_H        0      kJ/mol           #Not possible to calculate
it
```

```
#       Enthalpy of formation:

NiSiO3(s)
       NiSiO3 + 2.0000 H+ + 1.0000 H2O  =  + 1.0000 Si(OH)4 + 1.0000 Ni+2
        log_k           -2.09                   #89BAE/McK
        -delta_H        -0      kJ/mol          #Not possible to calculate
it
#       Enthalpy of formation:  -0 kJ/mol

Ni2SiO4(s)
       Ni2SiO4 + 4.0000 H+  =  + 1.0000 Si(OH)4 + 2.0000 Ni+2
        log_k           19.24                   #95ROB/HEM
        -delta_H        -168.906        kJ/mol  #95ROB/HEM
#       Enthalpy of formation:  -1396.254 kJ/mol

Ni3(PO4)2(cr)
       Ni3(PO4)2 + 4.0000 H+  =  + 2.0000 H2PO4- + 3.0000 Ni+2
        log_k           10.11                   #DGf 89BAE/McK, logK calc
        -delta_H        -185.500 kJ/mol                 #Not possible to
calculate it
#       Enthalpy of formation:  -2582.000 kJ/mol

Ni2P2O7(cr)
       Ni2P2O7 + 1.0000 H2O + 2.0000 H+  =  + 2.0000 H2PO4- + 2.0000 Ni+2
        log_k           7.89                    #DGf 89BAE/McK, logK calc
        -delta_H        0                       #Not possible to calculate
it
#       Enthalpy of formation:  0 kcal/mol

NiSO4:6H2O(alfa)
       NiSO4:6H2O  =  + 1.0000 Ni+2 + 1.0000 SO4-2 + 6.0000 H2O
        log_k           -2.25                   #Gamsjager et al. (2005)
#       -delta_H                kJ/mol          ##Not reviewed
#       Enthalpy of formation:   kJ/mol

NiSO4:6H2O(beta)
       NiSO4:6H2O  =  + 1.0000 Ni+2 + 1.0000 SO4-2 + 6.0000 H2O
        log_k           -2.15                   #Gamsjager et al. (2005)
#       -delta_H                kJ/mol          # Not reviewed
#       Enthalpy of formation:   kJ/mol


NiSO4:7H2O
        NiSO4:7H2O  =  + 1.0000 Ni+2 + 1.0000 SO4-2 + 7.0000 H2O
        log_k           -2.27                   #Gamsjager et al. (2005)
#       -delta_H                kJ/mol          #Not reviewed
#       Enthalpy of formation:   kJ/mol

NiSO4(cr)
       NiSO4  =  + 1.0000 Ni+2 + 1.0000 SO4-2
```

```
        log_k           4.75                    #Gamsjager et al. (2005)
#       -delta_H        kJ/mol                  #Not reviewed
#       Enthalpy of formation:  kJ/mol

 NiS(alfa)
        NiS + 1.0000 H+  =  + 1.0000 HS- + 1.0000 Ni+2
        log_k           -9.51                   #Gamsjager et al. 2005
#       -delta_H                kJ/mol          #DHf  Not reviewed
#       Enthalpy of formation:   kJ/mol

 NiS(beta)
        NiS + 1.0000 H+  =  + 1.0000 HS- + 1.0000 Ni+2
        log_k           -10.13          #Gamsjager et al. 2005
#       -delta_H                kJ/mol          #DHf  Not reviewed
#       Enthalpy of formation:   kJ/mol


 NiS2(cr)
        NiS2 + 2.0000 H+ + 2.0000 e-  =  + 2.0000 HS- + 1.0000 Ni+2
        log_k           -17.97          #Gamsjager et al. 2005
#       -delta_H                kJ/mol          #DHf not reviewed
#       Enthalpy of formation:   kJ/mol

Ni9S8(s)
        Ni9S8 + 8.0000 H+  =  + 8.0000 HS- + 9.0000 Ni+2 + 2.0000 e-
        log_k           -75.82          #Gamsjager et al. 2005
#       -delta_H                kJ/mol          #DHf not reviewed
#       Enthalpy of formation:   kJ/mol

Ni3S2(s)
        Ni3S2 + 2.0000 H+  =  + 2.0000 HS- + 3.0000 Ni+2 + 2.0000 e-
        log_k           -17.23          #Gamsjager et al. 2005
#       -delta_H                kJ/mol          #DHf not reviewed
#       Enthalpy of formation:   kJ/mol



NiF2:4H2O
       NiF2:4H2O  =  + 1.0000 Ni+2 + 2.0000 F- + 4.0000 H2O
        log_k           -4.19                   #DGf 89BAE/McK, logK calc
        -delta_H        0                       #Not possible to calculate
it
#       Enthalpy of formation:  0 kcal/mol

NiF2(s)
       NiF2  =  + 1.0000 Ni+2 + 2.0000 F-
        log_k           -0.17                   #DGf 89BAE/McK, logK calc
        -delta_H        -67.900 kJ/mol  #DHf 89BAE/McK, H calc
#       Enthalpy of formation:  -656.900 kJ/mol
```

```
NiCl2:2H2O
       NiCl2:2H2O  =  + 1.0000 Ni+2 + 2.0000 Cl- + 2.0000 H2O
        log_k           3.87                    #DGf 89BAE/McK, logK calc
        -delta_H        -37.720 kJ/mol  #DHf 89BAE/McK, H calc
#       Enthalpy of formation:  -922.200 kJ/mol

NiCl2:4H2O
       NiCl2:4H2O  =  + 1.0000 Ni+2 + 2.0000 Cl- + 4.0000 H2O
        log_k           3.78                    #DGf 89BAE/McK, logK calc
        -delta_H        -14.880 kJ/mol  #DHf 89BAE/McK, H calc
#       Enthalpy of formation:  -1516.70 kJ/mol

NiCl2:6H2O
        NiCl2:6H2O  =  + 1.0000 Ni+2 + 2.0000 Cl- + 6.0000 H2O
        log_k           3.08                    #DGf 89BAE/McK, logK calc
        -delta_H        -0.040  kJ/mol  #DHf 89BAE/McK, H calc
#       Enthalpy of formation:  -2103.200 kJ/mol

NiCl2(s)
       NiCl2  =  + 1.0000 Ni+2 + 2.0000 Cl-
        log_k           8.61                    #DGf 95ROB/HEM, logK calc
        -delta_H        -83.321 kJ/mol  #DHf 95ROB/HEM, H calc
#       Enthalpy of formation:  -304.939 kJ/mol

NiBr2(s)
       NiBr2  =  + 1.0000 Ni+2 + 2.0000 Br-
        log_k           9.60                    #DGf 89BAE/McK, logK calc
        -delta_H        -84.820 kJ/mol  #DHf 89BAE/McK, H calc
#       Enthalpy of formation:  -212.100 kJ/mol

NiI2(s)
       NiI2  =  + 1.0000 Ni+2 + 2.0000 I-
        log_k           11.97                   #DGf 89BAE/McK, logK calc
        -delta_H        -89.460 kJ/mol  #DHf 89BAE/McK, H calc
#       Enthalpy of formation:  -78.200 kJ/mol

Np
       Np  =  + 1.0000 Np+3 + 3.0000 e-
        log_k           89.85                   #Sf 01LEM/FUG, logK calc
        -delta_H        -527.184        kJ/mol  #DHf 01LEM/FUG, H calc
#       Enthalpy of formation:  0 kJ/mol

Np(OH)3(s)
       Np(OH)3 +3.0000 H+  =  + 1.0000 Np+3 + 3.0000 H2O
        log_k           18.00                   #80ALL/KIP
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction
#       Enthalpy of formation:  0 kcal/mol

NpCO3OH(s)
```

```
       NpCO3OH + 1.0000 H+  =  + 1.0000 Np+3 + 1.0000 H2O + 1.0000 CO3-2
        log_k           -6.06                   #estimated from
actinides(III) and lanthanides
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction
#       Enthalpy of formation:  0 kcal/mol

NpO2(s)
       NpO2 + 4.0000 H+  =  + 1.0000 Np+4 + 2.0000 H2O
        log_k           -9.75                   #DHf and Sf 01LEM/FUG, logK
calc
        -delta_H        -53.682 kJ/mol  #DHf 01LEM/FUG, H calc
#       Enthalpy of formation:  -1074.000 kJ/mol

NpO2:2H2O(am)
       NpO2:2H2O + 4.0000 H+  =  + 1.0000 Np+4 + 4.0000 H2O
        log_k           -0.70                   #03GUI/FAN
        -delta_H        -81.156 kJ/mol  #Sf 84LEM, H calc
#       Enthalpy of formation:  -1618.186 kJ/mol

Np(HPO4)2(s)
       Np(HPO4)2 + 2.0000 H+  =  + 1.0000 Np+4 + 2.0000 H2PO4-
        log_k           -16.06          #estimated from actinides(IV)
        -delta_H        0                               #Not possible to
calculate
#       Enthalpy of formation:  -0 kJ/mol

NpO2OH(am)(aged)
       NpO2OH + 1.0000 H+  =  + 1.0000 H2O + 1.0000 NpO2+
        log_k           4.70                    #01LEM/FUG
        -delta_H        -41.111 kJ/mol  #DHf 01LEM/FUG, H calc
#       Enthalpy of formation:  -1222.900 kJ/mol

NpO2OH(am)(fresh)
       NpO2OH + 1.0000 H+  =  + 1.0000 H2O + 1.0000 NpO2+
        log_k           5.30                    #01LEM/FUG
#       -delta_H        0 nonsense to estimate DH
#       Enthalpy of formation:

Np2O5(cr)
       Np2O5 + 2.0000 H+  =  + 1.0000 H2O + 2.0000 NpO2+
        log_k           3.70                    #DHf and Sf 01LEM/FUG, logK
calc
        -delta_H        -79.492 kJ/mol  #DHf 01LEM/FUG, H calc
#       Enthalpy of formation:  -2162.700 kJ/mol

NpO2CO3Na:3.5H2O
       NpO2CO3Na:3.5H2O  =  + 1.0000 CO3-2 + 1.0000 Na+ + 1.0000 NpO2+ +
3.5000 H2O
        log_k           -11.00          #01LEM/FUG
```

```
        -delta_H        30.995  kJ/mol  #Sf 84LEM, H calc
#       Enthalpy of formation:  -2926.042 kJ/mol

NpO2(CO3)2Na3(s)
       NpO2(CO3)2Na3  =  + 2.0000 CO3-2 + 3.0000 Na+ + 1.0000 NpO2+
        log_k           -14.22          #01LEM/FUG
        -delta_H        0                               # Not possible to
calculate
#       Enthalpy of formation:  -0 kJ/mol

NpO3:H2O(cr)
       NpO3:H2O + 2.0000 H+  =  + 2.0000 H2O + 1.0000 NpO2+2
        log_k           5.47                    #01LEM/FUG
        -delta_H        -52.240 kJ/mol  #Sf 84LEM, H calc
#       Enthalpy of formation:  -1380.153 kJ/mol

NpO2CO3(s)
       NpO2CO3  =  + 1.0000 NpO2+2 + 1.0000 CO3-2
        log_k           -14.60          #01LEM/FUG
        -delta_H        0                               #Not possible to
calculate
#       Enthalpy of formation:  -0 kJ/mol

(NH4)4NpO2(CO3)3(s)
       (NH4)4NpO2(CO3)3  =  + 1.0000 NpO2+2 + 3.0000 CO3-2 + 4.0000 NH3 +
4.0000 H+
        log_k           -63.76          #01LEM/FUG
        -delta_H        0                               #Not possible to
calculate
#       Enthalpy of formation:  -0 kJ/mol

K4NpO2(CO3)3(s)
       K4NpO2(CO3)3  =  + 1.0000 NpO2+2 + 3.0000 CO3-2 + 4.0000 K+
        log_k           -26.40          #01LEM/FUG
        -delta_H        0                               #Not possible to
calculate
#       Enthalpy of formation:  -0 kJ/mol


Pa(c)
       Pa  =  + 1.0000 Pa+4 + 4.0000 e-
        log_k           +98.75                  #Sf 85BAR/PAR, logK calc
        -delta_H        -620.000        kJ/mol          #Sf 85BAR/PAR,H
calc
#       Enthalpy of formation:  -0 kJ/mol

PaO2(s)
       PaO2 + 4.0000 H+  =  + 1.0000 Pa+4 + 2.0000 H2O
        log_k           +0.60                           #76BAE/MES
        -delta_H        0                               #Not possible to
```

```
calculate
#       Enthalpy of formation:  0 kcal/mol

Pa2O5(s)
       Pa2O5 + 2.0000 H+  =  + 2.0000 PaO2+ + 1.0000 H2O
        log_k           -4.00                           #76BAE/MES
        -delta_H        0                               #Not possible to
calculate
#       Enthalpy of formation:  0 kcal/mol

Pd
       Pd  =  + 2.0000 e- + 1.0000 Pd+2
        log_k           -33.03                  # Calculated internally, Sf
82WAG/EVA
        -delta_H        189.883 kJ/mol          # Calculated internally, Sf
82WAG/EVA
#       Enthalpy of formation:  0 kJ/mol        # Reference state

Pd(OH)2(s)
       Pd(OH)2 + 2.0000 H+  =  + 2.0000 H2O + 1.0000 Pd+2
        log_k           -1.61                   # 92PEA/BER
        -delta_H        13.223  kJ/mol          # Calculated internally,
DHf 82WAG/EVA
#       Enthalpy of formation:  -395.000 kJ/mol # 82WAG/EVA

PdO(s)
       PdO + 2.0000 H+  =  + 1.0000 H2O + 1.0000 Pd+2
        log_k           -6.02                   # Calculated internally,
DHf 82WAG/EVA, DGf 99LOT/OCH
        -delta_H        -10.547 kJ/mol          # Calculated internally,
DHf 82WAG/EVA, DGf 99LOT/OCH
#       Enthalpy of formation:  -85.4 kJ/mol    # 82WAG/EVA

# PdS(s)
#       PdS + 1.0000 H+  =  + 1.0000 HS- + 1.0000 Pd+2
#        log_k           -46.87                 # Calculated internally,
DHf and Sf 74 MIL
#       -delta_H        244.293 kJ/mol          # Calculated internally,
DHf and Sf 74 MIL
#       Enthalpy of formation:  -70.710 kJ/mol  # 74 MIL

PdCl2(cr)
       PdCl2  =  + 2.0000 Cl- + 1.0000 Pd+2
        log_k           -9.20                   # Calculated internally,
DGf 89BAE/MCK, DHf 82WAG/EVA
        -delta_H        54.423  kJ/mol          # Calculated internally,
DGf 89BAE/MCK, DHf 82WAG/EVA
#       Enthalpy of formation:  -198.700 kJ/mol # 82WAG/EVA

PdBr2(cr)
```

```
       PdBr2  =  + 2.0000 Br- + 1.0000 Pd+2
        log_k           -13.31                  # 89BAE/MCK
        -delta_H        51.263  kJ/mol          # Calculated internally,
DHf 82WAG/EVA
#       Enthalpy of formation:  -104.200 kJ/mol # 82WAG/EVA

PdI2(cr)
       PdI2  =  + 2.0000 I- + 1.0000 Pd+2
        log_k           -25.87                  # Calculated internally,
DGf,DHf 89BAE/MCK
        -delta_H        139.923kJ/mol           # Calculated internally,
DGf,DHf 89BAE/MCK
#       Enthalpy of formation:  -63.600 kJ/mol  # 89BAE/MCK
Pu(cr)
       Pu  =  + 1.0000 Pu+3 + 3.0000 e-
        log_k           101.43          #Sf 01LEM/FUG, logK calc
        -delta_H        -591.790        kJ/mol  #Sf 01LEM/FUG, H calc
#       Enthalpy of formation:  0 kJ/mol

Pu(OH)3(cr)
       Pu(OH)3 +3.0000 H+  =  + 1.0000 Pu+3 + 3.0000 H2O
        log_k           15.80                   #01LEM/FUG
        -delta_H        0                               # Not possible to
calculate
#       Enthalpy of formation:  -0 kJ/mol

Pu2O3(s)
       Pu2O3 +6.0000 H+  =  + 2.0000 Pu+3 + 3.0000 H2O
        log_k           50.63                   #DGf 01LEM/FUG, logK calc
        -delta_H        -385.070        kJ/mol  #DHf 01LEM/FUG, H calc
#       Enthalpy of formation:  -1656.000 kJ/mol

PuCO3OH(s)
       PuCO3OH +1.0000 H+  =  + 1.0000 Pu+3 + 1.0000 H2O + 1.0000 CO3-2
        log_k           -5.74                   #estimated from
actinides(III) and lanthanides
        -delta_H        0                               # Not possible to
calculate
#       Enthalpy of formation:  -0 kJ/mol

PuPO4(s,hyd)
       PuPO4 +2.0000 H+  =  + 1.0000 Pu+3 + 1.0000 H2PO4-
        log_k           -5.04                   #01LEM/FUG
        -delta_H        0                               #Not possible to
calculate
#       Enthalpy of formation:  -0 kJ/mol

Pu(OH)4(am)
       Pu(OH)4 +4.0000 H+  =  + 1.0000 Pu+4 + 4.0000 H2O
        log_k           -0.80                   #80LEM/GAR
```

```
        -delta_H        0                               #Not possible to
calculate
#       Enthalpy of formation:  -0 kJ/mol

PuO2:2H2O(am)
       PuO2:2H2O +4.0000 H+  =  + 1.0000 Pu+4 + 4.0000 H2O
        log_k           -2.37                   #03GUI/FAN
        -delta_H        -58.548 kJ/mol  #Sf 80LEM/TRE, H calc
#       Enthalpy of formation:  -1624.667 kJ/mol

Pu(HPO4)2(am,hyd)
       Pu(HPO4)2 + 2.0000 H+  =  + 1.0000 Pu+4 + 2.0000 H2PO4-
        log_k           -16.026         #01LEM/FUG
        -delta_H        -32.718 kJ/mol  #Sf 80LEM/TRE, H calc
#       Enthalpy of formation:  -3112.377 kJ/mol

PuO2OH(s)
       PuO2OH +1.0000 H+  =  + 1.0000 H2O + 1.0000 PuO2+
        log_k           5.00                    #01LEM/FUG
        -delta_H        -0              kJ/mol  #Not possible to calculate
#       Enthalpy of formation:  -1159.793 kJ/mol

PuO2(OH)2:H2O
       PuO2(OH)2:H2O +2.0000 H+  =  + 1.0000 PuO2+2 + 3.0000 H2O
        log_k           5.50                    #01LEM/FUG
        -delta_H        -46.718 kJ/mol  #01LEM/FUG
#       Enthalpy of formation:  -1632.808 kJ/mol

PuO2CO3(s)
       PuO2CO3  =  + 1.0000 CO3-2 + 1.0000 PuO2+2
        log_k           -14.65          #03GUI/FAN
        -delta_H        0                               #Not possible to
calculate
#       Enthalpy of formation:  -0 kJ/mol

RaCO3(cr)
RaCO3                  =  +1.000Ra+2                 +1.000CO3-2
    log_k      -8.3000                          #01HUM/BER
    -delta_h    11.7000         kJ/mol          #01HUM/BER
#    -a_e   -6.250212E+00 -0.000000E+00 -6.111444E+02 -0.000000E+00
0.000000E+00

RaSO4(cr)
RaSO4                  =  +1.000Ra+2                 +1.000SO4-2
    log_k     -10.2600                          #01HUM/BER
    -delta_h    39.3000         kJ/mol          #01HUM/BER
#    -a_e   -3.374813E+00 -0.000000E+00 -2.052818E+03 -0.000000E+00
0.000000E+00

Se(s)
```

```
       Se +1.0000 H+ + 2.0000 e-  =  + 1.0000 HSe-
        log_k           -7.69                   #Sf 92GRE/FUG, logK calc
        -delta_H        15.899  kJ/mol  #Sf 92GRE/FUG, H calc
#       Enthalpy of formation:  0 kJ/mol

Na2Se(sr)
       Na2Se + 1.0000 H+  =  + 1.0000 HSe- + 2.0000 Na+
        log_k          23.00                    #87ELR/ADR
        -delta_H        -123.381 kJ/mol       #DHf 82WAG/EVA, H calc
#       Enthalpy of formation:  -341.400 kJ/mol

K2Se(s)
       K2Se + 1.0000 H+  =  + 1.0000 HSe- + 2.0000 K+
        log_k           26.27                   #74MIL
        -delta_H        -103.453        kJ/mol  #74MIL
#       Enthalpy of formation:  -384.928 kJ/mol

CaSe(s)
       CaSe + 1.0000 H+  =  + 1.0000 HSe- + 1.0000 Ca+2
        log_k           25.53                   #DGf 82WAG/EVA, logK calc
        -delta_H        -158.901  kJ/mol                #DHf 82WAG/EVA, H
calc
#       Enthalpy of formation:  -368.200 kJ/mol

MgSe(s)
       MgSe + 1.0000 H+  =  + 1.0000 HSe- + 1.0000 Mg+2
        log_k           21.41                   #74MIL
        -delta_H        -158.221  kJ/mol                #74MIL
#       Enthalpy of formation:  -292.880 kJ/mol

SrSe(s)
       SrSe + 1.0000 H+  =  + 1.0000 HSe- + 1.0000 Sr+2
        log_k           32.41                   #87ELR/ADR
        -delta_H        -149.201  kJ/mol                #DHf 82WAG/EVA, H
calc
#       Enthalpy of formation:  -385.800 kJ/mol

BaSe(s)
       BaSe + 1.0000 H+  =  + 1.0000 HSe- + 1.0000 Ba+2
        log_k           35.86                   #87ELR/ADR
        -delta_H        -146.901  kJ/mol                #DHf 82WAG/EVA, H
calc
#       Enthalpy of formation:  -372.000 kJ/mol

Fe1.04Se(s)
        Fe1.04Se + 1.0000 H+  =  1.0400 Fe+2 + 1.0000 HSe- + 0.08 e-
        log_k           -3.3991                 #calculated 09ARC/PIQ
        -delta_H        -8.1000 kJ/mol          #calculated 09ARC/PIQ

FeSe2(s)
```

```
        FeSe2 + 2.0000 H+ + 2.0000 e-  =  + 1.0000 Fe+2 + 2.0000 HSe-
        log_k           -17.1256                #calculated 09ARC/PIQ
        -delta_H        +50.500 kJ/mol          #calculated 09ARC/PIQ
#       Enthalpy of formation:  -104.600 kJ/mol

NiSe(s)
        NiSe + 1.0000 H+  =  + 1.0000 Ni+2 + 1.0000 HSe-
        log_k           -18.700         #01SEB/POT
        -delta_H         20.799 kJ/mol          #DHf 82WAG/EVA, H calc
#       Enthalpy of formation:  -59.000 kJ/mol

PdSe(s)
       PdSe + 1.0000 H+  =  + 1.0000 Pd+2 + 1.0000 HSe-
        log_k           -59.40          #01SEB/POT
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction

MnSe(s)
       MnSe + 1.0000 H+  =  + 1.0000 Mn+2 + 1.0000 HSe-
        log_k           2.50                    #01SEB/POT
        -delta_H        -50.043 kJ/mol          #74MIL
#       Enthalpy of formation:  -154.808 kJ/mol

Cu2Se(s)
        Cu2Se + 1.0000 H+  =  + 2.0000 Cu+ + 1.0000 HSe-
        log_k           -46.80          #01SEB/POT
        -delta_H        218.639 kJ/mol          #DHf 82WAG/EVA, H calc
#       Enthalpy of formation:  -59.400 kJ/mol

CuSe(s)
        CuSe + 1.0000 H+  =  + 1.0000 Cu+2 + 1.0000 HSe-
        log_k           -35.00          #01SEB/POT
        -delta_H        122.639 kJ/mol          #74MIL
#       Enthalpy of formation:  -41.840  kJ/mol

Ag2Se(s)
        Ag2Se + 1.0000 H+  =  + 1.0000 HSe- + 2.0000 Ag+
        log_k           -48.20          #01SEB/POT
        -delta_H        265.479 kJ/mol          #DHf 82WAG/EVA, H calc
#       Enthalpy of formation:  -38.000 kJ/mol

ZnSe(s)
        ZnSe + 1.0000 H+  =  + 1.0000 HSe- + 1.0000 Zn+2
        log_k           -15.37          #01SEB/POT
        -delta_H        21.501  kJ/mol          #78VAU/CRA
#       Enthalpy of formation:  -158.992 kJ/mol

CdSe(s)
        CdSe + 1.0000 H+  =  + 1.0000 Cd+2 + 1.0000 HSe-
        log_k           -17.47          #01SEB/POT
```

```
        -delta_H        84.746 kJ/mol           #74MIL
#       Enthalpy of formation:  -144.766 kJ/mol

HgSe(s)
        HgSe + 1.0000 H+  =  + 1.0000 Hg+2 + 1.0000 HSe-
        log_k           -43.30          #01SEB/POT
        -delta_H        229.623  kJ/mol         #78VAU/CRA
#       Enthalpy of formation:  -43.514 kJ/mol

SnSe(s)
       SnSe + 1.0000 H+  =  + 1.0000 HSe- + 1.0000 Sn+2
        log_k           -24.40          #01SEB/POT
        -delta_H        95.700 kJ/mol           #79KUB/ALC
#       Enthalpy of formation:  -88.701 kJ/mol

PbSe(s)
        PbSe + 1.0000 H+  =  + 1.0000 Pb+2 + 1.0000 HSe-
        log_k           -24.00          #01SEB/POT
        -delta_H        119.719 kJ/mol          #DHf 82WAG/EVA, H calc
#       Enthalpy of formation:  -102.9 kJ/mol

USe2(alpha)
       USe2 + 2.0000 H+  =  + 1.0000 U+4 + 2.0000 HSe-
        log_k           2.63                    #92GRE/FUG
        -delta_H        -132.402        kJ/mol  #92GRE/FUG
#       Enthalpy of formation:  -427 kJ/mol

USe2(beta)
       USe2 + 2.0000 H+  =  + 1.0000 U+4 + 2.0000 HSe-
        log_k           2.47                    #92GRE/FUG
        -delta_H        -132.402        kJ/mol  #92GRE/FUG
#       Enthalpy of formation:  -427 kJ/mol

USe3(cr)
       USe3 + 2.0000 H2O  =  + 1.0000 UO2+2 + 3.0000 HSe- + 1.0000 H+
        log_k           -18.46          #92GRE/FUG
        -delta_H        52.358  kJ/mol  #92GRE/FUG
#       Enthalpy of formation:  -452 kJ/mol

MgSeO3:6H2O
       MgSeO3:6H2O  =  + 1.0000 Mg+2 + 1.0000 SeO3-2 + 6.0000 H2O
        log_k           -5.36                   #01SEB/POT
        -delta_H        15.877  kJ/mol  #DHf 82WAG/EVA, H calc
#       Enthalpy of formation:  -2707.050 kJ/mol

MgSeO3(cr)
       MgSeO3  =  + 1.0000 Mg+2 + 1.0000 SeO3-2
        log_k           -7.56                   #01SEB/POT
        -delta_H        -76.003 kJ/mol  #DHf 82WAG/EVA, H calc
#       Enthalpy of formation:  -900.190 kJ/mol
```

```
CaSeO3:2H2O(cr)
       CaSeO3:2H2O  =  + 1.0000 Ca+2 + 1.0000 SeO3-2 + 2.0000 H2O
        log_k           -7.06                   #DGf 82WAG/EVA, logK calc
        -delta_H        0                               # Not possible to
calculate

CaSeO3:H2O
       CaSeO3:H2O  =  + 1.0000 Ca+2 + 1.0000 SeO3-2 + 1.0000 H2O
        log_k           -7.76                   #01SEB/POT
        -delta_H        0                               # Not possible to
calculate

SrSeO3(cr)
       SrSeO3  =  + 1.0000 Sr+2 + 1.0000 SeO3-2
        log_k           -6.10                   #87ELR/ADR
        -delta_H        -12.393 kJ/mol  #DHf 82WAG/EVA, H calc
#       Enthalpy of formation:  -1047.700 kJ/mol

BaSeO3(s)
       BaSeO3  =  + 1.0000 Ba+2 + 1.0000 SeO3-2
        log_k           -6.57                   #01SEB/POT
        -delta_H        -3.393  kJ/mol  #DHf 82WAG/EVA, H calc
#       Enthalpy of formation:  -1040.600 kJ/mol

Fe2(SeO3)3:6H2O
       Fe2(SeO3)3:6H2O  =  + 2.0000 Fe+3 + 3.0000 SeO3-2 + 6.0000 H2O
        log_k           -41.58          #01SEB/POT
        -delta_H        0                               # Not possible to
calculate

NiSeO3(cr)
       NiSeO3  =  + 1.0000 Ni+2 + 1.0000 SeO3-2
        log_k           -5.15                   #01SEB/POT
        -delta_H        0                               # Not possible to
calculate

MnSeO3
       MnSeO3  =  + 1.0000 Mn+2 + 1.0000 SeO3-2
        log_k           -7.11                   #01SEB/POT
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction    MnSeO3

CuSeO3:2H2O
        CuSeO3:2H2O  =  + 1.0000 Cu+2 + 1.0000 SeO3-2 + 2.0000 H2O
        log_k           -7.78                   #76SMI/MAR
        -delta_H        0                               # Not possible to
calculate

CuSeO3(s)
```

```
       CuSeO3  =  + 1.0000 Cu+2 + 1.0000 SeO3-2
        log_k           -8.42                   #01SEB/POT
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction    CuSeO3
#       Enthalpy of formation:  0 kcal/mol

Ag2SeO3(s)
       Ag2SeO3  =  + 2.0000 Ag+ + 1.0000 SeO3-2
        log_k           -15.15          #01SEB/POT
        -delta_H        67.687  kJ/mol  #DHf 82WAG/EVA, H calc
#       Enthalpy of formation:  -365.300 kJ/mol

ZnSeO3:H2O
       ZnSeO3:H2O  =  + 1.0000 H2O + 1.0000 SeO3-2 + 1.0000 Zn+2
        log_k           -7.70                   #01SEB/POT
        -delta_H        -17.513 kJ/mol  #DHf 82WAG/EVA, H calc
#       Enthalpy of formation:  -930.900 kJ/mol

CdSeO3(s)
       CdSeO3  =  + 1.0000 Cd+2 + 1.0000 SeO3-2
        log_k           -10.29          #DGf 82WAG/EVA, logK calc
        -delta_H        -9.813  kJ/mol  #DHf 82WAG/EVA, H calc
#       Enthalpy of formation:  -575.300 kJ/mol

Hg2SeO3(s)
       Hg2SeO3  =  + 1.0000 Hg2+2 + 1.0000 SeO3-2
        log_k           -15.70          #DGf 82WAG/EVA, logK calc
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction    Hg2SeO3

HgSeO3(s)
       HgSeO3  =  + 1.0000 Hg+2 + 1.0000 SeO3-2
        log_k           -15.39          #DGf 82WAG/EVA, logK calc
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction    HgSeO3

PbSeO3(s)
       PbSeO3  =  + 1.0000 Pb+2 + 1.0000 SeO3-2
        log_k           -12.12          #87ELR/ADR
        -delta_H        29.327   kJ/mol         #DHf 82WAG/EVA, H calc
#       Enthalpy of formation:  -537.600 kJ/mol

Th(SeO3)2(s)
       Th(SeO3)2  =  + 1.0000 Th+4 + 2.0000 SeO3-2
        log_k           -19.87          #01SEB/POT
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction

UO2SeO3(cr)
       UO2SeO3  =  + 1.0000 UO2+2 + 1.0000 SeO3-2
```

```
        log_k           -10.42          #01SEB/POT
        -delta_H        -6.193    kJ/mol                #DHf 92GRE/FUG, H
calc
#       Enthalpy of formation:  -1522.000 kJ/mol

Na2SeO4(cr)
       Na2SeO4  =  + 1.0000 SeO4-2 + 2.0000 Na+
        log_k           -0.89                   #87ELR/ADR
        -delta_H        -10.829  kJ/mol         #DHf 82WAG/EVA, H calc
#       Enthalpy of formation:  -1069.000 kJ/mol

K2SeO4(cr)
       K2SeO4  =  + 1.0000 SeO4-2 + 2.0000 K+
        log_k           0.66                    #DGf 82WAG/EVA, logK calc
        -delta_H        6.591  kJ/mol           #DHf 82WAG/EVA, H calc
#       Enthalpy of formation:  -1110.020 kJ/mol

MgSeO4:6H2O
       MgSeO4:6H2O  =  + 1.0000 SeO4-2 + 1.0000 Mg+2 + 6.0000 H2O
        log_k           -1.13                   #01SEB/POT
        -delta_H        -2.129  kJ/mol          #DHf 82WAG/EVA, H calc
#       Enthalpy of formation:  -2779.000 kJ/mol

CaSeO4:2H2O
       CaSeO4:2H2O  =  + 1.0000 Ca+2 + 1.0000 SeO4-2 + 2.0000 H2O
        log_k           -3.09                   #01SEB/POT
        -delta_H        -7.109  kJ/mol  #DHf 82WAG/EVA, H calc
#       Enthalpy of formation:  -1706.700 kJ/mol

SrSeO4(s)
       SrSeO4  =  + 1.0000 SeO4-2 + 1.0000 Sr+2
        log_k           -4.4000         #01SEB/POT
        -delta_H        -7.349   kJ/mol         #DHf 82WAG/EVA, H calc
#       Enthalpy of formation:  -1142.700 kJ/mol

BaSeO4(cr)
       BaSeO4  =  + 1.0000 Ba+2 + 1.0000 SeO4-2
        log_k           -7.38                   #01SEB/POT
        -delta_H        12.451  kJ/mol  #DHf 82WAG/EVA, H calc
#       Enthalpy of formation:  -1146.400 kJ/mol

NiSeO4:6H2O
       NiSeO4:6H2O  =  + 1.0000 SeO4-2 + 1.0000 Ni+2 + 6.0000 H2O
        log_k           -1.49                   #01SEB/POT
        -delta_H        2.491  kJ/mol           #Sf in analogy to
NiSO4:6H2O, H calc
#       Enthalpy of formation:  -2370.830 kJ/mol

Ag2SeO4(s)
       Ag2SeO4  =  + 2.0000 Ag+ + 1.0000 SeO4-2
```

```
        log_k           -8.91                   #01SEB/POT
        -delta_H        32.931  kJ/mol  #DHf 82WAG/EVA, H calc
#       Enthalpy of formation:  -420.500 kJ/mol

ZnSeO4(s)
       ZnSeO4  =  + 1.0000 Zn+2 + 1.0000 SeO4-2
        log_k           -13.40          #64SIL/MAR
        -delta_H        -88.139 kJ/mol  #DHf 82WAG/EVA, H calc
#       Enthalpy of formation:  -664.400 kJ/mol

PbSeO4(s)
       PbSeO4  =  + 1.0000 Pb+2 + 1.0000 SeO4-2
        log_k           -6.84                   #01SEB/POT
        -delta_H        10.971  kJ/mol  #DHf 82WAG/EVA, H calc
#       Enthalpy of formation:  -609.200 kJ/mol

SeO2(cr)
        SeO2 +1.0000 H2O  =  + 1.0000 SeO3-2 + 2.0000 H+
        log_k           -8.24                   #74MIL
        -delta_H        1.736   kJ/mol          #74MIL
#       Enthalpy of formation:  -225.099 kJ/mol

SeCl4(cr)
       SeCl4 +3.0000 H2O  =  + 1.0000 SeO3-2 + 4.0000 Cl- + 6.0000 H+
        log_k           12.91                   #74MIL
        -delta_H        -131.324        kJ/mol  #74MIL
#       Enthalpy of formation:  -188.698 kJ/mol

Se2O5(s)
       Se2O5 +2.0000 H2O  =  + 1.0000 SeO3-2 + 1.0000 SeO4-2 + 4.0000 H+
        log_k           8.05                    #74MIL
        -delta_H        -123.302        kJ/mol  #74MIL
#       Enthalpy of formation:  -413.379 kJ/mol

SeO3(cr)
       SeO3 +1.0000 H2O  =  + 1.0000 SeO4-2 + 2.0000 H+
        log_k           19.24                   #74MIL
        -delta_H        -143.030        kJ/mol  #74MIL
#       Enthalpy of formation:  -170.289 kJ/mol

Sm(cr)
       Sm  =  + 3.0000 e- + 1.0000 Sm+3
        log_k           116.62          #Sf 79ROB/HEM, logK calc
        -delta_H        -691.199        kJ/mol  #Sf 79ROB/HEM, logK calc
#       Enthalpy of formation:  0 kJ/mol

Sm2O3(s)
       Sm2O3 +6.0000 H+  =  + 2.0000 Sm+3 + 3.0000 H2O
        log_k           43.11                   #DGf 79ROB/HEM, logK calc
        -delta_H  -355.039  kJ/mol              #Sf 79ROB/HEM, H calc
```

```
#       Enthalpy of formation:  -1884.849 kJ/mol

Sm(OH)3(s)
       Sm(OH)3 +3.0000 H+  =  + 1.0000 Sm+3 + 3.0000 H2O
        log_k           16.50                   #95SPA/BRU
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction    Sm(OH)3
#       Enthalpy of formation:  0 kcal/mol

Sm(OH)3(am)
       Sm(OH)3 +3.0000 H+  =  + 1.0000 Sm+3 + 3.0000 H2O
        log_k           18.60                   #95SPA/BRU
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction    Sm(OH)3(am)
#       Enthalpy of formation:  0 kcal/mol

Sm2(CO3)3(s)
       Sm2(CO3)3  =  + 2.0000 Sm+3 + 3.0000 CO3-2
        log_k           -34.50          #95SPA/BRU
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction    Sm2(CO3)3
#       Enthalpy of formation:  0 kcal/mol

SmOHCO3(s)
       SmOHCO3 + 1.0000 H+  =  + 1.0000 Sm+3 + 1.0000 CO3-2 + 1.0000 H2O
        log_k           -7.70                   #estimated from lanthanides
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction    Sm2(CO3)3
#       Enthalpy of formation:  0 kcal/mol

SmPO4:xH2O
       SmPO4 +2.0000 H+  =  + 1.0000 H2PO4- + 1.0000 Sm+3
        log_k           -4.94                   #95SPA/BRU
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction
#       Enthalpy of formation:  0 kcal/mol

SmPO4(s)
       SmPO4 +2.0000 H+  =  + 1.0000 H2PO4- + 1.0000 Sm+3
        log_k           -6.67                   #97LIU/BYR
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction
#       Enthalpy of formation:  0 kcal/mol

Sm2(SO4)3(s)
       Sm2(SO4)3  =  + 2.0000 Sm+3 + 3.0000 SO4-2
        log_k           -9.80                   #95SPA/BRU
        -delta_H        -211.318  kJ/mol                #DHf 82WAG/EVA, H
calc
#       Enthalpy of formation:  -3899.100 kJ/mol
```

```
SmF3:0.5H2O
       SmF3:0.5H2O  =  + 0.5000 H2O + 1.0000 Sm+3 + 3.0000 F-
        log_k           -17.50          #95SPA/BRU
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction    SmF3:.5H2O
#       Enthalpy of formation:  0 kcal/mol

SmCl3:6H2O
       SmCl3:6H2O  =  + 6.0000 H2O + 1.0000 Sm+3 + 3.0000 Cl-
        log_k           4.80                    #96FAL/REA
        -delta_H        -38.311 kJ/mol          #Sf 82WAG/EVA, H calc
#       Enthalpy of formation:  -2869.108 kJ/mol

Sn(cr)
       Sn  =  + 2.0000 e- + 1.0000 Sn+2
        log_k            4.84                   #Sf 89COX/WAG, logK calc
        -delta_H        -8.900  kJ/mol  #Sf 89COX/WAG, H calc

SnO(s)
        SnO +2.0000 H+  =  + 1.0000 H2O + 1.0000 Sn+2
        log_k           2.50                    #01HUM/BER
        -delta_H        -15.439 kJ/mol  #Sf 89COX/WAG, H calc
#       Enthalpy of formation:  -279.291 kJ/mol

# SnS(s)
#        SnS + 1.0000 H+  =  + 1.0000 HS- + 1.0000 Sn+2
#        log_k           -15.63          #DGf 95ROB/HEM, logK calc
#       -delta_H        81.020  kJ/mol  #Sf 95ROB/HEM, H calc
#       Enthalpy of formation:  -106.220 kJ/mol

SnOHCl(s)
       SnOHCl + 1.0000 H+  =  + 1.0000 Sn+2 + 1.0000 Cl- + 1.0000 H2O
        log_k           -2.42                   #99LOT/OCH
        -delta_H        0       kJ/mol          #Not possible to calculate
it

CaSn(OH)6(s)
        CaSn(OH)6 +6.0000 H+  =  + 6.0000 H2O + 1.0000 Sn+4 + 1.0000 Ca+2
        log_k           8.54                    #00LOT/OCH
        -delta_H        0       kJ/mol          #Not possible to calculate
it

Sn(OH)4(s)
        Sn(OH)4 +4.0000 H+  =  + 4.0000 H2O + 1.0000 Sn+4
        log_k           -1.43                   #average value 99SEB/DON,
01SEB/POT2
        -delta_H        -3.074  kJ/mol  #DHf 82WAG/EVA, H calc
#       Enthalpy of formation:  -1110.000 kJ/mol
```

```
SnO2(am)
        SnO2 +4.0000 H+  =  + 2.0000 H2O + 1.0000 Sn+4
        log_k           -6.77                   #01HUM/BER
        -delta_H        0       kJ/mol          #Not possible to calculate
enthalpy of reaction

SnO2(cr)
        SnO2 +4.0000 H+  =  + 2.0000 H2O + 1.0000 Sn+4
        log_k           -7.47                   #01HUM/BER
        -delta_H        35.948  kJ/mol  #DHf 92GRE/FUG, H calc
#       Enthalpy of formation:  -577.362 kJ/mol

# SnS2(s)
#        SnS2 + 2.0000 H+  =  + 2.0000 HS- + 1.0000 Sn+4
#        log_k           -30.00         #DGf 85JAC/HEL, logK calc
#       -delta_H        151.199 kJ/mol          #DHf 85JAC/HEL, H calc
#       Enthalpy of formation:  -153.553 kJ/mol

Celestite
SrSO4                   =  +1.000Sr+2                 +1.000SO4-2
    log_k      -6.6319                          #01HUM/BER
    -delta_h    -4.3389                         #01HUM/BER
#    -a_e   -1.480596E+04 -2.466092E+00  7.569685E+05  5.436359E+03
-4.055360E+07

Strontianite
SrCO3                   =  +1.000Sr+2                 -1.000H+
+1.000HCO3-
    log_k       1.0583                          #01HUM/BER
    -delta_h   -16.5756                         #01HUM/BER
#    -a_e    2.629176E+02  3.252849E-02 -1.239138E+04 -9.551199E+01
5.637139E+05

Tc(cr)
Tc + 3H2O = TcO(OH)2 + 4H+ + 4e-
        log_k    -25.08
        -delta_H        108.170 kJ/mol          # Calculated from data of
99RAR/RAN
  #     Enthalpy of formation:  0.00 kJ/mol # 99RAR/RAN

TcO2:1.6H2O(s)
TcO2:1.6(H2O)           =  +1.000TcO(OH)2             +0.600H2O
    log_k      -8.4000                          #01HUM/BER
#    -a_e   -8.400000E+00 -0.000000E+00 -0.000000E+00 -0.000000E+00
-0.000000E+00

TcO2(cr)
        TcO2  + H2O = TcO(OH)2
        log_k           -12.39                  # Calculated internally
        -delta_H        0 kJ/mol                # Not available
```

```
#       Enthalpy of formation:  -457.8  kJ/mol # 99RAR/RAN

Tc2O7(cr)
        Tc2O7 + H2O = 2 TcO4- + 2 H+
        log_k           15.31                   #calculated internally
        -delta_H        -46.470 kJ/mol          #calculated internally
#       Enthalpy of formation: 1126.500 kJ/mol  #99RAR/RAN

Tc2O7:H2O(cr)
        Tc2O7:H2O = 2 TcO4- + 2 H+
        log_k           14.11                   #calculated internally
        -delta_H        -44.654 kJ/mol          #calculated internally
#       Enthalpy of formation: 1414.146 kJ/mol  #99RAR/RAN

KTcO4(cr)
        KTcO4 = TcO4- + K+
        log_k           -2.28                   #calculated internally
        -delta_H        +53.560 kJ/mol          #calculated internally
#       Enthalpy of formation: -1035.100 kJ/mol #99RAR/RAN

NaTcO4:4H2O (cr)
        NaTcO4:4H2O = TcO4- + Na+ + 4H2O
        log_k           0.79                    #99RAR/RAN
        -delta_H        0  kJ/mol               #not available
#       Enthalpy of formation: 0 kJ/mol         #not available

Th(cr)
       Th  =  + 1.0000 Th+4 + 4.0000 e-
        log_k           123.44          #Sf 99RAR/RAN, logK calc
        -delta_H        -769.02 kJ/mol  #Sf 99RAR/RAN, H calc
#       Enthalpy of formation:  0 kJ/mol

ThO2(cr)
        ThO2 +4.0000 H+  =  + 1.0000 Th+4 + 2.0000 H2O
        log_k           1.80                    #03NEC/ALT
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction
#       Enthalpy of formation:  0 kcal/mol

ThO2:2H2O(am)
       ThO2:2H2O +4.0000 H+  =  + 1.0000 Th+4 + 4.0000 H2O
        log_k           9.00                    #03NEC/ALT, 02NEC/MUL
        -delta_H        0                       # Not possible to calculate
enthalpy of reaction
#       Enthalpy of formation:  0 kcal/mol

Th(HPO4)2(s)
       Th(HPO4)2 + 2.0000 H+  =  + 1.0000 Th+4 + 2.0000 H2PO4-
        log_k           -15.98          #estimated from actinides(IV)
        -delta_H        0                       # Not possible to calculate
```

```
enthalpy of reaction
#       Enthalpy of formation:  0 kcal/mol

U(cr)
        U  =  + 1.0000 U+4 + 4.0000 e-
        log_k           92.83  #92GRE/FUG
        -delta_H        -591.200        kJ/mol  # 92GRE/FUGCalculated
enthalpy of reaction
#       Enthalpy of formation:  -0 kJ/mol

UO2(cr)
        UO2 +4.0000 H+  =  + 1.0000 U+4 + 2.0000 H2O
        log_k           -4.85   #92GRE/FUG
        -delta_H        -77.860 kJ/mol  # 92GRE/FUG Calculated enthalpy of
reaction        Uraninite
#       Enthalpy of formation:  -1085 kJ/mol

UO2:2H2O(am)
       UO2:2H2O +4.0000 H+  =  + 1.0000 U+4 + 4.0000 H2O
        log_k           1.50   #03GUI/FAN
        -delta_H        0               # Not possible to calculate
enthalpy of reaction
#       Enthalpy of formation:  0 kcal/mol

UO2.25
       UO2.25 +4.5000 H+ + 0.5000 e-  =  + 1.0000 U+4 + 2.2500 H2O
        log_k           -1.00    #92GRE/FUG
        -delta_H        -106.318        kJ/mol  # 92GRE/FUG Calculated
enthalpy of reaction    UO2.25
#       Enthalpy of formation:  -1128.000 kJ/mol

UO2.34(b)
        UO2.34 + 4.6800 H+ + 0.6800 e-  =  + 1.0000 U+4 + 2.3400 H2O
        log_k           0.63   #03GUI/FAN
        -delta_H        -117.127        kJ/mol  # 92GRE/FUG Calculated
enthalpy of reaction    UO2.34
#       Enthalpy of formation:  -1141 kJ/mol

UO2.67
        UO2.67 + 5.3400 H+ + 1.3400 e-  =  + 1.0000 U+4 + 2.6700 H2O
        log_k           6.85
        -delta_H        -161.823        kJ/mol  # Calculated enthalpy of
reaction        UO2.67
#       Enthalpy of formation:  -1191.6 kJ/mol

U(OH)2SO4(cr)
       U(OH)2SO4 +2.0000 H+  =  + 1.0000 SO4-2 + 1.0000 U+4 + 2.0000 H2O
        log_k           -3.17   #92GRE/FUG
        -delta_H        0               # Not possible to calculate
enthalpy of reaction    U(OH)2SO4
```

```
#       Enthalpy of formation:  0 kcal/mol

U(SO4)2(cr)
       U(SO4)2  =  + 1.0000 U+4 + 2.0000 SO4-2
        log_k           -11.68  #92GRE/FUG
        -delta_H        -100.280        kJ/mol  #92GRE/FUG Calculated
enthalpy of reaction    U(SO4)2
#       Enthalpy of formation:  -2309.6 kJ/mol

U(SO4)2:4H2O(cr)
       U(SO4)2:4H2O  =  + 1.0000 U+4 + 2.0000 SO4-2 + 4.0000 H2O
        log_k           -11.72  #92GRE/FUG
        -delta_H        -70.0000        kJ/mol  # #92GRE/FUG Calculated
enthalpy of reaction    U(SO4)2:4H2O
#       Enthalpy of formation:  -3483.2 kJ/mol

U(SO4)2:8H2O(cr)
       U(SO4)2:8H2O  =  + 1.0000 U+4 + 2.0000 SO4-2 + 8.0000 H2O
        log_k          -12.77  #92GRE/FUG
        -delta_H        -33.920 kJ/mol  # 92GRE/FUG Calculated enthalpy of
reaction        U(SO4)2:8H2O
#       Enthalpy of formation:  -4662.6 kJ/mol

# US2(cr)
#       US2 +2.0000 H+  =  + 1.0000 U+4 + 2.0000 HS-
#        log_k           -2.43  #92GRE/FUG
#       -delta_H        -103.400        kJ/mol  # Calculated enthalpy of
reaction        US2
#       Enthalpy of formation:  -520.4 kJ/mol

UO3(a)
       UO3 +2.0000 H+  =  + 1.0000 H2O + 1.0000 UO2+2
        log_k           9.52   #92GRE/FUG
        -delta_H        -92.420 kJ/mol  # 92GRE/FUG Calculated enthalpy of
reaction        UO3(alpha)
#       Enthalpy of formation:  -1212.41 kJ/mol

UO3(b)
       UO3 +2.0000 H+  =  + 1.0000 H2O + 1.0000 UO2+2
        log_k           8.30  #92GRE/FUG
        -delta_H        -84.530 kJ/mol  # #92GRE/FUG Calculated enthalpy of
reaction        UO3(beta)
#       Enthalpy of formation:  -1220.3 kJ/mol

UO3:0.9H2O
        UO3:0.9H2O +2.0000 H+  =  + 1.0000 UO2+2 + 1.9000 H2O
        log_k           5.00  #92GRE/FUG
        -delta_H        -55.777 kJ/mol  # #92GRE/FUG Calculated enthalpy of
reaction        Schoepite-dehy(.9)
#       Enthalpy of formation:  -1506.3 kJ/mol
```

```
UO3:2H2O
        UO3:2H2O +2.0000 H+  =  + 1.0000 UO2+2 + 3.0000 H2O
        log_k           5.96    #92SAN/BRU APPROPPRIATED FOR GEOCH. CALC.
        -delta_H        0       kJ/mol  # Calculated NOT POSSIBLE TO
CALCULATE       Schoepite

UO2(OH)2(b)
       UO2(OH)2 +2.0000 H+  =  + 1.0000 UO2+2 + 2.0000 H2O
        log_k           4.93   #92GRE/FUG
        -delta_H        -56.860 kJ/mol  # 92GRE/FUG Calculated enthalpy of
reaction        UO2(OH)2(beta)
#       Enthalpy of formation:  -1533.8 kJ/mol

UO2CO3(cr)
        UO2CO3  =  + 1.0000 CO3-2 + 1.0000 UO2+2
        log_k           -14.63  #03GUI/FAN
        -delta_H        -2.929  kJ/mol  # Calculated enthalpy of reaction
        Rutherfordine
#       Enthalpy of formation:  -1691.301 kJ/mol

UO2(CO3)3Mg2:18H2O
       UO2(CO3)3Mg2:18H2O  =  + 1.0000 UO2+2 + 3.0000 CO3-2 + 2.0000 Mg+2 +
18.0000 H2O
        log_k           -29.01
        -delta_H        40.570  kJ/mol
#       Enthalpy of formation:  -9164.200 kJ/mol

UO2(CO3)3Na4
       UO2(CO3)3Na4  =  + 1.0000 UO2+2 + 3.0000 CO3-2 + 4.0000 Na+
        log_k           -26.94
        -delta_H        0               # Not possible to calculate
enthalpy of reaction    Na4UO2(CO3)3
#       Enthalpy of formation:  0 kcal/mol

USiO4(cr)_nea
        USiO4 + 4 H+ = U+4 + Si(OH)4
        log_k -8.06     #92GRE/FUG
        -delta_H -56.833                #calc. DGf i Sf de 92GRE/FUG
#       Enthalpy of formation:  0 kcal/mol

USiO4(am)
        USiO4 + 4 H+ = U+4 + Si(OH)4
        log_k -1.5         #veure skb-tdb
        -delta_H        0       #
#       Enthalpy of formation:  0 kcal/mol

Ca(UO2)2(SiO3OH)2.5aqnat(3)
        Ca(UO2)2(SiO3OH)2:5H2O + 6H+ = Ca+2 + 2 UO2+2 + 2 Si(OH)4 + 5 H2O
        log_k 9.42 #92NGU/SIL aquesta Ès la seleccionada
```

```
        -delta_H 0
#       Enthalpy of formation:  0 kcal/mol

Soddyite(2)
        (UO2)2SiO4:2H2O  + 4 H+ = 2UO2+2 + Si(OH)4 + 2 H2O
        log_k 3.90                      #97PER/CAS aquesta Ès la que fem
servir als c‡lculs
        -delta_H 0
#       Enthalpy of formation:  0 kcal/mol

Soddyite(3)
        (UO2)2SiO4:2H2O  + 4 H+ = 2UO2+2 + Si(OH)4 + 2 H2O
        log_k 5.74                      #92NGU/SIL
        -delta_H 0
#       Enthalpy of formation:  0 kcal/mol

U(HPO4)2.4aq
        U(HPO4)2:4H2O + 2 H+ = U+4 + 2 H2PO4- + 4H2O
        log_k -16.07                    #92GRE/FUG
        -delta_H -4.902 kJ/mol          #calc. logK i Sf de 92GRE/FUG
#       Enthalpy of formation:  -4334.819 kcal/mol

(UO2)(HPO4).4aq (cr)
        UO2(HPO4):4H2O + H+ = UO2+2 + H2PO4- + 4 H2O
        log_k -4.64                     #92GRE/FUG
        -delta_H 5.048 kJ/mol           #calc. logK i Sf de 92GRE/FUG
#       Enthalpy of formation:  -3469.968 kcal/mol

(UO2)3(PO4)2:6aq
        (UO2)3(PO4)2:6H2O + 4H+ = 3 UO2+2 + 2 H2PO4- + 6 H2O
        log_k -11.07                    #calc. DGf de 92GRE/FUG
        -delta_H 0 kJ/mol
#       Enthalpy of formation:  0 kcal/mol

(UO2)3(PO4)2:4aq(cr)
        (UO2)3(PO4)2:4H2O + 4 H+ = 3 UO2+2 + 2 H2PO4- + 4 H2O
        log_k -14.15                    #92SAN/BRU
        -delta_H 0            #not possible to calculate
#       Enthalpy of formation:

(UO2)3(PO4)2(cr)
        (UO2)3(PO4)2 + 4H+ = 3 UO2+2 + 2 H2PO4-
        log_k 2.80                      #calc. DHf i Sf de 92GRE/FUG
        -delta_H -170.900 kJ/mol              #calc. DHf i Sf de 92GRE/FUG
#       Enthalpy of formation:  0 kcal/mol

(UO2)(SO3)(cr)
        (UO2)(SO3)= UO2+2 + SO3-2
        log_k -15.83                    #calc. DHf i Sf de 92GRE/FUG
        -delta_H +6.450 kJ/mol        #calc. DHf i Sf de 92GRE/FUG
```

```
#       Enthalpy of formation:  -1661.0 kcal/mol

UO2(SO4):2.5aq cr
        UO2(SO4):2.5H2O = UO2+2 + SO4-2 + 2.5 H2O
        log_k -1.59                     #calc. DGf i DHf de 92GRE/FUG
        -delta_H -35.915 kJ/mol       #calc. DGf i DHf de 92GRE/FUG
#       Enthalpy of formation:  0 kcal/mol

UO2(SO4):3.5aq cr
        UO2(SO4):3.5H2O = UO2+2 + SO4-2 + 3.5 H2O
        log_k -1.59                     #calc. DGf i DHf de 92GRE/FUG
        -delta_H -27.145 kJ/mol       #calc. DGf i DHf de 92GRE/FUG
#       Enthalpy of formation:  2901.6 kcal/mol

UO2(SO4):3aq cr
        UO2(SO4):3H2O = UO2+2 + SO4-2 + 3H2O
        log_k -1.50                     #calc. DGf i DHf de 92GRE/FUG
        -delta_H -34.330 kJ/mol       #calc. DGf i DHf de 92GRE/FUG
#       Enthalpy of formation:  -2751.5 kcal/mol

UO2(SO4) cr
        UO2(SO4) = UO2+2 + SO4-2
        log_k 1.89               #calc. DHf i Sf de 92GRE/FUG
        -delta_H -83.200 kJ/mol       #calc. DHf i Sf de 92GRE/FUG
#       Enthalpy of formation:  -1845.14 kcal/mol

(U2O7)Na2 s
        U2O7Na2 + 6H+ = 2 UO2+2 + 3H2O + 2Na+
        log_k 22.60              #calc. DHf i Sf de 92GRE/FUG
        -delta_H -172.370 kJ/mol              #calc. DHf i Sf de 92GRE/FUG


(UO4)Ba s
        UO4Ba + 4H+ = UO2+2 + Ba+2 + 2 H2O
        log_k 17.64                             #calc. DHf i Sf de 92GRE/
FUG
        -delta_H -131.660 kJ/mol              #calc. DHf i Sf de 92GRE/FUG


(UO4)Ca(s)
        UO4Ca + 4H+ = UO2+2 + Ca+2 + 2 H2O
        log_k 15.93                                     #calc. DHf i Sf de
92GRE/FUG
        -delta_H -131.360 kJ/mol              #calc. DHf i Sf de 92GRE/FUG

(UO4)Li2 s
        UO4Li2 + 4H+ = UO2+2 + 2 Li+ + 2 H2O
        log_k 27.94                                     #calc. DHf i Sf de
92GRE/FUG
        -delta_H -179.400 kJ/mol              #calc. DHf i Sf de 92GRE/FUG
```

```
(UO4)Mg s
        UO4Mg + 4H+ = UO2+2 + Mg+2 + 2 H2O
        log_k 23.23                                     #calc. DHf i Sf de
92GRE/FUG
        -delta_H -200.360 kJ/mol              #calc. DHf i Sf de 92GRE/FUG


(UO4)Na2 s
        UO4Na2 + 4H+ = UO2+2 + 2 Na+ + 2 H2O
        log_k 30.03                                     #calc. DHf i Sf de
92GRE/FUG
        -delta_H -173.640 kJ/mol              #calc. DHf i Sf de 92GRE/FUG
#       Enthalpy of formation:  0 kcal/mol

(UO4)Sr s
        UO4Sr + 4H+ = UO2+2 + Sr+2 + 2 H2O
        log_k 19.16                                     #calc. DHf i Sf de
92GRE/FUG
        -delta_H -151.960 kJ/mol              #calc. DHf i Sf de 92GRE/FUG
#       Enthalpy of formation:  0 kcal/mol

Becquerelite(syn)
        Ca(UO2)6O4(OH)6:8H2O + 14 H+ = Ca+2 + 6 UO2+2 + 18 H2O
        log_k 40.5                                      #03GUI/FAN
        -delta_H 0
#       Enthalpy of formation:  0 kcal/mol

Becquerelite(nat)
        Ca(UO2)6O4(OH)6:8H2O + 14 H+ = Ca+2 + 6 UO2+2 + 18 H2O
        log_k 29.00                                     #97CAS/BRU
        -delta_H -378.310 kJ/mol              #calc. logK de 97CAS/BRU i
DHf estimada segons 99CHE/EWI
#       Enthalpy of formation:  -11423.63 kcal/mol

Zr
       Zr  =  + 4.0000 e- + 1.0000 Zr+4
        log_k           92.06                   # calculated internally, Sf
75DOB
        -delta_H        -560.194        kJ/mol  # calculated internally, Sf
75DOB
#       Enthalpy of formation:  0 kJ/mol        # reference state

Zr(OH)4(alpha)
       Zr(OH)4 + 4.0000 H+  =  + 4.0000 H2O + 1.0000 Zr+4
        log_k           -0.14                   # calculated in 03DOM/DUR
        -delta_H        0                               # no data available
#       Enthalpy of formation:  0 kJ/mol        # no data available
```

```
Zr(OH)4(beta)
       Zr(OH)4 + 4.0000 H+  =  + 4.0000 H2O + 1.0000 Zr+4
        log_k           -2.77                   # calculated in 03DOM/DUR
        -delta_H        -41.613 kJ/mol          # calculated internally
#       Enthalpy of formation:  -1661.900 kJ/mol# 92SLO/KRI

ZrO2(s)
       ZrO2 + 4.0000 H+  =  + 2.0000 H2O + 1.0000 Zr+4
        log_k           -7.54                   # calculated internally, Sf
92SLO/KRI
        -delta_H        -31.294 kJ/mol          # calculated internally, Sf
92SLO/KRI
#       Enthalpy of formation:  -1100.560 kJ/mol# 67KOR/USH

ZrSiO4(s)
       ZrSiO4 + 4.0000 H+  =  + 1.0000 Si(OH)4 + 1.0000 Zr+4
        log_k           -15.85                  # calculated internally,
DGf 76SCH/VER, Sf average reported entropies 03DOM/DUR
        -delta_H        20.858  kJ/mol          # calculated internally,
DGf 76SCH/VER, Sf average reported entropies 03DOM/DUR
#       Enthalpy of formation:  -2038.012 kJ/mol # calculated internally,
DGf 76SCH/VER, Sf average reported entropies 03DOM/DUR

Zr(SO3)2(cr)
       Zr(SO3)2   =  + 2.0000 SO3-2 + 1.0000 Zr+4
        log_k           -58.06                  # Brown et al. 2005
#       -delta_H                kJ/mol        # Not revised
#       Enthalpy of formation:  kJ/mol

Zr(SO4)2(cr)
       Zr(SO4)2   =  + 2.0000 SO4-2 + 1.0000 Zr+4
        log_k           1.24                    # Brown et al. 2005
#       -delta_H                kJ/mol        # Not revised
#       Enthalpy of formation:  kJ/mol

Zr(SO4)2:4H2O
       Zr(SO4)2:4H2O   =  + 2.0000 SO4-2 + 1.0000 Zr+4  +4.000H2O
        log_k           -7.65                   # Brown et al. 2005
#       -delta_H                kJ/mol        # Not revised
#       Enthalpy of formation:  kJ/mol


ZrS1.5(cr)
       ZrS1.5 + 1.5000 H+  =  + 1.5000 HS- + 1.0000 Zr+4        +1.000e-
        log_k           1.41                    # Brown et al. 2005
#       -delta_H                kJ/mol        # Not revised
#       Enthalpy of formation:  kJ/mol

ZrS2(cr)
       ZrS2 + 2.0000 H+  =  + 2.0000 HS- + 1.0000 Zr+4
```

```
        log_k           -10.81          # Brown et al. 2005
#       -delta_H                kJ/mol        # Not revised
#       Enthalpy of formation:  kJ/mol

ZrS3(cr)
       ZrS3 + 3.0000 H+ +2.000e-  =  + 3.0000 HS- + 1.0000 Zr+4
        log_k           -19.30          # Brown et al. 2005
#       -delta_H                kJ/mol        # Not revised
#       Enthalpy of formation:  kJ/mol


ZrCl(cr)
       ZrCl  =  + 1.0000 Cl- + 1.0000 Zr+4 + 3.00 e-
        log_k           67.17                   # calculated internally,
DHf, Sf 97VIS/COR
        -delta_H        -427.274        kJ/mol  # calculated internally,
DHf, Sf 97VIS/COR
#       Enthalpy of formation:  -300.000 kJ/mol # 97VIS/COR

ZrCl2(cr)
       ZrCl2  =  + 2.0000 Cl- + 1.0000 Zr+4 + 2.00 e-
        log_k           53.51                   # calculated internally,
DHf, Sf 97VIS/COR
        -delta_H        -363.354        kJ/mol  # calculated internally,
DHf, Sf 97VIS/COR
#       Enthalpy of formation:  -531.000 kJ/mol # 97VIS/COR

ZrCl3(cr)
       ZrCl3  =  + 3.0000 Cl- + 1.0000 Zr+4 + 1.00 e-
        log_k           40.31                   # calculated internally,
DHf, Sf 97VIS/COR
        -delta_H        -302.034        kJ/mol  # calculated internally,
DHf, Sf 97VIS/COR
#       Enthalpy of formation:  -759.400 kJ/mol # 97VIS/COR

ZrCl4(cr)
       ZrCl4  =  + 4.0000 Cl- + 1.0000 Zr+4
        log_k           27.98                   # calculated internally,
DHf, Sf 97VIS/COR
        -delta_H        -247.514        kJ/mol  # calculated internally,
DHf, Sf 97VIS/COR
#       Enthalpy of formation:  -981.000 kJ/mol # 97VIS/COR

ZrF(cr)
       ZrF  =  + 1.0000 F- + 1.0000 Zr+4 + 3.00 e-
        log_k           62.09                   # calculated internally,
DHf, Sf 97VIS/COR
        -delta_H        -417.544        kJ/mol  # calculated internally,
DHf, Sf 97VIS/COR
#       Enthalpy of formation:  -478.000 kJ/mol # 97VIS/COR
```

```
ZrF2(cr)
       ZrF2  =  + 2.0000 F- + 1.0000 Zr+4 + 2.00 e-
        log_k           31.03                   # calculated internally,
DHf, Sf 97VIS/COR
        -delta_H        -268.894        kJ/mol  # calculated internally,
DHf, Sf 97VIS/COR
#       Enthalpy of formation:  -962.000 kJ/mol # 97VIS/COR

ZrF3(cr)
       ZrF3  =  + 3.0000 F- + 1.0000 Zr+4 + 1.00 e-
        log_k           2.30                    # calculated internally,
DHf, Sf 97VIS/COR
        -delta_H        -133.244        kJ/mol  # calculated internally,
DHf, Sf 97VIS/COR
#       Enthalpy of formation:  -1433.000 kJ/mol# 97VIS/COR
ZrF4(cr)
       ZrF4  =  + 4.0000 F- + 1.0000 Zr+4
        log_k           -27.75                  # calculated internally,
DHf, Sf 97VIS/COR
        -delta_H        9.706   kJ/mol          # calculated internally,
DHf, Sf 97VIS/COR
#       Enthalpy of formation:  -1911.300 kJ/mol# 97VIS/COR

CaZrO3(s)
        CaZrO3 + 6.000 H+ = 1.000 Ca+2 + 1.000 Zr+4 + 3.0000 H2O
        log_k           19.05                   # calculated internally,
DHf, Sf 91YOK/SAK
        -delta_H        -193.784        kJ/mol  # calculated internally,
DHf, Sf 91YOK/SAK
#       Enthalpy of formation:  -1766.900 kJ/mol# 91YOK/SAK

BaZrO3(s)
        BaZrO3 + 6.000 H+ = 1.000 Ba+2 + 1.000 Zr+4 + 3.0000 H2O
        log_k           17.54                   # calculated internally,
DHf, Sf 91YOK/SAK
        -delta_H        -172.984        kJ/mol  # calculated internally,
DHf, Sf 91YOK/SAK
#       Enthalpy of formation:  -1779.500 kJ/mol# 91YOK/SAK

Ba2ZrO4(s)
        Ba2ZrO4 + 8.000 H+ = 2.000 Ba+2 + 1.000 Zr+4 + 4.0000 H2O
        log_k           61.23                   # calculated internally,
DHf, Sf 91YOK/SAK
        -delta_H        -422.114        kJ/mol  # calculated internally,
DHf, Sf 91YOK/SAK
#       Enthalpy of formation:  -2351.000 kJ/mol# 91YOK/SAK

SrZrO3(s)
        SrZrO3 + 6.000 H+ = 1.000 Sr+2 + 1.000 Zr+4 + 3.0000 H2O
```

```
        log_k           20.87                   # calculated internally,
DHf, Sf 91YOK/SAK
        -delta_H        -201.284        kJ/mol  # calculated internally,
DHf, Sf 91YOK/SAK
#       Enthalpy of formation:  -1767.300 kJ/mol# 91YOK/SAK

Sr2ZrO4(s)
        Sr2ZrO4 + 8.000 H+ = 2.000 Sr+2 + 1.000 Zr+4 + 4.0000 H2O
        log_k           61.98                   # calculated internally,
DHf, Sf 91YOK/SAK
        -delta_H        -440.714        kJ/mol  # calculated internally,
DHf, Sf 91YOK/SAK
#       Enthalpy of formation:  -2364.600 kJ/mol# 91YOK/SAK

Sr3Zr2O7(s)
        Sr3Zr2O7 + 14.000 H+ = 3.000 Sr+2 + 2.000 Zr+4 + 7.0000 H2O
        log_k           82.06                   # calculated internally,
DHf, Sf 91YOK/SAK
        -delta_H        -637.498        kJ/mol  # calculated internally,
DHf, Sf 91YOK/SAK
#       Enthalpy of formation:  -4136.400 kJ/mol# 91YOK/SAK

Sr4Zr3O10(s)
        Sr4Zr3O10 + 20.000 H+ = 4.000 Sr+2 + 3.000 Zr+4 + 10.0000 H2O
        log_k           102.48                  # calculated internally,
DHf, Sf 91YOK/SAK
        -delta_H        -836.281        kJ/mol  # calculated internally,
DHf, Sf 91YOK/SAK
#       Enthalpy of formation:  -5906.200 kJ/mol# 91YOK/SAK


# PMATCH GASES

CH4(g)
CH4                     =  +1.000CH4
    log_k      -2.8565
    delta_h   -13.7966
#    -a_e   -7.806599E+01 -6.229365E-05  3.957200E+03  2.503828E+01
-0.000000E+00

CO2(g)
CO2                     =  +1.000H+                    -1.000H2O
+1.000HCO3-
    log_k      -7.8198
    delta_h   -10.8748
#    -a_e   -2.479229E+02 -4.106888E-02  1.491484E+04  8.638236E+01
-1.015550E+06

H2(g)
H2                      =  +1.000H2
```

```
    log_k      -3.1056
    delta_h    -4.0394
#    -a_e   -7.645288E+01 -6.533210E-03  3.037284E+03  2.631230E+01
-0.000000E+00

N2(g)
N2                      =  +1.000N2
    log_k      -3.1864
    delta_h   -10.4374
#    -a_e   -6.990691E+01  3.663863E-03  3.662355E+03  2.155827E+01
-0.000000E+00

O2(g)
O2                      =  +1.000O2
    log_k      -2.8944
    delta_h   -12.0593
#    -a_e   -6.096651E+01  4.101330E-03  3.376712E+03  1.839764E+01
-0.000000E+00

 H2S(g)
 H2S                     =  +1.000HS-                  +1.000H+
    log_k      -8.0100       #Grenthe et al. (1992)
#    delta_h     4.3000      #Hf not reviewed
#    -a_e   -7.256659E+00 -0.000000E+00 -2.246086E+02 -0.000000E+00
0.000000E+00

 SO2(g)
 SO2            +5.000H+                +6.000e-                    =
+1.000HS-                  +2.000H2O
    log_k      28.37       #Grenthe et al. (1992)
#    delta_h            #not reviewed
#       Enthalpy of formation: kJ/mol


END
```