Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) mbH

Forschungsvorhaben

Chemisch-toxische Stoffe in einem Endlager für hochradioaktive Abfälle

Kurztitel: CHEMOTOX

AP V: Methoden der Stoffbewertung und Identifizierung relevanter Stoffe, Anlagen

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Autoren dieses Berichts:

Horst-Jürgen Herbert (GRS mbH)

Helge Moog (GRS mbH)

Mingliang Xie (GRS mbH)

Federführung des Arbeitspakets AP V:

GRS mbH

Koordinator des Forschungsprojekts:

Öko-Institut e.V.

Kooperationspartner des Verbundprojekts:

DBE TECHNOLOGY GmbH

GRS mbH

Öko-Institut e.V.

GRS mbH
Theodor-Heuss-Str. 4
38122 Braunschweig
Telefon +49 (0) 531 – 8012 – 0
Fax +49 (0) 531 – 80 12 - 200

AP V: Methoden der Stoffbewertung und Identifizierung relevanter Stoffe, Anlagen

Das diesem Bericht zugrunde liegende FE-Vorhaben wurde im Auftrag des Bundesministeriums für Wirtschaft und Technologie unter den Kennzeichen 02E10387, 02E10397 und 02E10407 durchgeführt. Die Verantwortung für den Inhalt dieser Veröffentlichung liegt bei den Autoren.

Anlagenverzeichnis

Anlage 1: Verwendete thermodynamische Datenbasis

```
################################################################################
 Date:                January 2009
 Editor:              Moog (GRS)
 Serial No:           tdb-hmw-118.1.1.1
 Status:              For internal use only
********************************************************************************
### Source
This parameterfile was created from tdb-hmw-118#1.xls

### Purpose
Calculate reaction of BSK3+3SF with Opalinus, saturated NaCl- and IP21-
solution.

### Data
It contains the most recent values for
- Pitzer parameters
-- for the oceanic system (data0,hmw)
-- for radionulclide (INE)
-- Si, Al: Reardon, E, J, (1990): An ion interaction model for the determination of
      chemical equilibria in cement/water systems, Cement and Concrete Research (20),
      175-192,
-- Zn (KODA), I, Se (ISe-project), and Fe (FeS-project)
- Gibbs energies of formation
-- from the Chemical Thermodynamics series (NEA)
-- calculated from solubility constants (INE)
-- calculated from data in KODA
Some solids were added from a database for Geochemist's Workbench
Some addional elements …
For detailed information please consult the references below.

There is a strong probability that data in this file are in part inconsistent. One
      example is, that carbonate data originate in part from the
HMW-database including Pitzer parameters, others were taken from different sources.

###History of changes
118,1,1,1
First version issued

###References
1     CO2(g)
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = -394373 +/- 133, Reference: NEA-9
      V0 [cm3 mol-1] =  +/- unknown, Reference:
      Remark: dG^0_f value adopted from NEA-9 deviates from that given in data0,ypf
      (for 298,15 K) by 36 J only
2     H2
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = 0 +/- , Reference: by convention
      V0 [cm3 mol-1] =  +/- unknown, Reference:
      Remark:
```

```
3     H2O(g)
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = -228582 +/- 40, Reference: NEA-6
      V0 [cm3 mol-1] =  +/- unknown, Reference:
      Remark:
4     H2S(g)
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = -33443 +/- 500, Reference: NEA-6
      V0 [cm3 mol-1] =  +/- unknown, Reference:
      Remark:
5     O2(g)
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = 0 +/- unknown, Reference: by convention
      V0 [cm3 mol-1] =  +/- unknown, Reference:
      Remark:
6     Hg(g)
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = 31842 +/- 54, Reference: NEA-7
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
7     I2(g)
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = 19323 +/- 120, Reference: NEA-6
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
8     H2Se(g)
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = 15217 +/- 2003, Reference: NEA-7
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
##AQUEOUS
1     H2O
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = -237140 +/- 41, Reference: NEA-9
      V0 [cm3 mol-1] = 18,06862038 +/- unknown, Reference: HbChemPhys
      Remark:
2     H<+>
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = 0 +/- unknown, Reference: by convention
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
3     OH<->
      Gibbs Free Energy of Formation calculated from logK for reaction
      deltaG_0^f [J mol-1] = -157246,238 +/- unknown, Reaction: 0 = +1OH<->+1H<+>-
      1H2O, logK(298,15K) = -13,9967 +/- unknown, Reference: HMW
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
4     O2(aq)
      Gibbs Free Energy of Formation calculated from logK for reaction
```

```
      deltaG_0^f [J mol-1] = 16543,62 +/- unknown, Reaction: 0 = +1O2(aq)+1O2(g),
      logK(298,15K) = -2,8983 +/- , Reference:
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
5     (CO2)<0>
      Gibbs Free Energy of Formation calculated from logK for reaction
      deltaG_0^f [J mol-1] = -385879,15 +/- unknown, Reaction: 0 = +1(CO2)<0>+1H2O-
      1H<+>-1(HCO3)<->, logK(298,15K) = 6,3374 +/- unknown, Reference: HMW
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
6     (CO3)<2->
      Gibbs Free Energy of Formation calculated from logK for reaction
      deltaG_0^f [J mol-1] = -527827,834 +/- unknown, Reaction: 0 = +1(CO3)<2-
      >+1H<+>-1(HCO3)<->, logK(298,15K) = -10,3393 +/- unknown, Reference: HMW
      V0 [cm3 mol-1] = -4,07 +/- unknown, Reference: KPP1996
      Remark:
7     (HCO3)<->
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = -586845 +/- 251, Reference: NEA-9
      V0 [cm3 mol-1] = 24,38 +/- unknown, Reference: KPP1996
      Remark:
8     (HSO4)<->
      Gibbs Free Energy of Formation calculated from logK for reaction
      deltaG_0^f [J mol-1] = -755297,933 +/- unknown, Reaction: 0 = +1(HSO4)<->-
      1H<+>-1(SO4)<2->, logK(298,15K) = 1,9786 +/- unknown, Reference: HMW
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
9     (SO4)<2->
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = -744004 +/- 418, Reference: NEA-5
      V0 [cm3 mol-1] = 14,18 +/- unknown, Reference: KPP1996
      Remark:
10    Ca(CO3)<0>
      Gibbs Free Energy of Formation calculated from logK for reaction
      deltaG_0^f [J mol-1] = -1098621,589 +/- unknown, Reaction: 0 =
      +1Ca(CO3)<0>+1H<+>-1Ca<2+>-1(HCO3)<->, logK(298,15K) = -7,188 +/- unknown,
      Reference: HMW
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
11    Ca<2+>
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = -552806 +/- 1050, Reference: NEA-5
      V0 [cm3 mol-1] = -18,03 +/- unknown, Reference: KPP1996
      Remark:
12    Cl<->
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = -131217 +/- 117, Reference: NEA-5
      V0 [cm3 mol-1] = 17,82 +/- unknown, Reference: KPP1996
      Remark:
13    K<+>
      Gibbs Free Energy of Formation directly entered
```

deltaG_0^f [J mol-1] = -282510 +/- 116, Reference: NEA-5

V0 [cm3 mol-1] = 9,02 +/- unknown, Reference: KPP1996

Remark:

14 Mg(CO3)<0>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -999918,837 +/- unknown, Reaction: 0 = +1Mg(CO3)<0>+1H<+>-1(HCO3)<->-1Mg<2+>, logK(298,15K) = -7,4108 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = dummy value 0,001

Remark:

15 Mg(OH)<+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -625108,153 +/- unknown, Reaction: 0 = +1Mg(OH)<+>+1H<+>-1H2O-1Mg<2+>, logK(298,15K) = -11,8091 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = dummy value 0,001

Remark:

16 Mg<2+>

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -455375 +/- 1335, Reference: NEA-5

V0 [cm3 mol-1] = -21,56 +/- unknown, Reference: KPP1996

Remark:

17 Na<+>

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -261953 +/- 96, Reference: NEA-5

V0 [cm3 mol-1] = -1,2 +/- unknown, Reference: KPP1996

Remark:

18 H2S<0>

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -27648 +/- 2115, Reference: NEA-6

V0 [cm3 mol-1] = dummy value 0,001

Remark:

19 HS<->

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = 12243 +/- 2115, Reference: NEA-6

V0 [cm3 mol-1] = dummy value 0,001

Remark:

20 H2SiO4<2->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1178373,256 +/- unknown, Reaction: 0 = +1H2SiO4<2->+2H<+>-1SiO2<0>-2H2O, logK(298,15K) = -22,9119 +/- unknown, Reference: INTGRS

V0 [cm3 mol-1] = dummy value 0,001

Remark: Grambow-Data0

21 H3SiO4<->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1253139,483 +/- unknown, Reaction: 0 = +1H3SiO4<->+1H<+>-1SiO2<0>-2H2O, logK(298,15K) = -9,8135 +/- unknown, Reference: INTGRS

V0 [cm3 mol-1] = dummy value 0,001

Remark: Grambow-Data0

22 SiO2<0>

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -834875,36 +/- unknown, Reference: Solids_j_Mg_TJW_1,xls

V0 [cm3 mol-1] = dummy value 0,001

Remark:

23 Al(OH)4<->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1313595,61 +/- unknown, Reaction: 0 = +1Al(OH)4<->+4H<+>-1Al<3+>-4H2O, logK(298,15K) = -22,1567 +/- unknown, Reference: REA90

V0 [cm3 mol-1] = dummy value 0,001

Remark:

24 Al<3+>

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -491507 +/- 3338, Reference: NEA-5

V0 [cm3 mol-1] = dummy value 0,001

Remark:

25 Pb<2+>

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -24238 +/- 399, Reference: NEA-5

V0 [cm3 mol-1] = dummy value 0,001

Remark:

26 Fe<2+>

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -90500 +/- 1000, Reference: PK1995

V0 [cm3 mol-1] = dummy value 0,001

Remark: referenced value for 1 atm

27 Fe<3+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = 72395,235 +/- 1100, Reaction: 0 = +1Fe<3+>+0,5H2O-0,25O2(g)-1Fe<2+>-1H<+>, logK(298,15K) = -7,7654 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = dummy value 0,001

Remark: referenced value for 1 atm

28 Am|+II|<2+>

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -376780 +/- 15236, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

29 Am|+III|(CO3)<+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1172190,176 +/- 5289, Reaction: 0 = +1Am|+III|(CO3)<+>-1Am|+III|<3+>-1(CO3)<2->, logK(298,15K) = 8 +/- 0,4, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

30 Am|+III|(CO3)2<->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1727987,419 +/- 5911, Reaction: 0 = +1Am|+III|(CO3)2<->-1Am|+III|<3+>-2(CO3)<2->, logK(298,15K) = 12,9 +/- 0,6, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

31 Am|+III|(CO3)3<3->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2267802,143 +/- 7521, Reaction: 0 = +1Am|+III|(CO3)3<3->-1Am|+III|<3+>-3(CO3)<2->, logK(298,15K) = 15 +/- 1, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

32 Am|+III|(CO3)5<6->

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -3210230 +/- 7919, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

33 Am|+III|(H2PO4)<2+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1752974,128 +/- 5763, Reaction: 0 = +1Am|+III|(H2PO4)<2+>-1Am|+III|<3+>-1(H2PO4)<->, logK(298,15K) = 3 +/- 0,5, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

34 Am|+III|(HCO3)<2+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1203237,932 +/- 5060, Reaction: 0 = +1Am|+III|(HCO3)<2+>-1Am|+III|<3+>-1(HCO3)<->, logK(298,15K) = 3,1 +/- 0,3, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

35 Am|+III|(OH)<2+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -794740,092 +/- 5546, Reaction: 0 = +1Am|+III|(OH)<2+>+1H<+>-1Am|+III|<3+>-1H2O, logK(298,15K) = -7,2 +/- 0,5, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

36 Am|+III|(OH)2<+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -986786,555 +/- 6211, Reaction: 0 = +1Am|+III|(OH)2<+>+2H<+>-1Am|+III|<3+>-2H2O, logK(298,15K) = -15,1 +/- 0,7, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

37 Am|+III|(OH)3<0>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1160567,281 +/- 5547, Reaction: 0 = +1Am|+III|(OH)3<0>+3H<+>-1Am|+III|<3+>-3H2O, logK(298,15K) = -26,2 +/- 0,5, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

38 Am|+III|(SO4)<+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1361538,541 +/- 4849, Reaction: 0 = +1Am|+III|(SO4)<+>-1Am|+III|<3+>-1(SO4)<2->, logK(298,15K) = 3,3 +/- 0,15, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

39 Am|+III|(SO4)2<->

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      Gibbs Free Energy of Formation calculated from logK for reaction
      deltaG_0^f [J mol-1] = -2107825,758 +/- 4903, Reaction: 0 = +1Am|+III|(SO4)2<->-1Am|+III|<3+>-2(SO4)<2->, logK(298,15K) = 3,7 +/- 0,15, Reference: FZK-INE 002/04
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
40    Am|+III|<3+>
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = -598698 +/- 4755, Reference: FZK-INE 002/04
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
41    Am|+III|Cl<2+>
      Gibbs Free Energy of Formation calculated from logK for reaction
      deltaG_0^f [J mol-1] = -731284,93 +/- 4759, Reaction: 0 = +1Am|+III|Cl<2+>-1Am|+III|<3+>-1Cl<->, logK(298,15K) = 0,24 +/- 0,03, Reference: FZK-INE 002/04
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
42    Am|+III|Cl2<+>
      Gibbs Free Energy of Formation calculated from logK for reaction
      deltaG_0^f [J mol-1] = -856908,048 +/- 4769, Reaction: 0 = +1Am|+III|Cl2<+>-1Am|+III|<3+>-2Cl<->, logK(298,15K) = -0,74 +/- 0,05, Reference: FZK-INE 002/04
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
43    Am|+IV|<4+>
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = -346358 +/- 8692, Reference: FZK-INE 002/04
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
44    (Am|+V|O2)(CO3)<->
      Gibbs Free Energy of Formation calculated from logK for reaction
      deltaG_0^f [J mol-1] = -1296734,852 +/- 6844, Reaction: 0 = +1(Am|+V|O2)(CO3)<->-1(Am|+V|O2)<+>-1(CO3)<2->, logK(298,15K) = 5,1 +/- 0,5, Reference: FZK-INE 002/04
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
45    (Am|+V|O2)(CO3)2<3->
      Gibbs Free Energy of Formation calculated from logK for reaction
      deltaG_0^f [J mol-1] = -1833695,554 +/- 7746, Reaction: 0 = +1(Am|+V|O2)(CO3)2<3->-1(Am|+V|O2)<+>-2(CO3)<2->, logK(298,15K) = 6,7 +/- 0,8, Reference: FZK-INE 002/04
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
46    (Am|+V|O2)(CO3)3<5->
      Gibbs Free Energy of Formation calculated from logK for reaction
      deltaG_0^f [J mol-1] = -2352390,52 +/- 8514, Reaction: 0 = +1(Am|+V|O2)(CO3)3<5->-1(Am|+V|O2)<+>-3(CO3)<2->, logK(298,15K) = 5,1 +/- 1, Reference: FZK-INE 002/04
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
47    (Am|+V|O2)<+>
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = -739796 +/- 6208, Reference: FZK-INE 002/04
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```
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
48    (Am|+VI|O2)<2+>
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = -585801 +/- 5715, Reference: FZK-INE 002/04
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
49    Am(SiO)(OH)3<2+>
      Gibbs Free Energy of Formation calculated from logK for reaction
      deltaG_0^f [J mol-1] = -1898263,848 +/- 5000, Reaction: 0 =
      +1Am(SiO)(OH)3<2+>+1H<+>-1Am|+III|<3+>-1SiO2<0>-2H2O, logK(298,15K) = -1,68 +/-
      0,18, Reference: FZK-INE 002/04
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
50    (AsO4)<3->
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = -647500 +/- unknown, Reference: /BPJ 1985/
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
51    (H2AsO4)<->
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = -748500 +/- unknown, Reference: /BPJ 1985/
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
52    (HAsO4)<2->
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = -707100 +/- unknown, Reference: /BPJ 1985/
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
53    H2AsO3<->
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = -587500 +/- unknown, Reference: /BPJ 1985/
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
54    HAsO2<0>
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = -402700 +/- unknown, Reference: /BPJ 1985/
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
55    B(OH)3<0>
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = -969268 +/- unknown, Reference: NTB 02-16
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
56    Ba<2+>
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = -557656 +/- 2582, Reference: NEA-7
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
57    Cd<2+>
```

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      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = -77733 +/- 750, Reference: NEA 9
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
58    CdSeO4<0>
      Gibbs Free Energy of Formation calculated from logK for reaction
      deltaG_0^f [J mol-1] = -530175,182 +/- 1652, Reaction: 0 = +1CdSeO4<0>-1Cd<2+>-
      1SeO4<2->, logK(298,15K) = 2,27 +/- 0,06, Reference: NEA-7
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
59    Cm(CO3)<+>
      Gibbs Free Energy of Formation calculated from logK for reaction
      deltaG_0^f [J mol-1] = -1169292,176 +/- unknown, Reaction: 0 = +1Cm(CO3)<+>-
      1Cm<3+>-1(CO3)<2->, logK(298,15K) = 8 +/- 0,4, Reference: FZK-INE 002/04
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
60    Cm(CO3)2<->
      Gibbs Free Energy of Formation calculated from logK for reaction
      deltaG_0^f [J mol-1] = -1725089,419 +/- unknown, Reaction: 0 = +1Cm(CO3)2<->-
      1Cm<3+>-2(CO3)<2->, logK(298,15K) = 12,9 +/- 0,6, Reference: FZK-INE 002/04
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
61    Cm(CO3)3<3->
      Gibbs Free Energy of Formation calculated from logK for reaction
      deltaG_0^f [J mol-1] = -2264904,143 +/- unknown, Reaction: 0 = +1Cm(CO3)3<3->-
      1Cm<3+>-3(CO3)<2->, logK(298,15K) = 15 +/- 1, Reference: FZK-INE 002/04
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
62    Cm(CO3)4<5->
      Gibbs Free Energy of Formation calculated from logK for reaction
      deltaG_0^f [J mol-1] = -2781315,891 +/- unknown, Reaction: 0 = +1Cm(CO3)4<5->-
      1Cm<3+>-4(CO3)<2->, logK(298,15K) = 13 +/- 0,5, Reference: FZK-INE 002/04
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
63    Cm(HCO3)<2+>
      Gibbs Free Energy of Formation calculated from logK for reaction
      deltaG_0^f [J mol-1] = -1200339,932 +/- unknown, Reaction: 0 = +1Cm(HCO3)<2+>-
      1Cm<3+>-1(HCO3)<->, logK(298,15K) = 3,1 +/- 0,3, Reference: FZK-INE 002/04
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
64    Cm(OH)<2+>
      Gibbs Free Energy of Formation calculated from logK for reaction
      deltaG_0^f [J mol-1] = -791842,092 +/- 6900, Reaction: 0 = +1Cm(OH)<2+>+1H<+>-
      1Cm<3+>-1H2O, logK(298,15K) = -7,2 +/- 0,5, Reference: FZK-INE 002/04
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
65    Cm(OH)2<+>
      Gibbs Free Energy of Formation calculated from logK for reaction
      deltaG_0^f [J mol-1] = -983888,555 +/- 7500, Reaction: 0 = +1Cm(OH)2<+>+2H<+>-
      1Cm<3+>-2H2O, logK(298,15K) = -15,1 +/- 0,7, Reference: FZK-INE 002/04
      V0 [cm3 mol-1] = dummy value 0,001
```

```
      Remark:
66    Cm(OH)3<0>
      Gibbs Free Energy of Formation calculated from logK for reaction
      deltaG_0^f [J mol-1] = -1157669,281 +/- 6900, Reaction: 0 = +1Cm(OH)3<0>+3H<+>-
      1Cm<3+>-3H2O, logK(298,15K) = -26,2 +/- 0,5, Reference: FZK-INE 002/04
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
67    Cm(SO4)<+>
      Gibbs Free Energy of Formation calculated from logK for reaction
      deltaG_0^f [J mol-1] = -1358640,541 +/- unknown, Reaction: 0 = +1Cm(SO4)<+>-
      1Cm<3+>-1(SO4)<2->, logK(298,15K) = 3,3 +/- 0,15, Reference: FZK-INE 002/04
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
68    Cm(SO4)2<->
      Gibbs Free Energy of Formation calculated from logK for reaction
      deltaG_0^f [J mol-1] = -2104927,758 +/- unknown, Reaction: 0 = +1Cm(SO4)2<->-
      1Cm<3+>-2(SO4)<2->, logK(298,15K) = 3,7 +/- 0,15, Reference: FZK-INE 002/04
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
69    Cm<3+>
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = -595800 +/- 6300, Reference: FZK-INE 002/04
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
70    CmCl<2+>
      Gibbs Free Energy of Formation calculated from logK for reaction
      deltaG_0^f [J mol-1] = -728386,93 +/- unknown, Reaction: 0 = +1CmCl<2+>-
      1Cm<3+>-1Cl<->, logK(298,15K) = 0,24 +/- 0,03, Reference: FZK-INE 002/04
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
71    CmCl2<+>
      Gibbs Free Energy of Formation calculated from logK for reaction
      deltaG_0^f [J mol-1] = -854010,048 +/- unknown, Reaction: 0 = +1CmCl2<+>-
      1Cm<3+>-2Cl<->, logK(298,15K) = -0,74 +/- 0,05, Reference: FZK-INE 002/04
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
72    Cm(SiO)(OH)3<2+>
      Gibbs Free Energy of Formation calculated from logK for reaction
      deltaG_0^f [J mol-1] = -1895365,848 +/- unknown, Reaction: 0 =
      +1Cm(SiO)(OH)3<2+>+1H<+>-1Cm<3+>-1SiO2<0>-2H2O, logK(298,15K) = -1,68 +/- 0,18,
      Reference: FZK-INE 002/04
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
73    Co<2+>
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = -53555,2 +/- unknown, Reference: /BPJ 1985/
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
74    Co(OH)2
      Gibbs Free Energy of Formation calculated from logK for reaction
```

```
      deltaG_0^f [J mol-1] = -634004,795 +/- unknown, Reaction: 0 = +1Co(OH)2-
      1Co<2+>-2H2O+2H<+>, logK(298,15K) = 18,6 +/- 0,4, Reference: Koda
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
75    Co(OH)3<->
      Gibbs Free Energy of Formation calculated from logK for reaction
      deltaG_0^f [J mol-1] = -945920,154 +/- unknown, Reaction: 0 = +1Co(OH)3<->-
      1Co<2+>-3H2O+3H<+>, logK(298,15K) = 31,7 +/- 0,5, Reference: Koda
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
76    Co(OH)4<2->
      Gibbs Free Energy of Formation calculated from logK for reaction
      deltaG_0^f [J mol-1] = -1267082,543 +/- unknown, Reaction: 0 = +1Co(OH)4<2->-
      1Co<2+>-4H2O+4H<+>, logK(298,15K) = 46,42 +/- 0,43, Reference: Koda
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
77    Co2(OH)<3+>
      Gibbs Free Energy of Formation calculated from logK for reaction
      deltaG_0^f [J mol-1] = -400360,46 +/- unknown, Reaction: 0 = +1Co2(OH)<3+>-
      2Co<2+>-1H2O+1H<+>, logK(298,15K) = 9,83 +/- 0,39, Reference: Koda
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
78    Co4(OH)4<4+>
      Gibbs Free Energy of Formation calculated from logK for reaction
      deltaG_0^f [J mol-1] = -1333337,116 +/- unknown, Reaction: 0 = +1Co4(OH)4<4+>-
      4Co<2+>-4H2O+4H<+>, logK(298,15K) = 29,88 +/- 0,35, Reference: Koda
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
79    CoOH<+>
      Gibbs Free Energy of Formation calculated from logK for reaction
      deltaG_0^f [J mol-1] = -343380,434 +/- unknown, Reaction: 0 = +1CoOH<+>-
      1Co<2+>+1H<+>-1H2O, logK(298,15K) = 9,23 +/- 0,72, Reference: Koda
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
80    Cr<3+>
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = -215000 +/- unknown, Reference: /BPJ 1985/
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
81    CrO4<2->
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = -727800 +/- unknown, Reference: /BPJ 1985/
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
82    Cs<+>
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = -291456 +/- 553, Reference: NEA 9
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
83    Cu<+>
      Gibbs Free Energy of Formation directly entered
```

deltaG_0^f [J mol-1] = 50300 +/- unknown, Reference: /BPJ/

V0 [cm3 mol-1] = dummy value 0,001

Remark:

84 Cu<2+>

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = 65700 +/- 1557, Reference: /BPJ/

V0 [cm3 mol-1] = dummy value 0,001

Remark:

85 Cu(CO3)2<2->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -931162,828 +/- unknown, Reaction: 0 = +1Cu(CO3)2<2->-1Cu<2+>-2(CO3)<2->, logK(298,15K) = -10,3 +/- 0,1, Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

86 Cu(HCO3)<->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -510642,201 +/- unknown, Reaction: 0 = +1Cu(HCO3)<->-1Cu<2+>-1(HCO3)<->, logK(298,15K) = -1,84 +/- 0,1, Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

87 Cu(OH)<+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -126061,06 +/- unknown, Reaction: 0 = +1Cu(OH)<+>+1H<+>-1Cu<2+>-1H2O, logK(298,15K) = -7,95 +/- 0,16, Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

88 Cu(OH)2(aq)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -316109,708 +/- unknown, Reaction: 0 = +1Cu(OH)2(aq)+2H<+>-1Cu<2+>-2H2O, logK(298,15K) = -16,2 +/- 0,2, Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

89 Cu(OH)3<->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -493886,064 +/- unknown, Reaction: 0 = +1Cu(OH)3<->+3H<+>-1Cu<2+>-3H2O, logK(298,15K) = -26,6 +/- 0,09, Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

90 Cu(OH)4<2->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -656022,382 +/- unknown, Reaction: 0 = +1Cu(OH)4<2->+4H<+>-1Cu<2+>-4H2O, logK(298,15K) = -39,74 +/- 0,18, Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

91 Cu2(OH)<3+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -69208,527 +/- unknown, Reaction: 0 = +1Cu2(OH)<3+>+1H<+>-2Cu<2+>-1H2O, logK(298,15K) = -6,4 +/- 0,12, Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

92 Cu2(OH)2<2+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -283345,114 +/- unknown, Reaction: 0 = +1Cu2(OH)2<2+>+2H<+>-2Cu<2+>-2H2O, logK(298,15K) = -10,43 +/- 0,07, Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

93 Cu3(OH)4<2+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -631020,299 +/- unknown, Reaction: 0 = +1Cu3(OH)4<2+>+4H<+>-3Cu<2+>-4H2O, logK(298,15K) = -21,1 +/- 0,2, Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

94 CuCO3<0>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -500657,122 +/- unknown, Reaction: 0 = +1CuCO3<0>-1Cu<2+>-1(CO3)<2->, logK(298,15K) = 6,75 +/- 0,03, Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

95 Hg<2+>

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = 164667 +/- 313, Reference: NEA-7

V0 [cm3 mol-1] = dummy value 0,001

Remark:

96 Hg2<2+>

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = 153567 +/- 559, Reference: NEA-7

V0 [cm3 mol-1] = dummy value 0,001

Remark:

97 Hg(OH)<+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -91880,345 +/- unknown, Reaction: 0 = +1Hg(OH)<+>+1H<+>-1Hg<2+>-1H2O, logK(298,15K) = 3,4 +/- 0,08, Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

98 Hg(OH)2

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -343747,095 +/- unknown, Reaction: 0 = +1Hg(OH)2+2H<+>-1Hg<2+>-2H2O, logK(298,15K) = 5,98 +/- 0,06, Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

99 Hg(OH)3<->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -667249,782 +/- unknown, Reaction: 0 = +1Hg(OH)3<->+3H<+>-1Hg<2+>-3H2O, logK(298,15K) = 21,11 +/- , Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

100 Hg(SeO3)2<2->

Gibbs Free Energy of Formation calculated from logK for reaction

```
      deltaG_0^f [J mol-1] = -644878,058 +/- 6291, Reaction: 0 = +1Hg(SeO3)2<2->-
      1HgSeO3-1SeO3<2->, logK(298,15K) = -1,35 +/- 0,15, Reference: NAE-7
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
101   HgSe2<2->
      Gibbs Free Energy of Formation calculated from logK for reaction
      deltaG_0^f [J mol-1] = 65334,758 +/- 5641, Reaction: 0 = +1HgSe2<2->+1H<+>-
      1HSe<->-1alpha-HgSe, logK(298,15K) = -12,8 +/- 0,6, Reference: NAE-7
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
102   I<->
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = -51724 +/- 112, Reference: NEA-6
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
103   IO3<->
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = -126338 +/- 779, Reference: NEA-6
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
104   Li<+>
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = -292918 +/- 0,109, Reference: NEA 9
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
105   Mn<2+>
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = -228100 +/- unknown, Reference: BPJ
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
106   MoO4<2->
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = -853535,058 +/- unknown, Reference: /DHH1976/
      V0 [cm3 mol-1] = dummy value 0,001
      Remark: DFG calculated from DFG=-204kcal/mol
107   (NH4)<+>
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = -79398 +/- unknown, Reference: /NEA-9/
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
108   NO3<->
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = -110794 +/- unknown, Reference: /NEA-9/
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
109   Nd<3+>
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = -672000 +/- unknown, Reference: BPJ
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
```

110 Ni<2+>

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -45773 +/- 771, Reference: NEA-6

V0 [cm3 mol-1] = dummy value 0,001

Remark:

111 HNi(P2O7)<->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2064270,34 +/- 4766, Reaction: 0 = +1HNi(P2O7)<->-1Ni<2+>-1(HP2O7)<3->, logK(298,15K) = 5,14 +/- 0,25, Reference: NEA-6

V0 [cm3 mol-1] = dummy value 0,001

Remark:

112 Ni(HPO4)<0>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1159167,53 +/- 1820, Reaction: 0 = +1Ni(HPO4)<0>-1Ni<2+>-1(HPO4)<2->, logK(298,15K) = 3,05 +/- 0,09, Reference: NEA-6

V0 [cm3 mol-1] = dummy value 0,001

Remark:

113 Ni(P2O7)<2->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2031107,213 +/- 4843, Reaction: 0 = +1Ni(P2O7)<2->-1Ni<2+>-1(P2O7)<4->, logK(298,15K) = 8,73 +/- 0,25, Reference:

V0 [cm3 mol-1] = dummy value 0,001

Remark:

114 Np|+III|(CO3)3<3->

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -2185950 +/- 15451, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

115 Np|+III|(OH)<2+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -711190,527 +/- 5922, Reaction: 0 = +1Np|+III|(OH)<2+>+1H<+>-1H2O-1Np|+III|<3+>, logK(298,15K) = -6,8 +/- 0,3, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

116 Np|+III|<3+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -512865,218 +/- 5669, Reaction: 0 = +1Np|+III|<3+>+1H<+>-0,5H2-1Np|+IV|<4+>, logK(298,15K) = 3,695 +/- 0,169, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

117 Np|+IV|(CO3)4<4->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2812456,343 +/- 8240, Reaction: 0 = +1Np|+IV|(CO3)4<4->-4(CO3)<2->-1Np|+IV|<4+>, logK(298,15K) = 36,68 +/- 1,06, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

118 Np|+IV|(CO3)5<6->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -3334176,571 +/- 8425, Reaction: 0 = +1Np|+IV|(CO3)5<6->-5(CO3)<2->-1Np|+IV|<4+>, logK(298,15K) = 35,61 +/- 1,1, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

119 Np|+IV|(OH)<3+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -732053,423 +/- 5702, Reaction: 0 = +1Np|+IV|(OH)<3+>+1H<+>-1H2O-1Np|+IV|<4+>, logK(298,15K) = 0,55 +/- 0,2, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

120 Np|+IV|(OH)2(CO3)2<2->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2118498,665 +/- unknown, Reaction: 0 = +1Np|+IV|(OH)2(CO3)2<2->+2OH<->-1Np|+IV|(OH)4(am)-2(CO3)<2->, logK(298,15K) = -11,75 +/- unknown, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

121 Np|+IV|(OH)2<2+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -968051,815 +/- 5844, Reaction: 0 = +1Np|+IV|(OH)2<2+>+2H<+>-2H2O-1Np|+IV|<4+>, logK(298,15K) = 0,35 +/- 0,3, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

122 Np|+IV|(OH)3<+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1187211,48 +/- 8000, Reaction: 0 = +1Np|+IV|(OH)3<+>+3H<+>-3H2O-1Np|+IV|<4+>, logK(298,15K) = -2,8 +/- 1, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

123 Np|+IV|(OH)4(CO3)<2->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1935130,532 +/- unknown, Reaction: 0 = +1Np|+IV|(OH)4(CO3)<2->-1(CO3)<2->-1Np|+IV|(OH)4(am), logK(298,15K) = -6,5 +/- 0,4, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

124 Np|+IV|(OH)4(CO3)2<4->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2460675,149 +/- unknown, Reaction: 0 = +1Np|+IV|(OH)4(CO3)2<4->-2(CO3)<2->-1Np|+IV|(OH)4(am), logK(298,15K) = -6,9 +/- 0,4, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

125 Np|+IV|(OH)4<0>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1392957,245 +/- 8409, Reaction: 0 = +1Np|+IV|(OH)4<0>+4H<+>-4H2O-1Np|+IV|<4+>, logK(298,15K) = -8,3 +/- 1,1, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

126 Np|+IV|(SO4)<2+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1274870,101 +/- 5809, Reaction: 0 = +1Np|+IV|(SO4)<2+>+1H<+>-1Np|+IV|<4+>-1(HSO4)<->, logK(298,15K) = 4,87 +/- 0,15, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

127 Np|+IV|(SO4)2<0>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2042839,89 +/- 6360, Reaction: 0 = +1Np|+IV|(SO4)2<0>+2H<+>-1Np|+IV|<4+>-2(HSO4)<->, logK(298,15K) = 7,09 +/- 0,25, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

128 Np|+IV|<4+>

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -491774 +/- 5586, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

129 Np|+IV|Cl<3+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -631553,064 +/- 5844, Reaction: 0 = +1Np|+IV|Cl<3+>-1Np|+IV|<4+>-1Cl<->, logK(298,15K) = 1,5 +/- 0,3, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

130 (Np|+V|O2)(CO3)<->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1463916,142 +/- 5652, Reaction: 0 = +1(Np|+V|O2)(CO3)<->-1(CO3)<2->-1(Np|+V|O2)<+>, logK(298,15K) = 4,962 +/- 0,061, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

131 (Np|+V|O2)(CO3)2(OH)<4->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2170298,338 +/- 8785, Reaction: 0 = +1(Np|+V|O2)(CO3)2(OH)<4->+1(CO3)<2->-1(Np|+V|O2)(CO3)3<5->-1OH<->, logK(298,15K) = 3,195 +/- 1,164, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

132 (Np|+V|O2)(CO3)2<3->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2000694,187 +/- 5685, Reaction: 0 = +1(Np|+V|O2)(CO3)2<3->-2(CO3)<2->-1(Np|+V|O2)<+>, logK(298,15K) = 6,53 +/- 0,1, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

133 (Np|+V|O2)(CO3)3<5->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2522642,737 +/- 5733, Reaction: 0 = +1(Np|+V|O2)(CO3)3<5->-3(CO3)<2->-1(Np|+V|O2)<+>, logK(298,15K) = 5,5 +/- 0,15, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

134 (Np|+V|O2)(HPO4)<->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2020588,726 +/- 5870, Reaction: 0 = +1(Np|+V|O2)(HPO4)<->-1(HPO4)<2->-1(Np|+V|O2)<+>, logK(298,15K) = 2,95 +/- 0,1, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

135 (Np|+V|O2)(HPO4)2<2->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -3042135,406 +/- 8598, Reaction: 0 = +1(Np|+V|O2)(HPO4)2<2->-2(HPO4)<2->-1(Np|+VI|O2)<2+>, logK(298,15K) = 9,5 +/- 1, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

136 (Np|+V|O2)(OH)<0>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1080404,117 +/- 6902, Reaction: 0 = +1(Np|+V|O2)(OH)<0>+1H<+>-1H2O-1(Np|+V|O2)<+>, logK(298,15K) = -11,3 +/- 0,7, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

137 (Np|+V|O2)(OH)2<->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1247335,192 +/- 6311, Reaction: 0 = +1(Np|+V|O2)(OH)2<->+2H<+>-2H2O-1(Np|+V|O2)<+>, logK(298,15K) = -23,6 +/- 0,5, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

138 (Np|+V|O2)(PO4)<2->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1973212,299 +/- unknown, Reaction: 0 = +1(Np|+V|O2)(PO4)<2->-1(PO4)<3->-1(Np|+V|O2)<+>, logK(298,15K) = 7 +/- 0,2, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

139 (Np|+V|O2)(SO4)<->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1654280,539 +/- 5850, Reaction: 0 = +1(Np|+V|O2)(SO4)<->-1(SO4)<2->-1(Np|+V|O2)<+>, logK(298,15K) = 0,44 +/- 0,27, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

140 (Np|+V|O2)<+>

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -907765 +/- 5628, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

141 (Np|+VI|O2)(CO3)<0>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1376965,792 +/- 6617, Reaction: 0 = +1(Np|+VI|O2)(CO3)<0>-1(CO3)<2->-1(Np|+VI|O2)<2+>, logK(298,15K) = 9,32 +/- 0,61, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

142 (Np|+VI|O2)(CO3)2<2->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1945868,701 +/- 7033, Reaction: 0 = +1(Np|+VI|O2)(CO3)2<2->-2(CO3)<2->-1(Np|+VI|O2)<2+>, logK(298,15K) = 16,516 +/- 0,729, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

143 (Np|+VI|O2)(CO3)3<4->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2489992,732 +/- 5759, Reaction: 0 = +1(Np|+VI|O2)(CO3)3<4->-1(Np|+V|O2)(CO3)3<5->, logK(298,15K) = -5,72 +/- 0,095, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

144 (Np|+VI|O2)(H2PO4)<+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1952041,702 +/- 6491, Reaction: 0 = +1(Np|+VI|O2)(H2PO4)<+>-1(H2PO4)<->-1(Np|+VI|O2)<2+>, logK(298,15K) = 3,32 +/- 0,5, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

145 (Np|+VI|O2)(HPO4)<0>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1927313,865 +/- 7067, Reaction: 0 = +1(Np|+VI|O2)(HPO4)<0>-1(HPO4)<2->-1(Np|+VI|O2)<2+>, logK(298,15K) = 6,2 +/- 0,7, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

146 (Np|+VI|O2)(OH)<+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1003967,982 +/- 6062, Reaction: 0 = +1(Np|+VI|O2)(OH)<+>+1H<+>-1H2O-1(Np|+VI|O2)<2+>, logK(298,15K) = -5,1 +/- 0,4, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

147 (Np|+VI|O2)(SO4)<0>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1558665,38 +/- 5641, Reaction: 0 = +1(Np|+VI|O2)(SO4)<0>-1(SO4)<2->-1(Np|+VI|O2)<2+>, logK(298,15K) = 3,28 +/- 0,06, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

148 (Np|+VI|O2)(SO4)2<2->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2310774,801 +/- 5705, Reaction: 0 = +1(Np|+VI|O2)(SO4)2<2->-2(SO4)<2->-1(Np|+VI|O2)<2+>, logK(298,15K) = 4,7 +/- 0,1, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

149 (Np|+VI|O2)<2+>

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -795939 +/- 5615, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

150 (Np|+VI|O2)2(CO3)(OH)3<->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2814482,093 +/- 14665, Reaction: 0 = +1(Np|+VI|O2)2(CO3)(OH)3<->+5CO2(g)+2H2O-7H<+>-2(Np|+VI|O2)(CO3)3<4->, logK(298,15K) = 49,166 +/- 1,586, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

151 (Np|+VI|O2)2(OH)2<2+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2030368,572 +/- 11294, Reaction: 0 = +1(Np|+VI|O2)2(OH)2<2+>+2H<+>-2H2O-2(Np|+VI|O2)<2+>, logK(298,15K) = -6,27 +/- 0,21, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

152 (Np|+VI|O2)3(CO3)6<6->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -5839277,766 +/- 19185, Reaction: 0 = +1(Np|+VI|O2)3(CO3)6<6->+3(CO3)<2->-3(Np|+VI|O2)(CO3)3<4->, logK(298,15K) = -8,272 +/- 1,447, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

153 (Np|+VI|O2)3(OH)5<+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -3475795,309 +/- 16893, Reaction: 0 = +1(Np|+VI|O2)3(OH)5<+>+5H<+>-5H2O-3(Np|+VI|O2)<2+>, logK(298,15K) = -17,12 +/- 0,22, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

154 (Np|+VI|O2)Cl<+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -929439,217 +/- 5699, Reaction: 0 = +1(Np|+VI|O2)Cl<+>-1Cl<->-1(Np|+VI|O2)<2+>, logK(298,15K) = 0,4 +/- 0,17, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

155 (H2P2O7)<2->

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -2027117 +/- 4445, Reference: NEA-6

V0 [cm3 mol-1] = dummy value 0,001

Remark:

156 (H2PO4)<->

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -1137152 +/- 1567, Reference: NEA-6

V0 [cm3 mol-1] = dummy value 0,001

Remark:

157 (H3P2O7)<->

```
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = -2039960 +/- 4362, Reference: NEA-6
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
158   (HP2O7)<3->
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = -1989158 +/- 4482, Reference: NEA-6
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
159   (HPO4)<2->
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = -1095985 +/- 1567, Reference: NEA-6
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
160   (P2O7)<4->
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = -1935503 +/- 4563, Reference: NEA-6
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
161   (PO4)<3->
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = -1025491 +/- 1576, Reference: NEA-6
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
162   H3PO4<0>
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = -1149367 +/- 1576, Reference: NEA-6
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
163   H4P2O7<0>
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = -2045668 +/- 3299, Reference: NEA-6
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
164   Pu|+III|(OH)<2+>
      Gibbs Free Energy of Formation calculated from logK for reaction
      deltaG_0^f [J mol-1] = -776738,505 +/- 3187, Reaction: 0 =
      +1Pu|+III|(OH)<2+>+1H<+>-1H2O-1Pu|+III|<3+>, logK(298,15K) = -6,9 +/- 0,3,
      Reference: FZK-INE 002/04
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
165   Pu|+III|(SO4)<+>
      Gibbs Free Energy of Formation calculated from logK for reaction
      deltaG_0^f [J mol-1] = -1345298,456 +/- 4599, Reaction: 0 =
      +1Pu|+III|(SO4)<+>+1H<+>-1(HSO4)<->-1Pu|+III|<3+>, logK(298,15K) = 1,93 +/-
      0,61, Reference: FZK-INE 002/04
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
166   Pu|+III|(SO4)2<->
      Gibbs Free Energy of Formation calculated from logK for reaction
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deltaG_0^f [J mol-1] = -2099511,861 +/- 5766, Reaction: 0 = +1Pu|+III|(SO4)2<->+2H<+>-2(HSO4)<->-1Pu|+III|<3+>, logK(298,15K) = 1,74 +/- 0,76, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

167 Pu|+III|<3+>

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -578984 +/- 2688, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark: in forming reaction given by INE species PuCl3*6H2O(c) is not defined

168 Pu|+IV|(CO3)4<4->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2800496,916 +/- 7013, Reaction: 0 = +1Pu|+IV|(CO3)4<4->-4(CO3)<2->-1Pu|+IV|<4+>, logK(298,15K) = 37 +/- 1,1, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

169 Pu|+IV|(CO3)5<6->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -3320618,893 +/- 7261, Reaction: 0 = +1Pu|+IV|(CO3)5<6->-5(CO3)<2->-1Pu|+IV|<4+>, logK(298,15K) = 35,65 +/- 1,13, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

170 Pu|+IV|(OH)<3+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -718552,826 +/- 2936, Reaction: 0 = +1Pu|+IV|(OH)<3+>+1H<+>-1H2O-1Pu|+IV|<4+>, logK(298,15K) = 0,6 +/- 0,2, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

171 Pu|+IV|(OH)2(CO3)2<2->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2112076,04 +/- unknown, Reaction: 0 = +1Pu|+IV|(OH)2(CO3)2<2->+2OH<->-1Pu|+IV|(OH)4(am)-2(CO3)<2->, logK(298,15K) = -12,09 +/- unknown, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

172 Pu|+IV|(OH)2<2+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -955692,826 +/- 3203, Reaction: 0 = +1Pu|+IV|(OH)2<2+>+2H<+>-2H2O-1Pu|+IV|<4+>, logK(298,15K) = 0,6 +/- 0,3, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

173 Pu|+IV|(OH)3<+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1176279,502 +/- 3542, Reaction: 0 = +1Pu|+IV|(OH)3<+>+3H<+>-3H2O-1Pu|+IV|<4+>, logK(298,15K) = -2,3 +/- 0,4, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

174 Pu|+IV|(OH)4(CO3)<2->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1925511,404 +/- unknown, Reaction: 0 = +1Pu|+IV|(OH)4(CO3)<2->-1Pu|+IV|(OH)4(am)-1(CO3)<2->, logK(298,15K) = -7,4 +/- 0,3, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

175 Pu|+IV|(OH)4(CO3)2<4->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2461330,497 +/- unknown, Reaction: 0 = +1Pu|+IV|(OH)4(CO3)2<4->-1Pu|+IV|(OH)4(am)-2(CO3)<2->, logK(298,15K) = -6 +/- 0,3, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

176 Pu|+IV|(OH)4<0>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1378029,637 +/- 3936, Reaction: 0 = +1Pu|+IV|(OH)4<0>+4H<+>-4H2O-1Pu|+IV|<4+>, logK(298,15K) = -8,5 +/- 0,5, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

177 Pu|+IV|(SO4)<2+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1261312,423 +/- 3270, Reaction: 0 = +1Pu|+IV|(SO4)<2+>+1H<+>-1(HSO4)<->-1Pu|+IV|<4+>, logK(298,15K) = 4,91 +/- 0,22, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

178 Pu|+IV|(SO4)2<0>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2029567,613 +/- 4225, Reaction: 0 = +1Pu|+IV|(SO4)2<0>+2H<+>-2(HSO4)<->-1Pu|+IV|<4+>, logK(298,15K) = 7,18 +/- 0,32, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

179 Pu|+IV|<4+>

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -477988 +/- 2705, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

180 Pu|+IV|Cl<3+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -619479,477 +/- 3204, Reaction: 0 = +1Pu|+IV|Cl<3+>-1Cl<->-1Pu|+IV|<4+>, logK(298,15K) = 1,8 +/- 0,3, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

181 (Pu|+V|O2)(CO3)<->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1409701,54 +/- 3002, Reaction: 0 = +1(Pu|+V|O2)(CO3)<->-1(CO3)<2->-1(Pu|+V|O2)<+>, logK(298,15K) = 5,12 +/- 0,14, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

182 (Pu|+V|O2)(CO3)3<5->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2464814,944 +/- 6096, Reaction: 0 = +1(Pu|+V|O2)(CO3)3<5->-3(CO3)<2->-1(Pu|+V|O2)<+>, logK(298,15K) = 5,025 +/- 0,92, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

183 (Pu|+V|O2)(OH)<0>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1034249,272 +/- unknown, Reaction: 0 = +1(Pu|+V|O2)(OH)<0>+1H<+>-1H2O-1(Pu|+V|O2)<+>, logK(298,15K) = -9,73 +/- unknown, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

184 (Pu|+V|O2)<+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -852648,528 +/- 2868, Reaction: 0 = +1(Pu|+V|O2)<+>+1H<+>-0,5H2-1(Pu|+VI|O2)<2+>, logK(298,15K) = 15,819 +/- 0,09, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

185 Pu|+V|(H3PO4)<4+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1641054,303 +/- 3569, Reaction: 0 = +1Pu|+V|(H3PO4)<4+>-1H3PO4<0>-1Pu|+IV|<4+>, logK(298,15K) = 2,4 +/- 0,3, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

186 (Pu|+VI|O2)(CO3)<0>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1344407,24 +/- 4032, Reaction: 0 = +1(Pu|+VI|O2)(CO3)<0>-1(CO3)<2->-1(Pu|+VI|O2)<2+>, logK(298,15K) = 9,5 +/- 0,5, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

187 (Pu|+VI|O2)(CO3)2<2->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1901916,896 +/- 4088, Reaction: 0 = +1(Pu|+VI|O2)(CO3)2<2->-2(CO3)<2->-1(Pu|+VI|O2)<2+>, logK(298,15K) = 14,7 +/- 0,5, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

188 (Pu|+VI|O2)(CO3)3<4->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2448581,271 +/- 4180, Reaction: 0 = +1(Pu|+VI|O2)(CO3)3<4->-3(CO3)<2->-1(Pu|+VI|O2)<2+>, logK(298,15K) = 18 +/- 0,5, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

189 (Pu|+VI|O2)(OH)<+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -968098,765 +/- 4013, Reaction: 0 = +1(Pu|+VI|O2)(OH)<+>+1H<+>-1H2O-1(Pu|+VI|O2)<2+>, logK(298,15K) = -5,5 +/- 0,5, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

190 (Pu|+VI|O2)(OH)2<0>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1161286,836 +/- 9015, Reaction: 0 = +1(Pu|+VI|O2)(OH)2<0>+2H<+>-2H2O-1(Pu|+VI|O2)<2+>, logK(298,15K) = -13,2 +/- 1,5, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

191 (Pu|+VI|O2)(SO4)<0>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1525650,184 +/- 3072, Reaction: 0 = +1(Pu|+VI|O2)(SO4)<0>-1(Pu|+VI|O2)<2+>-1(SO4)<2->, logK(298,15K) = 3,38 +/- 0,2, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

192 (Pu|+VI|O2)(SO4)2<2->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2275476,388 +/- 3156, Reaction: 0 = +1(Pu|+VI|O2)(SO4)2<2->-1(Pu|+VI|O2)<2+>-2(SO4)<2->, logK(298,15K) = 4,4 +/- 0,2, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

193 (Pu|+VI|O2)<2+>

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -762353 +/- 2821, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

194 (Pu|+VI|O2)2(OH)2<2+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1956175,68 +/- 8026, Reaction: 0 = +1(Pu|+VI|O2)2(OH)2<2+>+2H<+>-2H2O-2(Pu|+VI|O2)<2+>, logK(298,15K) = -7,5 +/- 1, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

195 (Pu|+VI|O2)3(OH)5<+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -3354602,516 +/- unknown, Reaction: 0 = +1(Pu|+VI|O2)3(OH)5<+>+5H<+>-5H2O-3(Pu|+VI|O2)<2+>, logK(298,15K) = -20,7 +/- 0,6, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

196 (Pu|+VI|O2)Cl<+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -894882,85 +/- 2829, Reaction: 0 = +1(Pu|+VI|O2)Cl<+>-1Cl<->-1(Pu|+VI|O2)<2+>, logK(298,15K) = 0,23 +/- 0,03, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

197 (Pu|+VI|O2)Cl2<0>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1018222,751 +/- 3308, Reaction: 0 = +1(Pu|+VI|O2)Cl2<0>-2Cl<->-1(Pu|+VI|O2)<2+>, logK(298,15K) = -1,15 +/- 0,3, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

198 Ra<2+>

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -561500 +/- unknown, Reference: NTB 02-16

V0 [cm3 mol-1] = dummy value 0,001

Remark:

199 RaCl<+>

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -692146 +/- unknown, Reference: NTB 02-16

V0 [cm3 mol-1] = dummy value 0,001

Remark:

200 RaCO3<0>

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -1103688 +/- unknown, Reference: NTB 02-16

V0 [cm3 mol-1] = dummy value 0,001

Remark:

201 RaOH<+>

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -721584 +/- unknown, Reference: NTB 02-16

V0 [cm3 mol-1] = dummy value 0,001

Remark:

202 RaSO4<0>

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -1321201 +/- unknown, Reference: NTB 02-16

V0 [cm3 mol-1] = dummy value 0,001

Remark: 0

203 H2Se<0>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = 21495,847 +/- 2003, Reaction: 0 = +1H2Se<0>-1H2Se(g), logK(298,15K) = -1,1 +/- 0,01, Reference: NEA-7

V0 [cm3 mol-1] = dummy value 0,001

Remark:

204 H2SeO3<0>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -425178,782 +/- 849, Reaction: 0 = +1H2SeO3<0>+2H2-1Se(cr)-3H2O, logK(298,15K) = -50,147 +/- 0,147, Reference: NEA-7

V0 [cm3 mol-1] = dummy value 0,001

Remark:

205 HSe<->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = 43471,811 +/- 2024, Reaction: 0 = +1HSe<->+1H<+>-1H2Se<0>, logK(298,15K) = -3,85 +/- 0,05, Reference: NEA-7

V0 [cm3 mol-1] = dummy value 0,001

Remark:

206 HSeO3<->
Gibbs Free Energy of Formation calculated from logK for reaction
deltaG_0^f [J mol-1] = -410109,549 +/- 1166, Reaction: 0 = +1HSeO3<->+1H<+>-1H2SeO3<0>, logK(298,15K) = -2,64 +/- 0,14, Reference: NEA-7
V0 [cm3 mol-1] = dummy value 0,001
Remark:

207 HSeO4<->
Gibbs Free Energy of Formation directly entered
deltaG_0^f [J mol-1] = -449474 +/- 1312, Reference: NEA-7
V0 [cm3 mol-1] = dummy value 0,001
Remark:

208 Se<2->
Gibbs Free Energy of Formation directly entered
deltaG_0^f [J mol-1] = 128600 +/- 3000, Reference: NEA-7
V0 [cm3 mol-1] = dummy value 0,001
Remark:

209 Se2<2->
Gibbs Free Energy of Formation directly entered
deltaG_0^f [J mol-1] = 112670 +/- 6294, Reference: NEA-7
V0 [cm3 mol-1] = dummy value 0,001
Remark:

210 Se3<2->
Gibbs Free Energy of Formation directly entered
deltaG_0^f [J mol-1] = 100590 +/- 9198, Reference: NEA-7
V0 [cm3 mol-1] = dummy value 0,001
Remark:

211 Se4<2->
Gibbs Free Energy of Formation directly entered
deltaG_0^f [J mol-1] = 97580 +/- 12149, Reference: NEA-7
V0 [cm3 mol-1] = dummy value 0,001
Remark:

212 SeO3<2->
Gibbs Free Energy of Formation calculated from logK for reaction
deltaG_0^f [J mol-1] = -362390,312 +/- 1756, Reaction: 0 = +1SeO3<2->+1H<+>-1HSeO3<->, logK(298,15K) = -8,36 +/- 0,23, Reference: NEA-7
V0 [cm3 mol-1] = dummy value 0,001
Remark:

213 SeO4<2->
Gibbs Free Energy of Formation calculated from logK for reaction
deltaG_0^f [J mol-1] = -439484,925 +/- 1431, Reaction: 0 = +1SeO4<2->+1H<+>-1HSeO4<->, logK(298,15K) = -1,75 +/- 0,1, Reference: NEA-7
V0 [cm3 mol-1] = dummy value 0,001
Remark:

214 ZnSeO4<0>
Gibbs Free Energy of Formation calculated from logK for reaction
deltaG_0^f [J mol-1] = -599017,298 +/- 1493, Reaction: 0 = +1ZnSeO4<0>-1Zn<2+>-1SeO4<2->, logK(298,15K) = 2,16 +/- 0,06, Reference: NEA-7
V0 [cm3 mol-1] = dummy value 0,001
Remark:

215 Sn(OH)6<2->

Gibbs Free Energy of Formation directly entered
deltaG_0^f [J mol-1] = -1299000 +/- unknown, Reference: /BPJ 1985/
V0 [cm3 mol-1] = dummy value 0,001
Remark:

216 Sn<2+>
Gibbs Free Energy of Formation directly entered
deltaG_0^f [J mol-1] = -27240 +/- unknown, Reference:
V0 [cm3 mol-1] = dummy value 0,001
Remark:

217 Sn<4+>
Gibbs Free Energy of Formation directly entered
deltaG_0^f [J mol-1] = 2720 +/- unknown, Reference: /BPJ 1985/
V0 [cm3 mol-1] = dummy value 0,001
Remark:

218 SnO3<2->
Gibbs Free Energy of Formation directly entered
deltaG_0^f [J mol-1] = -574965 +/- unknown, Reference: /BPJ 1985/
V0 [cm3 mol-1] = dummy value 0,001
Remark:

219 Sr<2+>
Gibbs Free Energy of Formation directly entered
deltaG_0^f [J mol-1] = -563864 +/- 781, Reference: NEA-9
V0 [cm3 mol-1] = dummy value 0,001
Remark:

220 SrSO4<0>
Gibbs Free Energy of Formation calculated from logK for reaction
deltaG_0^f [J mol-1] = -1320939,418 +/- unknown, Reaction: 0 = +1SrSO4<0>-1Sr<2+>-1(SO4)<2->, logK(298,15K) = 2,29 +/- unknown, Reference: /PSI/NAGRA/
V0 [cm3 mol-1] = dummy value 0,001
Remark:

221 (TcO)(OH)<+>
Gibbs Free Energy of Formation calculated from logK for reaction
deltaG_0^f [J mol-1] = -345378,096 +/- 9009, Reaction: 0 = +1(TcO)(OH)<+>+1H2O-1H<+>-1(TcO)(OH)2<0>, logK(298,15K) = 2,5 +/- 0,3, Reference: FZK-INE 002/04
V0 [cm3 mol-1] = dummy value 0,001
Remark:

222 (TcO)(OH)2<0>
Gibbs Free Energy of Formation calculated from logK for reaction
deltaG_0^f [J mol-1] = -568247,989 +/- 8845, Reaction: 0 = +1(TcO)(OH)2<0>+0,6H2O-1TcO2*1,6H2O(s), logK(298,15K) = -8,4 +/- 0,5, Reference: FZK-INE 002/04
V0 [cm3 mol-1] = dummy value 0,001
Remark:

223 (TcO)(OH)3<->
Gibbs Free Energy of Formation calculated from logK for reaction
deltaG_0^f [J mol-1] = -743170,324 +/- 9135, Reaction: 0 = +1(TcO)(OH)3<->+1H<+>-1H2O-1(TcO)(OH)2<0>, logK(298,15K) = -10,9 +/- 0,4, Reference: FZK-INE 002/04
V0 [cm3 mol-1] = dummy value 0,001
Remark:

224 (TcO)<2+>

```
      Gibbs Free Energy of Formation calculated from logK for reaction
      deltaG_0^f [J mol-1] = -116800,16 +/- unknown, Reaction: 0 = +1(TcO)<2+>+2H2O-
      2H<+>-1(TcO)(OH)2<0>, logK(298,15K) = 4 +/- unknown, Reference: FZK-INE 002/04
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
225   (TcO4)<->
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = -637406 +/- 7616, Reference: FZK-INE 002/04
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
226   (TcO4)<2->
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = -575759 +/- 8133, Reference: FZK-INE 002/04
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
227   Tc(CO3)(OH)2<0>
      Gibbs Free Energy of Formation calculated from logK for reaction
      deltaG_0^f [J mol-1] = -968899,836 +/- 9010, Reaction: 0 = +1Tc(CO3)(OH)2<0>-
      1CO2(g)-1(TcO)(OH)2<0>, logK(298,15K) = 1,1 +/- 0,3, Reference: FZK-INE 002/04
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
228   Tc(CO3)(OH)3<->
      Gibbs Free Energy of Formation calculated from logK for reaction
      deltaG_0^f [J mol-1] = -1158663,082 +/- 9486, Reaction: 0 = +1Tc(CO3)(OH)3<-
      >+1H<+>-1CO2(g)-1H2O-1(TcO)(OH)2<0>, logK(298,15K) = -7,2 +/- 0,6, Reference:
      FZK-INE 002/04
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
229   H2TeO4
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = -550857 +/- unknown, Reference: /BPJ 1985/
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
230   HTeO2<+>
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = -216540 +/- unknown, Reference: /BPJ 1985/
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
231   HTeO3<->
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = -436590 +/- unknown, Reference: /BPJ 1985/
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
232   HTeO4<->
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = -515753 +/- unknown, Reference: /BPJ 1985/
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
233   TeO3<2->
      Gibbs Free Energy of Formation directly entered
```

deltaG_0^f [J mol-1] = -392420 +/- unknown, Reference: /BPJ 1985/

V0 [cm3 mol-1] = dummy value 0,001

Remark:

234 TeO4<2->

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -456424 +/- unknown, Reference: /BPJ 1985/

V0 [cm3 mol-1] = dummy value 0,001

Remark:

235 Th(CO3)5<6->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -3506989,191 +/- unknown, Reaction: 0 = +1Th(CO3)5<6->+4OH<->-1Th(OH)4(am)-5(CO3)<2->, logK(298,15K) = -18,4 +/- unknown, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

236 Th(HPO4)<2+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1874789,555 +/- unknown, Reaction: 0 = +1Th(HPO4)<2+>-1Th<4+>-1(HPO4)<2->, logK(298,15K) = 13 +/- 1, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

237 Th(OH)(CO3)4<5->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -3172939,069 +/- unknown, Reaction: 0 = +1Th(OH)(CO3)4<5->+3OH<->-1Th(OH)4(am)-4(CO3)<2->, logK(298,15K) = -12 +/- 0,1, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

238 Th(OH)<3+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -929182,306 +/- 5600, Reaction: 0 = +1Th(OH)<3+>+1H<+>-1H2O-1Th<4+>, logK(298,15K) = -2,2 +/- 0,2, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

239 Th(OH)2(CO3)<0>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1717590,788 +/- unknown, Reaction: 0 = +1Th(OH)2(CO3)<0>+2OH<->-1Th(OH)4(am)-1(CO3)<2->, logK(298,15K) = -17,1 +/- 0,2, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

240 Th(OH)2(CO3)2<2->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2281379,291 +/- unknown, Reaction: 0 = +1Th(OH)2(CO3)2<2->+2OH<->-1Th(OH)4(am)-2(CO3)<2->, logK(298,15K) = -10,8 +/- 0,1, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

241 Th(OH)2<2+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1144631,744 +/- 6400, Reaction: 0 = +1Th(OH)2<2+>+2H<+>-2H2O-1Th<4+>, logK(298,15K) = -6 +/- 0,6, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

242 Th(OH)3(CO3)<->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1919359,76 +/- unknown, Reaction: 0 = +1Th(OH)3(CO3)<->+1OH<->-1Th(OH)4(am)-1(CO3)<2->, logK(298,15K) = -9,3 +/- 0,5, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

243 Th(OH)3<+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1353231,53 +/- 7900, Reaction: 0 = +1Th(OH)3<+>+3H<+>-3H2O-1Th<4+>, logK(298,15K) = -11 +/- 1, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

244 Th(OH)4(CO3)<2->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2089163,692 +/- unknown, Reaction: 0 = +1Th(OH)4(CO3)<2->-1Th(OH)4(am)-1(CO3)<2->, logK(298,15K) = -7,1 +/- 0,2, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

245 Th(OH)4<0>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1553269,252 +/- 7900, Reaction: 0 = +1Th(OH)4<0>+4H<+>-4H2O-1Th<4+>, logK(298,15K) = -17,5 +/- 1, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

246 Th(SO4)<2+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1491985,125 +/- unknown, Reaction: 0 = +1Th(SO4)<2+>-1Th<4+>-1(SO4)<2->, logK(298,15K) = 7,6 +/- 0,5, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

247 Th(SO4)2<0>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2258821,296 +/- unknown, Reaction: 0 = +1Th(SO4)2<0>-1Th<4+>-2(SO4)<2->, logK(298,15K) = 11,6 +/- unknown, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

248 Th(SO4)3<2->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -3007391,73 +/- unknown, Reaction: 0 = +1Th(SO4)3<2->-1Th<4+>-3(SO4)<2->, logK(298,15K) = 12,4 +/- unknown, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

249 Th<4+>

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -704600 +/- 5400, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

250 Th2(OH)2<6+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1850944,157 +/- 10800, Reaction: 0 = +1Th2(OH)2<6+>+2H<+>-2Th<4+>-2H2O, logK(298,15K) = -5,7 +/- unknown, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

251 Th4(OH)12<4+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -5511675,259 +/- 21600, Reaction: 0 = +1Th4(OH)12<4+>+12H<+>-4Th<4+>-12H2O, logK(298,15K) = -26,7 +/- unknown, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

252 Th4(OH)8<8+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -4599075,929 +/- 21600, Reaction: 0 = +1Th4(OH)8<8+>+8H<+>-4Th<4+>-8H2O, logK(298,15K) = -20,4 +/- unknown, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

253 Ti(OH)4<0>

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = 0 +/- unknown, Reference: gesetzt

V0 [cm3 mol-1] = dummy value 0,001

Remark:

254 (UO2)(H2PO4)(H3PO4)<+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -3260703,27 +/- 3659, Reaction: 0 = +1(UO2)(H2PO4)(H3PO4)<+>+1H<+>-1(U|+VI|O2)<2+>-2H3PO4<0>, logK(298,15K) = 1,65 +/- 0,11, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

255 (UO2)(H2PO4)<+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2108311,008 +/- 2378, Reaction: 0 = +1(UO2)(H2PO4)<+>+1H<+>-1(U|+VI|O2)<2+>-1H3PO4<0>, logK(298,15K) = 1,12 +/- 0,06, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

256 (UO2)(H2PO4)2<0>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -3254938,147 +/- 3659, Reaction: 0 = +1(UO2)(H2PO4)2<0>+2H<+>-1(U|+VI|O2)<2+>-2H3PO4<0>, logK(298,15K) = 0,64 +/- 0,11, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

257 (UO2)(H3PO4)<2+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2106256,112 +/- 2504, Reaction: 0 = +1(UO2)(H3PO4)<2+>-1H3PO4<0>-1(U|+VI|O2)<2+>, logK(298,15K) = 0,76 +/- 0,15, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

258 (UO2)(HAsO4)<0>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1707133,881 +/- 4717, Reaction: 0 = +1(UO2)(HAsO4)<0>-1(AsO4)<3->-1(U|+VI|O2)<2+>-1H<+>, logK(298,15K) = 18,76 +/- 0,31, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

259 (UO2)(HPO4)<0>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2089862,229 +/- 2777, Reaction: 0 = +1(UO2)(HPO4)<0>-1(HPO4)<2->-1(U|+VI|O2)<2+>, logK(298,15K) = 7,24 +/- 0,26, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

260 U|+III|<3+>

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -476473 +/- 1810, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

261 U|+IV|(CO3)4<4->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2841637,796 +/- 5958, Reaction: 0 = +1U|+IV|(CO3)4<4->+1(CO3)<2->-1U|+IV|(CO3)5<6->, logK(298,15K) = 1,12 +/- 0,25, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

262 U|+IV|(CO3)5<6->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -3363072,622 +/- 5772, Reaction: 0 = +1U|+IV|(CO3)5<6->-5(CO3)<2->-1U|+IV|<4+>, logK(298,15K) = 34 +/- 0,9, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

263 U|+IV|(OH)<3+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -763917,657 +/- 1798, Reaction: 0 = +1U|+IV|(OH)<3+>+1H<+>-1H2O-1U|+IV|<4+>, logK(298,15K) = -0,54 +/- 0,06, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

264 U|+IV|(OH)2(CO3)2<2->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2141972,076 +/- unknown, Reaction: 0 = +1U|+IV|(OH)2(CO3)2<2->+2OH<->-2(CO3)<2->-1U|+IV|(OH)4(am), logK(298,15K) = -12,11 +/- unknown, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

265 U|+IV|(OH)2<2+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -997861,153 +/- 6000, Reaction: 0 = +1U|+IV|(OH)2<2+>+2H<+>-2H2O-1U|+IV|<4+>, logK(298,15K) = -1,1 +/- 1, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

266 U|+IV|(OH)3<+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1214452,199 +/- 6000, Reaction: 0 = +1U|+IV|(OH)3<+>+3H<+>-3H2O-1U|+IV|<4+>, logK(298,15K) = -4,7 +/- 1, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

267 U|+IV|(OH)4<0>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1421414,919 +/- 8189, Reaction: 0 = +1U|+IV|(OH)4<0>-4OH<->-1U|+IV|<4+>, logK(298,15K) = 46 +/- 1,4, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

268 U|+IV|(SO4)<2+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1311422,921 +/- 2113, Reaction: 0 = +1U|+IV|(SO4)<2+>-1U|+IV|<4+>-1(SO4)<2->, logK(298,15K) = 6,58 +/- 0,19, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

269 U|+IV|(SO4)2<0>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2077859,529 +/- 2262, Reaction: 0 = +1U|+IV|(SO4)2<0>-2(SO4)<2->-1U|+IV|<4+>, logK(298,15K) = 10,51 +/- 0,2, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

270 U|+IV|<4+>

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -529860 +/- 1765, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

271 U|+IV|Cl<3+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -670894,833 +/- 1918, Reaction: 0 = +1U|+IV|Cl<3+>-1U|+IV|<4+>-1Cl<->, logK(298,15K) = 1,72 +/- 0,13, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

272 (U|+V|O2)(CO3)3<5->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2584175,399 +/- 2943, Reaction: 0 = +1(U|+V|O2)(CO3)3<5->-3(CO3)<2->-1(U|+V|O2)<+>, logK(298,15K) = 6,95 +/- 0,36, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

273 (U|+V|O2)<+>

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -961021 +/- 1752, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

274 (U|+VI|O2)(CO3)<0>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1537116,779 +/- 1799, Reaction: 0 = +1(U|+VI|O2)(CO3)<0>-1(U|+VI|O2)<2+>-1(CO3)<2->, logK(298,15K) = 9,94 +/- 0,03, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

275 (U|+VI|O2)(CO3)2<2->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2103017,257 +/- 1982, Reaction: 0 = +1(U|+VI|O2)(CO3)2<2->-1(U|+VI|O2)<2+>-2(CO3)<2->, logK(298,15K) = 16,61 +/- 0,09, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

276 (U|+VI|O2)(CO3)3<4->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2660698,155 +/- 2116, Reaction: 0 = +1(U|+VI|O2)(CO3)3<4->-1(U|+VI|O2)<2+>-3(CO3)<2->, logK(298,15K) = 21,84 +/- 0,04, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

277 (U|+VI|O2)(H2AsO4)<+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1725399,618 +/- 4582, Reaction: 0 = +1(U|+VI|O2)(H2AsO4)<+>-1(AsO4)<3->-1(U|+VI|O2)<2+>-2H<+>, logK(298,15K) = 21,96 +/- 0,24, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

278 (U|+VI|O2)(H2AsO4)2<0>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2484606,014 +/- 8283, Reaction: 0 = +1(U|+VI|O2)(H2AsO4)2<0>-2(AsO4)<3->-1(U|+VI|O2)<2+>-4H<+>, logK(298,15K) = 41,53 +/- 0,2, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

279 (U|+VI|O2)(OH)<+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1159723,776 +/- 2221, Reaction: 0 = +1(U|+VI|O2)(OH)<+>+1H<+>-1(U|+VI|O2)<2+>-1H2O, logK(298,15K) = -5,25 +/- 0,24, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

280 (U|+VI|O2)(OH)2<0>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1357478,281 +/- 1794, Reaction: 0 = +1(U|+VI|O2)(OH)2<0>+2H<+>-1(U|+VI|O2)<2+>-2H2O, logK(298,15K) = -12,15 +/- 0,07, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

281 (U|+VI|O2)(OH)3<->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1548383,135 +/- 2969, Reaction: 0 = +1(U|+VI|O2)(OH)3<->+3H<+>-1(U|+VI|O2)<2+>-3H2O, logK(298,15K) = -20,25 +/- 0,42, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

282 (U|+VI|O2)(OH)4<2->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1718910,276 +/- 4260, Reaction: 0 = +1(U|+VI|O2)(OH)4<2->+4H<+>-1(U|+VI|O2)<2+>-4H2O, logK(298,15K) = -31,92 +/- 0,33, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

283 (U|+VI|O2)(PO4)<->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2053559,405 +/- 2504, Reaction: 0 = +1(U|+VI|O2)(PO4)<->-1(PO4)<3->-1(U|+VI|O2)<2+>, logK(298,15K) = 13,23 +/- 0,15, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

284 (U|+VI|O2)(SO4)<0>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1714535,335 +/- 1800, Reaction: 0 = +1(U|+VI|O2)(SO4)<0>-1(U|+VI|O2)<2+>-1(SO4)<2->, logK(298,15K) = 3,15 +/- 0,02, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

285 (U|+VI|O2)(SO4)2<2->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2464190,297 +/- 1978, Reaction: 0 = +1(U|+VI|O2)(SO4)2<2->-1(U|+VI|O2)<2+>-2(SO4)<2->, logK(298,15K) = 4,14 +/- 0,07, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

286 (U|+VI|O2)(SO4)3<4->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -3201801,289 +/- 3054, Reaction: 0 = +1(U|+VI|O2)(SO4)3<4->-1(U|+VI|O2)<2+>-3(SO4)<2->, logK(298,15K) = 3,02 +/- 0,38, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

287 (U|+VI|O2)<2+>

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -952551 +/- 1747, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

288 (U|+VI|O2)11(CO3)6(OH)12<2->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -16698985,903 +/- 22383, Reaction: 0 = +1(U|+VI|O2)11(CO3)6(OH)12<2->+24H<+>-18H2O-11(U|+VI|O2)<2+>-6CO2(g), logK(298,15K) = -72,5 +/- 2, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

289 (U|+VI|O2)2(CO3)(OH)3<->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -3139525,108 +/- 4517, Reaction: 0 = +1(U|+VI|O2)2(CO3)(OH)3<->+5H<+>-4H2O-2(U|+VI|O2)<2+>-1CO2(g), logK(298,15K) = -19,01 +/- 0,5, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

290 (U|+VI|O2)2(OH)<3+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2126830,285 +/- 6693, Reaction: 0 = +1(U|+VI|O2)2(OH)<3+>+1H<+>-1H2O-2(U|+VI|O2)<2+>, logK(298,15K) = -2,7 +/- 1, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

291 (U|+VI|O2)2(OH)2<2+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2347302,8 +/- 3503, Reaction: 0 = +1(U|+VI|O2)2(OH)2<2+>+2H<+>-2H2O-2(U|+VI|O2)<2+>, logK(298,15K) = -5,62 +/- 0,04, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

292 (U|+VI|O2)3(CO3)6<6->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -5716385,697 +/- 8096, Reaction: 0 = +1(U|+VI|O2)3(CO3)6<6->-6(CO3)<2->-3(U|+VI|O2)<2+>, logK(298,15K) = -54 +/- 1, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

293 (U|+VI|O2)3(OH)4<2+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -3738287,292 +/- 5517, Reaction: 0 = +1(U|+VI|O2)3(OH)4<2+>+4H<+>-4H2O-3(U|+VI|O2)<2+>, logK(298,15K) = -11,9 +/- 0,3, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

294 (U|+VI|O2)3(OH)5<+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -3954592,936 +/- 5291, Reaction: 0 = +1(U|+VI|O2)3(OH)5<+>+5H<+>-5H2O-3(U|+VI|O2)<2+>, logK(298,15K) = -15,55 +/- 0,12, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

295 (U|+VI|O2)3(OH)7<->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -4333834,024 +/- 6958, Reaction: 0 = +1(U|+VI|O2)3(OH)7<->+7H<+>-7H2O-3(U|+VI|O2)<2+>, logK(298,15K) = -32,2 +/- 0,8, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

296 (U|+VI|O2)3O(OH)2(HCO3)<+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -4100695,252 +/- 5973, Reaction: 0 = +1(U|+VI|O2)3O(OH)2(HCO3)<+>+5H<+>-4H2O-3(U|+VI|O2)<2+>-1CO2(g), logK(298,15K) = -17,5 +/- 0,5, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

297 (U|+VI|O2)4(OH)7<+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -5345177,864 +/- 9029, Reaction: 0 = +1(U|+VI|O2)4(OH)7<+>+7H<+>-7H2O-4(U|+VI|O2)<2+>, logK(298,15K) = -21,9 +/- 1, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

298 (U|+VI|O2)Cl<+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1084738,367 +/- 1755, Reaction: 0 = +1(U|+VI|O2)Cl<+>-1(U|+VI|O2)<2+>-1Cl<->, logK(298,15K) = 0,17 +/- 0,02, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

299 (U|+VI|O2)Cl2<0>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1208706,153 +/- 2885, Reaction: 0 = +1(U|+VI|O2)Cl2<0>-1(U|+VI|O2)<2+>-2Cl<->, logK(298,15K) = -1,1 +/- 0,4, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

300 (U|+VI|O2)SiO(OH)3<+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2251203,561 +/- 2172, Reaction: 0 = +1(U|+VI|O2)SiO(OH)3<+>+1H<+>-1(U|+VI|O2)<2+>-1SiO2<0>-2H2O, logK(298,15K) = -1,84 +/- 0,1, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

301 V<2+>

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -218000 +/- unknown, Reference: /BPJ 1985/

V0 [cm3 mol-1] = dummy value 0,001

Remark:

302 V<3+>

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -251300 +/- unknown, Reference: /BPJ 1985/

V0 [cm3 mol-1] = dummy value 0,001

Remark:

303 VO<2+>

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -446400 +/- unknown, Reference: /BPJ 1985/

V0 [cm3 mol-1] = dummy value 0,001

Remark:

304 VO2<+>

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = 0 +/- unknown, Reference: gesetzt

V0 [cm3 mol-1] = dummy value 0,001

Remark:

305 Zn(OH)<+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -341532,68 +/- unknown, Reaction: 0 = +1Zn(OH)<+>+1H<+>-1Zn<2+>-1H2O, logK(298,15K) = -7,5 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

306 Zn(OH)2<0>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -527871,099 +/- unknown, Reaction: 0 = +1Zn(OH)2<0>+2H<+>-1Zn<2+>-2H2O, logK(298,15K) = -16,4 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

307 Zn(OH)3<->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -697656,195 +/- unknown, Reaction: 0 = +1Zn(OH)3<->+3H<+>-1Zn<2+>-3H2O, logK(298,15K) = -28,2 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

308 Zn(OH)4<2->

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -860020,836 +/- unknown, Reaction: 0 = +1Zn(OH)4<2->+4H<+>-1Zn<2+>-4H2O, logK(298,15K) = -41,3 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

309 Zn<2+>

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -147203 +/- 254, Reference: NEA 9

V0 [cm3 mol-1] = dummy value 0,001

Remark:

310 ZnCO3<0>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -702429,439 +/- unknown, Reaction: 0 = +1ZnCO3<0>+1H<+>-1Zn<2+>-1(HCO3)<->, logK(298,15K) = -5,5393 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

311 Zr(OH)<3+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -767476,275 +/- , Reaction: 0 = +1Zr(OH)<3+>+1H<+>-1Zr<4+>-1H2O, logK(298,15K) = 0,32 +/- 0,22, Reference: NEA-8

V0 [cm3 mol-1] = dummy value 0,001

Remark:

312 Zr(OH)2<2+>

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1008383,583 +/- , Reaction: 0 = +1Zr(OH)2<2+>+2H<+>-1Zr<4+>-2H2O, logK(298,15K) = 0,98 +/- 1,06, Reference: NEA-8

V0 [cm3 mol-1] = dummy value 0,001

```
      Remark:
313   Zr(OH)4<0>
      Gibbs Free Energy of Formation calculated from logK for reaction
      deltaG_0^f [J mol-1] = -1464569,087 +/- , Reaction: 0 = +1Zr(OH)4<0>+4H<+>-
      1Zr<4+>-4H2O, logK(298,15K) = -2,19 +/- 1,7, Reference: NEA-8
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
314   Zr<4+>
      Gibbs Free Energy of Formation calculated from logK for reaction
      deltaG_0^f [J mol-1] = -528509,701 +/- , Reaction: 0 = +1Zr<4+>+2H2O-4H<+>-
      1ZrO2(monoclinic), logK(298,15K) = -7 +/- 1,6, Reference: NEA-8
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
315   Ag<+>
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = 77096 +/- 156, Reference: NEA-8
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
316   AgCl<0>
      Gibbs Free Energy of Formation calculated from logK for reaction
      deltaG_0^f [J mol-1] = -72337,429 +/- unknown, Reaction: 0 = +1AgCl<0>-
      1AgCl(cr), logK(298,15K) = -6,50863830616573 +/- 0,0969100130080562, Reference:
      /FRI1985/
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
317   AgCl2<->
      Gibbs Free Energy of Formation calculated from logK for reaction
      deltaG_0^f [J mol-1] = -214437,259 +/- unknown, Reaction: 0 = +1AgCl2<->-
      1AgCl(cr)-1Cl<->, logK(298,15K) = -4,60205999132796 +/- 0,0969100130080562,
      Reference: /FRI1985/
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
318   AgCl3<2->
      Gibbs Free Energy of Formation calculated from logK for reaction
      deltaG_0^f [J mol-1] = -345101,093 +/- unknown, Reaction: 0 = +1AgCl3<2->-
      1AgCl(cr)-2Cl<->, logK(298,15K) = -4,69897000433602 +/- 0,0969100130080562,
      Reference: /FRI1985/
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
319   AgCl4<3->
      Gibbs Free Energy of Formation calculated from logK for reaction
      deltaG_0^f [J mol-1] = -468275,829 +/- unknown, Reaction: 0 = +1AgCl4<3->-
      1AgCl(cr)-3Cl<->, logK(298,15K) = -6,10790539730952 +/- 0,0969100130080562,
      Reference: /FRI1985/
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
##MIXED-SOLID-PHASES
Automatic generation of references not yet implemented
##SOLIDS
1     Ca(CO3)_Aragonite
      Gibbs Free Energy of Formation calculated from logK for reaction
```

deltaG_0^f [J mol-1] = -1127551,091 +/- unknown, Reaction: 0 = +1Ca(CO3)_Aragonite+1H<+>-1Ca<2+>-1(HCO3)<->, logK(298,15K) = -2,1198 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = 34,15 +/- unknown, Reference: YPF

Remark:

2 Ca(CO3)_Calcite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1128617,353 +/- unknown, Reaction: 0 = +1Ca(CO3)_Calcite+1H<+>-1Ca<2+>-1(HCO3)<->, logK(298,15K) = -1,933 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = 36,934 +/- unknown, Reference: YPF

Remark:

3 Ca(OH)2_Portlandite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -896922,648 +/- unknown, Reaction: 0 = +1Ca(OH)2_Portlandite+2H<+>-1Ca<2+>-2H2O, logK(298,15K) = -22,8035 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = 33,056 +/- unknown, Reference: YPF

Remark:

4 Ca(SO4):2H2O_Gypsum

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1797235,69 +/- unknown, Reaction: 0 = +1Ca(SO4):2H2O_Gypsum-1Ca<2+>-1(SO4)<2->-2H2O, logK(298,15K) = 4,5805 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = 74,69 +/- unknown, Reference: YPF

Remark:

5 Ca(SO4)_Anhydrite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1321709,053 +/- unknown, Reaction: 0 = +1Ca(SO4)_Anhydrite-1Ca<2+>-1(SO4)<2->, logK(298,15K) = 4,3621 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = 45,94 +/- unknown, Reference: YPF

Remark:

6 Ca2Cl2(OH)2:H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1928024,206 +/- unknown, Reaction: 0 = +1Ca2Cl2(OH)2:H2O+2H<+>-2Ca<2+>-2Cl<->-3H2O, logK(298,15K) = -26,5313 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = dummy value 0,001

Remark:

7 Ca4Cl2(OH)6:13H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -6586979,679 +/- unknown, Reaction: 0 = +1Ca4Cl2(OH)6:13H2O+6H<+>-4Ca<2+>-2Cl<->-19H2O, logK(298,15K) = -68,7343 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = 354,662925 +/- unknown, Reference:

Remark:

8 CaCl2:4H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1731167,12 +/- unknown, Reaction: 0 = +1CaCl2:4H2O-1Ca<2+>-2Cl<->-4H2O, logK(298,15K) = -5,717 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = dummy value 0,001

Remark:

9 CaCl2:6H2O_Antarcticite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2214428,154 +/- unknown, Reaction: 0 = +1CaCl2:6H2O_Antarcticite-1Ca<2+>-2Cl<->-6H2O, logK(298,15K) = -4,1436 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = 128,11 +/- unknown, Reference:

Remark: V0 calculated from http://webmineral,com/data/Antarcticite,shtml: rho = 1,71 g/cm3

10 CaMg(CO3)2_Dolomite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2161344,878 +/- unknown, Reaction: 0 = +1CaMg(CO3)2_Dolomite+2H<+>-1Ca<2+>-1Mg<2+>-2(HCO3)<->, logK(298,15K) = -3,596 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = 64,365 +/- unknown, Reference: YPF

Remark:

11 CaNa2(CO3)2:5H2O_Gaylussite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -3371843,138 +/- unknown, Reaction: 0 = +1CaNa2(CO3)2:5H2O_Gaylussite+2H<+>-1Ca<2+>-2Na<+>-2(HCO3)<->-5H2O, logK(298,15K) = -11,2576 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = 148,15 +/- unknown, Reference: YPF

Remark:

12 K(HCO3)_Kalicinite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -867748,757 +/- unknown, Reaction: 0 = +1K(HCO3)_Kalicinite-1K<+>-1(HCO3)<->, logK(298,15K) = -0,2814 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = 46,14 +/- unknown, Reference: YPF

Remark:

13 K(HSO4)_Mercallite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1034513,822 +/- unknown, Reaction: 0 = +1K(HSO4)_Mercallite-1K<+>-1H<+>-1(SO4)<2->, logK(298,15K) = 1,4015 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = 58,59 +/- unknown, Reference: YPF

Remark:

14 K2(CO3):1,5H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1431247,053 +/- unknown, Reaction: 0 = +1K2(CO3):1,5H2O+1H<+>-2K<+>-1(HCO3)<->-1,5H2O, logK(298,15K) = -13,372 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = 80,88 +/- unknown, Reference: YPF

Remark:

15 K2(SO4)_Arcanite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1319163,196 +/- unknown, Reaction: 0 = +1K2(SO4)_Arcanite-2K<+>-1(SO4)<2->, logK(298,15K) = 1,7763 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = 65,5 +/- unknown, Reference: YPF

Remark:

16 K2Ca(SO4)2:H2O_Syngenite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2885489,785 +/- unknown, Reaction: 0 = +1K2Ca(SO4)2:H2O_Syngenite-2K<+>-1Ca<2+>-2(SO4)<2->-1H2O, logK(298,15K) = 7,4484 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = 124,2 +/- unknown, Reference: YPF

Remark:

17 K2Mg(SO4)2:4H2O_Leonite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -3479675,302 +/- unknown, Reaction: 0 = +1K2Mg(SO4)2:4H2O_Leonite-2K<+>-1Mg<2+>-2(SO4)<2->-4H2O, logK(298,15K) = 3,979 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = 166,3 +/- unknown, Reference: YPF

Remark:

18 K2Mg(SO4)2:6H2O_Picromerite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -3955945,696 +/- unknown, Reaction: 0 = +1K2Mg(SO4)2:6H2O_Picromerite-2K<+>-1Mg<2+>-2(SO4)<2->-6H2O, logK(298,15K) = 4,3277 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = 197,5 +/- unknown, Reference:

Remark:

19 K2MgCa2(SO4)4:2H2O_Polyhalite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -5654754,91 +/- unknown, Reaction: 0 = +1K2MgCa2(SO4)4:2H2O_Polyhalite-2K<+>-1Mg<2+>-2Ca<2+>-4(SO4)<2->-2H2O, logK(298,15K) = 13,7441 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = 218,1 +/- unknown, Reference: YPF

Remark:

20 K2Na(HCO3)(CO3):2H2O_Trona-K

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2408868,41 +/- unknown, Reaction: 0 = +1K2Na(HCO3)(CO3):2H2O_Trona-K+1H<+>-2K<+>-1Na<+>-2(HCO3)<->-2H2O, logK(298,15K) = -11,5757 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = dummy value 0,001

Remark:

21 K3(HSO4)(SO4)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2355758,741 +/- unknown, Reaction: 0 = +1K3(HSO4)(SO4)-3K<+>-1H<+>-2(SO4)<2->, logK(298,15K) = 3,5425 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = dummy value 0,001

Remark:

22 K8(HCO3)4(CO3)2:3H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -6334529,138 +/- unknown, Reaction: 0 = +1K8(HCO3)4(CO3)2:3H2O+2H<+>-8K<+>-6(HCO3)<->-3H2O, logK(298,15K) = -27,6874 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = dummy value 0,001

Remark:

23 K8(HSO4)6(SO4)_Misenite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -7529789,68 +/- unknown, Reaction: 0 = +1K8(HSO4)6(SO4)_Misenite-8K<+>-6H<+>-7(SO4)<2->, logK(298,15K) = 10,8061 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = dummy value 0,001

Remark:

24 KCl_Sylvite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -408590,332 +/- unknown, Reaction: 0 = +1KCl_Sylvite-1K<+>-1Cl<->, logK(298,15K) = -0,8999 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = 37,524 +/- unknown, Reference: YPF

Remark:

25 KMgCl(SO4):3H2O_Kainite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2325625,369 +/- unknown, Reaction: 0 = +1KMgCl(SO4):3H2O_Kainite-1K<+>-1Mg<2+>-1Cl<->-1(SO4)<2->-3H2O, logK(298,15K) = 0,1926 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = 115,797553488372 +/- unknown, Reference:

Remark:

26 KMgCl3:6H2O_Carnallite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2529657,892 +/- unknown, Reaction: 0 = +1KMgCl3:6H2O_Carnallite-1K<+>-1Mg<2+>-3Cl<->-6H2O, logK(298,15K) = -4,3304 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = 172,58 +/- unknown, Reference: YPF

Remark:

27 KNa(CO3):6H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2495792,967 +/- unknown, Reaction: 0 = +1KNa(CO3):6H2O+1H<+>-1(HCO3)<->-1K<+>-1Na<+>-6H2O, logK(298,15K) = -10,2233 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = dummy value 0,001

Remark:

28 Mg(CO3):3H2O_Nesquehonite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1724116,861 +/- unknown, Reaction: 0 = +1Mg(CO3):3H2O_Nesquehonite+1H<+>-1Mg<2+>-1(HCO3)<->-3H2O, logK(298,15K) = -5,1722 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = 74,79 +/- unknown, Reference: YPF

Remark: poor G-fit from data0,ypf

29 Mg(CO3)_Magnesite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1027919,07 +/- unknown, Reaction: 0 = +1Mg(CO3)_Magnesite+1H<+>-1Mg<2+>-1(HCO3)<->, logK(298,15K) = -2,5054 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = 28,018 +/- unknown, Reference: YPF

Remark:

30 Mg(OH)2_Brucite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -831996,097 +/- unknown, Reaction: 0 = +1Mg(OH)2_Brucite+2H<+>-1Mg<2+>-2H2O, logK(298,15K) = -17,109 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = 24,63 +/- unknown, Reference: YPF

Remark:

31 Mg(SO4):6H2O_Hexahydrite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2631552,221 +/- unknown, Reaction: 0 = +1Mg(SO4):6H2O_Hexahydrite-1Mg<2+>-1(SO4)<2->-6H2O, logK(298,15K) = 1,6351 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = 132,58 +/- unknown, Reference: YPF

Remark:

32 Mg(SO4):7H2O_Epsomite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2870096,399 +/- unknown, Reaction: 0 = +1Mg(SO4):7H2O_Epsomite-1Mg<2+>-1(SO4)<2->-7H2O, logK(298,15K) = 1,8811 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = 146,8 +/- unknown, Reference: YPF

Remark:

33 Mg(SO4):H2O_Kieserite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1437219,377 +/- unknown, Reaction: 0 = +1Mg(SO4):H2O_Kieserite-1Mg<2+>-1(SO4)<2->-1H2O, logK(298,15K) = 0,1227 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = 56,6 +/- unknown, Reference: YPF

Remark:

34 Mg2CaCl6:12H2O_Tachyhydrite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -4997309,956 +/- unknown, Reaction: 0 = +1Mg2CaCl6:12H2O_Tachyhydrite-2Mg<2+>-1Ca<2+>-6Cl<->-12H2O, logK(298,15K) = -17,3839 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = 203,78 +/- unknown, Reference: YPF

Remark:

35 Mg2Cl(OH)3:4H2O_Oxychloride-Mg

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2313687,076 +/- unknown, Reaction: 0 = +1Mg2Cl(OH)3:4H2O_Oxychloride-Mg-2Mg<2+>-1Cl<->-3OH<->-4H2O, logK(298,15K) = -26,0297 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = 86,3108916666667 +/- unknown, Reference:

Remark:

36 MgCl2:6H2O_Bischoffite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2115217,386 +/- unknown, Reaction: 0 = +1MgCl2:6H2O_Bischoffite-1Mg<2+>-2Cl<->-6H2O, logK(298,15K) = -4,4554 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = 129,57 +/- unknown, Reference: YPF

Remark:

37 Na(HCO3)_Nahcolite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -851098,341 +/- unknown, Reaction: 0 = +1Na(HCO3)_Nahcolite-1Na<+>-1(HCO3)<->, logK(298,15K) = 0,403 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = 38,62 +/- unknown, Reference: YPF

Remark:

38 Na2(CO3):10H2O_Natron

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -3427841,828 +/- unknown, Reaction: 0 = +1Na2(CO3):10H2O_Natron+1H<+>-1(HCO3)<->-2Na<+>-10H2O, logK(298,15K) = -9,5145 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = 195,99 +/- unknown, Reference: YPF

Remark:

39 Na2(CO3):7H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2714340,675 +/- unknown, Reaction: 0 = +1Na2(CO3):7H2O+1H<+>-2Na<+>-1(HCO3)<->-7H2O, logK(298,15K) = -9,8791 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = 153,71 +/- unknown, Reference: YPF

Remark:

40 Na2(CO3):H2O_Thermonatrit

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1286123,699 +/- unknown, Reaction: 0 = +1Na2(CO3):H2O_Thermonatrit+1H<+>-2Na<+>-1(HCO3)<->-1H2O, logK(298,15K) = -10,8211 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = 54,92 +/- unknown, Reference: YPF

Remark:

41 Na2(SO4):10H2O_Mirabilite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -3646318,335 +/- unknown, Reaction: 0 = +1Na2(SO4):10H2O_Mirabilite-2Na<+>-1(SO4)<2->-10H2O, logK(298,15K) = 1,2278 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = 219,8 +/- unknown, Reference: YPF

Remark:

42 Na2(SO4)_Thenardite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1269551,062 +/- unknown, Reaction: 0 = +1Na2(SO4)_Thenardite-2Na<+>-1(SO4)<2->, logK(298,15K) = 0,2875 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = 53,33 +/- unknown, Reference: YPF

Remark:

43 Na2Ca(CO3)2:2H2O_Pirssonite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2659408,248 +/- unknown, Reaction: 0 = +1Na2Ca(CO3)2:2H2O_Pirssonite+2H<+>-2Na<+>-1Ca<2+>-2(HCO3)<->-2H2O, logK(298,15K) = -11,4354 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = 102,3 +/- unknown, Reference: YPF

Remark:

44 Na2Ca(SO4)2_Glauberite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2594655,83 +/- unknown, Reaction: 0 = +1Na2Ca(SO4)2_Glauberite-2Na<+>-1Ca<2+>-2(SO4)<2->, logK(298,15K) = 5,2445 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = 101,12 +/- unknown, Reference: YPF

Remark:

45 Na2Mg(SO4)2:4H2O_Bloedite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -3429245,205 +/- unknown, Reaction: 0 = +1Na2Mg(SO4)2:4H2O_Bloedite-2Na<+>-1Mg<2+>-2(SO4)<2->-4H2O, logK(298,15K) = 2,3469 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = 149,98 +/- unknown, Reference: YPF

Remark:

46 Na3(CO3)(HCO3):2H2O_Trona

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2380773,885 +/- unknown, Reaction: 0 = +1Na3(CO3)(HCO3):2H2O_Trona+1H<+>-3Na<+>-2(HCO3)<->-2H2O, logK(298,15K) = -9,2948 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = 106,115588732394 +/- unknown, Reference:

Remark: V0 calculated from density 2,11 - 2,17, Average = 2,13, according to http://webmineral,com/data/Trona,shtml

47 Na3(HSO4)(SO4)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2278515,059 +/- unknown, Reaction: 0 = +1Na3(HSO4)(SO4)-3Na<+>-1H<+>-2(SO4)<2->, logK(298,15K) = 0,8143 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = dummy value 0,001

Remark:

48 Na4Ca(SO4)3:2H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -4339287,731 +/- unknown, Reaction: 0 = +1Na4Ca(SO4)3:2H2O-4Na<+>-1Ca<2+>-3(SO4)<2->-2H2O, logK(298,15K) = 5,6723 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = dummy value 0,001

Remark:

49 Na6(CO3)(SO4)2_Burkeite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -3591961,585 +/- unknown, Reaction: 0 = +1Na6(CO3)(SO4)2_Burkeite+1H<+>-6Na<+>-1(HCO3)<->-2(SO4)<2->, logK(298,15K) = -9,5671 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = 151,19 +/- unknown, Reference: YPF

Remark:

50 NaCl_Halite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -384206,09 +/- unknown, Reaction: 0 = +1NaCl_Halite-1Na<+>-1Cl<->, logK(298,15K) = -1,5704 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = 27,015 +/- unknown, Reference: YPF

Remark:

51 NaK3(SO4)2_Glaserite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2619196,974 +/- unknown, Reaction: 0 = +1NaK3(SO4)2_Glaserite-1Na<+>-3K<+>-2(SO4)<2->, logK(298,15K) = 3,8027 +/- unknown, Reference: HMW

V0 [cm3 mol-1] = 246,23 +/- unknown, Reference: YPF

Remark: Value for V0 is twice as high as in hnv !

52 2Pb(CO3):Pb(OH)2_Hydrocerussite_(Schock)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1708697,11 +/- unknown, Reaction: 0 = +12Pb(CO3):Pb(OH)2_Hydrocerussite_(Schock)+4H<+>-3Pb<2+>-2(HCO3)<->-2H2O, logK(298,15K) = -2,1 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

53 2PbCl2:KCl

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1047085,361 +/- unknown, Reaction: 0 = +12PbCl2:KCl-2Pb<2+>-1K<+>-5Cl<->, logK(298,15K) = 10,514 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

54 3Pb(OH)2:Pb(SO4)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2177604,555 +/- unknown, Reaction: 0 = +13Pb(OH)2:Pb(SO4)+6H<+>-4Pb<2+>-1(SO4)<2->-6H2O, logK(298,15K) = -15,1 +/- unknown, Reference: HAG1998

V0 [cm3 mol-1] = dummy value 0,001

Remark:

55 3Pb(OH)2:PbCl2

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1688614,099 +/- unknown, Reaction: 0 = +13Pb(OH)2:PbCl2+6H<+>-4Pb<2+>-2Cl<->-6H2O, logK(298,15K) = -16,4 +/- unknown, Reference: HAG1998

V0 [cm3 mol-1] = dummy value 0,001

Remark:

56 3PbCl2:3KCl:H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2424134,59 +/- unknown, Reaction: 0 = +13PbCl2:3KCl:H2O-3Pb<2+>-3K<+>-9Cl<->-1H2O, logK(298,15K) = 15,031 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

57 NaPb2(CO3)2(OH)_Auerbachs_Salz

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1700281,943 +/- unknown, Reaction: 0 = +1NaPb2(CO3)2(OH)_Auerbachs_Salz+3H<+>-2Pb<2+>-1Na<+>-2(HCO3)<->-1H2O, logK(298,15K) = -3,675 +/- unknown, Reference: HAG1998

V0 [cm3 mol-1] = dummy value 0,001

Remark:

58 Pb

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = 0 +/- unknown, Reference:

V0 [cm3 mol-1] = 18,267 +/- unknown, Reference: COM

Remark:

59 Pb(CO3):PbCl2_Phosgenite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -956547,84 +/- unknown, Reaction: 0 = +1Pb(CO3):PbCl2_Phosgenite+1H<+>-2Pb<2+>-1(HCO3)<->-2Cl<->, logK(298,15K) = 10,3 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

60 Pb(CO3)_Cerussite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -629708,343 +/- unknown, Reaction: 0 = +1Pb(CO3)_Cerussite+1H<+>-1Pb<2+>-1(HCO3)<->, logK(298,15K) = 3,263 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

61 Pb(OH)2:Pb(SO4)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1261622,762 +/- unknown, Reaction: 0 = +1Pb(OH)2:Pb(SO4)+2H<+>-2Pb<2+>-1(SO4)<2->-2H2O, logK(298,15K) = -0,9 +/- unknown, Reference: HAG1998

V0 [cm3 mol-1] = dummy value 0,001

Remark:

62 Pb(OH)Cl_Laurionite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -390939,668 +/- unknown, Reaction: 0 = +1Pb(OH)Cl_Laurionite+1H<+>-1Pb<2+>-1Cl<->-1H2O, logK(298,15K) = -0,29 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

63 Pb(SO4):K2(SO4)_Palmierite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2150249,034 +/- unknown, Reaction: 0 = +1Pb(SO4):K2(SO4)_Palmierite-1Pb<2+>-2K<+>-2(SO4)<2->, logK(298,15K) = 12,786 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

64 Pb(SO4)_Anglesite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -813012,462 +/- unknown, Reaction: 0 = +1Pb(SO4)_Anglesite-1Pb<2+>-1(SO4)<2->, logK(298,15K) = 7,8434 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

65 Pb2(O)(SO4)_Lanarkite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1026708,898 +/- unknown, Reaction: 0 = +1Pb2(O)(SO4)_Lanarkite+2H<+>-2Pb<2+>-1(SO4)<2->-1H2O, logK(298,15K) = -0,51 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

66 Pb3(CO3)2(OH)2_Hydrocerussite_(RIC)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1701169,344 +/- unknown, Reaction: 0 = +1Pb3(CO3)2(OH)2_Hydrocerussite_(RIC)+4H<+>-3Pb<2+>-2(HCO3)<->-2H2O, logK(298,15K) = -3,4188 +/- unknown, Reference: HAG1998

V0 [cm3 mol-1] = dummy value 0,001

Remark:

67 Pb3O4_Minium

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -602116,505 +/- unknown, Reaction: 0 = +1Pb3O4_Minium+8H<+>-1Pb<4+>-2Pb<2+>-4H2O, logK(298,15K) = -16,2585 +/- unknown, Reference: COM

V0 [cm3 mol-1] = 76,81 +/- unknown, Reference: COM

Remark:

68 PbCl2:3MgCl2:19H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -6909444,432 +/- unknown, Reaction: 0 = +1PbCl2:3MgCl2:19H2O-1Pb<2+>-3Mg<2+>-8Cl<->-19H2O, logK(298,15K) = -6,362 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

69 PbCl2:Pb(SO4):2Na2(SO4):5w

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -4866792,316 +/- unknown, Reaction: 0 = +1PbCl2:Pb(SO4):2Na2(SO4):5w-2Pb<2+>-4Na<+>-2Cl<->-3(SO4)<2->-5H2O, logK(298,15K) = 15,83 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

70 PbCl2_Cotunnite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -313891,373 +/- unknown, Reaction: 0 = +1PbCl2_Cotunnite-1Pb<2+>-2Cl<->, logK(298,15K) = 4,7686 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = 46,5059197324415 +/- unknown, Reference:

Remark: V0 calculated from rho=5,98 g/cc taken from http://www,matweb,com/search/SpecificMaterial,asp?bassnum=EINOR0401

71 PbO_Litharge

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -189205,508 +/- unknown, Reaction: 0 = +1PbO_Litharge+2H<+>-1H2O-1Pb<2+>, logK(298,15K) = -12,644 +/- unknown, Reference: COM

V0 [cm3 mol-1] = 23,91 +/- unknown, Reference: COM

Remark:

72 PbO_Massicot

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -188205,459 +/- unknown, Reaction: 0 = +1PbO_Massicot+2H<+>-1H2O-1Pb<2+>, logK(298,15K) = -12,8192 +/- unknown, Reference: COM

V0 [cm3 mol-1] = 23,15 +/- unknown, Reference: COM

Remark:

73 Fe(OH)2(cr)

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -486975 +/- unknown, Reference: Barin

V0 [cm3 mol-1] = dummy value 0,001

Remark:

74 Fe(OH)2_precipitated

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -483324 +/- unknown, Reference: calc, From emf (Moog)

V0 [cm3 mol-1] = 26,43 +/- unknown, Reference: ymp

Remark:

75 Fe(SO4):7H2O_Melanterite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2507304,264 +/- unknown, Reaction: 0 = +1Fe(SO4):7H2O_Melanterite-1Fe<2+>-1(SO4)<2->-7H2O, logK(298,15K) = 2,246 +/- 0,009, Reference: MoHa

V0 [cm3 mol-1] = dummy value 0,001

Remark:

76 FeAl2O4_Hercynite

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -1879669 +/- unknown, Reference: Barin

V0 [cm3 mol-1] = dummy value 0,001

Remark:

77 FeCl2:4H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1284285,964 +/- unknown, Reaction: 0 = +1FeCl2:4H2O-1Fe<2+>-2Cl<->-4H2O, logK(298,15K) = -3,0147 +/- 0,03, Reference: MoHa

V0 [cm3 mol-1] = dummy value 0,001

Remark:

78 FeK2(SO4)2:6H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -3591070,696 +/- unknown, Reaction: 0 = +1FeK2(SO4)2:6H2O-1Fe<2+>-2K<+>-2(SO4)<2->-6H2O, logK(298,15K) = 4,3277 +/- unknown, Reference: MoHa

V0 [cm3 mol-1] = dummy value 0,001

Remark: logK: value for Picromerite in data0,hmw

79 FeNa2(SO4)2:4H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -3069987,49 +/- unknown, Reaction: 0 = +1FeNa2(SO4)2:4H2O-1Fe<2+>-2Na<+>-2(SO4)<2->-4H2O, logK(298,15K) = 3,331 +/- 0,03, Reference: MoHa

V0 [cm3 mol-1] = dummy value 0,001

Remark:

80 FeS

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -101965 +/- unknown, Reference: Barin

V0 [cm3 mol-1] = dummy value 0,001

Remark:

81 FeS2

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -160076 +/- unknown, Reference: Barin

V0 [cm3 mol-1] = dummy value 0,001

Remark:

82 Fe3O4_Magnetite

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -1015227 +/- unknown, Reference: Barin

V0 [cm3 mol-1] = 44,524 +/- unknown, Reference: YMP

Remark:

83 Fe(OH)3(cr)

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -696486 +/- unknown, Reference: Barin

V0 [cm3 mol-1] = 34,36 +/- unknown, Reference: YPF

Remark:

84 Fe2(SO4)3

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -2262753 +/- unknown, Reference: Barin

V0 [cm3 mol-1] = 130,77 +/- unknown, Reference: YPF

Remark:

85 KFe3(SO4)2(OH)6_Jarosite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -3029660,08 +/- unknown, Reaction: 0 = +1KFe3(SO4)2(OH)6_Jarosite+6H<+>-1K<+>-2(SO4)<2->-3Fe<3+>-6H2O, logK(298,15K) = 9,3706 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 156,75 +/- unknown, Reference: YPF

Remark:

86 NaFe3(SO4)2(OH)6_Jarosite-Na

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2986713,854 +/- unknown, Reaction: 0 = +1NaFe3(SO4)2(OH)6_Jarosite-Na+6H<+>-1Na<+>-2(SO4)<2->-3Fe<3+>-6H2O, logK(298,15K) = 5,4482 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 168,42 +/- unknown, Reference: YPF

Remark:

87 Fe2(SiO4)_Fayalite

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -1378985 +/- unknown, Reference: Barin

V0 [cm3 mol-1] = dummy value 0,001

Remark:

88 FeSiO3(cr)

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -1117463 +/- unknown, Reference: Barin

V0 [cm3 mol-1] = dummy value 0,001

Remark:

89 Am|+III|(CO3)(OH)(am,hyd)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1399074,535 +/- unknown, Reaction: 0 = +1Am|+III|(CO3)(OH)(am,hyd)-1Am|+III|<3+>-1(CO3)<2->-1OH<->, logK(298,15K) = 20,2 +/- 1, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

90 Am|+III|(CO3)(OH):0,5H2O(c)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1530202,229 +/- 5560, Reaction: 0 = +1Am|+III|(CO3)(OH):0,5H2O(c)-1Am|+III|<3+>-1(CO3)<2->-0,5H2O-1OH<->, logK(298,15K) = 22,4 +/- 0,5, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

91 Am|+III|(OH)3(am)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1213652,078 +/- unknown, Reaction: 0 = +1Am|+III|(OH)3(am)+3H<+>-3H2O-1Am|+III|<3+>, logK(298,15K) = -16,9 +/- 0,8, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

92 Am|+III|(OH)3(c)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1221072,534 +/- 5861, Reaction: 0 = +1Am|+III|(OH)3(c)+3H<+>-3H2O-1Am|+III|<3+>, logK(298,15K) = -15,6 +/- 0,6, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

93 Am|+III|(PO4)(am,hyd)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1765691,379 +/- unknown, Reaction: 0 = +1Am|+III|(PO4)(am,hyd)-1Am|+III|<3+>-1(PO4)<3->, logK(298,15K) = 24,79 +/- 0,6, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

94 Am|+III|2(CO3)3(am,hyd)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2876203,815 +/- unknown, Reaction: 0 = +1Am|+III|2(CO3)3(am,hyd)-3(CO3)<2->-2Am|+III|<3+>, logK(298,15K) = 16,7 +/- 1,1, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

95 NaAm|+III|(CO3)2:5H2O(c)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -3221875,565 +/- 5605, Reaction: 0 = +1NaAm|+III|(CO3)2:5H2O(c)-1Am|+III|<3+>-2(CO3)<2->-5H2O-1Na<+>, logK(298,15K) = 21 +/- 0,5, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

96 (Am|+V|O2)(OH)(am)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -946683,374 +/- unknown, Reaction: 0 = +1(Am|+V|O2)(OH)(am)+1H<+>-1H2O-1(Am|+V|O2)<+>, logK(298,15K) = -5,3 +/- 0,5, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

97 Na(Am|+V|O2)(CO3)(s)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1591794,5 +/- 6627, Reaction: 0 = +1Na(Am|+V|O2)(CO3)(s)-1(Am|+V|O2)<+>-1(CO3)<2->-1Na<+>, logK(298,15K) = 10,9 +/- 0,4, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

98 K2HAsO4:3H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1991494,158 +/- unknown, Reaction: 0 = +1K2HAsO4:3H2O-2K<+>-1(HAsO4)<2->-3H2O, logK(298,15K) = 1,3935 +/- , Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

99 K3AsO4:7H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -3156410,183 +/- unknown, Reaction: 0 = +1K3AsO4:7H2O-3K<+>-1(AsO4)<3->-7H2O, logK(298,15K) = 0,2453 +/- , Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

100 KH2AsO4

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1029378,641 +/- unknown, Reaction: 0 = +1KH2AsO4-1K<+>-1(H2AsO4)<->, logK(298,15K) = -0,2858 +/- , Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

101 Na2HAsO4:7H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1937259,651 +/- unknown, Reaction: 0 = +1Na2HAsO4:7H2O-2Na<+>-1(HAsO4)<2->-3H2O, logK(298,15K) = -0,9051 +/- , Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

102 Na3AsO4:12H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -4262084,972 +/- unknown, Reaction: 0 = +1Na3AsO4:12H2O-3Na<+>-1(AsO4)<3->-12H2O, logK(298,15K) = -2,9702 +/- , Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

103 NaH2AsO4:H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1258950,863 +/- unknown, Reaction: 0 = +1NaH2AsO4:H2O-1Na<+>-1(H2AsO4)<->-1H2O, logK(298,15K) = 1,9898 +/- , Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

104 Na2[B4O5(OH)4]:8H2O_Borax

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -5517956,02 +/- unknown, Reaction: 0 = +1Na2[B4O5(OH)4]:8H2O_Borax+2H<+>-2Na<+>-4B(OH)3<0>-5H2O, logK(298,15K) = -12,0395 +/- unknown, Reference: /WEP1982/

V0 [cm3 mol-1] = dummy value 0,001

Remark:

105 BaSeO3

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -957148,59 +/- 3400, Reaction: 0 = +1BaSeO3-1Ba<2+>-1SeO3<2->, logK(298,15K) = 6,5 +/- 0,25, Reference: NEA-7

V0 [cm3 mol-1] = dummy value 0,001

Remark:

106 BaSeO4

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1040293,728 +/- 3007, Reaction: 0 = +1BaSeO4-1Ba<2+>-1SeO4<2->, logK(298,15K) = 7,56 +/- 0,1, Reference: NEA-7

V0 [cm3 mol-1] = dummy value 0,001

Remark:

107 (CdCl2)2:5H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1889151,573 +/- unknown, Reaction: 0 = +1(CdCl2)2:5H2O-2Cd<2+>-4Cl<->-5H2O, logK(298,15K) = 4,05 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

108 (CdSO4)3:8H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -4395768,714 +/- unknown, Reaction: 0 = +1(CdSO4)3:8H2O-3Cd<2+>-3(SO4)<2->-8H2O, logK(298,15K) = 5,858 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

109 2CdSO4:2K2SO4:3H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -5025284,752 +/- unknown, Reaction: 0 = +12CdSO4:2K2SO4:3H2O-4K<+>-2Cd<2+>-4(SO4)<2->-3H2O, logK(298,15K) = 9,17 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

110 3CdSO4:K2SO4:5H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -5012448,993 +/- unknown, Reaction: 0 = +13CdSO4:K2SO4:5H2O-2K<+>-3Cd<2+>-4(SO4)<2->-5H2O, logK(298,15K) = 9,2 +/- unknown, Reference:

V0 [cm3 mol-1] = dummy value 0,001

Remark:

111 CdCl2:H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -587216,162 +/- unknown, Reaction: 0 = +1CdCl2:H2O-1Cd<2+>-2Cl<->-1H2O, logK(298,15K) = 1,736 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

112 CdCO3

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -669587,378 +/- unknown, Reaction: 0 = +1CdCO3+1H<+>-1Cd<2+>-1(HCO3)<->, logK(298,15K) = 0,8776 +/- unknown, Reference:

V0 [cm3 mol-1] = dummy value 0,001

Remark:

113 K4CdCl6

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2000897,204 +/- unknown, Reaction: 0 = +1K4CdCl6-4K<+>-1Cd<2+>-6Cl<->, logK(298,15K) = 1,02 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

114 KCd3Cl7:4H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2430878,26 +/- unknown, Reaction: 0 = +1KCd3Cl7:4H2O-1K<+>-3Cd<2+>-7Cl<->-4H2O, logK(298,15K) = 8,425 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

115 KCdCl3:H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1008614,772 +/- unknown, Reaction: 0 = +1KCdCl3:H2O-1K<+>-1Cd<2+>-3Cl<->-1H2O, logK(298,15K) = 3,08 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

116 Mg2CdCl6:12H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -4583352,399 +/- unknown, Reaction: 0 = +1Mg2CdCl6:12H2O-2Mg<2+>-1Cd<2+>-6Cl<->-12H2O, logK(298,15K) = -6,677 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

117 MgCd2Cl6:12H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -4251397,573 +/- unknown, Reaction: 0 = +1MgCd2Cl6:12H2O-1Mg<2+>-2Cd<2+>-6Cl<->-12H2O, logK(298,15K) = 1,327 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

118 Na2Cd(SO4)2:2H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2582535,219 +/- unknown, Reaction: 0 = +1Na2Cd(SO4)2:2H2O-2Na<+>-1Cd<2+>-2(SO4)<2->-2H2O, logK(298,15K) = 3,26 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

119 Na2CdCl4:3H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1845347,456 +/- unknown, Reaction: 0 = +1Na2CdCl4:3H2O-2Na<+>-1Cd<2+>-4Cl<->-3H2O, logK(298,15K) = 1,3 +/- unknown, Reference:

V0 [cm3 mol-1] = dummy value 0,001

Remark:

120 Na3Cd4Cl11:14H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -5897240,278 +/- unknown, Reaction: 0 = +1Na3Cd4Cl11:14H2O-3Na<+>-4Cd<2+>-11Cl<->-14H2O, logK(298,15K) = 6,5 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

121 alpha-CdSe

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -140897 +/- 1918, Reference: NEA-7

V0 [cm3 mol-1] = dummy value 0,001

Remark:

122 CdSeO3

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -493432 +/- 6467, Reference: NEA-7

V0 [cm3 mol-1] = dummy value 0,001

Remark:

123 Co(OH)2(cr)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -458197,079 +/- unknown, Reaction: 0 = +1Co(OH)2(cr)-1Co<2+>-2H2O+2H<+>, logK(298,15K) = -12,2 +/- 0,2, Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

124 CoCl2:6H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1753219,176 +/- unknown, Reaction: 0 = +1CoCl2:6H2O-1Co<2+>-2Cl<->-6H2O, logK(298,15K) = 2,521 +/- , Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

125 CoCl2:MgCl2:8H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2981148,976 +/- unknown, Reaction: 0 = +1CoCl2:MgCl2:8H2O-1Co<2+>-4Cl<->-8H2O-1Mg<2+>, logK(298,15K) = 8,8 +/- 0,09, Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

126 CoSO4:7H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2444165,256 +/- unknown, Reaction: 0 = +1CoSO4:7H2O-1Co<2+>-1(SO4)<2->-7H2O, logK(298,15K) = -2,343 +/- , Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

127 CoSO4:K2SO4:6H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -3499912,619 +/- unknown, Reaction: 0 = +1CoSO4:K2SO4:6H2O-1Co<2+>-2(SO4)<2->-6H2O-2K<+>, logK(298,15K) = -5,17 +/- 0,04, Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

128 CoSO4:Na2SO4:4H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2995078,498 +/- unknown, Reaction: 0 = +1CoSO4:Na2SO4:4H2O-1Co<2+>-2(SO4)<2->-4H2O-2Na<+>, logK(298,15K) = -3,32 +/- 0,03, Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

129 K2CrO4

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1292510,03 +/- unknown, Reaction: 0 = +1K2CrO4-2K<+>-1CrO4<2->, logK(298,15K) = -0,054304 +/- , Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

130 K2CrO4:MgCrO4

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2488552,694 +/- unknown, Reaction: 0 = +1K2CrO4:MgCrO4-2K<+>-1Mg<2+>-2CrO4<2->, logK(298,15K) = 2,2 +/- 0,2, Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

131 MgCrO4

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1181614,25 +/- unknown, Reaction: 0 = +1MgCrO4-1Mg<2+>-1CrO4<2->, logK(298,15K) = -0,27343 +/- , Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

132 MgCrO4:5H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2369758,091 +/- unknown, Reaction: 0 = +1MgCrO4:5H2O-1Mg<2+>-1CrO4<2->-5H2O, logK(298,15K) = 0,15471 +/- , Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

133 Na2CrO4:4H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2194693,01 +/- unknown, Reaction: 0 = +1Na2CrO4:4H2O-2Na<+>-1CrO4<2->-4H2O, logK(298,15K) = -0,97634 +/- , Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

134 Na2CrO4:6H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2670986,636 +/- unknown, Reaction: 0 = +1Na2CrO4:6H2O-2Na<+>-1CrO4<2->-6H2O, logK(298,15K) = -0,62357 +/- , Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

135 Na2CrO4:MgCrO4:2H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2949704,196 +/- unknown, Reaction: 0 = +1Na2CrO4:MgCrO4:2H2O-2K<+>-1Mg<2+>-2CrO4<2->-2H2O, logK(298,15K) = -0,1 +/- 0,2, Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

136 Cs2SeO4

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1018766,61 +/- 1800, Reaction: 0 = +1Cs2SeO4-2Cs<+>-1SeO4<2->, logK(298,15K) = -0,636 +/- 0,065, Reference: NEA-7

V0 [cm3 mol-1] = dummy value 0,001

Remark:

137 Cu(OH)2(s)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -458068,73 +/- unknown, Reaction: 0 = +1Cu(OH)2(s)+2H<+>-1Cu<2+>-2H2O, logK(298,15K) = 8,67 +/- 0,05, Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

138 Cu2CO3(OH)2(s)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -521641,614 +/- unknown, Reaction: 0 = +1Cu2CO3(OH)2(s)-2Cu<2+>-1(CO3)<2->-2OH<->, logK(298,15K) = -33,16 +/- 0,08, Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

139 Cu3(CO3)2(OH)2(s)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -916757,027 +/- unknown, Reaction: 0 = +1Cu3(CO3)2(OH)2(s)-3Cu<2+>-2(CO3)<2->-2OH<->, logK(298,15K) = -44,9 +/- 0,2, Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

140 CuO(s)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -215049,446 +/- unknown, Reaction: 0 = +1CuO(s)+2H<+>-1Cu<2+>-1H2O, logK(298,15K) = 7,64 +/- 0,06, Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

141 FeCO3_Siderite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -678035,673 +/- unknown, Reaction: 0 = +1FeCO3_Siderite+1H<+>-1Fe<2+>-1(HCO3)<->, logK(298,15K) = 0,121 +/- unknown, Reference: PSI/NAGRA

V0 [cm3 mol-1] = dummy value 0,001

Remark:

142 Hg(liquid)

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = 0 +/- 0, Reference: Convention

V0 [cm3 mol-1] = dummy value 0,001

Remark:

143 Hg2Cl2

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -210725 +/- 471, Reference: NEA-7

V0 [cm3 mol-1] = dummy value 0,001

Remark:

144 Hg2SO4

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -625780 +/- 411, Reference: NEA-7

V0 [cm3 mol-1] = dummy value 0,001

Remark:

145 HgO(red)

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -58523 +/- 154, Reference: NEA-7

V0 [cm3 mol-1] = dummy value 0,001

Remark:

146 HgO(s)(hx)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = 388164,778 +/- unknown, Reaction: 0 = +1HgO(s)(hx)+3H2O-1Hg(OH)2, logK(298,15K) = -3,59 +/- 0,05, Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

147 HgO(s)(O-rh,red)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -85943,981 +/- unknown, Reaction: 0 = +1HgO(s)(O-rh,red)+1H2O-1Hg(OH)2, logK(298,15K) = -3,62 +/- 0,05, Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

148 HgO(s)(O-rh,yellow)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = 151253,1 +/- unknown, Reaction: 0 = +1HgO(s)(O-rh,yellow)+2H2O-1Hg(OH)2, logK(298,15K) = -3,63 +/- 0,05, Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

149 alpha-HgSe

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -51200 +/- 4000, Reference: NEA-7

V0 [cm3 mol-1] = dummy value 0,001

Remark:

150 Hg2SeO3

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -295585,561 +/- 5998, Reaction: 0 = +1Hg2SeO3-1Hg2<2+>-1SeO3<2->, logK(298,15K) = 15,2 +/- 1, Reference: NAE-7

V0 [cm3 mol-1] = dummy value 0,001

Remark:

151 HgSeO3

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -290193,604 +/- 5,98, Reaction: 0 = +1HgSeO3-1Hg<2+>-1SeO3<2->, logK(298,15K) = 16,2 +/- 1, Reference: NEA-7

V0 [cm3 mol-1] = dummy value 0,001

Remark:

152 I2(cr)

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = 0 +/- 0, Reference: Convention

V0 [cm3 mol-1] = 51,3783279352227 +/- unknown, Reference:

Remark: V0 calculated from rho = 4,94 g/cm3

153 KI

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -324244,925 +/- unknown, Reaction: 0 = +1KI-1K<+>-1I<->, logK(298,15K) = -1,75 +/- unknown, Reference: I/Se-AB

V0 [cm3 mol-1] = dummy value 0,001

Remark:

154 MgI2:8H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2426609,368 +/- unknown, Reaction: 0 = +1MgI2:8H2O-1Mg<2+>-2I<->-8H2O, logK(298,15K) = -5,139 +/- unknown, Reference: I/Se-AB

V0 [cm3 mol-1] = dummy value 0,001

Remark:

155 NaI:2H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -771002,401 +/- unknown, Reaction: 0 = +1NaI:2H2O-1Na<+>-1I<->-2H2O, logK(298,15K) = -2,9703 +/- unknown, Reference: I/Se-AB

V0 [cm3 mol-1] = dummy value 0,001

Remark:

156 beta-Ni(IO3)2

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -323735,629 +/- 1743, Reaction: 0 = +1beta-Ni(IO3)2-1Ni<2+>-2IO3<->, logK(298,15K) = 4,43 +/- 0,02, Reference: NEA-6

V0 [cm3 mol-1] = dummy value 0,001

Remark:

157 Ni(IO3)2:2H2O(cr)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -802068,34 +/- 1832, Reaction: 0 = +1Ni(IO3)2:2H2O(cr)-1Ni<2+>-2IO3<->-2H2O, logK(298,15K) = 5,14 +/- 0,1, Reference: NEA-6

V0 [cm3 mol-1] = dummy value 0,001

Remark:

158 NiI2(cr)

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -94360 +/- 898, Reference: NEA-6

V0 [cm3 mol-1] = dummy value 0,001

Remark:

159 Li2SeO4:H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1252403,354 +/- 1500, Reaction: 0 = +1Li2SeO4:H2O-2Li<+>-1SeO4<2->-1H2O, logK(298,15K) = -1,762 +/- 0,065, Reference: NEA-7

V0 [cm3 mol-1] = dummy value 0,001

Remark:

160 Anatase_TiO2

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = 425427,146 +/- unknown, Reaction: 0 = +1Anatase_TiO2+2H2O-1Ti(OH)4<0>, logK(298,15K) = 8,5586 +/- , Reference: Min-GWB

V0 [cm3 mol-1] = dummy value 0,001

Remark:

161 Bassanite_CaSO4:0,5H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1436279,998 +/- unknown, Reaction: 0 = +1Bassanite_CaSO4:0,5H2O-0,5H2O-1Ca<2+>-1(SO4)<2->, logK(298,15K) = 3,6615 +/- , Reference: Min-GWB

V0 [cm3 mol-1] = dummy value 0,001

Remark:

162 CaSO4:0,5H2O(beta)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1435320,476 +/- unknown, Reaction: 0 = +1CaSO4:0,5H2O(beta)-0,5H2O-1Ca<2+>-1(SO4)<2->, logK(298,15K) = 3,4934 +/- , Reference: Min-GWB

V0 [cm3 mol-1] = dummy value 0,001

Remark:

163 Cassiterite_SnO2

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -519615,416 +/- unknown, Reaction: 0 = +1Cassiterite_SnO2+2H<+>-0,5O2(aq)-1H2O-1Sn<2+>, logK(298,15K) = 46,1642 +/- , Reference: Min-GWB

V0 [cm3 mol-1] = dummy value 0,001

Remark:

164 Chalcedony-SiO2

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -856155,514 +/- unknown, Reaction: 0 = +1Chalcedony-SiO2-1SiO2<0>, logK(298,15K) = 3,7281 +/- , Reference: Min-GWB

V0 [cm3 mol-1] = dummy value 0,001

Remark:

165 Coesite_SiO2

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -853080,021 +/- unknown, Reaction: 0 = +1Coesite_SiO2-1SiO2<0>, logK(298,15K) = 3,1893 +/- , Reference: Min-GWB

V0 [cm3 mol-1] = dummy value 0,001

Remark:

166 Dawsonite_NaAlCO3(OH)2

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1793683,289 +/- unknown, Reaction: 0 = +1Dawsonite_NaAlCO3(OH)2+3H<+>-1Al<3+>-1(HCO3)<->-1Na<+>-2H2O, logK(298,15K) = -3,6618 +/- , Reference: Min-GWB

V0 [cm3 mol-1] = dummy value 0,001

Remark:

167 Delafossite_CuFeO2

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -388214,417 +/- unknown, Reaction: 0 = +1Delafossite_CuFeO2+4H<+>-1Cu<+>-1Fe<3+>-2H2O, logK(298,15K) = 6,4172 +/- , Reference: Min-GWB

V0 [cm3 mol-1] = dummy value 0,001

Remark:

168 Dolomite-dis_CaMg(CO3)2

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2158708,333 +/- unknown, Reaction: 0 = +1Dolomite-dis_CaMg(CO3)2+2H<+>-1Ca<2+>-1Mg<2+>-2(HCO3)<->, logK(298,15K) = -4,0579 +/- , Reference: Min-GWB

V0 [cm3 mol-1] = dummy value 0,001

Remark:

169 Dolomite-ord_CaMg(CO3)2

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2167523,835 +/- unknown, Reaction: 0 = +1Dolomite-ord_CaMg(CO3)2+2H<+>-1Ca<2+>-1Mg<2+>-2(HCO3)<->, logK(298,15K) = -2,5135 +/- , Reference: Min-GWB

V0 [cm3 mol-1] = dummy value 0,001

Remark:

170 Eskolaite_Cr2O3

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1051056,585 +/- unknown, Reaction: 0 = +1Eskolaite_Cr2O3+2H2O+1,5O2(aq)-2CrO4<2->-4H<+>, logK(298,15K) = 7,8698 +/- , Reference: Min-GWB

V0 [cm3 mol-1] = dummy value 0,001

Remark:

171 Gibbsite_Al(OH)3

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1163161,35 +/- unknown, Reaction: 0 = +1Gibbsite_Al(OH)3+3H<+>-1Al<3+>-3H2O, logK(298,15K) = -6,9666 +/- , Reference: Min-GWB

V0 [cm3 mol-1] = dummy value 0,001

Remark:

172 Goethite_FeOOH

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -398833,816 +/- unknown, Reaction: 0 = +1Goethite_FeOOH+3H<+>-1Fe<3+>-2H2O, logK(298,15K) = -0,5345 +/- , Reference: Min-GWB

V0 [cm3 mol-1] = dummy value 0,001

Remark:

173 Hematite_Fe2O3

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -566009,637 +/- unknown, Reaction: 0 = +1Hematite_Fe2O3+6H<+>-2Fe<3+>-3H2O, logK(298,15K) = -0,1086 +/- , Reference: Min-GWB

V0 [cm3 mol-1] = dummy value 0,001

Remark:

174 MnHPO4

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1397987,029 +/- unknown, Reaction: 0 = +1MnHPO4-1(HPO4)<2->-1Mn<2+>, logK(298,15K) = 12,947 +/- , Reference: Min-GWB

V0 [cm3 mol-1] = dummy value 0,001

Remark:

175 Morenosite_NiSO4:7H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2461252,998 +/- unknown, Reaction: 0 = +1Morenosite_NiSO4:7H2O-1Ni<2+>-1(SO4)<2->-7H2O, logK(298,15K) = 2,014 +/- , Reference: Min-GWB

V0 [cm3 mol-1] = dummy value 0,001

Remark:

176 Ni2SiO4

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1318838,895 +/- unknown, Reaction: 0 = +1Ni2SiO4+4H<+>-1SiO2<0>-2H2O-2Ni<2+>, logK(298,15K) = -14,3416 +/- , Reference: Min-GWB

V0 [cm3 mol-1] = dummy value 0,001

Remark:

177 NiCO3

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -612572,496 +/- unknown, Reaction: 0 = +1NiCO3+1H<+>-1(HCO3)<->-1Ni<2+>, logK(298,15K) = -3,5118 +/- , Reference: Min-GWB

V0 [cm3 mol-1] = dummy value 0,001

Remark:

178 NiSO4:6H2O(alpha)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2224074,183 +/- unknown, Reaction: 0 = +1NiSO4:6H2O(alpha)-1Ni<2+>-1(SO4)<2->-6H2O, logK(298,15K) = 2,0072 +/- , Reference: Min-GWB

V0 [cm3 mol-1] = dummy value 0,001

Remark:

179 Rhodochrosite_MnCO3

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -813535,113 +/- unknown, Reaction: 0 = +1Rhodochrosite_MnCO3+1H<+>-1(HCO3)<->-1Mn<2+>, logK(298,15K) = -0,247 +/- , Reference: Min-GWB

V0 [cm3 mol-1] = dummy value 0,001

Remark:

180 Rutile-TiO2

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = 419224,786 +/- unknown, Reaction: 0 = +1Rutile-TiO2+2H2O-1Ti(OH)4<0>, logK(298,15K) = 9,6452 +/- , Reference: Min-GWB

V0 [cm3 mol-1] = dummy value 0,001

Remark:

181 SiO2(am)-GWB

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -850364,705 +/- unknown, Reaction: 0 = +1SiO2(am)-GWB-1SiO2<0>, logK(298,15K) = 2,7136 +/- , Reference: Min-GWB

V0 [cm3 mol-1] = dummy value 0,001

Remark:

182 Trevorite_NiFe2O4

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -793674,491 +/- unknown, Reaction: 0 = +1Trevorite_NiFe2O4+8H<+>-1Ni<2+>-2Fe<3+>-4H2O, logK(298,15K) = -9,7876 +/- , Reference: Min-GWB

V0 [cm3 mol-1] = dummy value 0,001

Remark:

183 Tridymite_SiO2

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -856724,606 +/- unknown, Reaction: 0 = +1Tridymite_SiO2-1SiO2<0>, logK(298,15K) = 3,8278 +/- , Reference: Min-GWB

V0 [cm3 mol-1] = dummy value 0,001

Remark:

184 V2O4

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1318151,229 +/- unknown, Reaction: 0 = +1V2O4+4H<+>-2H2O-2VO<2+>, logK(298,15K) = -8,5719 +/- , Reference: Min-GWB

V0 [cm3 mol-1] = dummy value 0,001

Remark:

185 2MgCl2:MnCl2:12H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -4692718,528 +/- unknown, Reaction: 0 = +12MgCl2:MnCl2:12H2O-1Mn<2+>-6Cl<->-12H2O-2Mg<2+>, logK(298,15K) = -13,86 +/- 0,07, Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

186 CaCl2:MnCl2:8H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -3160654,484 +/- unknown, Reaction: 0 = +1CaCl2:MnCl2:8H2O -1Mn<2+>-4Cl<->-8H2O-1Ca<2+>, logK(298,15K) = -7,4 +/- 0,1, Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

187 MgCl2:2MnCl2:12H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -4481197,726 +/- unknown, Reaction: 0 = +1MgCl2:2MnCl2:12H2O-2Mn<2+>-6Cl<->-12H2O-1Mg<2+>, logK(298,15K) = -11,1 +/- 0,1, Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

188 MgCl2:MnCl2:8H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -3057915,004 +/- unknown, Reaction: 0 = +1MgCl2:MnCl2:8H2O-1Mn<2+>-4Cl<->-8H2O-1Mg<2+>, logK(298,15K) = -8,33 +/- 0,06, Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

189 Mn(OH)2

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -683930,228 +/- unknown, Reaction: 0 = +1Mn(OH)2-2Mn<2+>-2OH<->, logK(298,15K) = -15,2 +/- 0,1, Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

190 MnCl2:4H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1422580,632 +/- unknown, Reaction: 0 = +1MnCl2:4H2O-1Mn<2+>-2Cl<->-4H2O, logK(298,15K) = -2,893 +/- , Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

191 MnCl2:KCl:2H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1356165,473 +/- unknown, Reaction: 0 = +1MnCl2:KCl:2H2O -1Mn<2+>-3Cl<->-2H2O-1K<+>, logK(298,15K) = -3,92 +/- 0,05, Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

192 MnSO4:4H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1929882,489 +/- unknown, Reaction: 0 = +1MnSO4:4H2O-1Mn<2+>-1(SO4)<2->-4H2O, logK(298,15K) = 1,615 +/- , Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

193 MnSO4:5H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2167416,344 +/- unknown, Reaction: 0 = +1MnSO4:5H2O-1Mn<2+>-1(SO4)<2->-5H2O, logK(298,15K) = 1,684 +/- , Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

194 MnSO4:H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1217292,34 +/- unknown, Reaction: 0 = +1MnSO4:H2O-1Mn<2+>-1(SO4)<2->-1H2O, logK(298,15K) = 1,41 +/- , Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

195 MnSO4:K2SO4:4H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -3253661,779 +/- unknown, Reaction: 0 = +1MnSO4:K2SO4:4H2O-1Mn<2+>-2(SO4)<2->-4H2O-2K<+>, logK(298,15K) = 4,2 +/- 0,3, Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

196 MnSO4:Na2SO4:2H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2469293,887 +/- unknown, Reaction: 0 = +1MnSO4:Na2SO4:2H2O-1Mn<2+>-2(SO4)<2->-2H2O-1Na<+>, logK(298,15K) = 2,97 +/- 0,02, Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

197 CaMoO4_Powellite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1451777,078 +/- unknown, Reaction: 0 = +1CaMoO4_Powellite-1Ca<2+>-1MoO4<2->, logK(298,15K) = 7,96 +/- unknown, Reference: /GMR1992/

V0 [cm3 mol-1] = dummy value 0,001

Remark: logK value valid for 22C

198 MgMoO4:5H2O(s)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2505169,937 +/- unknown, Reaction: 0 = +1MgMoO4:5H2O(s)-1Mg<2+>-1MoO4<2->-5H2O, logK(298,15K) = 1,85 +/- 0,03, Reference: /GMR1992/

V0 [cm3 mol-1] = dummy value 0,001

Remark:

199 Na0,5Nd0,5MoO4(s)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1371541,46 +/- unknown, Reaction: 0 = +1Na0,5Nd0,5MoO4(s)-0,5Na<+>-0,5Nd<3+>-1MoO4<2->, logK(298,15K) = 8,94 +/- 0,13, Reference: /GMR1992/

V0 [cm3 mol-1] = dummy value 0,001

Remark: logK-value valid for 22C

200 Nd(OH)3

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1298712,075 +/- unknown, Reaction: 0 = +1Nd(OH)3-1Nd<3+>-3OH<->, logK(298,15K) = 27,15 +/- 0,3, Reference: SM8097

V0 [cm3 mol-1] = dummy value 0,001

Remark:

201 Nd2(CO3)3

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -3124981,78 +/- unknown, Reaction: 0 = +1Nd2(CO3)3-2Nd<3+>-3(CO3)<2->, logK(298,15K) = 34,6 +/- 0,1, Reference: SM8097

V0 [cm3 mol-1] = dummy value 0,001

Remark: logK: Alternatively 34,8

202 NdO(HCO3)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1479796,991 +/- unknown, Reaction: 0 = +1NdO(HCO3)-1Nd<3+>-1OH<->-1(CO3)<2->, logK(298,15K) = 21,5 +/- 0,3, Reference: SM8097

V0 [cm3 mol-1] = dummy value 0,001

Remark: logK: Alternatively 21,65

203 alpha-NiS

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = 8733,305 +/- 1007, Reaction: 0 = +1alpha-NiS, logK(298,15K) = -1,53 +/- 0,3, Reference:

V0 [cm3 mol-1] = dummy value 0,001

Remark:

204 alpha-NiSO4:6H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2225871,075 +/- 1059, Reaction: 0 = +1alpha-NiSO4:6H2O-1Ni<2+>-1(SO4)<2->-6H2O, logK(298,15K) = 2,322 +/- , Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

205 beta-Ni(OH)2

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = 62902,631 +/- 1400, Reaction: 0 = +1beta-Ni(OH)2, logK(298,15K) = -11,02 +/- 0,2, Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

206 beta-NiS

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = 11986,89 +/- 1007, Reaction: 0 = +1beta-NiS, logK(298,15K) = -2,1 +/- 0,3, Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

207 beta-NiSO4:6H2O

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -2224915 +/- 1815, Reference: NEA-6

V0 [cm3 mol-1] = dummy value 0,001

Remark:

208 K2Ni(SO4)2:6H2O(cr)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -3560455,69 +/- unknown, Reaction: 0 = +1K2Ni(SO4)2:6H2O(cr)-2K<+>-1Ni<2+>-2(SO4)<2->, logK(298,15K) = 6,8 +/- 0,1, Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

209 Na2Ni(SO4)2:4H2O(cr)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -3026168,069 +/- unknown, Reaction: 0 = +1Na2Ni(SO4)2:4H2O(cr)-2Na<+>-1Ni<2+>-2(SO4)<2->, logK(298,15K) = 3,49 +/- 0,03, Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

210 Ni(CO3)(cr)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -636416,414 +/- 1292, Reaction: 0 = +1Ni(CO3)(cr)+2H<+>-1Ni<2+>-1H2O-1CO2(g), logK(298,15K) = -7,16 +/- 0,18, Reference: NEA-6

V0 [cm3 mol-1] = dummy value 0,001

Remark:

211 Ni(CO3):5,5H2O(cr)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1920879,506 +/- 1004, Reaction: 0 = +1Ni(CO3):5,5H2O(cr)+2H<+>-1Ni<2+>-6,5H2O-1CO2(g), logK(298,15K) = -10,63 +/- 0,1, Reference: NEA-6

V0 [cm3 mol-1] = dummy value 0,001

Remark:

212 Ni(cr)

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = 0 +/- 0, Reference: NEA-6

V0 [cm3 mol-1] = dummy value 0,001

Remark:

213 Ni(OH)2(cr)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -460118,551 +/- unknown, Reaction: 0 = +1Ni(OH)2(cr)-1Ni<2+>-2H2O+2H<+>, logK(298,15K) = -10,5 +/- 1,3, Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark:

214 Ni3S2(cr)

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -211172 +/- 1624, Reference: NEA-6

V0 [cm3 mol-1] = dummy value 0,001

Remark:

215 Ni9S8(cr)

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -746803 +/- 9255, Reference: NEA-6

V0 [cm3 mol-1] = dummy value 0,001

Remark:

216 NiCl2(cr)

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -258743 +/- 154, Reference: NEA-6

V0 [cm3 mol-1] = dummy value 0,001

Remark:

217 NiCl2:2H2O(cr)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -753430,642 +/- 1256, Reaction: 0 = +1NiCl2:2H2O(cr)+2H2O(g)-1NiCl2:4H2O(cr), logK(298,15K) = -4,099 +/- 0,123, Reference: NEA-6

V0 [cm3 mol-1] = dummy value 0,001

Remark:

218 NiCl2:4H2O(cr)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1233991,91 +/- 1040, Reaction: 0 = +1NiCl2:4H2O(cr)-1Ni<2+>-2Cl<->-4H2O, logK(298,15K) = -3,99 +/- unknown, Reference: Koda

V0 [cm3 mol-1] = dummy value 0,001

Remark: log K (NEA 6): -3,777±0,105

219 NiCl2:6H2O(cr)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1713421,706 +/- 846, Reaction: 0 = +1NiCl2:6H2O(cr)-1Ni<2+>-2Cl<->-6H2O, logK(298,15K) = -3,0878 +/- unknown, Reference: /BC1999/

V0 [cm3 mol-1] = dummy value 0,001

Remark: log K (NEA 6): -3,045±0,014

220 NiO(cr)

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -211660 +/- 422, Reference: NEA-6

V0 [cm3 mol-1] = dummy value 0,001

Remark:

221 NiS2(cr)

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -123832 +/- 7396, Reference: NEA-6

V0 [cm3 mol-1] = dummy value 0,001

Remark:

222 NiSO4(cr)

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -762688 +/- 1572, Reference: NEA-6

V0 [cm3 mol-1] = dummy value 0,001

Remark:

223 NiSO4:7H2O(cr)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2463011,075 +/- 929, Reaction: 0 = +1NiSO4:7H2O(cr)-1Ni<2+>-1(SO4)<2->-7H2O, logK(298,15K) = 2,322 +/- unknown, Reference: /BC1999/

V0 [cm3 mol-1] = dummy value 0,001

Remark:

224 NiSe2

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -112355 +/- 7017, Reference: NEA-7

V0 [cm3 mol-1] = dummy value 0,001

Remark:

225 NiSeO3:2H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -915549,96 +/- 6022, Reaction: 0 = +1NiSeO3:2H2O-1Ni<2+>-1SeO3<2->-2H2O, logK(298,15K) = 5,8 +/- 1, Reference: NEA-7

V0 [cm3 mol-1] = dummy value 0,001

Remark:

226 NiSeO4:6H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1915980,732 +/- unknown, Reaction: 0 = +1NiSeO4:6H2O-1Ni<2+>-1SeO4<2->-6H2O, logK(298,15K) = 1,381 +/- 0,045, Reference: NEA-7

V0 [cm3 mol-1] = dummy value 0,001

Remark:

227 Ni2(SiO4)(oliv)

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -1288441 +/- 5002, Reference: NEA-6

V0 [cm3 mol-1] = dummy value 0,001

Remark:

228 Np|+IV|(OH)4(am)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1444404,976 +/- unknown, Reaction: 0 = +1Np|+IV|(OH)4(am)-1Np|+IV|<4+>-4OH<->, logK(298,15K) = 56,7 +/- 0,5, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

229 (Np|+V|O2)(OH)(am,aged)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1118077,199 +/- 6310, Reaction: 0 = +1(Np|+V|O2)(OH)(am,aged)+1H<+>-1H2O-1(Np|+V|O2)<+>, logK(298,15K) = -4,7 +/- 0,5, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

230 (Np|+V|O2)(OH)(am,fresh)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1114652,374 +/- 5743, Reaction: 0 = +1(Np|+V|O2)(OH)(am,fresh)+1H<+>-1H2O-1(Np|+V|O2)<+>, logK(298,15K) = -5,3 +/- 0,2, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

231 K(Np|+V|O2)(CO3)(s)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1793163,596 +/- 5746, Reaction: 0 = +1K(Np|+V|O2)(CO3)(s)-1(Np|+V|O2)<+>-1(CO3)<2->-1K<+>, logK(298,15K) = 13,15 +/- 0,19, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

232 K3(Np|+V|O2)(CO3)2(s)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2899197,008 +/- 5765, Reaction: 0 = +1K3(Np|+V|O2)(CO3)2(s)-1(Np|+V|O2)<+>-2(CO3)<2->-3K<+>, logK(298,15K) = 15,46 +/- 0,16, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

233 Na(Np|+V|O2)(CO3):3,5H2O(c)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2590324,304 +/- 5808, Reaction: 0 = +1Na(Np|+V|O2)(CO3):3,5H2O(c)-1(Np|+V|O2)<+>-1(CO3)<2->-3,5H2O-1Na<+>, logK(298,15K) = 11 +/- 0,24, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

234 Na3(Np|+V|O2)(CO3)2(c)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2830448,035 +/- 6365, Reaction: 0 = +1Na3(Np|+V|O2)(CO3)2(c)-1(Np|+V|O2)<+>-2(CO3)<2->-3Na<+>, logK(298,15K) = 14,22 +/- 0,5, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

235 Np|+V|2O5(c)

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -2031570 +/- 11226, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

236 Np|+V|O2,5(s,hyd)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1007517,296 +/- unknown, Reaction: 0 = +1Np|+V|O2,5(s,hyd)+0,5H2O-1(Np|+V|O2)<+>-1OH<->, logK(298,15K) = 10,7 +/- 1, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = 24,212 +/- unknown, Reference: HbChemPhys

Remark: V0: chapter B-101, for NpO2 rho=11,11 and Mw=269,0g/mol

237 (Np|+VI|O2)(CO3)(s)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1407081,425 +/- 6233, Reaction: 0 = +1(Np|+VI|O2)(CO3)(s)-1(CO3)<2->-1(Np|+VI|O2)<2+>, logK(298,15K) = 14,596 +/- 0,469, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

238 K4(Np|+VI|O2)(CO3)3(s)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -3660177,397 +/- 7641, Reaction: 0 = +1K4(Np|+VI|O2)(CO3)3(s)-4K<+>-1(Np|+VI|O2)(CO3)3<4->, logK(298,15K) = 7,033 +/- 0,876, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

239 Np|+VI|O3:H2O(c)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1238996,006 +/- 6062, Reaction: 0 = +1Np|+VI|O3:H2O(c)+2H<+>-2H2O-1(Np|+VI|O2)<2+>, logK(298,15K) = -5,47 +/- 0,4, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

240 PbSe

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -97936 +/- 7694, Reference: NEA-7

V0 [cm3 mol-1] = dummy value 0,001

Remark:

241 PbSeO3

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -457978,846 +/- 5985, Reaction: 0 = +1PbSeO3-1Pb<2+>-1SeO3<2->, logK(298,15K) = 12,5 +/- 1, Reference: NEA-7

V0 [cm3 mol-1] = dummy value 0,001

Remark:

242 PbSeO4

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -503108,42 +/- 2060, Reaction: 0 = +1PbSeO4-1Pb<2+>-1SeO4<2->, logK(298,15K) = 6,9 +/- 0,25, Reference: NEA-7

V0 [cm3 mol-1] = dummy value 0,001

Remark:

243 Pu|+III|(OH)3(c)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1200216,925 +/- 8975, Reaction: 0 = +1Pu|+III|(OH)3(c)+3H<+>-3H2O-1Pu|+III|<3+>, logK(298,15K) = -15,8 +/- 1,5, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

244 Pu|+III|(PO4)(s,hyd)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1744892,851 +/- 5528, Reaction: 0 = +1Pu|+III|(PO4)(s,hyd)-1(PO4)<3->-1Pu|+III|<3+>, logK(298,15K) = 24,6 +/- 0,8, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

245 Pu|+IV|(HPO4)2(am,hyd)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2843767,901 +/- unknown, Reaction: 0 = +1Pu|+IV|(HPO4)2(am,hyd)-2(HPO4)<2->-1Pu|+IV|<4+>, logK(298,15K) = 30,45 +/- 0,51, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

246 Pu|+IV|(OH)4(am)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1439923,086 +/- unknown, Reaction: 0 = +1Pu|+IV|(OH)4(am)-4OH<->-1Pu|+IV|<4+>, logK(298,15K) = 58,33 +/- 0,52, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark: logK: in INE-Report from 2000: 58,5

247 (Pu|+V|O2)(OH)(am)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1061248,314 +/- 4046, Reaction: 0 = +1(Pu|+V|O2)(OH)(am)+1H<+>-1H2O-1(Pu|+V|O2)<+>, logK(298,15K) = -5 +/- 0,5, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

248 (Pu|+VI|O2)(CO3)(s)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1373803,66 +/- 3912, Reaction: 0 = +1(Pu|+VI|O2)(CO3)(s)-1(CO3)<2->-1(Pu|+VI|O2)<2+>, logK(298,15K) = 14,65 +/- 0,47, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

249 (Pu|+VI|O2)(OH)2:H2O(c)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1442378,765 +/- 6368, Reaction: 0 = +1(Pu|+VI|O2)(OH)2:H2O(c)+2H<+>-3H2O-1(Pu|+VI|O2)<2+>, logK(298,15K) = -5,5 +/- 1, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

250 RaCO3(cr)
Gibbs Free Energy of Formation directly entered
deltaG_0^f [J mol-1] = -1136794 +/- unknown, Reference: NTB 02-16
V0 [cm3 mol-1] = dummy value 0,001
Remark:

251 RaSO4(cr)
Gibbs Free Energy of Formation directly entered
deltaG_0^f [J mol-1] = -1364069 +/- unknown, Reference: NTB 02-16
V0 [cm3 mol-1] = dummy value 0,001
Remark:

252 3MgSeO4:2Na2SeO4:18H2O
Gibbs Free Energy of Formation calculated from logK for reaction
deltaG_0^f [J mol-1] = -8902371,315 +/- unknown, Reaction: 0 = +13MgSeO4:2Na2SeO4:18H2O-4Na<+>-3Mg<2+>-5SeO4<2->-18H2O, logK(298,15K) = 3,94 +/- unknown, Reference: I/SE-AB
V0 [cm3 mol-1] = dummy value 0,001
Remark:

253 CaSeO3
Gibbs Free Energy of Formation calculated from logK for reaction
deltaG_0^f [J mol-1] = -950586,177 +/- unknown, Reaction: 0 = +1CaSeO3-1Ca<2+>-1SeO3<2->, logK(298,15K) = 6,2 +/- 0,3, Reference: I/SE-AB
V0 [cm3 mol-1] = dummy value 0,001
Remark:

254 CaSeO4:2H2O
Gibbs Free Energy of Formation calculated from logK for reaction
deltaG_0^f [J mol-1] = -1481868,48 +/- 2300, Reaction: 0 = +1CaSeO4:2H2O-1Ca<2+>-1SeO4<2->-2H2O, logK(298,15K) = 2,68 +/- 0,25, Reference: NEA-7
V0 [cm3 mol-1] = dummy value 0,001
Remark:

255 K2Mg(SeO4)2:6H2O
Gibbs Free Energy of Formation calculated from logK for reaction
deltaG_0^f [J mol-1] = -3338575,517 +/- unknown, Reaction: 0 = +1K2Mg(SeO4)2:6H2O-2K<+>-1Mg<2+>-2SeO4<2->-6H2O, logK(298,15K) = 2,868 +/- unknown, Reference: I/SE-AB
V0 [cm3 mol-1] = dummy value 0,001
Remark:

256 K2SeO4
Gibbs Free Energy of Formation calculated from logK for reaction
deltaG_0^f [J mol-1] = -997158,674 +/- unknown, Reaction: 0 = +1K2SeO4-2K<+>-1SeO4<2->, logK(298,15K) = -1,287 +/- unknown, Reference: I/SE-AB
V0 [cm3 mol-1] = dummy value 0,001
Remark:

257 MgSeO3
Gibbs Free Energy of Formation calculated from logK for reaction
deltaG_0^f [J mol-1] = -851442,764 +/- unknown, Reaction: 0 = +1MgSeO3-1Mg<2+>-1SeO3<2->, logK(298,15K) = 5,9 +/- 0,3, Reference: I/SE-AB
V0 [cm3 mol-1] = dummy value 0,001
Remark:

258 MgSeO4:6H2O
Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2324349,795 +/- 2000, Reaction: 0 = +1MgSeO4:6H2O-1Mg<2+>-1SeO4<2->-6H2O, logK(298,15K) = 1,165 +/- unknown, Reference: I/SE-AB

V0 [cm3 mol-1] = dummy value 0,001

Remark:

259 Na2SeO3

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = 10731,12 +/- 967, Reaction: 0 = +1Na2SeO3, logK(298,15K) = -1,88 +/- unknown, Reference: I/SE-AB

V0 [cm3 mol-1] = dummy value 0,001

Remark:

260 Na2SeO3:5H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2067771,79 +/- unknown, Reaction: 0 = +1Na2SeO3:5H2O-2Na<+>-1SeO3<2->-5H2O, logK(298,15K) = -0,7401 +/- unknown, Reference: I/SE-AB

V0 [cm3 mol-1] = dummy value 0,001

Remark:

261 Na2SeO4(cr)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -958583,612 +/- unknown, Reaction: 0 = +1Na2SeO4(cr)-2Na<+>-1SeO4<2->, logK(298,15K) = -0,8422 +/- unknown, Reference: I/SE-AB

V0 [cm3 mol-1] = dummy value 0,001

Remark:

262 Na2SeO4:10H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -3338186,64 +/- 1600, Reaction: 0 = +1Na2SeO4:10H2O-2Na<+>-1SeO4<2->-10H2O, logK(298,15K) = 0,5949 +/- unknown, Reference: I/SE-AB

V0 [cm3 mol-1] = dummy value 0,001

Remark:

263 Se(cr)

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = 0 +/- 0, Reference: NEA-7

V0 [cm3 mol-1] = dummy value 0,001

Remark:

264 Se(mono)

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = 1281 +/- 184, Reference: NEA-7

V0 [cm3 mol-1] = dummy value 0,001

Remark:

265 SeCl4

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -85902 +/- 3114, Reference: NEA-7

V0 [cm3 mol-1] = dummy value 0,001

Remark:

266 SeO2(cr)

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -171797 +/- 620, Reference: NEA-7

V0 [cm3 mol-1] = dummy value 0,001

Remark:

267 SeO3(cr)

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -86154 +/- 2222, Reference: NEA-7

V0 [cm3 mol-1] = dummy value 0,001

Remark:

268 SrSeO3

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -962214,981 +/- 3400, Reaction: 0 = +1SrSeO3-1Sr<2+>-1SeO3<2->, logK(298,15K) = 6,3 +/- 0,5, Reference: NEA-7

V0 [cm3 mol-1] = dummy value 0,001

Remark:

269 USe

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -273255 +/- 18006, Reference: NEA-7

V0 [cm3 mol-1] = dummy value 0,001

Remark:

270 alpha-ZnSe

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -172488 +/- 4013, Reference: NEA-7

V0 [cm3 mol-1] = dummy value 0,001

Remark:

271 ZnSeO4:6H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2018306,895 +/- 1524, Reaction: 0 = +1ZnSeO4:6H2O-1Zn<2+>-1SeO4<2->-6H2O, logK(298,15K) = 1,538 +/- 0,068, Reference: NEA-7

V0 [cm3 mol-1] = dummy value 0,001

Remark:

272 SnO2(cr)_Cassiterite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -519615,416 +/- , Reaction: 0 = +1SnO2(cr)_Cassiterite-0,5O2(aq)-1H2O-1Sn<2+>+2H<+>, logK(298,15K) = 46,1642 +/- , Reference: Min-GWB

V0 [cm3 mol-1] = dummy value 0,001

Remark:

273 SnS_Herzenbergite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -104171,468 +/- unknown, Reaction: 0 = +1SnS_Herzenbergite-1HS<->-1Sn<2+>+1H<+>, logK(298,15K) = 15,6226 +/- , Reference: Min-GWB

V0 [cm3 mol-1] = dummy value 0,001

Remark:

274 SrCO3(s)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1144669,891 +/- unknown, Reaction: 0 = +1SrCO3(s)+1H<+>-1Sr<2+>-1(HCO3)<->, logK(298,15K) = -1,058 +/- unknown, Reference: /PSI/NAGRA/

V0 [cm3 mol-1] = dummy value 0,001

Remark:

275 K(TcO4)(c)

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -932921 +/- 7604, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

276 TcO2:1,6H2O(s)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -758479,548 +/- 8372, Reaction: 0 = +1TcO2:1,6H2O(s)+0,4H2O-1(TcO4)<->-1,5H2-1H<+>, logK(298,15K) = 37,829 +/- 0,609, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

277 Th(OH)4(am)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1601862,962 +/- unknown, Reaction: 0 = +1Th(OH)4(am)-1Th<4+>-4OH<->, logK(298,15K) = 47 +/- 0,8, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

278 UO2(OH)2:2H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1634859,982 +/- unknown, Reaction: 0 = +1UO2(OH)2:2H2O+2H<+>-1(U|+VI|O2)<2+>-3H2O, logK(298,15K) = -5,1 +/- unknown, Reference:

V0 [cm3 mol-1] = dummy value 0,001

Remark:

279 U|+IV|(OH)2(SO4)(c)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1766276,168 +/- 3385, Reaction: 0 = +1U|+IV|(OH)2(SO4)(c)-2OH<->-1(SO4)<2->-1U|+IV|<4+>, logK(298,15K) = 31,17 +/- 0,5, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

280 U|+IV|(OH)4(am)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1469933,282 +/- unknown, Reaction: 0 = +1U|+IV|(OH)4(am)-4OH<->-1U|+IV|<4+>, logK(298,15K) = 54,5 +/- 1, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

281 U|+IV|(SiO4)(c)_Coffinit

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1885022,184 +/- 4000, Reaction: 0 = +1U|+IV|(SiO4)(c)_Coffinit+4H<+>-1U|+IV|<4+>-1SiO2<0>-2H2O, logK(298,15K) = 8,06 +/- 0,77, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

282 (U|+VI|O2)(CO3)(c)_Rutherfordit

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1564629,544 +/- 1794, Reaction: 0 = +1(U|+VI|O2)(CO3)(c)_Rutherfordit-1(CO3)<2->-1(U|+VI|O2)<2+>, logK(298,15K) = 14,76 +/- 0,02, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

283 (U|+VI|O2)3(PO4)2:4H2O(c)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -6138966,935 +/- 6355, Reaction: 0 = +1(U|+VI|O2)3(PO4)2:4H2O(c)+6H<+>-4H2O-2H3PO4<0>-3(U|+VI|O2)<2+>, logK(298,15K) = 5,96 +/- 0,3, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

284 Ca(U|+VI|6O19):11H2O(c)_Bequerelit

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -10305456,27 +/- 13964, Reaction: 0 = +1Ca(U|+VI|6O19):11H2O(c)_Bequerelit+14H<+>-18H2O-6(U|+VI|O2)<2+>-1Ca<2+>, logK(298,15K) = -40,5 +/- 1,6, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

285 K2(U|+VI|6O19):11H2O(c)_Compreignacit

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -10337077,615 +/- 10956, Reaction: 0 = +1K2(U|+VI|6O19):11H2O(c)_Compreignacit+14H<+>-18H2O-2K<+>-6(U|+VI|O2)<2+>, logK(298,15K) = -37,1 +/- 0,54, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

286 Na(U|+VI|O2)(OH)3(c)_Clarkeit

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1619202,388 +/- unknown, Reaction: 0 = +1Na(U|+VI|O2)(OH)3(c)_Clarkeit+1H2O-1Na<+>-1(U|+VI|O2)<2+>-3OH<->, logK(298,15K) = 29,8 +/- 0,2, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

287 Na2(U|+VI|2O7)(c)

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -3011450 +/- 4015, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

288 Na4(U|+VI|O2)(CO3)3(c)

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -3738991,103 +/- 2342, Reaction: 0 = +1Na4(U|+VI|O2)(CO3)3(c)-1(U|+VI|O2)(CO3)3<4->-4Na<+>, logK(298,15K) = 5,34 +/- 0,16, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

289 U|+VI|O3:2H2O(c)_Metaschoepit

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1633470,645 +/- unknown, Reaction: 0 = +1U|+VI|O3:2H2O(c)_Metaschoepit-1(U|+VI|O2)<2+>-2OH<->-1H2O, logK(298,15K) = 22,65 +/- 0,13, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

290 U|+VI|O3:2H2O(c)_Schoepit

Gibbs Free Energy of Formation directly entered

deltaG_0^f [J mol-1] = -1636510 +/- 1705, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

291 (U|+VI|O2)2(SiO4):2H2O(c)_Soddyit

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -3653147,495 +/- unknown, Reaction: 0 = +1(U|+VI|O2)2(SiO4):2H2O(c)_Soddyit+4H<+>-2(U|+VI|O2)<2+>-1SiO2<0>-2H2O-2H2O, logK(298,15K) = -6,2 +/- 1, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

292 Ca(U|+VI|O2)2(SiO3OH)2:5H2O(c)_Uranophan

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -6208148,958 +/- unknown, Reaction: 0 = +1Ca(U|+VI|O2)2(SiO3OH)2:5H2O(c)_Uranophan+6H<+>-5H2O-1Ca<2+>-2(U|+VI|O2)<2+>-2SiO2<0>, logK(298,15K) = -9,42 +/- 0,48, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

293 Na2(U|+VI|O2)2(Si2O5)3:4H2O(c)_Na-weeksite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -9089678,096 +/- unknown, Reaction: 0 = +1Na2(U|+VI|O2)2(Si2O5)3:4H2O(c)_Na-weeksite+5H2O+6H<+>-2Na<+>-2(U|+VI|O2)<2+>-6SiO2<0>, logK(298,15K) = -1,5 +/- 0,08, Reference: FZK-INE 002/04

V0 [cm3 mol-1] = dummy value 0,001

Remark:

294 Al2O3_Corundum

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1583736,215 +/- unknown, Reaction: 0 = +1Al2O3_Corundum+6H<+>-2Al<3+>-3H2O, logK(298,15K) = -19,3933 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 25,575 +/- unknown, Reference: YPF

Remark:

295 AlOOH_Boehmite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -916689,841 +/- unknown, Reaction: 0 = +1AlOOH_Boehmite+3H<+>-1Al<3+>-2H2O, logK(298,15K) = -8,6014 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 19,535 +/- unknown, Reference: YPF

Remark:

296 Beidellite-Ca_Ca,165Al2,33Si3,67O10(OH)2

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -5377318,939 +/- unknown, Reaction: 0 = +1Beidellite-Ca_Ca,165Al2,33Si3,67O10(OH)2+7,32H<+>-0,165Ca<2+>-2,33Al<3+>-3,67SiO2<0>-4,66H2O, logK(298,15K) = -4,9352 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 129,766 +/- unknown, Reference: YPF

Remark:

297 Beidellite-H_H,33Al2,33Si3,67O10(OH)2

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -5291573,683 +/- unknown, Reaction: 0 = +1Beidellite-H_H,33Al2,33Si3,67O10(OH)2+6,99H<+>-2,33Al<3+>-3,67SiO2<0>-4,66H2O, logK(298,15K) = -3,9773 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 128,913 +/- unknown, Reference: YPF

Remark:

298 Beidellite-K_K,33Al2,33Si3,67O10(OH)2

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -5380949,625 +/- unknown, Reaction: 0 = +1Beidellite-K_K,33Al2,33Si3,67O10(OH)2+7,32H<+>-0,33K<+>-2,33Al<3+>-3,67SiO2<0>-4,66H2O, logK(298,15K) = -4,6522 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 134,152 +/- unknown, Reference: YPF

Remark:

299 Beidellite-Mg_Mg,165Al2,33Si3,67O10(OH)2

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -5361460,3 +/- unknown, Reaction: 0 = +1Beidellite-Mg_Mg,165Al2,33Si3,67O10(OH)2+7,32H<+>-0,165Mg<2+>-2,33Al<3+>-3,67SiO2<0>-4,66H2O, logK(298,15K) = -4,8971 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 128,725 +/- unknown, Reference: YPF

Remark:

300 Beidellite-Na_Na,33Al2,33Si3,67O10(OH)2

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -5372231,359 +/- unknown, Reaction: 0 = +1Beidellite-Na_Na,33Al2,33Si3,67O10(OH)2+7,32H<+>-0,33Na<+>-2,33Al<3+>-3,67SiO2<0>-4,66H2O, logK(298,15K) = -4,9911 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 130,727 +/- unknown, Reference: YPF

Remark:

301 Chabazite_K0,6Na0,2Ca1,55Al3,8Si8,2O24:10,0H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -13879273,758 +/- unknown, Reaction: 0 = +1Chabazite_K0,6Na0,2Ca1,55Al3,8Si8,2O24:10,0H2O+15,2H<+>-0,2Na<+>-1,5Ca<2+>-3,8Al<3+>-8,2SiO2<0>-0,6K<+>, logK(298,15K) = -10,3714 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 499,4 +/- unknown, Reference: YPF

Remark:

302 Chamosite-7A_Fe2Al2SiO5(OH)4

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -3472687,847 +/- unknown, Reaction: 0 = +1Chamosite-7A_Fe2Al2SiO5(OH)4+10H<+>-1SiO2<0>-2Al<3+>-2Fe<2+>-7H2O, logK(298,15K) = -32,6174 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 106,2 +/- unknown, Reference: YPF

Remark:

303 Clinoptilolite-Ca_Ca1,7335Al3,45Fe,017Si14,533O36:10,922H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -19052582,422 +/- unknown, Reaction: 0 = +1Clinoptilolite-Ca_Ca1,7335Al3,45Fe,017Si14,533O36:10,922H2O+13,868H<+>-0,017Fe<3+>-1,7335Ca<2+>-3,45Al<3+>-14,533SiO2<0>, logK(298,15K) = 5,6428 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 632,05 +/- unknown, Reference: YPF

Remark:

304 Clinoptilolite-Cs_Cs3,467Al3,45Fe,017Si14,533O36:10,922H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -19139295,699 +/- unknown, Reaction: 0 = +1Clinoptilolite-Cs_Cs3,467Al3,45Fe,017Si14,533O36:10,922H2O+13,868H<+>-0,017Fe<3+>-3,467Cs<+>-3,45Al<3+>-14,533SiO2<0>, logK(298,15K) = 11,6912 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 632,05 +/- unknown, Reference: YPF

Remark:

305 Clinoptilolite-K_K3,467Al3,45Fe,017Si14,533O36:10,922H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -19096239,942 +/- unknown, Reaction: 0 = +1Clinoptilolite-K_K3,467Al3,45Fe,017Si14,533O36:10,922H2O+13,868H<+>-0,017Fe<3+>-3,467K<+>-3,45Al<3+>-14,533SiO2<0>, logK(298,15K) = 9,5819 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 632,05 +/- unknown, Reference: YPF

Remark:

306 Clinoptilolite-Na_Na3,467Al3,45Fe,017Si14,533O36:10,922H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -19003208,052 +/- unknown, Reaction: 0 = +1Clinoptilolite-Na_Na3,467Al3,45Fe,017Si14,533O36:10,922H2O+13,868H<+>-0,017Fe<3+>-3,467Na<+>-3,45Al<3+>-14,533SiO2<0>, logK(298,15K) = 5,7696 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 632,05 +/- unknown, Reference: YPF

Remark:

307 Clinoptilolite-NH4_(NH4)3,467Al3,45Fe,017Si14,533O36:10,922H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -18389152,665 +/- unknown, Reaction: 0 = +1Clinoptilolite-NH4_(NH4)3,467Al3,45Fe,017Si14,533O36:10,922H2O+13,868H<+>-0,017Fe<3+>-3,467(NH4)<+>-3,45Al<3+>-14,533SiO2<0>, logK(298,15K) = 9,0742 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = dummy value 0,001

Remark:

308 Cronstedtite-7A_Fe2Fe2SiO5(OH)4

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2431884,223 +/- unknown, Reaction: 0 = +1Cronstedtite-7A_Fe2Fe2SiO5(OH)4+10H<+>-1SiO2<0>-2Fe<2+>-2Fe<3+>-7H2O, logK(298,15K) = -17,3756 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 110,9 +/- unknown, Reference: YPF

Remark:

309 Daphnite-7A_Fe5AlAlSi3O10(OH)8

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -6471810,946 +/- unknown, Reaction: 0 = +1Daphnite-7A_Fe5AlAlSi3O10(OH)8+16H<+>-2Al<3+>-3SiO2<0>-5Fe<2+>-12H2O, logK(298,15K) = -55,0117 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 221,2 +/- unknown, Reference: YPF

Remark:

310 Erionite_K1,5Na0,9Ca0,9Al4,2Si13,8O36:13,0H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -19845021,031 +/- unknown, Reaction: 0 = +1Erionite_K1,5Na0,9Ca0,9Al4,2Si13,8O36:13,0H2O+16,8H<+>-1,5K<+>-4,2Al<3+>-0,9Ca<2+>-13,8SiO2<0>-0,9Na<+>, logK(298,15K) = 4,8296 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 672 +/- unknown, Reference: YPF

Remark:

311 Fe3Si2O5(OH)4_Greenalite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2994738,751 +/- unknown, Reaction: 0 = +1Fe3Si2O5(OH)4_Greenalite+6H<+>-2SiO2<0>-3Fe<2+>-5H2O, logK(298,15K) = -23,1624 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 115 +/- unknown, Reference: YPF

Remark:

312 Ferroaluminoceladonite_KFeAlSi4O10(OH)2

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -5126466,999 +/- unknown, Reaction: 0 = +1Ferroaluminoceladonite_KFeAlSi4O10(OH)2+6H<+>-1Al<3+>-1K<+>-1Fe<2+>-4H2O, logK(298,15K) = -4,5745 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 153,678 +/- unknown, Reference: YPF

Remark:

313 Ferroceladonite_KFeFeSi4O10(OH)2

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -4606065,186 +/- unknown, Reaction: 0 = +1Ferroceladonite_KFeFeSi4O10(OH)2+6H<+>-1Fe<3+>-1K<+>-1Fe<2+>-4H2O, logK(298,15K) = 3,0464 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 156,72 +/- unknown, Reference: YPF

Remark:

314 Illite_K0,6Mg0,25Al1,8Al0,5Si3,5O10(OH)2

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -5473799,868 +/- unknown, Reaction: 0 = +1Illite_K0,6Mg0,25Al1,8Al0,5Si3,5O10(OH)2+8H<+>-0,25Mg<2+>-0,6K<+>-2,3Al<3+>-3,5SiO2<0>, logK(298,15K) = -8,3706 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 139,346 +/- unknown, Reference: YPF

Remark:

315 K2Si4O9

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -4058816,05 +/- unknown, Reaction: 0 = +1K2Si4O9+2H<+>-2K<+>-4SiO2<0>-1H2O, logK(298,15K) = -14,5138 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = dummy value 0,001

Remark:

316 K3AlCl6

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1945935,168 +/- unknown, Reaction: 0 = +1K3AlCl6-3K<+>-1Al<3+>-6Cl<->, logK(298,15K) = -31,6052 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = dummy value 0,001

Remark:

317 KAl(SO4)2

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2246653,812 +/- unknown, Reaction: 0 = +1KAl(SO4)2-1K<+>-1Al<3+>-2(SO4)<2->, logK(298,15K) = -2,6929 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = dummy value 0,001

Remark:

318 KAl(SO4)2:12H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -5147168,695 +/- unknown, Reaction: 0 = +1KAl(SO4)2:12H2O-1K<+>-1Al<3+>-2(SO4)<2->-12H2O, logK(298,15K) = 6,9137 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = dummy value 0,001

Remark:

319 KAl(SO4)2:3H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2981412,857 +/- unknown, Reaction: 0 = +1KAl(SO4)2:3H2O-1K<+>-1Al<3+>-2(SO4)<2->-3H2O, logK(298,15K) = 1,3959 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = dummy value 0,001

Remark:

320 KAl3(OH)6(SO4)2_Alunite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -4681588,577 +/- unknown, Reaction: 0 = +1KAl3(OH)6(SO4)2_Alunite+6H<+>-1K<+>-2(SO4)<2->-3Al<3+>-6H2O, logK(298,15K) = 2,4018 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 293,6 +/- unknown, Reference: YPF

Remark:

321 KAlCl4

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1102052,851 +/- unknown, Reaction: 0 = +1KAlCl4-1K<+>-1Al<3+>-4Cl<->, logK(298,15K) = -34,4833 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = dummy value 0,001

Remark:

322 Kaolinite_Al2Si2O5(OH)4

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -3804479,604 +/- unknown, Reaction: 0 = +1Kaolinite_Al2Si2O5(OH)4+6H<+>-2Al<3+>-2SiO2<0>-5H2O, logK(298,15K) = -5,9539 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 99,52 +/- unknown, Reference: YPF

Remark:

323 KMgAlSi4O10(OH)2_Celadonite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -5472718,368 +/- unknown, Reaction: 0 = +1KMgAlSi4O10(OH)2_Celadonite+6H<+>-1Al<3+>-1K<+>-1Mg<2+>-4H2O, logK(298,15K) = -7,8372 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 157,1 +/- unknown, Reference: YPF

Remark:

324 Laumontite_K0,2Na0,2Ca1,8Al4Si8,0O24:8,0H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -13461785,055 +/- unknown, Reaction: 0 = +1Laumontite_K0,2Na0,2Ca1,8Al4Si8,0O24:8,0H2O+16H<+>-1,8Ca<2+>-4Al<3+>-0,2K<+>-8SiO2<0>-0,2Na<+>, logK(298,15K) = -14,2657 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 406,4 +/- unknown, Reference: YPF

Remark:

325 Maximum-Microcline_KAlSi3O8

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -3754009,321 +/- unknown, Reaction: 0 = +1Maximum-Microcline_KAlSi3O8+4H<+>-1Al<3+>-1K<+>-2H2O-3SiO2<0>, logK(298,15K) = 0,1903 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 108,741 +/- unknown, Reference: YPF

Remark: together with K-Feldspar questionable

326 Mesolite_Na,676Ca,657Al1,99Si3,01O10:2,647H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -5528504,225 +/- unknown, Reaction: 0 = +1Mesolite_Na,676Ca,657Al1,99Si3,01O10:2,647H2O+7,96H<+>-0,657Ca<2+>-0,676Na<+>-1,99Al<3+>-3,01SiO2<0>, logK(298,15K) = -13,029 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 171,7 +/- unknown, Reference: YPF

Remark:

327 Mg2Al2SiO5(OH)4_Amesit-7A

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -4165191,156 +/- unknown, Reaction: 0 = +1Mg2Al2SiO5(OH)4_Amesit-7A+10H<+>-1SiO2<0>-2Al<3+>-2Mg<2+>-7H2O, logK(298,15K) = -39,1427 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 103 +/- unknown, Reference: YPF

Remark:

328 Mg4Al4Si2O10(OH)8_Amesit-14A

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -8368892,764 +/- unknown, Reaction: 0 = +1Mg4Al4Si2O10(OH)8_Amesit-14A+20H<+>-2SiO2<0>-4Al<3+>-4Mg<2+>-14H2O, logK(298,15K) = -71,5387 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 205,4 +/- unknown, Reference: YPF

Remark:

329 Minnesotaite_Fe3Si4O10(OH)2

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -4473939,658 +/- unknown, Reaction: 0 = +1Minnesotaite_Fe3Si4O10(OH)2+6H<+>-3Fe<2+>-4H2O-4SiO2<0>, logK(298,15K) = -15,0002 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 147,86 +/- unknown, Reference: YPF

Remark:

330 Montmorillonite-Ca_Ca0,165Mg0,33Al1,67Si4O10(OH)2

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -5336651,868 +/- unknown, Reaction: 0 = +1Montmorillonite-Ca_Ca0,165Mg0,33Al1,67Si4O10(OH)2+6H<+>-0,33Mg<2+>-4SiO2<0>-1,67Al<3+>-4H2O, logK(298,15K) = -2,4024 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 133,07 +/- unknown, Reference: YPF

Remark:

331 Montmorillonite-H_H0,33Mg0,33Al1,67Si4O10(OH)2

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -5250906,612 +/- unknown, Reaction: 0 = +1Montmorillonite-H_H0,33Mg0,33Al1,67Si4O10(OH)2+5,67H<+>-0,33Mg<2+>-4SiO2<0>-1,67Al<3+>-4H2O, logK(298,15K) = -1,4445 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 132,216 +/- unknown, Reference: YPF

Remark:

332 Montmorillonite-K_K0,33Mg0,33Al1,67Si4O10(OH)2

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -5340282,554 +/- unknown, Reaction: 0 = +1Montmorillonite-K_K0,33Mg0,33Al1,67Si4O10(OH)2+6H<+>-0,33Mg<2+>-4SiO2<0>-1,67Al<3+>-4H2O, logK(298,15K) = -2,1194 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 137,455 +/- unknown, Reference: YPF

Remark:

333 Montmorillonite-Mg_Mg0,495Al1,67Si4O10(OH)2

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -5320793,23 +/- unknown, Reaction: 0 = +1Montmorillonite-Mg_Mg0,495Al1,67Si4O10(OH)2+6H<+>-0,495Mg<2+>-4SiO2<0>-1,67Al<3+>-4H2O, logK(298,15K) = -2,3643 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 132,029 +/- unknown, Reference: YPF

Remark:

334 Montmorillonite-Na_Na0,33Mg0,33Al1,67Si4O10(OH)2

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -5331564,289 +/- unknown, Reaction: 0 = +1Montmorillonite-Na_Na0,33Mg0,33Al1,67Si4O10(OH)2+6H<+>-0,33Mg<2+>-4SiO2<0>-1,67Al<3+>-4H2O, logK(298,15K) = -2,4583 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 134,03 +/- unknown, Reference: YPF

Remark:

335 Mordenite_Ca,2895Na,361Al,94Si5,06O12:3,468H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -6235240,634 +/- unknown, Reaction: 0 = +1Mordenite_Ca,2895Na,361Al,94Si5,06O12:3,468H2O+3,76H<+>-0,2895Ca<2+>-0,361Na<+>-0,94Al<3+>-5,06SiO2<0>, logK(298,15K) = 4,5423 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = dummy value 0,001

Remark:

336 Na,96Al,96Si2,04O6:H2O_Analcim

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -3084635,342 +/- unknown, Reaction: 0 = +1Na,96Al,96Si2,04O6:H2O_Analcim+3,84H<+>-0,96Al<3+>-0,96Na<+>-2,04SiO2<0>-2,92H2O, logK(298,15K) = -6,0057 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = dummy value 0,001

Remark:

337 Na,96Al,96Si2,04O6_Analcime-dehy

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2811176,208 +/- unknown, Reaction: 0 = +1Na,96Al,96Si2,04O6_Analcime-dehy+3,84H<+>-0,96Al<3+>-0,96Na<+>-2,04SiO2<0>-1,92H2O, logK(298,15K) = -12,3685 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 89,1 +/- unknown, Reference: YPF

Remark:

338 Nontronite-Ca_Ca,165Fe2Al,33Si3,67H2O12

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -4341044,646 +/- unknown, Reaction: 0 = +1Nontronite-Ca_Ca,165Fe2Al,33Si3,67H2O12+7,32H<+>-0,165Ca<2+>-0,33Al<3+>-2Fe<3+>-3,67SiO2<0>, logK(298,15K) = 11,1001 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 135,85 +/- unknown, Reference: YPF

Remark:

339 Nontronite-H_H,33Fe2Al,33Si3,67H2O12

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -4259340,685 +/- unknown, Reaction: 0 = +1Nontronite-H_H,33Fe2Al,33Si3,67H2O12+6,99H<+>, logK(298,15K) = 12,766 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = dummy value 0,001

Remark:

340 Nontronite-K_K,33Fe2Al,33Si3,67H2O12

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -4344675,332 +/- unknown, Reaction: 0 = +1Nontronite-K_K,33Fe2Al,33Si3,67H2O12+7,32H<+>-0,33K<+>-0,33Al<3+>-2Fe<3+>-3,67SiO2<0>, logK(298,15K) = 11,3831 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 140,235 +/- unknown, Reference: YPF

Remark:

341 Nontronite-Mg_Mg,165Fe2Al,33Si3,67H2O12

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -4325186,008 +/- unknown, Reaction: 0 = +1Nontronite-Mg_Mg,165Fe2Al,33Si3,67H2O12+7,32H<+>-0,165Mg<2+>-0,33Al<3+>-2Fe<3+>-3,67SiO2<0>, logK(298,15K) = 11,1382 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 134,809 +/- unknown, Reference: YPF

Remark:

342 Nontronite-Na_Na,33Fe2Al,33Si3,67H2O12

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -4335957,067 +/- unknown, Reaction: 0 = +1Nontronite-Na_Na,33Fe2Al,33Si3,67H2O12+7,32H<+>-0,33Na<+>-0,33Al<3+>-2Fe<3+>-3,67SiO2<0>, logK(298,15K) = 11,0442 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 136,81 +/- unknown, Reference: YPF

Remark:

343 Phillipsite_K0,7Na0,7Ca1,1Al3,6Si12,4O32:12,6H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -17845058,436 +/- unknown, Reaction: 0 = +1Phillipsite_K0,7Na0,7Ca1,1Al3,6Si12,4O32:12,6H2O+14,4H<+>-1,1Ca<2+>-

3,6Al<3+>-0,7K<+>-12,4SiO2<0>-0,7Na<+>, logK(298,15K) = 6,7617 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 609,2 +/- unknown, Reference: YPF

Remark:

344 Pyrophyllite_Al2Si4O10(OH)2

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -5270523,472 +/- unknown, Reaction: 0 = +1Pyrophyllite_Al2Si4O10(OH)2+6H<+>-2Al<3+>-4H2O-4SiO2<0>, logK(298,15K) = -0,0967 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 126,6 +/- unknown, Reference: YPF

Remark:

345 Ripidolite-14A_Mg3Fe2Al2Si3O10(OH)8

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -7542655,67 +/- unknown, Reaction: 0 = +1Ripidolite-14A_Mg3Fe2Al2Si3O10(OH)8+16H<+>-2Al<3+>-2Fe<2+>-3Mg<2+>-3SiO2<0>, logK(298,15K) = -59,1778 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 209,634 +/- unknown, Reference: YPF

Remark: Phase should not be used simultaneously with ss-chlorite

346 Ripidolite-7A_Mg3Fe2Al2Si3O10(OH)8

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -7523400,729 +/- unknown, Reaction: 0 = +1Ripidolite-7A_Mg3Fe2Al2Si3O10(OH)8+16H<+>-2Al<3+>-2Fe<2+>-3Mg<2+>-3SiO2<0>, logK(298,15K) = -62,5511 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 215,38 +/- unknown, Reference: YPF

Remark: Phase should not be used simultaneously with ss-chlorite

347 Saponite-Ca_Ca,165Mg3Al,33Si3,67O10(OH)2

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -5634464,852 +/- unknown, Reaction: 0 = +1Saponite-Ca_Ca,165Mg3Al,33Si3,67O10(OH)2+7,32H<+>-0,33Al<3+>-3Mg<2+>-3,67SiO2<0>-4,66H2O, logK(298,15K) = -27,0032 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 134,359 +/- unknown, Reference: YPF

Remark:

348 Saponite-H_H,33Mg3Al,33Si3,67O10(OH)2

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -5548719,596 +/- unknown, Reaction: 0 = +1Saponite-H_H,33Mg3Al,33Si3,67O10(OH)2+6,99H<+>-0,33Al<3+>-3Mg<2+>-3,67SiO2<0>-4,66H2O, logK(298,15K) = -26,0453 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 133,506 +/- unknown, Reference: YPF

Remark:

349 Saponite-K_K,33Mg3Al,33Si3,67O10(OH)2

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -5638095,538 +/- unknown, Reaction: 0 = +1Saponite-K_K,33Mg3Al,33Si3,67O10(OH)2+7,32H<+>-0,33Al<3+>-3Mg<2+>-3,67SiO2<0>-4,66H2O, logK(298,15K) = -26,7202 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 138,745 +/- unknown, Reference: YPF

Remark:

350 Saponite-Mg_Mg3,165Al,33Si3,67O10(OH)2

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -5618606,214 +/- unknown, Reaction: 0 = +1Saponite-Mg_Mg3,165Al,33Si3,67O10(OH)2+7,32H<+>-0,33Al<3+>-3,165Mg<2+>-3,67SiO2<0>-4,66H2O, logK(298,15K) = -26,9651 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 132,602 +/- unknown, Reference: YPF

Remark:

351 Saponite-Na_Na,33Mg3Al,33Si3,67O10(OH)2

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -5629377,273 +/- unknown, Reaction: 0 = +1Saponite-Na_Na,33Mg3Al,33Si3,67O10(OH)2+7,32H<+>-0,33Al<3+>-3Mg<2+>-3,67SiO2<0>-4,66H2O, logK(298,15K) = -27,0591 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 135,32 +/- unknown, Reference: YPF

Remark:

352 Scolecite_CaAl2Si3O10:3H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -5613223,17 +/- unknown, Reaction: 0 = +1Scolecite_CaAl2Si3O10:3H2O+8H<+>-1Ca<2+>-2Al<3+>-3SiO2<0>-7H2O, logK(298,15K) = -15,2772 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = dummy value 0,001

Remark: a Ca-zeolite (Natrolite = Na-zeolite)

353 Sepiolite_Mg4Si6O15(OH)2:6H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -9265517,078 +/- unknown, Reaction: 0 = +1Sepiolite_Mg4Si6O15(OH)2:6H2O+8H<+>-4Mg<2+>-6SiO2<0>-11H2O, logK(298,15K) = -30,4439 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 285,6 +/- unknown, Reference: YPF

Remark:

354 Smectite-high-Fe-Mg_Ca,025Na,1K,2Fe++,5Fe+++,2Mg1,15Al1,25Si3,5H

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -5273457,591 +/- unknown, Reaction: 0 = +1Smectite-high-Fe-Mg_Ca,025Na,1K,2Fe++,5Fe+++,2Mg1,15Al1,25Si3,5H+8H<+>-0,025Ca<2+>-0,1Na<+>-0,2Fe<3+>-0,2K<+>-1,15Mg<2+>-1,25Al<3+>-3,5SiO2<0>-5H2O, logK(298,15K) = -17,4595 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 139,51 +/- unknown, Reference: YPF

Remark:

355 Smectite-low-Fe-Mg_Ca,02Na,15K,2Fe++,29Fe+++,16Mg,9Al1,25Si3,7

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -5279978,603 +/- unknown, Reaction: 0 = +1Smectite-low-Fe-Mg_Ca,02Na,15K,2Fe++,29Fe+++,16Mg,9Al1,25Si3,7+7H<+>-0,02Ca<2+>-0,15Na<+>-0,16Fe<3+>-0,2K<+>-0,9Mg<2+>-1,25Al<3+>-3,75SiO2<0>-4,5H2O, logK(298,15K) = -11,1541 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 139,602 +/- unknown, Reference: YPF

Remark:

356 Stellerite_Ca2,0Al4,0Si14,0O36:14,0H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -20027116,77 +/- unknown, Reaction: 0 = +1Stellerite_Ca2,0Al4,0Si14,0O36:14,0H2O+16H<+>-2Ca<2+>-4Al<3+>-22H2O-14SiO2<0>, logK(298,15K) = 8,7844 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 665,5 +/- unknown, Reference: YPF

Remark:

357 Stilbite_Ca1,019Na,136K,006Al2,18Si6,82O18:7,33H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -10130643,987 +/- unknown, Reaction: 0 = +1Stilbite_Ca1,019Na,136K,006Al2,18Si6,82O18:7,33H2O+8,72H<+>-0,006K<+>-0,136Na<+>-1,019Ca<2+>-2,18Al<3+>-11,69H2O, logK(298,15K) = -1,3118 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = dummy value 0,001

Remark:

358 Talc_Mg3Si4O10(OH)2

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -5527669,956 +/- unknown, Reaction: 0 = +1Talc_Mg3Si4O10(OH)2+6H<+>-3Mg<2+>-4H2O-4SiO2<0>, logK(298,15K) = -22,1646 +/- unknown, Reference: YPF

V0 [cm3 mol-1] = 136,25 +/- unknown, Reference: YPF

Remark:

359 C2AH8_Ca2Al2O5:8H2O_Dicalciumaluminathydrat

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -4831760,378 +/- , Reaction: 0 = +1C2AH8_Ca2Al2O5:8H2O_Dicalciumaluminathydrat+10H<+>-2Ca<2+>-2Al<3+>-13H2O, logK(298,15K) = -59,51 +/- unknown, Reference: /RAR1997a/

V0 [cm3 mol-1] = dummy value 0,001

Remark:

360 C2ASH8_Ca2Al2SiO7:8H2O_Gehlenithydrat

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -5722802,878 +/- , Reaction: 0 = +1C2ASH8_Ca2Al2SiO7:8H2O_Gehlenithydrat+10H<+>-2Ca<2+>-2Al<3+>-13H2O-1SiO2<0>, logK(298,15K) = -49,67 +/- unknown, Reference: /RAR1997a/

V0 [cm3 mol-1] = dummy value 0,001

Remark:

361 C3AH6_Ca3Al2O6:6H2O_Hydrogarnet

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -5038117,36 +/- , Reaction: 0 = +1C3AH6_Ca3Al2O6:6H2O_Hydrogarnet+12H<+>-3Ca<2+>-2Al<3+>-12H2O, logK(298,15K) = -78,66 +/- unknown, Reference: /RAR1997a/

V0 [cm3 mol-1] = dummy value 0,001

Remark:

362 C3AS(0,5)_Ca3Al2Si(0,5)O7_Tricalciumalumohemisilikat

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -4058629,554 +/- , Reaction: 0 = +1C3AS(0,5)_Ca3Al2Si(0,5)O7_Tricalciumalumohemisilikat+12H<+>-3Ca<2+>-2Al<3+>-6H2O-0,5SiO2<0>, logK(298,15K) = -74,12 +/- unknown, Reference: /RAR1997a/

V0 [cm3 mol-1] = dummy value 0,001

Remark:

363 C3ASH4_Ca3Al2SiO8:4H2O_Si-Hydrogarnet

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -5451740,437 +/- , Reaction: 0 = +1C3ASH4_Ca3Al2SiO8:4H2O_Si-Hydrogarnet+12H<+>-3Ca<2+>-2Al<3+>-10H2O-1SiO2<0>, logK(298,15K) = -69,37 +/- unknown, Reference: /RAR1997a/

V0 [cm3 mol-1] = dummy value 0,001

Remark:

364 C9S6H16_Ca9Si6O21:16H2O_Jennit

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -15073353,076 +/- , Reaction: 0 = +1C9S6H16_Ca9Si6O21:16H2O_Jennit+18H<+>-9Ca<2+>, logK(298,15K) = -147,1 +/- unknown, Reference: /RAR1997a/

V0 [cm3 mol-1] = dummy value 0,001

Remark:

365 Ca4Al2Cl2O6:10H2O_Friedelsches_Salz_Monochlorid

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -6839704,603 +/- , Reaction: 0 = +1Ca4Al2Cl2O6:10H2O_Friedelsches_Salz_Monochlorid+12H<+>-4Ca<2+>-2Al<3+>-16H2O-2Cl<->, logK(298,15K) = -72,04 +/- unknown, Reference: /RAR1997a/

V0 [cm3 mol-1] = dummy value 0,001

Remark:

366 Ca6Al2(SO4)3(OH)12:26H2O_Ettringit

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -15227966,757 +/- , Reaction: 0 = +1Ca6Al2(SO4)3(OH)12:26H2O_Ettringit+12H<+>-6Ca<2+>-2Al<3+>-38H2O-3(SO4)<2->, logK(298,15K) = -55,223 +/- unknown, Reference: /RAR1997a/

V0 [cm3 mol-1] = dummy value 0,001

Remark:

367 CSH(0,8)_Ca0,8SiO2,8_H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1640727,047 +/- , Reaction: 0 = +1CSH(0,8)_Ca0,8SiO2,8_H2O+1,6H<+>-0,8Ca<2+>, logK(298,15K) = -11,08 +/- unknown, Reference: /RAR1997a/

V0 [cm3 mol-1] = dummy value 0,001

Remark:

368 CSH(1,1)_Ca(1,1)SiO(3,1):3H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2319797,486 +/- , Reaction: 0 = +1CSH(1,1)_Ca(1,1)SiO(3,1):3H2O+2,2H<+>-1,1Ca<2+>, logK(298,15K) = -16,72 +/- unknown, Reference: /RAR1997a/

V0 [cm3 mol-1] = dummy value 0,001

Remark:

369 CSH(1,8)_Ca(1,8)SiO(3,8):5H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -3256395,967 +/- , Reaction: 0 = +1CSH(1,8)_Ca(1,8)SiO(3,8):5H2O+3,6H<+>-1,8Ca<2+>, logK(298,15K) = -32,6 +/- unknown, Reference: /RAR1997a/

V0 [cm3 mol-1] = dummy value 0,001

Remark:

370 Mg4Al2O7:10H2O_Hydrotalcit

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -6405279,257 +/- , Reaction: 0 = +1Mg4Al2O7:10H2O_Hydrotalcit+14H<+>-4Mg<2+>-2Al<3+>-17H2O, logK(298,15K) = -75,44 +/- unknown, Reference: /RAR1997a/

V0 [cm3 mol-1] = dummy value 0,001

Remark:

371 Ca2Zn2(OH)2(HSiO4)2_Clinohedrite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -4784175,542 +/- unknown, Reaction: 0 = +1Ca2Zn2(OH)2(HSiO4)2_Clinohedrite+8H<+>-2Zn<2+>-2SiO2<0>-6H2O-2Ca<2+>, logK(298,15K) = 51,08 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

372 Ca2ZnSi2O7:2H2O_Hardystonite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -3880628,976 +/- unknown, Reaction: 0 = +1Ca2ZnSi2O7:2H2O_Hardystonite+6H<+>-1Zn<2+>-2SiO2<0>-5H2O-2Ca<2+>, logK(298,15K) = -39,88 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

373 CaZn2(OH)6:2H2O_Calziumzinkat

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2493748,925 +/- unknown, Reaction: 0 = +1CaZn2(OH)6:2H2O_Calziumzinkat+6H<+>-2Zn<2+>-1Ca<2+>-8H2O, logK(298,15K) = -43,9 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

374 Goslarite_ZnSO4:7H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2562168,703 +/- unknown, Reaction: 0 = +1Goslarite_ZnSO4:7H2O-7H2O-1Zn<2+>-1(SO4)<2->, logK(298,15K) = 1,9239 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

375 K2Zn(SO4)2:6H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -3654973,251 +/- unknown, Reaction: 0 = +1K2Zn(SO4)2:6H2O-2K<+>-1Zn<2+>-2(SO4)<2->-6H2O, logK(298,15K) = 5,589 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

376 K2ZnCl4

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1226582,493 +/- unknown, Reaction: 0 = +1K2ZnCl4-2K<+>-1Zn<2+>-4Cl<->, logK(298,15K) = -1,841 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

377 KZnCl3:2H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1292190,536 +/- unknown, Reaction: 0 = +1KZnCl3:2H2O-1K<+>-1Zn<2+>-3Cl<->-2H2O, logK(298,15K) = -0,9554 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

378 MgZnCl4:5H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2280301,922 +/- unknown, Reaction: 0 = +1MgZnCl4:5H2O-1Mg<2+>-1Zn<2+>-4Cl<->-5H2O, logK(298,15K) = -5,754 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

379 Na2Zn(SO4)2:4H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -3127187,09 +/- unknown, Reaction: 0 = +1Na2Zn(SO4)2:4H2O-2Na<+>-1Zn<2+>-2(SO4)<2->-4H2O, logK(298,15K) = 3,418 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

380 Na2ZnCl4:3H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1892027,524 +/- unknown, Reaction: 0 = +1Na2ZnCl4:3H2O-2Na<+>-1Zn<2+>-4Cl<->-3H2O, logK(298,15K) = -2,6926 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

381 Zn(OH)2

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -555726,348 +/- unknown, Reaction: 0 = +1Zn(OH)2+2H<+>-1Zn<2+>-2H2O, logK(298,15K) = -11,52 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

382 Zn2(PO4)OH_Tarbuttit

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1628958,338 +/- unknown, Reaction: 0 = +1Zn2(PO4)OH_Tarbuttit+1H<+>-2Zn<2+>-1(PO4)<3->-1H2O, logK(298,15K) = 12,6 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

383 Zn2Ca(PO4)2:2H2O_Scholzit

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -3567118,257 +/- unknown, Reaction: 0 = +1Zn2Ca(PO4)2:2H2O_Scholzit-1Ca<2+>-2Zn<2+>-2(PO4)<3->-2H2O, logK(298,15K) = 34,1 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

384 Zn2SiO4_Willemit

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1524162,486 +/- unknown, Reaction: 0 = +1Zn2SiO4_Willemit+4H<+>-2Zn<2+>-1SiO2<0>-2H2O, logK(298,15K) = -13,91 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

385 Zn3(PO4)2_Zn-Orthophosphat

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2675613,682 +/- unknown, Reaction: 0 = +1Zn3(PO4)2_Zn-Orthophosphat, logK(298,15K) = 32,064 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

386 Zn4(PO4)(OH)2:3H2O_Spencerit

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -3967053,459 +/- unknown, Reaction: 0 = +1Zn4(PO4)(OH)2:3H2O_Spencerit+2H<+>-4Zn<2+>-2(PO4)<3->-5H2O, logK(298,15K) = 24,8 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

387 Zn5(OH)6(CO3)2

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -3140765,039 +/- unknown, Reaction: 0 = +1Zn5(OH)6(CO3)2+8H<+>-5Zn<2+>-2(HCO3)<->-6H2O, logK(298,15K) = -33,5982 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

388 Zn5(PO4)3OH

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -4329892,897 +/- unknown, Reaction: 0 = +1Zn5(PO4)3OH+1H<+>-5Zn<2+>-3(PO4)<3->-1H2O, logK(298,15K) = 49,1 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

389 ZnAl6(PO4)4(OH)8:4H2O_Faustit

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -10419078,648 +/- unknown, Reaction: 0 = +1ZnAl6(PO4)4(OH)8:4H2O_Faustit+8H<+>-1Zn<2+>-4(PO4)<3->-12H2O-6Al<3+>, logK(298,15K) = 65,73 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

390 ZnCl2:4Zn(OH)2

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2661539,249 +/- unknown, Reaction: 0 = +1ZnCl2:4Zn(OH)2+8H<+>-5Zn<2+>-8H2O-2Cl<->, logK(298,15K) = -41 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

391 ZnCO3

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -731403,464 +/- unknown, Reaction: 0 = +1ZnCO3+1H<+>-1Zn<2+>-1(HCO3)<->, logK(298,15K) = -0,4633 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

392 ZnCO3:H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -970495,044 +/- unknown, Reaction: 0 = +1ZnCO3:H2O+1H<+>-1Zn<2+>-1(HCO3)<->-1H2O, logK(298,15K) = -0,1214 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

393 ZnO-aktiv

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -319670,876 +/- unknown, Reaction: 0 = +1ZnO-aktiv-1H2O-1Zn<2+>+2H<+>, logK(298,15K) = -11,33 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

394 ZnSO4:2H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1369351,345 +/- unknown, Reaction: 0 = +1ZnSO4:2H2O-2H2O-1Zn<2+>-1(SO4)<2->, logK(298,15K) = 0,677 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

395 ZnSO4:6H2O

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -2324149,094 +/- unknown, Reaction: 0 = +1ZnSO4:6H2O-6H2O-1Zn<2+>-1(SO4)<2->, logK(298,15K) = 1,7698 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

Remark:

396 ZnSO4:H2O_Gunningite

Gibbs Free Energy of Formation calculated from logK for reaction

deltaG_0^f [J mol-1] = -1132363,179 +/- unknown, Reaction: 0 = +1ZnSO4:H2O_Gunningite-1H2O-1Zn<2+>-1(SO4)<2->, logK(298,15K) = 0,7036 +/- unknown, Reference: ULT

V0 [cm3 mol-1] = dummy value 0,001

```
      Remark:
397   ZrO2(monoclinic)
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = -1042746 +/- 1313, Reference: NEA-8
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
398   BSK3+3SF
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = 0 +/- , Reference: gesetzt
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
399   HAW-Kokille
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = 0 +/- , Reference: gesetzt
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
400   SpentFuel
      Gibbs Free Energy of Formation directly entered
      deltaG_0^f [J mol-1] = 0 +/- unknown, Reference: gesetzt
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
401   NaOH
      Gibbs Free Energy of Formation calculated from logK for reaction
      deltaG_0^f [J mol-1] = -379766,367 +/- unknown, Reaction: 0 = +1NaOH+1H<+>-
      1Na<+>-1H2O, logK(298,15K) = -20,905 +/- unknown, Reference: YPF
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
402   AgCl(cr)
      Gibbs Free Energy of Formation calculated from logK for reaction
      deltaG_0^f [J mol-1] = -109489,014 +/- unknown, Reaction: 0 = +1AgCl(cr)-
      1Ag<+>-1Cl<->, logK(298,15K) = 9,7 +/- 0,1, Reference: /BR1973a/
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
403   AgI(cr)
      Gibbs Free Energy of Formation calculated from logK for reaction
      deltaG_0^f [J mol-1] = -65956,683 +/- unknown, Reaction: 0 = +1AgI(cr)-1Ag<+>-
      1I<->, logK(298,15K) = 16 +/- 0,1, Reference: /BR1973a/
      V0 [cm3 mol-1] = dummy value 0,001
      Remark:
##Pitzer-Parameters
1     beta0 (Pb<2+> Cl<->)
      Value in this parameterfile (chemapp) = -4,7625519008 = R * -0,5728; Reference:
      HAG1998
      Remark: Value was actually copied from a data file for EQ36, Though
      calculations with the given Pitzer parameters for Pb compare very well with
      experiments, all Pitzer parameters for Pb are still preliminary until a final
      release by Hagemann,
2     beta1 (Pb<2+> Cl<->)
      Value in this parameterfile (chemapp) = -4,61347271857 = R * -0,55487, alpha1 =
      2; Reference: HAG1998
```

Remark: Value was actually copied from a data file for EQ36, Though calculations with the given Pitzer parameters for Pb compare very well with experiments, all Pitzer parameters for Pb are still preliminary until a final release by Hagemann,

3 beta2 (Pb<2+> Cl<->)

Value in this parameterfile (chemapp) = -210,7104950175 = R * -25,3425, alpha2 = 14; Reference: HAG1998

Remark: Value was actually copied from a data file for EQ36, Though calculations with the given Pitzer parameters for Pb compare very well with experiments, all Pitzer parameters for Pb are still preliminary until a final release by Hagemann,

4 cphi (Pb<2+> Cl<->)

Value in this parameterfile (chemapp) = 2,01668464305 = R * 0,24255; Reference: HAG1998

Remark: Value was actually copied from a data file for EQ36, Though calculations with the given Pitzer parameters for Pb compare very well with experiments, all Pitzer parameters for Pb are still preliminary until a final release by Hagemann,

5 beta0 (Pb<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = 0,73891059257 = R * 0,08887; Reference: HAG1998

Remark: Value was actually copied from a data file for EQ36, Though calculations with the given Pitzer parameters for Pb compare very well with experiments, all Pitzer parameters for Pb are still preliminary until a final release by Hagemann,

6 beta1 (Pb<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = 11,28827900426 = R * 1,35766, alpha1 = 1,4; Reference: HAG1998

Remark: Value was actually copied from a data file for EQ36, Though calculations with the given Pitzer parameters for Pb compare very well with experiments, all Pitzer parameters for Pb are still preliminary until a final release by Hagemann,

7 beta2 (Pb<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = -1213,918606 = R * -146, alpha2 = 12; Reference: HAG1998

Remark: Value was actually copied from a data file for EQ36, Though calculations with the given Pitzer parameters for Pb compare very well with experiments, all Pitzer parameters for Pb are still preliminary until a final release by Hagemann,

8 cphi (Pb<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = -8,3369601797 = R * -1,0027; Reference: HAG1998

Remark: Value was actually copied from a data file for EQ36, Though calculations with the given Pitzer parameters for Pb compare very well with experiments, all Pitzer parameters for Pb are still preliminary until a final release by Hagemann,

9 psi (Pb<2+> Na<+> Cl<->)

Value in this parameterfile (chemapp) = -1,57335491653 = R * -0,18923; Reference: HAG1998

Remark: Value was actually copied from a data file for EQ36, Though calculations with the given Pitzer parameters for Pb compare very well with experiments, all Pitzer parameters for Pb are still preliminary until a final release by Hagemann,

10 psi (Pb<2+> K<+> Cl<->)

Value in this parameterfile (chemapp) = -1,32333757076 = R * -0,15916; Reference: HAG1998

Remark: Value was actually copied from a data file for EQ36, Though calculations with the given Pitzer parameters for Pb compare very well with experiments, all Pitzer parameters for Pb are still preliminary until a final release by Hagemann,

11 psi (Pb<2+> Mg<2+> Cl<->)

Value in this parameterfile (chemapp) = -3,04618739507 = R * -0,36637; Reference: HAG1998

Remark: Value was actually copied from a data file for EQ36, Though calculations with the given Pitzer parameters for Pb compare very well with experiments, all Pitzer parameters for Pb are still preliminary until a final release by Hagemann,

12 psi (Pb<2+> Ca<2+> Cl<->)

Value in this parameterfile (chemapp) = -2,89943627592 = R * -0,34872; Reference: HAG1998

Remark: Value was actually copied from a data file for EQ36, Though calculations with the given Pitzer parameters for Pb compare very well with experiments, all Pitzer parameters for Pb are still preliminary until a final release by Hagemann,

13 theta (Pb<2+> Na<+>)

Value in this parameterfile (chemapp) = 1,47324820409 = R * 0,17719; Reference: HAG1998

Remark: Value was actually copied from a data file for EQ36, Though calculations with the given Pitzer parameters for Pb compare very well with experiments, all Pitzer parameters for Pb are still preliminary until a final release by Hagemann,

14 theta (Pb<2+> K<+>)

Value in this parameterfile (chemapp) = 0,11856492686 = R * 0,01426; Reference: HAG1998

Remark: Value was actually copied from a data file for EQ36, Though calculations with the given Pitzer parameters for Pb compare very well with experiments, all Pitzer parameters for Pb are still preliminary until a final release by Hagemann,

15 theta (Pb<2+> Mg<2+>)

Value in this parameterfile (chemapp) = -0,3250973801 = R * -0,0391; Reference: HAG1998

Remark: Value was actually copied from a data file for EQ36, Though calculations with the given Pitzer parameters for Pb compare very well with experiments, all Pitzer parameters for Pb are still preliminary until a final release by Hagemann,

16 psi (Pb<2+> Na<+> (SO4)<2->)

Value in this parameterfile (chemapp) = 3,0688860101 = R * 0,3691; Reference: HAG1998

Remark: Value was actually copied from a data file for EQ36, Though calculations with the given Pitzer parameters for Pb compare very well with experiments, all Pitzer parameters for Pb are still preliminary until a final release by Hagemann,

17 psi (Pb<2+> K<+> (SO4)<2->)

Value in this parameterfile (chemapp) = -0,4082424901 = R * -0,0491; Reference: HAG1998

Remark: Value was actually copied from a data file for EQ36, Though calculations with the given Pitzer parameters for Pb compare very well with experiments, all Pitzer parameters for Pb are still preliminary until a final release by Hagemann,

18 psi (Pb<2+> Mg<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = 8,39150337186 = R * 1,00926; Reference: HAG1998

Remark: Value was actually copied from a data file for EQ36, Though calculations with the given Pitzer parameters for Pb compare very well with experiments, all Pitzer parameters for Pb are still preliminary until a final release by Hagemann,

19 psi (Pb<2+> Cl<-> (SO4)<2->)

Value in this parameterfile (chemapp) = -1,25657204743 = R * -0,15113; Reference: HAG1998

Remark: Value was actually copied from a data file for EQ36, Though calculations with the given Pitzer parameters for Pb compare very well with experiments, all Pitzer parameters for Pb are still preliminary until a final release by Hagemann,

20 beta0 (Fe<2+> Cl<->)

Value in this parameterfile (chemapp) = 3,10330808564 = R * 0,37324; Reference: MoHa

Remark:

21 beta1 (Fe<2+> Cl<->)

Value in this parameterfile (chemapp) = 9,43688683989 = R * 1,13499, alpha1 = 2; Reference: MoHa

Remark:

22 cphi (Fe<2+> Cl<->)

Value in this parameterfile (chemapp) = -0,17901142183 = R * -0,02153; Reference: MoHa

Remark:

23 beta0 (Fe<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = 2,39981730993 = R * 0,28863; Reference: MoHa

Remark:

24 beta1 (Fe<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = 22,50413861771 = R * 2,70661, alpha1 = 1,4; Reference: MoHa

Remark:

25 beta2 (Fe<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = -349,209462 = R * -42, alpha2 = 12; Reference: MoHa

Remark:

26 cphi (Fe<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = 0,06219254228 = R * 0,00748; Reference: MoHa

Remark:

27 theta (Fe<2+> Na<+>)

Value in this parameterfile (chemapp) = 1,07722804516 = R * 0,12956; Reference: MoHa

Remark:

28 psi (Fe<2+> Na<+> Cl<->)

Value in this parameterfile (chemapp) = -0,17618448809 = R * -0,02119; Reference: MoHa

Remark:

29 psi (Fe<2+> Na<+> (SO4)<2->)

Value in this parameterfile (chemapp) = -0,5446004705 = R * -0,0655; Reference: MoHa

Remark:

30 theta (Fe<2+> K<+>)

Value in this parameterfile (chemapp) = -0,310685678407767 = R * -0,03737; Reference: INTGRS

Remark:

31 psi (Fe<2+> K<+> Cl<->)

Value in this parameterfile (chemapp) = -0,106525336812285 = R * -0,01281; Reference: INTGRS

Remark:

32 psi (Fe<2+> K<+> (SO4)<2->)

Value in this parameterfile (chemapp) = -0,139617438206258 = R * -0,01679; Reference: INTGRS

Remark:

33 theta (Fe<2+> Mg<2+>)

Value in this parameterfile (chemapp) = 0,90910863274 = R * 0,10934; Reference: MoHa

Remark:

34 psi (Fe<2+> Mg<2+> Cl<->)

Value in this parameterfile (chemapp) = -0,25043307132 = R * -0,03012; Reference: MoHa

Remark:

35 psi (Fe<2+> Mg<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = 0,20927624187 = R * 0,02517; Reference: MoHa

Remark:

36 theta (Fe<2+> Ca<2+>)

Value in this parameterfile (chemapp) = -0,06352286404 = R * -0,00764; Reference: MoHa

Remark:

37 psi (Fe<2+> Ca<2+> Cl<->)

Value in this parameterfile (chemapp) = -0,07557890499 = R * -0,00909; Reference: MoHa

Remark:

38 psi (Fe<2+> Cl<-> (SO4)<2->)

Value in this parameterfile (chemapp) = 0,10734033701 = R * 0,01291; Reference: MoHa

Remark:

39 beta0 (Fe<3+> Cl<->)

Value in this parameterfile (chemapp) = 4,52342656444 = R * 0,54404; Reference: MoHa

Remark:

40 beta1 (Fe<3+> Cl<->)

Value in this parameterfile (chemapp) = 50,94018196326 = R * 6,12666, alpha1 = 2; Reference: MoHa

Remark:

41 beta2 (Fe<3+> Cl<->)

Value in this parameterfile (chemapp) = 757,73838700395 = R * 91,13445, alpha2 = 12; Reference: MoHa

Remark:

42 cphi (Fe<3+> Cl<->)

Value in this parameterfile (chemapp) = -0,52248387124 = R * -0,06284; Reference: MoHa

Remark:

43 beta0 (Fe<3+> (SO4)<2->)

```
      Value in this parameterfile (chemapp) = 4,95752718375 = R * 0,59625; Reference:
      MoHa
      Remark:
44    beta1 (Fe<3+> (SO4)<2->)
      Value in this parameterfile (chemapp) = 163,58018828466 = R * 19,67406, alpha1
      = 1,559; Reference: MoHa
      Remark:
45    beta2 (Fe<3+> (SO4)<2->)
      Value in this parameterfile (chemapp) = 615,82556494996 = R * 74,06636, alpha2
      = 5,268; Reference: MoHa
      Remark:
46    cphi (Fe<3+> (SO4)<2->)
      Value in this parameterfile (chemapp) = -0,26830926997 = R * -0,03227;
      Reference: MoHa
      Remark:
47    theta (Fe<3+> Na<+>)
      Value in this parameterfile (chemapp) = 2,04029785429 = R * 0,24539; Reference:
      MoHa
      Remark:
48    psi (Fe<3+> Na<+> Cl<->)
      Value in this parameterfile (chemapp) = -0,22790074651 = R * -0,02741;
      Reference: MoHa
      Remark:
49    theta (Fe<3+> K<+>)
      Value in this parameterfile (chemapp) = 1,24085762164 = R * 0,14924; Reference:
      MoHa
      Remark:
50    psi (Fe<3+> K<+> Cl<->)
      Value in this parameterfile (chemapp) = -0,29757634869 = R * -0,03579;
      Reference: MoHa
      Remark:
51    theta (Fe<3+> Mg<2+>)
      Value in this parameterfile (chemapp) = 1,2787717918 = R * 0,1538; Reference:
      MoHa
      Remark:
52    psi (Fe<3+> Mg<2+> Cl<->)
      Value in this parameterfile (chemapp) = -0,64146452365 = R * -0,07715;
      Reference: MoHa
      Remark:
53    theta (Fe<3+> Ca<2+>)
      Value in this parameterfile (chemapp) = 1,35451698701 = R * 0,16291; Reference:
      MoHa
      Remark:
54    psi (Fe<3+> Ca<2+> Cl<->)
      Value in this parameterfile (chemapp) = -0,4082424901 = R * -0,0491; Reference:
      MoHa
      Remark:
55    beta0 ((TcO)(OH)<+> (SO4)<2->)
      Value in this parameterfile (chemapp) = 0,8314511 = R * 0,1; Reference: FZK-INE
      002/04
      Remark:
56    beta1 ((TcO)(OH)<+> (SO4)<2->)
```

Value in this parameterfile (chemapp) = 8,314511 = R * 1, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

57 beta0 ((TcO)(OH)<+> Cl<->)

Value in this parameterfile (chemapp) = 0,8314511 = R * 0,1; Reference: FZK-INE 002/04

Remark:

58 beta1 ((TcO)(OH)<+> Cl<->)

Value in this parameterfile (chemapp) = 1,6629022 = R * 0,2, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

59 beta0 ((TcO)<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = 1,6629022 = R * 0,2; Reference: FZK-INE 002/04

Remark:

60 beta1 ((TcO)<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = 24,943533 = R * 3, alpha1 = 1,4; Reference: FZK-INE 002/04

Remark:

61 beta2 ((TcO)<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = -332,58044 = R * -40, alpha2 = 12; Reference: FZK-INE 002/04

Remark:

62 beta0 ((TcO)<2+> Cl<->)

Value in this parameterfile (chemapp) = 2,4943533 = R * 0,3; Reference: FZK-INE 002/04

Remark:

63 beta1 ((TcO)<2+> Cl<->)

Value in this parameterfile (chemapp) = 14,1346687 = R * 1,7, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

64 psi ((TcO4)<-> (SO4)<2-> Na<+>)

Value in this parameterfile (chemapp) = -0,024943533 = R * -0,003; Reference: FZK-INE 002/04

Remark:

65 psi ((TcO4)<-> (SO4)<2-> K<+>)

Value in this parameterfile (chemapp) = 0,016629022 = R * 0,002; Reference: FZK-INE 002/04

Remark:

66 psi ((TcO4)<-> (SO4)<2-> Ca<2+>)

Value in this parameterfile (chemapp) = -0,24943533 = R * -0,03; Reference: FZK-INE 002/04

Remark:

67 theta ((TcO4)<-> (SO4)<2->)

Value in this parameterfile (chemapp) = 1,488297469 = R * 0,179; Reference: FZK-INE 002/04

Remark:

68 psi ((TcO4)<-> Cl<-> Na<+>)

Value in this parameterfile (chemapp) = -0,0706733435 = R * -0,0085; Reference: FZK-INE 002/04

Remark:

69 psi ((TcO4)<-> Cl<-> K<+>)

```
      Value in this parameterfile (chemapp) = -0,091459621 = R * -0,011; Reference:
      FZK-INE 002/04
      Remark:
70    psi ((TcO4)<-> Cl<-> Mg<2+>)
      Value in this parameterfile (chemapp) = -0,274378863 = R * -0,033; Reference:
      FZK-INE 002/04
      Remark:
71    psi ((TcO4)<-> Cl<-> Ca<2+>)
      Value in this parameterfile (chemapp) = -0,0956168765 = R * -0,0115; Reference:
      FZK-INE 002/04
      Remark:
72    theta ((TcO4)<-> Cl<->)
      Value in this parameterfile (chemapp) = 0,557072237 = R * 0,067; Reference:
      FZK-INE 002/04
      Remark:
73    beta0 (Ca<2+> (TcO)(OH)3<->)
      Value in this parameterfile (chemapp) = 2,4943533 = R * 0,3; Reference: FZK-INE
      002/04
      Remark:
74    beta1 (Ca<2+> (TcO)(OH)3<->)
      Value in this parameterfile (chemapp) = 14,1346687 = R * 1,7, alpha1 = 2;
      Reference: FZK-INE 002/04
      Remark:
75    beta0 (Ca<2+> (TcO4)<->)
      Value in this parameterfile (chemapp) = 2,4644210604 = R * 0,2964; Reference:
      FZK-INE 002/04
      Remark:
76    beta1 (Ca<2+> (TcO4)<->)
      Value in this parameterfile (chemapp) = 13,810402771 = R * 1,661, alpha1 = 2;
      Reference: FZK-INE 002/04
      Remark:
77    beta0 (Ca<2+> Tc(CO3)(OH)3<->)
      Value in this parameterfile (chemapp) = 2,4943533 = R * 0,3; Reference: FZK-INE
      002/04
      Remark:
78    beta1 (Ca<2+> Tc(CO3)(OH)3<->)
      Value in this parameterfile (chemapp) = 14,1346687 = R * 1,7, alpha1 = 2;
      Reference: FZK-INE 002/04
      Remark:
79    beta0 (Cs<+> (TcO4)<->)
      Value in this parameterfile (chemapp) = -1,5664538724 = R * -0,1884; Reference:
      FZK-INE 002/04
      Remark:
80    beta1 (Cs<+> (TcO4)<->)
      Value in this parameterfile (chemapp) = -1,3203443468 = R * -0,1588, alpha1 =
      2; Reference: FZK-INE 002/04
      Remark:
81    beta1 (K<+> (TcO)(OH)3<->)
      Value in this parameterfile (chemapp) = 0,8314511 = R * 0,1, alpha1 = 2;
      Reference: FZK-INE 002/04
      Remark:
82    beta0 (K<+> (TcO4)<->)
```

Value in this parameterfile (chemapp) = -0,4805787358 = R * -0,0578; Reference: FZK-INE 002/04

Remark:

83 beta1 (K<+> (TcO4)<->)

Value in this parameterfile (chemapp) = 0,049887066 = R * 0,006, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

84 beta1 (K<+> Tc(CO3)(OH)3<->)

Value in this parameterfile (chemapp) = 2,4943533 = R * 0,3, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

85 beta0 (Mg<2+> (TcO)(OH)3<->)

Value in this parameterfile (chemapp) = 2,4943533 = R * 0,3; Reference: FZK-INE 002/04

Remark:

86 beta1 (Mg<2+> (TcO)(OH)3<->)

Value in this parameterfile (chemapp) = 14,1346687 = R * 1,7, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

87 beta0 (Mg<2+> (TcO4)<->)

Value in this parameterfile (chemapp) = 2,6090935518 = R * 0,3138; Reference: FZK-INE 002/04

Remark:

88 beta1 (Mg<2+> (TcO4)<->)

Value in this parameterfile (chemapp) = 15,29870024 = R * 1,84, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

89 cphi (Mg<2+> (TcO4)<->)

Value in this parameterfile (chemapp) = 0,0947854254 = R * 0,0114; Reference: FZK-INE 002/04

Remark:

90 beta0 (Mg<2+> Tc(CO3)(OH)3<->)

Value in this parameterfile (chemapp) = 2,4943533 = R * 0,3; Reference: FZK-INE 002/04

Remark:

91 beta1 (Mg<2+> Tc(CO3)(OH)3<->)

Value in this parameterfile (chemapp) = 14,1346687 = R * 1,7, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

92 beta1 (Na<+> (TcO)(OH)3<->)

Value in this parameterfile (chemapp) = 0,8314511 = R * 0,1, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

93 beta0 (Na<+> (TcO4)<->)

Value in this parameterfile (chemapp) = 0,09237421721 = R * 0,01111; Reference: FZK-INE 002/04

Remark:

94 beta1 (Na<+> (TcO4)<->)

Value in this parameterfile (chemapp) = 1,3261645045 = R * 0,1595, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

95 cphi (Na<+> (TcO4)<->)

Value in this parameterfile (chemapp) = 0,01962224596 = R * 0,00236; Reference: FZK-INE 002/04

Remark:

96 psi (Na<+> Mg<2+> (TcO4)<->)

Value in this parameterfile (chemapp) = -0,16629022 = R * -0,02; Reference: FZK-INE 002/04

Remark:

97 beta1 (Na<+> Tc(CO3)(OH)3<->)

Value in this parameterfile (chemapp) = 2,4943533 = R * 0,3, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

98 beta0 (K<+> Th(CO3)5<6->)

Value in this parameterfile (chemapp) = 10,89200941 = R * 1,31; Reference: FZK-INE 002/04

Remark:

99 beta1 (K<+> Th(CO3)5<6->)

Value in this parameterfile (chemapp) = 249,43533 = R * 30, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

100 beta1 (K<+> Th(OH)(CO3)4<5->)

Value in this parameterfile (chemapp) = 191,233753 = R * 23, alpha1 = 2; Reference: FZK-INE 002/04

Remark: Schätzwert [siehe Kapitel 3,6]

101 beta1 (K<+> Th(OH)2(CO3)2<2->)

Value in this parameterfile (chemapp) = 16,629022 = R * 2, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

102 beta1 (K<+> Th(OH)3(CO3)<->)

Value in this parameterfile (chemapp) = 1,6629022 = R * 0,2, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

103 beta1 (K<+> Th(OH)4(CO3)<2->)

Value in this parameterfile (chemapp) = 16,629022 = R * 2, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

104 beta0 (Na<+> Th(CO3)5<6->)

Value in this parameterfile (chemapp) = 10,89200941 = R * 1,31; Reference: FZK-INE 002/04

Remark:

105 beta1 (Na<+> Th(CO3)5<6->)

Value in this parameterfile (chemapp) = 249,43533 = R * 30, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

106 beta1 (Na<+> Th(OH)(CO3)4<5->)

Value in this parameterfile (chemapp) = 191,233753 = R * 23, alpha1 = 2; Reference: FZK-INE 002/04

Remark: Schätzwert [siehe Kapitel 3,6]

107 beta1 (Na<+> Th(OH)2(CO3)2<2->)

Value in this parameterfile (chemapp) = 16,629022 = R * 2, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

108 beta1 (Na<+> Th(OH)3(CO3)<->)

Value in this parameterfile (chemapp) = 1,6629022 = R * 0,2, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

109 beta1 (Na<+> Th(OH)4(CO3)<2->)

Value in this parameterfile (chemapp) = 16,629022 = R * 2, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

110 psi (Th(CO3)5<6-> Cl<-> Na<+>)

Value in this parameterfile (chemapp) = 2,4943533 = R * 0,3; Reference: FZK-INE 002/04

Remark: Keine qcc'-Parameter und ycc'a–Parameter für Th4+ und kationische Th-Komplexe bekannt, alle Werte gleich Null gesetzt,

111 theta (Th(CO3)5<6-> Cl<->)

Value in this parameterfile (chemapp) = 14,9661198 = R * 1,8; Reference: FZK-INE 002/04

Remark:

112 beta0 (Th(OH)<3+> Cl<->)

Value in this parameterfile (chemapp) = 4,9887066 = R * 0,6; Reference: FZK-INE 002/04

Remark:

113 beta1 (Th(OH)<3+> Cl<->)

Value in this parameterfile (chemapp) = 49,0556149 = R * 5,9, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

114 beta0 (Th(OH)2<2+> Cl<->)

Value in this parameterfile (chemapp) = 1,91233753 = R * 0,23; Reference: FZK-INE 002/04

Remark:

115 beta1 (Th(OH)2<2+> Cl<->)

Value in this parameterfile (chemapp) = 16,04700623 = R * 1,93, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

116 beta0 (Th(OH)3<+> Cl<->)

Value in this parameterfile (chemapp) = 0,66516088 = R * 0,08; Reference: FZK-INE 002/04

Remark:

117 beta1 (Th(OH)3<+> Cl<->)

Value in this parameterfile (chemapp) = 3,24265929 = R * 0,39, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

118 beta0 (Th<4+> Cl<->)

Value in this parameterfile (chemapp) = 8,430914154 = R * 1,014; Reference: FZK-INE 002/04

Remark:

119 beta1 (Th<4+> Cl<->)

Value in this parameterfile (chemapp) = 110,83243163 = R * 13,33, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

120 cphi (Th<4+> Cl<->)

Value in this parameterfile (chemapp) = -0,8597204374 = R * -0,1034; Reference: FZK-INE 002/04

Remark:

121 beta0 ((U|+VI|O2)(OH)<+> Cl<->)

Value in this parameterfile (chemapp) = 1,24717665 = R * 0,15; Reference: FZK-INE 002/04

Remark:

122 beta1 ((U|+VI|O2)(OH)<+> Cl<->)

Value in this parameterfile (chemapp) = 2,4943533 = R * 0,3, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

123 beta0 ((U|+VI|O2)<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = 2,677272542 = R * 0,322; Reference: FZK-INE 002/04

Remark:

124 beta1 ((U|+VI|O2)<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = 15,190611597 = R * 1,827, alpha1 = 1,4; Reference: FZK-INE 002/04

Remark:

125 cphi ((U|+VI|O2)<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = -0,1463353936 = R * -0,0176; Reference: FZK-INE 002/04

Remark:

126 beta0 ((U|+VI|O2)<2+> Cl<->)

Value in this parameterfile (chemapp) = 3,55320627585 = R * 0,42735; Reference: FZK-INE 002/04

Remark:

127 beta1 ((U|+VI|O2)<2+> Cl<->)

Value in this parameterfile (chemapp) = 13,669056084 = R * 1,644, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

128 cphi ((U|+VI|O2)<2+> Cl<->)

Value in this parameterfile (chemapp) = -0,30647287546 = R * -0,03686; Reference: FZK-INE 002/04

Remark:

129 theta ((U|+VI|O2)<2+> Na<+>)

Value in this parameterfile (chemapp) = 0,1920652041 = R * 0,0231; Reference: FZK-INE 002/04

Remark: nur gültig in Kombination mit den binären Parametern für UO22+/ClO4- aus Kim und Frederick, 1988,

130 beta0 ((U|+VI|O2)2(OH)2<2+> Cl<->)

Value in this parameterfile (chemapp) = 4,1572555 = R * 0,5; Reference: FZK-INE 002/04

Remark:

131 beta1 ((U|+VI|O2)2(OH)2<2+> Cl<->)

Value in this parameterfile (chemapp) = 13,3032176 = R * 1,6, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

132 beta0 ((U|+VI|O2)3(OH)4<2+> Cl<->)

Value in this parameterfile (chemapp) = 0,58201577 = R * 0,07; Reference: FZK-INE 002/04

Remark:

133 beta1 ((U|+VI|O2)3(OH)4<2+> Cl<->)

Value in this parameterfile (chemapp) = 13,3032176 = R * 1,6, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

134 theta ((U|+VI|O2)3(OH)4<2+> Na<+>)

Value in this parameterfile (chemapp) = 0,41572555 = R * 0,05; Reference: FZK-INE 002/04

Remark:

135 beta0 ((U|+VI|O2)3(OH)5<+> Cl<->)

Value in this parameterfile (chemapp) = 2,57749841 = R * 0,31; Reference: FZK-INE 002/04

Remark:

136 beta1 ((U|+VI|O2)3(OH)5<+> Cl<->)

Value in this parameterfile (chemapp) = 2,4943533 = R * 0,3, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

137 psi ((U|+VI|O2)3(OH)5<+> Mg<2+> Cl<->)

Value in this parameterfile (chemapp) = -0,66516088 = R * -0,08; Reference: FZK-INE 002/04

Remark:

138 beta0 ((U|+VI|O2)4(OH)7<+> Cl<->)

Value in this parameterfile (chemapp) = 1,91233753 = R * 0,23; Reference: FZK-INE 002/04

Remark:

139 beta1 ((U|+VI|O2)4(OH)7<+> Cl<->)

Value in this parameterfile (chemapp) = 2,4943533 = R * 0,3, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

140 beta0 (K<+> U|+IV|(CO3)4<4->)

Value in this parameterfile (chemapp) = 8,314511 = R * 1; Reference: FZK-INE 002/04

Remark:

141 beta1 (K<+> U|+IV|(CO3)4<4->)

Value in this parameterfile (chemapp) = 108,088643 = R * 13, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

142 beta0 (K<+> U|+IV|(CO3)5<6->)

Value in this parameterfile (chemapp) = 12,4717665 = R * 1,5; Reference: FZK-INE 002/04

Remark:

143 beta1 (K<+> U|+IV|(CO3)5<6->)

Value in this parameterfile (chemapp) = 260,2441943 = R * 31,3, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

144 beta1 (K<+> U|+IV|(OH)2(CO3)2<2->)

Value in this parameterfile (chemapp) = 16,629022 = R * 2, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

145 beta0 (Mg<2+> (U|+VI|O2)(OH)3<->)

Value in this parameterfile (chemapp) = 1,6629022 = R * 0,2; Reference: FZK-INE 002/04

Remark:

146 beta1 (Mg<2+> (U|+VI|O2)(OH)3<->)

Value in this parameterfile (chemapp) = 13,3032176 = R * 1,6, alpha1 = 2; Reference: FZK-INE 002/04

```
      Remark:
147   beta1 (Mg<2+> (U|+VI|O2)(OH)4<2->)
      Value in this parameterfile (chemapp) = 24,943533 = R * 3, alpha1 = 1,4;
      Reference: FZK-INE 002/04
      Remark:
148   beta2 (Mg<2+> (U|+VI|O2)(OH)4<2->)
      Value in this parameterfile (chemapp) = -332,58044 = R * -40, alpha2 = 12;
      Reference: FZK-INE 002/04
      Remark:
149   beta0 (Mg<2+> (U|+VI|O2)3(OH)7<->)
      Value in this parameterfile (chemapp) = 1,6629022 = R * 0,2; Reference: FZK-INE
      002/04
      Remark:
150   beta1 (Mg<2+> (U|+VI|O2)3(OH)7<->)
      Value in this parameterfile (chemapp) = 13,3032176 = R * 1,6, alpha1 = 2;
      Reference: FZK-INE 002/04
      Remark:
151   beta0 (Na<+> (U|+VI|O2)(CO3)2<2->)
      Value in this parameterfile (chemapp) = -0,99774132 = R * -0,12; Reference:
      FZK-INE 002/04
      Remark:
152   beta1 (Na<+> (U|+VI|O2)(CO3)2<2->)
      Value in this parameterfile (chemapp) = 20,7862775 = R * 2,5, alpha1 = 2;
      Reference: FZK-INE 002/04
      Remark:
153   beta0 (Na<+> (U|+VI|O2)(CO3)3<4->)
      Value in this parameterfile (chemapp) = 7,31676968 = R * 0,88; Reference: FZK-
      INE 002/04
      Remark:
154   beta1 (Na<+> (U|+VI|O2)(CO3)3<4->)
      Value in this parameterfile (chemapp) = 98,1112298 = R * 11,8, alpha1 = 2;
      Reference: FZK-INE 002/04
      Remark:
155   beta0 (Na<+> (U|+VI|O2)(OH)3<->)
      Value in this parameterfile (chemapp) = -1,99548264 = R * -0,24; Reference:
      FZK-INE 002/04
      Remark:
156   beta1 (Na<+> (U|+VI|O2)(OH)3<->)
      Value in this parameterfile (chemapp) = 2,4943533 = R * 0,3, alpha1 = 2;
      Reference: FZK-INE 002/04
      Remark:
157   beta0 (Na<+> (U|+VI|O2)(OH)4<2->)
      Value in this parameterfile (chemapp) = 1,33032176 = R * 0,16; Reference: FZK-
      INE 002/04
      Remark:
158   beta1 (Na<+> (U|+VI|O2)(OH)4<2->)
      Value in this parameterfile (chemapp) = 13,3032176 = R * 1,6, alpha1 = 2;
      Reference: FZK-INE 002/04
      Remark:
159   beta0 (Na<+> (U|+VI|O2)3(OH)7<->)
      Value in this parameterfile (chemapp) = -1,99548264 = R * -0,24; Reference:
      FZK-INE 002/04
```

Remark:

160 beta1 (Na<+> (U|+VI|O2)3(OH)7<->)

Value in this parameterfile (chemapp) = 2,4943533 = R * 0,3, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

161 beta0 (Na<+> U|+IV|(CO3)4<4->)

Value in this parameterfile (chemapp) = 8,314511 = R * 1; Reference: FZK-INE 002/04

Remark:

162 beta1 (Na<+> U|+IV|(CO3)4<4->)

Value in this parameterfile (chemapp) = 108,088643 = R * 13, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

163 beta0 (Na<+> U|+IV|(CO3)5<6->)

Value in this parameterfile (chemapp) = 12,4717665 = R * 1,5; Reference: FZK-INE 002/04

Remark:

164 beta1 (Na<+> U|+IV|(CO3)5<6->)

Value in this parameterfile (chemapp) = 260,2441943 = R * 31,3, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

165 beta1 (Na<+> U|+IV|(OH)2(CO3)2<2->)

Value in this parameterfile (chemapp) = 16,629022 = R * 2, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

166 beta0 (U|+IV|(OH)<3+> Cl<->)

Value in this parameterfile (chemapp) = 4,9887066 = R * 0,6; Reference: FZK-INE 002/04

Remark:

167 beta1 (U|+IV|(OH)<3+> Cl<->)

Value in this parameterfile (chemapp) = 49,0556149 = R * 5,9, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

168 beta0 (U|+IV|(OH)2<2+> Cl<->)

Value in this parameterfile (chemapp) = 1,91233753 = R * 0,23; Reference: FZK-INE 002/04

Remark:

169 beta1 (U|+IV|(OH)2<2+> Cl<->)

Value in this parameterfile (chemapp) = 16,04700623 = R * 1,93, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

170 beta0 (U|+IV|(OH)3<+> Cl<->)

Value in this parameterfile (chemapp) = 0,66516088 = R * 0,08; Reference: FZK-INE 002/04

Remark:

171 beta1 (U|+IV|(OH)3<+> Cl<->)

Value in this parameterfile (chemapp) = 3,24265929 = R * 0,39, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

172 beta0 (U|+IV|<4+> Cl<->)

Value in this parameterfile (chemapp) = 10,55942897 = R * 1,27; Reference: FZK-INE 002/04

```
      Remark:
173   beta1 (U|+IV|<4+> Cl<->)
      Value in this parameterfile (chemapp) = 112,2458985 = R * 13,5, alpha1 = 2;
      Reference: FZK-INE 002/04
      Remark:
174   theta ((Np|+V|O2)(CO3)<-> Cl<->)
      Value in this parameterfile (chemapp) = -2,07862775 = R * -0,25; Reference:
      FZK-INE 002/04
      Remark:
175   theta ((Np|+V|O2)(CO3)2<3-> Cl<->)
      Value in this parameterfile (chemapp) = -2,07862775 = R * -0,25; Reference:
      FZK-INE 002/04
      Remark:
176   theta ((Np|+V|O2)(CO3)3<5-> (CO3)<2->)
      Value in this parameterfile (chemapp) = -6,90104413 = R * -0,83; Reference:
      FZK-INE 002/04
      Remark:
177   theta ((Np|+V|O2)(CO3)3<5-> Cl<->)
      Value in this parameterfile (chemapp) = -2,07862775 = R * -0,25; Reference:
      FZK-INE 002/04
      Remark:
178   lambda ((Np|+V|O2)(OH)<0> Cl<->)
      Value in this parameterfile (chemapp) = -1,57975709 = R * -0,19; Reference:
      FZK-INE 002/04
      Remark:
179   theta ((Np|+V|O2)(OH)2<-> Cl<->)
      Value in this parameterfile (chemapp) = -1,99548264 = R * -0,24; Reference:
      FZK-INE 002/04
      Remark:
180   theta ((Np|+V|O2)<+> Ca<2+>)
      Value in this parameterfile (chemapp) = 0,41572555 = R * 0,05; Reference: FZK-
      INE 002/04
      Remark:
181   beta0 ((Np|+V|O2)<+> Cl<->)
      Value in this parameterfile (chemapp) = 1,1765033065 = R * 0,1415; Reference:
      FZK-INE 002/04
      Remark:
182   beta1 ((Np|+V|O2)<+> Cl<->)
      Value in this parameterfile (chemapp) = 2,336377591 = R * 0,281, alpha1 = 2;
      Reference: FZK-INE 002/04
      Remark:
183   theta ((Np|+V|O2)<+> Mg<2+>)
      Value in this parameterfile (chemapp) = 0,41572555 = R * 0,05; Reference: FZK-
      INE 002/04
      Remark:
184   lambda ((Np|+VI|O2)(CO3)<0> Cl<->)
      Value in this parameterfile (chemapp) = -2,07862775 = R * -0,25; Reference:
      FZK-INE 002/04
      Remark:
185   beta0 ((Np|+VI|O2)(OH)<+> Cl<->)
      Value in this parameterfile (chemapp) = 1,24717665 = R * 0,15; Reference: FZK-
      INE 002/04
```

Remark:

186 beta1 ((Np|+VI|O2)(OH)<+> Cl<->)

Value in this parameterfile (chemapp) = 2,4943533 = R * 0,3, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

187 beta0 ((Np|+VI|O2)<2+> Cl<->)

Value in this parameterfile (chemapp) = 3,5536220014 = R * 0,4274; Reference: FZK-INE 002/04

Remark:

188 beta1 ((Np|+VI|O2)<2+> Cl<->)

Value in this parameterfile (chemapp) = 13,669056084 = R * 1,644, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

189 cphi ((Np|+VI|O2)<2+> Cl<->)

Value in this parameterfile (chemapp) = -0,3059740048 = R * -0,0368; Reference: FZK-INE 002/04

Remark:

190 beta0 ((Np|+VI|O2)2(OH)2<2+> Cl<->)

Value in this parameterfile (chemapp) = 4,1572555 = R * 0,5; Reference: FZK-INE 002/04

Remark:

191 beta1 ((Np|+VI|O2)2(OH)2<2+> Cl<->)

Value in this parameterfile (chemapp) = 13,3032176 = R * 1,6, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

192 beta0 ((Np|+VI|O2)3(OH)5<+> Cl<->)

Value in this parameterfile (chemapp) = 2,57749841 = R * 0,31; Reference: FZK-INE 002/04

Remark:

193 beta1 ((Np|+VI|O2)3(OH)5<+> Cl<->)

Value in this parameterfile (chemapp) = 2,4943533 = R * 0,3, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

194 beta0 (K<+> (Np|+V|O2)(CO3)<->)

Value in this parameterfile (chemapp) = 0,8314511 = R * 0,1; Reference: FZK-INE 002/04

Remark:

195 beta1 (K<+> (Np|+V|O2)(CO3)<->)

Value in this parameterfile (chemapp) = 2,82693374 = R * 0,34, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

196 beta0 (K<+> (Np|+V|O2)(CO3)2<3->)

Value in this parameterfile (chemapp) = 3,99096528 = R * 0,48; Reference: FZK-INE 002/04

Remark:

197 beta1 (K<+> (Np|+V|O2)(CO3)2<3->)

Value in this parameterfile (chemapp) = 36,5838484 = R * 4,4, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

198 beta0 (K<+> (Np|+V|O2)(CO3)3<5->)

Value in this parameterfile (chemapp) = 14,9661198 = R * 1,8; Reference: FZK-INE 002/04

```
      Remark:
199   beta1 (K<+> (Np|+V|O2)(CO3)3<5->)
      Value in this parameterfile (chemapp) = 188,7393997 = R * 22,7, alpha1 = 2;
      Reference: FZK-INE 002/04
      Remark:
200   beta2 (K<+> (Np|+V|O2)(CO3)3<5->)
      Value in this parameterfile (chemapp) = -790,7099961 = R * -95,1, alpha2 = 12;
      Reference: FZK-INE 002/04
      Remark:
201   cphi (K<+> (Np|+V|O2)(CO3)3<5->)
      Value in this parameterfile (chemapp) = -1,820877909 = R * -0,219; Reference:
      FZK-INE 002/04
      Remark:
202   beta0 (K<+> Np|+IV|(CO3)4<4->)
      Value in this parameterfile (chemapp) = 8,314511 = R * 1; Reference: FZK-INE
      002/04
      Remark:
203   beta1 (K<+> Np|+IV|(CO3)4<4->)
      Value in this parameterfile (chemapp) = 108,088643 = R * 13, alpha1 = 2;
      Reference: FZK-INE 002/04
      Remark:
204   beta0 (K<+> Np|+IV|(CO3)5<6->)
      Value in this parameterfile (chemapp) = 12,4717665 = R * 1,5; Reference: FZK-
      INE 002/04
      Remark:
205   beta1 (K<+> Np|+IV|(CO3)5<6->)
      Value in this parameterfile (chemapp) = 260,2441943 = R * 31,3, alpha1 = 2;
      Reference: FZK-INE 002/04
      Remark:
206   beta1 (K<+> Np|+IV|(OH)2(CO3)2<2->)
      Value in this parameterfile (chemapp) = 16,629022 = R * 2, alpha1 = 2;
      Reference: FZK-INE 002/04
      Remark:
207   beta1 (K<+> Np|+IV|(OH)4(CO3)<2->)
      Value in this parameterfile (chemapp) = 16,629022 = R * 2, alpha1 = 2;
      Reference: FZK-INE 002/04
      Remark:
208   beta0 (K<+> Np|+IV|(OH)4(CO3)2<4->)
      Value in this parameterfile (chemapp) = 8,314511 = R * 1; Reference: FZK-INE
      002/04
      Remark:
209   beta1 (K<+> Np|+IV|(OH)4(CO3)2<4->)
      Value in this parameterfile (chemapp) = 108,088643 = R * 13, alpha1 = 2;
      Reference: FZK-INE 002/04
      Remark:
210   beta0 (Mg<2+> (Np|+V|O2)(CO3)<->)
      Value in this parameterfile (chemapp) = 3,3258044 = R * 0,4; Reference: FZK-INE
      002/04
      Remark:
211   beta1 (Mg<2+> (Np|+V|O2)(CO3)<->)
      Value in this parameterfile (chemapp) = 14,1346687 = R * 1,7, alpha1 = 2;
      Reference: FZK-INE 002/04
```

Remark:

212 beta0 (Mg<2+> (Np|+V|O2)(OH)2<->)

Value in this parameterfile (chemapp) = 3,3258044 = R * 0,4; Reference: FZK-INE 002/04

Remark:

213 beta1 (Mg<2+> (Np|+V|O2)(OH)2<->)

Value in this parameterfile (chemapp) = 14,1346687 = R * 1,7, alpha1 = 1,4; Reference: FZK-INE 002/04

Remark:

214 beta0 (Na<+> (Np|+V|O2)(CO3)<->)

Value in this parameterfile (chemapp) = 0,8314511 = R * 0,1; Reference: FZK-INE 002/04

Remark:

215 beta1 (Na<+> (Np|+V|O2)(CO3)<->)

Value in this parameterfile (chemapp) = 2,82693374 = R * 0,34, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

216 beta0 (Na<+> (Np|+V|O2)(CO3)2<3->)

Value in this parameterfile (chemapp) = 3,99096528 = R * 0,48; Reference: FZK-INE 002/04

Remark:

217 beta1 (Na<+> (Np|+V|O2)(CO3)2<3->)

Value in this parameterfile (chemapp) = 36,5838484 = R * 4,4, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

218 beta0 (Na<+> (Np|+V|O2)(CO3)3<5->)

Value in this parameterfile (chemapp) = 14,9661198 = R * 1,8; Reference: FZK-INE 002/04

Remark:

219 beta1 (Na<+> (Np|+V|O2)(CO3)3<5->)

Value in this parameterfile (chemapp) = 188,7393997 = R * 22,7, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

220 lambda (Na<+> (Np|+VI|O2)(CO3)<0>)

Value in this parameterfile (chemapp) = 0,41572555 = R * 0,05; Reference: FZK-INE 002/04

Remark:

221 beta0 (Na<+> (Np|+VI|O2)(CO3)2<2->)

Value in this parameterfile (chemapp) = 1,762676332 = R * 0,212; Reference: FZK-INE 002/04

Remark:

222 beta1 (Na<+> (Np|+VI|O2)(CO3)2<2->)

Value in this parameterfile (chemapp) = 20,7862775 = R * 2,5, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

223 beta0 (Na<+> (Np|+VI|O2)(CO3)3<4->)

Value in this parameterfile (chemapp) = 10,39313875 = R * 1,25; Reference: FZK-INE 002/04

Remark:

224 beta1 (Na<+> (Np|+VI|O2)(CO3)3<4->)

Value in this parameterfile (chemapp) = 96,4483276 = R * 11,6, alpha1 = 2; Reference: FZK-INE 002/04

```
      Remark:
225   beta0 (Na<+> Np|+IV|(CO3)4<4->)
      Value in this parameterfile (chemapp) = 8,314511 = R * 1; Reference: FZK-INE
      002/04
      Remark:
226   beta1 (Na<+> Np|+IV|(CO3)4<4->)
      Value in this parameterfile (chemapp) = 108,088643 = R * 13, alpha1 = 2;
      Reference: FZK-INE 002/04
      Remark:
227   beta0 (Na<+> Np|+IV|(CO3)5<6->)
      Value in this parameterfile (chemapp) = 12,4717665 = R * 1,5; Reference: FZK-
      INE 002/04
      Remark:
228   beta1 (Na<+> Np|+IV|(CO3)5<6->)
      Value in this parameterfile (chemapp) = 260,2441943 = R * 31,3, alpha1 = 2;
      Reference: FZK-INE 002/04
      Remark:
229   beta1 (Na<+> Np|+IV|(OH)2(CO3)2<2->)
      Value in this parameterfile (chemapp) = 16,629022 = R * 2, alpha1 = 2;
      Reference: FZK-INE 002/04
      Remark:
230   beta1 (Na<+> Np|+IV|(OH)4(CO3)<2->)
      Value in this parameterfile (chemapp) = 16,629022 = R * 2, alpha1 = 2;
      Reference: FZK-INE 002/04
      Remark:
231   beta0 (Na<+> Np|+IV|(OH)4(CO3)2<4->)
      Value in this parameterfile (chemapp) = 8,314511 = R * 1; Reference: FZK-INE
      002/04
      Remark:
232   beta1 (Na<+> Np|+IV|(OH)4(CO3)2<4->)
      Value in this parameterfile (chemapp) = 108,088643 = R * 13, alpha1 = 2;
      Reference: FZK-INE 002/04
      Remark:
233   beta0 (Np|+IV|(OH)<3+> Cl<->)
      Value in this parameterfile (chemapp) = 4,9887066 = R * 0,6; Reference: FZK-INE
      002/04
      Remark:
234   beta1 (Np|+IV|(OH)<3+> Cl<->)
      Value in this parameterfile (chemapp) = 49,0556149 = R * 5,9, alpha1 = 2;
      Reference: FZK-INE 002/04
      Remark:
235   beta0 (Np|+IV|(OH)2<2+> Cl<->)
      Value in this parameterfile (chemapp) = 1,91233753 = R * 0,23; Reference: FZK-
      INE 002/04
      Remark:
236   beta1 (Np|+IV|(OH)2<2+> Cl<->)
      Value in this parameterfile (chemapp) = 15,7975709 = R * 1,9, alpha1 = 2;
      Reference: FZK-INE 002/04
      Remark:
237   beta0 (Np|+IV|(OH)3<+> Cl<->)
      Value in this parameterfile (chemapp) = 0,66516088 = R * 0,08; Reference: FZK-
      INE 002/04
```

Remark:

238 beta1 (Np|+IV|(OH)3<+> Cl<->)

Value in this parameterfile (chemapp) = 3,24265929 = R * 0,39, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

239 beta0 (Np|+IV|<4+> Cl<->)

Value in this parameterfile (chemapp) = 10,97515452 = R * 1,32; Reference: FZK-INE 002/04

Remark:

240 beta1 (Np|+IV|<4+> Cl<->)

Value in this parameterfile (chemapp) = 112,2458985 = R * 13,5, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

241 theta ((Pu|+V|O2)(CO3)<-> Cl<->)

Value in this parameterfile (chemapp) = -1,74604731 = R * -0,21; Reference: FZK-INE 002/04

Remark:

242 theta ((Pu|+V|O2)(CO3)3<5-> (CO3)<2->)

Value in this parameterfile (chemapp) = -6,90104413 = R * -0,83; Reference: FZK-INE 002/04

Remark:

243 theta ((Pu|+V|O2)(CO3)3<5-> Cl<->)

Value in this parameterfile (chemapp) = -2,16177286 = R * -0,26; Reference: FZK-INE 002/04

Remark:

244 theta ((Pu|+V|O2)<+> Ca<2+>)

Value in this parameterfile (chemapp) = 0,41572555 = R * 0,05; Reference: FZK-INE 002/04

Remark:

245 beta0 ((Pu|+V|O2)<+> Cl<->)

Value in this parameterfile (chemapp) = 1,1765033065 = R * 0,1415; Reference: FZK-INE 002/04

Remark:

246 beta1 ((Pu|+V|O2)<+> Cl<->)

Value in this parameterfile (chemapp) = 2,336377591 = R * 0,281, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

247 theta ((Pu|+V|O2)<+> Mg<2+>)

Value in this parameterfile (chemapp) = 0,41572555 = R * 0,05; Reference: FZK-INE 002/04

Remark:

248 beta0 ((Pu|+VI|O2)(OH)<+> Cl<->)

Value in this parameterfile (chemapp) = 1,24717665 = R * 0,15; Reference: FZK-INE 002/04

Remark:

249 beta1 ((Pu|+VI|O2)(OH)<+> Cl<->)

Value in this parameterfile (chemapp) = 2,4943533 = R * 0,3, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

250 beta0 ((Pu|+VI|O2)<2+> Cl<->)

Value in this parameterfile (chemapp) = 3,55320627585 = R * 0,42735; Reference: FZK-INE 002/04

Remark:

251 beta1 ((Pu|+VI|O2)<2+> Cl<->)

Value in this parameterfile (chemapp) = 13,669056084 = R * 1,644, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

252 cphi ((Pu|+VI|O2)<2+> Cl<->)

Value in this parameterfile (chemapp) = -0,30647287546 = R * -0,03686; Reference: FZK-INE 002/04

Remark:

253 beta0 ((Pu|+VI|O2)2(OH)2<2+> Cl<->)

Value in this parameterfile (chemapp) = 4,1572555 = R * 0,5; Reference: FZK-INE 002/04

Remark:

254 beta1 ((Pu|+VI|O2)2(OH)2<2+> Cl<->)

Value in this parameterfile (chemapp) = 13,3032176 = R * 1,6, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

255 beta0 ((Pu|+VI|O2)3(OH)5<+> Cl<->)

Value in this parameterfile (chemapp) = 2,57749841 = R * 0,31; Reference: FZK-INE 002/04

Remark:

256 beta1 ((Pu|+VI|O2)3(OH)5<+> Cl<->)

Value in this parameterfile (chemapp) = 2,4943533 = R * 0,3, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

257 beta0 (K<+> (Pu|+V|O2)(CO3)<->)

Value in this parameterfile (chemapp) = 0,8314511 = R * 0,1; Reference: FZK-INE 002/04

Remark:

258 beta1 (K<+> (Pu|+V|O2)(CO3)<->)

Value in this parameterfile (chemapp) = 2,82693374 = R * 0,34, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

259 beta0 (K<+> (Pu|+V|O2)(CO3)3<5->)

Value in this parameterfile (chemapp) = 14,9661198 = R * 1,8; Reference: FZK-INE 002/04

Remark:

260 beta1 (K<+> (Pu|+V|O2)(CO3)3<5->)

Value in this parameterfile (chemapp) = 188,7393997 = R * 22,7, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

261 beta2 (K<+> (Pu|+V|O2)(CO3)3<5->)

Value in this parameterfile (chemapp) = -790,7099961 = R * -95,1, alpha2 = 12; Reference: FZK-INE 002/04

Remark:

262 cphi (K<+> (Pu|+V|O2)(CO3)3<5->)

Value in this parameterfile (chemapp) = -1,820877909 = R * -0,219; Reference: FZK-INE 002/04

Remark:

263 beta0 (K<+> Pu|+IV|(CO3)4<4->)

Value in this parameterfile (chemapp) = 8,314511 = R * 1; Reference: FZK-INE 002/04

Remark:

264 beta1 (K<+> Pu|+IV|(CO3)4<4->)

Value in this parameterfile (chemapp) = 108,088643 = R * 13, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

265 beta0 (K<+> Pu|+IV|(CO3)5<6->)

Value in this parameterfile (chemapp) = 12,4717665 = R * 1,5; Reference: FZK-INE 002/04

Remark:

266 beta1 (K<+> Pu|+IV|(CO3)5<6->)

Value in this parameterfile (chemapp) = 260,2441943 = R * 31,3, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

267 beta1 (K<+> Pu|+IV|(OH)2(CO3)2<2->)

Value in this parameterfile (chemapp) = 16,629022 = R * 2, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

268 beta1 (K<+> Pu|+IV|(OH)4(CO3)<2->)

Value in this parameterfile (chemapp) = 16,629022 = R * 2, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

269 beta0 (K<+> Pu|+IV|(OH)4(CO3)2<4->)

Value in this parameterfile (chemapp) = 8,314511 = R * 1; Reference: FZK-INE 002/04

Remark:

270 beta1 (K<+> Pu|+IV|(OH)4(CO3)2<4->)

Value in this parameterfile (chemapp) = 108,088643 = R * 13, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

271 beta0 (Mg<2+> (Pu|+V|O2)(CO3)<->)

Value in this parameterfile (chemapp) = 3,3258044 = R * 0,4; Reference: FZK-INE 002/04

Remark:

272 beta1 (Mg<2+> (Pu|+V|O2)(CO3)<->)

Value in this parameterfile (chemapp) = 14,1346687 = R * 1,7, alpha1 = 2; Reference: FZK-INE 002/04

Remark: INE-FZK 002/04)

273 beta0 (Na<+> (Pu|+V|O2)(CO3)<->)

Value in this parameterfile (chemapp) = 0,8314511 = R * 0,1; Reference: FZK-INE 002/04

Remark:

274 beta1 (Na<+> (Pu|+V|O2)(CO3)<->)

Value in this parameterfile (chemapp) = 2,82693374 = R * 0,34, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

275 beta0 (Na<+> (Pu|+V|O2)(CO3)3<5->)

Value in this parameterfile (chemapp) = 14,9661198 = R * 1,8; Reference: FZK-INE 002/04

Remark:

276 beta1 (Na<+> (Pu|+V|O2)(CO3)3<5->)

Value in this parameterfile (chemapp) = 188,7393997 = R * 22,7, alpha1 = 2; Reference: FZK-INE 002/04

```
      Remark:
277   beta0 (Na<+> (Pu|+VI|O2)(CO3)2<2->)
      Value in this parameterfile (chemapp) = 1,762676332 = R * 0,212; Reference:
      FZK-INE 002/04
      Remark:
278   beta1 (Na<+> (Pu|+VI|O2)(CO3)2<2->)
      Value in this parameterfile (chemapp) = 20,7862775 = R * 2,5, alpha1 = 2;
      Reference: FZK-INE 002/04
      Remark:
279   beta0 (Na<+> (Pu|+VI|O2)(CO3)3<4->)
      Value in this parameterfile (chemapp) = 10,39313875 = R * 1,25; Reference: FZK-
      INE 002/04
      Remark:
280   beta1 (Na<+> (Pu|+VI|O2)(CO3)3<4->)
      Value in this parameterfile (chemapp) = 96,4483276 = R * 11,6, alpha1 = 2;
      Reference: FZK-INE 002/04
      Remark:
281   beta0 (Na<+> Pu|+IV|(CO3)4<4->)
      Value in this parameterfile (chemapp) = 8,314511 = R * 1; Reference: FZK-INE
      002/04
      Remark:
282   beta1 (Na<+> Pu|+IV|(CO3)4<4->)
      Value in this parameterfile (chemapp) = 108,088643 = R * 13, alpha1 = 2;
      Reference: FZK-INE 002/04
      Remark:
283   beta0 (Na<+> Pu|+IV|(CO3)5<6->)
      Value in this parameterfile (chemapp) = 12,4717665 = R * 1,5; Reference: FZK-
      INE 002/04
      Remark:
284   beta1 (Na<+> Pu|+IV|(CO3)5<6->)
      Value in this parameterfile (chemapp) = 260,2441943 = R * 31,3, alpha1 = 2;
      Reference: FZK-INE 002/04
      Remark:
285   beta1 (Na<+> Pu|+IV|(OH)2(CO3)2<2->)
      Value in this parameterfile (chemapp) = 16,629022 = R * 2, alpha1 = 2;
      Reference: FZK-INE 002/04
      Remark:
286   beta1 (Na<+> Pu|+IV|(OH)4(CO3)<2->)
      Value in this parameterfile (chemapp) = 16,629022 = R * 2, alpha1 = 2;
      Reference: FZK-INE 002/04
      Remark:
287   beta0 (Na<+> Pu|+IV|(OH)4(CO3)2<4->)
      Value in this parameterfile (chemapp) = 8,314511 = R * 1; Reference: FZK-INE
      002/04
      Remark:
288   beta1 (Na<+> Pu|+IV|(OH)4(CO3)2<4->)
      Value in this parameterfile (chemapp) = 108,088643 = R * 13, alpha1 = 2;
      Reference: FZK-INE 002/04
      Remark:
289   beta0 (Pu|+III|(OH)<2+> Cl<->)
      Value in this parameterfile (chemapp) = 0,457298105 = R * 0,055; Reference:
      FZK-INE 002/04
```

```
      Remark: INE-FZK 002/04)
290   beta1 (Pu|+III|(OH)<2+> Cl<->)
      Value in this parameterfile (chemapp) = 15,04926491 = R * 1,81, alpha1 = 2;
      Reference: FZK-INE 002/04
      Remark:
291   theta (Pu|+III|<3+> Ca<2+>)
      Value in this parameterfile (chemapp) = 1,6629022 = R * 0,2; Reference: FZK-INE
      002/04
      Remark:
292   beta0 (Pu|+III|<3+> Cl<->)
      Value in this parameterfile (chemapp) = 4,8689776416 = R * 0,5856; Reference:
      FZK-INE 002/04
      Remark:
293   beta1 (Pu|+III|<3+> Cl<->)
      Value in this parameterfile (chemapp) = 46,5612616 = R * 5,6, alpha1 = 2;
      Reference: FZK-INE 002/04
      Remark:
294   cphi (Pu|+III|<3+> Cl<->)
      Value in this parameterfile (chemapp) = -0,157975709 = R * -0,019; Reference:
      FZK-INE 002/04
      Remark: Unter Vernachlässigung von Chloridkomplexen,
295   theta (Pu|+III|<3+> K<+>)
      Value in this parameterfile (chemapp) = 0,8314511 = R * 0,1; Reference: FZK-INE
      002/04
      Remark: a) analog zu Na+,
296   theta (Pu|+III|<3+> Mg<2+>)
      Value in this parameterfile (chemapp) = 1,6629022 = R * 0,2; Reference: FZK-INE
      002/04
      Remark: b) analog zu Ca2+,
297   theta (Pu|+III|<3+> Na<+>)
      Value in this parameterfile (chemapp) = 0,8314511 = R * 0,1; Reference: FZK-INE
      002/04
      Remark:
298   beta0 (Pu|+IV|(OH)<3+> Cl<->)
      Value in this parameterfile (chemapp) = 4,9887066 = R * 0,6; Reference: FZK-INE
      002/04
      Remark:
299   beta1 (Pu|+IV|(OH)<3+> Cl<->)
      Value in this parameterfile (chemapp) = 49,0556149 = R * 5,9, alpha1 = 2;
      Reference: FZK-INE 002/04
      Remark:
300   beta0 (Pu|+IV|(OH)2<2+> Cl<->)
      Value in this parameterfile (chemapp) = 1,91233753 = R * 0,23; Reference: FZK-
      INE 002/04
      Remark:
301   beta1 (Pu|+IV|(OH)2<2+> Cl<->)
      Value in this parameterfile (chemapp) = 15,7975709 = R * 1,9, alpha1 = 2;
      Reference: FZK-INE 002/04
      Remark:
302   beta0 (Pu|+IV|(OH)3<+> Cl<->)
      Value in this parameterfile (chemapp) = 0,66516088 = R * 0,08; Reference: FZK-
      INE 002/04
```

```
      Remark:
303   beta1 (Pu|+IV|(OH)3<+> Cl<->)
      Value in this parameterfile (chemapp) = 3,24265929 = R * 0,39, alpha1 = 2;
      Reference: FZK-INE 002/04
      Remark:
304   beta0 (Pu|+IV|<4+> Cl<->)
      Value in this parameterfile (chemapp) = 10,97515452 = R * 1,32; Reference: FZK-
      INE 002/04
      Remark:
305   beta1 (Pu|+IV|<4+> Cl<->)
      Value in this parameterfile (chemapp) = 112,2458985 = R * 13,5, alpha1 = 2;
      Reference: FZK-INE 002/04
      Remark:
306   theta ((Am|+V|O2)(CO3)<-> Cl<->)
      Value in this parameterfile (chemapp) = -1,74604731 = R * -0,21; Reference:
      FZK-INE 002/04
      Remark:
307   theta ((Am|+V|O2)(CO3)2<3-> Cl<->)
      Value in this parameterfile (chemapp) = -2,16177286 = R * -0,26; Reference:
      FZK-INE 002/04
      Remark:
308   theta ((Am|+V|O2)(CO3)3<5-> (CO3)<2->)
      Value in this parameterfile (chemapp) = -6,90104413 = R * -0,83; Reference:
      FZK-INE 002/04
      Remark:
309   theta ((Am|+V|O2)(CO3)3<5-> Cl<->)
      Value in this parameterfile (chemapp) = -2,16177286 = R * -0,26; Reference:
      FZK-INE 002/04
      Remark:
310   theta ((Am|+V|O2)<+> Ca<2+>)
      Value in this parameterfile (chemapp) = 0,41572555 = R * 0,05; Reference: FZK-
      INE 002/04
      Remark:
311   beta0 ((Am|+V|O2)<+> Cl<->)
      Value in this parameterfile (chemapp) = 1,1765033065 = R * 0,1415; Reference:
      FZK-INE 002/04
      Remark:
312   beta1 ((Am|+V|O2)<+> Cl<->)
      Value in this parameterfile (chemapp) = 2,336377591 = R * 0,281, alpha1 = 2;
      Reference: FZK-INE 002/04
      Remark:
313   theta ((Am|+V|O2)<+> Mg<2+>)
      Value in this parameterfile (chemapp) = 0,41572555 = R * 0,05; Reference: FZK-
      INE 002/04
      Remark:
314   beta0 (Am|+III|(CO3)<+> Cl<->)
      Value in this parameterfile (chemapp) = -0,598644792 = R * -0,072; Reference:
      FZK-INE 002/04
      Remark:
315   beta1 (Am|+III|(CO3)<+> Cl<->)
      Value in this parameterfile (chemapp) = 3,350747933 = R * 0,403, alpha1 = 2;
      Reference: FZK-INE 002/04
```

Remark:

316 cphi (Am|+III|(CO3)<+> Cl<->)

Value in this parameterfile (chemapp) = 0,3226030268 = R * 0,0388; Reference: FZK-INE 002/04

Remark:

317 beta0 (Am|+III|(OH)<2+> Cl<->)

Value in this parameterfile (chemapp) = 0,457298105 = R * 0,055; Reference: FZK-INE 002/04

Remark:

318 beta1 (Am|+III|(OH)<2+> Cl<->)

Value in this parameterfile (chemapp) = 15,04926491 = R * 1,81, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

319 beta0 (Am|+III|(OH)2<+> Cl<->)

Value in this parameterfile (chemapp) = -3,442207554 = R * -0,414; Reference: FZK-INE 002/04

Remark:

320 lambda (Am|+III|(OH)3<0> Cl<->)

Value in this parameterfile (chemapp) = -1,6629022 = R * -0,2; Reference: FZK-INE 002/04

Remark: l = -0,2

321 beta0 (Am|+III|<3+> (SO4)<2->)

Value in this parameterfile (chemapp) = 14,899603712 = R * 1,792; Reference: FZK-INE 002/04

Remark:

322 beta1 (Am|+III|<3+> (SO4)<2->)

Value in this parameterfile (chemapp) = 125,083503484 = R * 15,044, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

323 cphi (Am|+III|<3+> (SO4)<2->)

Value in this parameterfile (chemapp) = -4,9887066 = R * -0,6; Reference: FZK-INE 002/04

Remark:

324 theta (Am|+III|<3+> Ca<2+>)

Value in this parameterfile (chemapp) = 1,6629022 = R * 0,2; Reference: FZK-INE 002/04

Remark:

325 beta0 (Am|+III|<3+> Cl<->)

Value in this parameterfile (chemapp) = 4,8689776416 = R * 0,5856; Reference: FZK-INE 002/04

Remark:

326 beta1 (Am|+III|<3+> Cl<->)

Value in this parameterfile (chemapp) = 46,5612616 = R * 5,6, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

327 cphi (Am|+III|<3+> Cl<->)

Value in this parameterfile (chemapp) = -0,133032176 = R * -0,016; Reference: FZK-INE 002/04

Remark: b) Unter Einbeziehung von Chloridkomplexen,

328 theta (Am|+III|<3+> K<+>)

Value in this parameterfile (chemapp) = 0,8314511 = R * 0,1; Reference: FZK-INE 002/04

```
      Remark: a) analog zu Na+,
329   theta (Am|+III|<3+> Mg<2+>)
      Value in this parameterfile (chemapp) = 1,6629022 = R * 0,2; Reference: FZK-INE
      002/04
      Remark: b) analog zu Ca2+,
330   theta (Am|+III|<3+> Na<+>)
      Value in this parameterfile (chemapp) = 0,8314511 = R * 0,1; Reference: FZK-INE
      002/04
      Remark:
331   theta (Am|+III|Cl<2+> Ca<2+>)
      Value in this parameterfile (chemapp) = -0,116403154 = R * -0,014; Reference:
      FZK-INE 002/04
      Remark:
332   beta0 (Am|+III|Cl<2+> Cl<->)
      Value in this parameterfile (chemapp) = 4,930505023 = R * 0,593; Reference:
      FZK-INE 002/04
      Remark:
333   beta1 (Am|+III|Cl<2+> Cl<->)
      Value in this parameterfile (chemapp) = 26,19070965 = R * 3,15, alpha1 = 2;
      Reference: FZK-INE 002/04
      Remark:
334   cphi (Am|+III|Cl<2+> Cl<->)
      Value in this parameterfile (chemapp) = -0,049887066 = R * -0,006; Reference:
      FZK-INE 002/04
      Remark:
335   theta (Am|+III|Cl<2+> Mg<2+>)
      Value in this parameterfile (chemapp) = -0,116403154 = R * -0,014; Reference:
      FZK-INE 002/04
      Remark: b) analog zu Ca2+,
336   theta (Am|+III|Cl2<+> Ca<2+>)
      Value in this parameterfile (chemapp) = -1,629644156 = R * -0,196; Reference:
      FZK-INE 002/04
      Remark:
337   beta0 (Am|+III|Cl2<+> Cl<->)
      Value in this parameterfile (chemapp) = 4,290287676 = R * 0,516; Reference:
      FZK-INE 002/04
      Remark:
338   beta1 (Am|+III|Cl2<+> Cl<->)
      Value in this parameterfile (chemapp) = 14,55039425 = R * 1,75, alpha1 = 2;
      Reference: FZK-INE 002/04
      Remark:
339   cphi (Am|+III|Cl2<+> Cl<->)
      Value in this parameterfile (chemapp) = 0,08314511 = R * 0,01; Reference: FZK-
      INE 002/04
      Remark:
340   theta (Am|+III|Cl2<+> Mg<2+>)
      Value in this parameterfile (chemapp) = -1,629644156 = R * -0,196; Reference:
      FZK-INE 002/04
      Remark: b) analog zu Ca2+,
341   beta0 (K<+> (Am|+V|O2)(CO3)<->)
      Value in this parameterfile (chemapp) = 0,8314511 = R * 0,1; Reference: FZK-INE
      002/04
```

Remark:

342 beta1 (K<+> (Am|+V|O2)(CO3)<->)

Value in this parameterfile (chemapp) = 2,82693374 = R * 0,34, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

343 beta0 (K<+> (Am|+V|O2)(CO3)2<3->)

Value in this parameterfile (chemapp) = 3,99096528 = R * 0,48; Reference: FZK-INE 002/04

Remark:

344 beta1 (K<+> (Am|+V|O2)(CO3)2<3->)

Value in this parameterfile (chemapp) = 36,5838484 = R * 4,4, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

345 beta0 (K<+> (Am|+V|O2)(CO3)3<5->)

Value in this parameterfile (chemapp) = 14,9661198 = R * 1,8; Reference: FZK-INE 002/04

Remark:

346 beta1 (K<+> (Am|+V|O2)(CO3)3<5->)

Value in this parameterfile (chemapp) = 188,7393997 = R * 22,7, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

347 beta2 (K<+> (Am|+V|O2)(CO3)3<5->)

Value in this parameterfile (chemapp) = -790,7099961 = R * -95,1, alpha2 = 12; Reference: FZK-INE 002/04

Remark:

348 cphi (K<+> (Am|+V|O2)(CO3)3<5->)

Value in this parameterfile (chemapp) = -1,820877909 = R * -0,219; Reference: FZK-INE 002/04

Remark:

349 beta0 (Mg<2+> (Am|+V|O2)(CO3)<->)

Value in this parameterfile (chemapp) = 3,3258044 = R * 0,4; Reference: FZK-INE 002/04

Remark:

350 beta1 (Mg<2+> (Am|+V|O2)(CO3)<->)

Value in this parameterfile (chemapp) = 14,1346687 = R * 1,7, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

351 beta0 (Na<+> (Am|+V|O2)(CO3)<->)

Value in this parameterfile (chemapp) = 0,8314511 = R * 0,1; Reference: FZK-INE 002/04

Remark:

352 beta1 (Na<+> (Am|+V|O2)(CO3)<->)

Value in this parameterfile (chemapp) = 2,82693374 = R * 0,34, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

353 beta0 (Na<+> (Am|+V|O2)(CO3)2<3->)

Value in this parameterfile (chemapp) = 3,99096528 = R * 0,48; Reference: FZK-INE 002/04

Remark:

354 beta1 (Na<+> (Am|+V|O2)(CO3)2<3->)

Value in this parameterfile (chemapp) = 36,5838484 = R * 4,4, alpha1 = 2; Reference: FZK-INE 002/04

```
      Remark:
355   beta0 (Na<+> (Am|+V|O2)(CO3)3<5->)
      Value in this parameterfile (chemapp) = 14,9661198 = R * 1,8; Reference: FZK-
      INE 002/04
      Remark:
356   beta1 (Na<+> (Am|+V|O2)(CO3)3<5->)
      Value in this parameterfile (chemapp) = 188,7393997 = R * 22,7, alpha1 = 2;
      Reference: FZK-INE 002/04
      Remark:
357   beta0 (Na<+> Am|+III|(CO3)2<->)
      Value in this parameterfile (chemapp) = -1,99548264 = R * -0,24; Reference:
      FZK-INE 002/04
      Remark:
358   beta1 (Na<+> Am|+III|(CO3)2<->)
      Value in this parameterfile (chemapp) = 1,862450464 = R * 0,224, alpha1 = 2;
      Reference: FZK-INE 002/04
      Remark:
359   cphi (Na<+> Am|+III|(CO3)2<->)
      Value in this parameterfile (chemapp) = 0,2361321124 = R * 0,0284; Reference:
      FZK-INE 002/04
      Remark:
360   beta0 (Na<+> Am|+III|(CO3)3<3->)
      Value in this parameterfile (chemapp) = 1,039313875 = R * 0,125; Reference:
      FZK-INE 002/04
      Remark:
361   beta1 (Na<+> Am|+III|(CO3)3<3->)
      Value in this parameterfile (chemapp) = 39,32763703 = R * 4,73, alpha1 = 2;
      Reference: FZK-INE 002/04
      Remark:
362   cphi (Na<+> Am|+III|(CO3)3<3->)
      Value in this parameterfile (chemapp) = 0,0058201577 = R * 0,0007; Reference:
      FZK-INE 002/04
      Remark:
363   beta0 (Cm(CO3)<+> Cl<->)
      Value in this parameterfile (chemapp) = -0,598644792 = R * -0,072; Reference:
      FZK-INE 002/04
      Remark:
364   beta1 (Cm(CO3)<+> Cl<->)
      Value in this parameterfile (chemapp) = 3,350747933 = R * 0,403, alpha1 = 2;
      Reference: FZK-INE 002/04
      Remark:
365   cphi (Cm(CO3)<+> Cl<->)
      Value in this parameterfile (chemapp) = 0,3226030268 = R * 0,0388; Reference:
      FZK-INE 002/04
      Remark:
366   beta0 (Cm(OH)<2+> Cl<->)
      Value in this parameterfile (chemapp) = 0,457298105 = R * 0,055; Reference:
      FZK-INE 002/04
      Remark:
367   beta1 (Cm(OH)<2+> Cl<->)
      Value in this parameterfile (chemapp) = 15,04926491 = R * 1,81, alpha1 = 2;
      Reference: FZK-INE 002/04
```

Remark:

368 beta0 (Cm(OH)2<+> Cl<->)

Value in this parameterfile (chemapp) = -3,442207554 = R * -0,414; Reference: FZK-INE 002/04

Remark:

369 beta0 (Cm(SO4)<+> Cl<->)

Value in this parameterfile (chemapp) = -0,756620501 = R * -0,091; Reference: FZK-INE 002/04

Remark:

370 beta1 (Cm(SO4)<+> Cl<->)

Value in this parameterfile (chemapp) = -3,24265929 = R * -0,39, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

371 cphi (Cm(SO4)<+> Cl<->)

Value in this parameterfile (chemapp) = 0,399096528 = R * 0,048; Reference: FZK-INE 002/04

Remark:

372 beta0 (Cm<3+> (SO4)<2->)

Value in this parameterfile (chemapp) = 14,899603712 = R * 1,792; Reference: FZK-INE 002/04

Remark:

373 beta1 (Cm<3+> (SO4)<2->)

Value in this parameterfile (chemapp) = 125,083503484 = R * 15,044, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

374 cphi (Cm<3+> (SO4)<2->)

Value in this parameterfile (chemapp) = -4,9887066 = R * -0,6; Reference: FZK-INE 002/04

Remark:

375 theta (Cm<3+> Ca<2+>)

Value in this parameterfile (chemapp) = 1,6629022 = R * 0,2; Reference: FZK-INE 002/04

Remark:

376 beta0 (Cm<3+> Cl<->)

Value in this parameterfile (chemapp) = 4,8689776416 = R * 0,5856; Reference: FZK-INE 002/04

Remark:

377 beta1 (Cm<3+> Cl<->)

Value in this parameterfile (chemapp) = 46,5612616 = R * 5,6, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

378 cphi (Cm<3+> Cl<->)

Value in this parameterfile (chemapp) = -0,133032176 = R * -0,016; Reference: FZK-INE 002/04

Remark: b) Unter Einbeziehung von Chloridkomplexen,

379 theta (Cm<3+> K<+>)

Value in this parameterfile (chemapp) = 0,8314511 = R * 0,1; Reference: FZK-INE 002/04

Remark: a) analog zu Na+,

380 theta (Cm<3+> Mg<2+>)

Value in this parameterfile (chemapp) = 1,6629022 = R * 0,2; Reference: FZK-INE 002/04

```
      Remark: b) analog zu Ca2+,
381   theta (Cm<3+> Na<+>)
      Value in this parameterfile (chemapp) = 0,8314511 = R * 0,1; Reference: FZK-INE
      002/04
      Remark:
382   theta (CmCl<2+> Ca<2+>)
      Value in this parameterfile (chemapp) = -0,116403154 = R * -0,014; Reference:
      FZK-INE 002/04
      Remark:
383   beta0 (CmCl<2+> Cl<->)
      Value in this parameterfile (chemapp) = 4,930505023 = R * 0,593; Reference:
      FZK-INE 002/04
      Remark:
384   beta1 (CmCl<2+> Cl<->)
      Value in this parameterfile (chemapp) = 26,19070965 = R * 3,15, alpha1 = 2;
      Reference: FZK-INE 002/04
      Remark:
385   cphi (CmCl<2+> Cl<->)
      Value in this parameterfile (chemapp) = -0,049887066 = R * -0,006; Reference:
      FZK-INE 002/04
      Remark:
386   theta (CmCl<2+> Mg<2+>)
      Value in this parameterfile (chemapp) = -0,116403154 = R * -0,014; Reference:
      FZK-INE 002/04
      Remark: b) analog zu Ca2+,
387   theta (CmCl2<+> Ca<2+>)
      Value in this parameterfile (chemapp) = -1,629644156 = R * -0,196; Reference:
      FZK-INE 002/04
      Remark:
388   beta0 (CmCl2<+> Cl<->)
      Value in this parameterfile (chemapp) = 4,290287676 = R * 0,516; Reference:
      FZK-INE 002/04
      Remark:
389   beta1 (CmCl2<+> Cl<->)
      Value in this parameterfile (chemapp) = 14,55039425 = R * 1,75, alpha1 = 2;
      Reference: FZK-INE 002/04
      Remark:
390   cphi (CmCl2<+> Cl<->)
      Value in this parameterfile (chemapp) = 0,08314511 = R * 0,01; Reference: FZK-
      INE 002/04
      Remark:
391   theta (CmCl2<+> Mg<2+>)
      Value in this parameterfile (chemapp) = -1,629644156 = R * -0,196; Reference:
      FZK-INE 002/04
      Remark: b) analog zu Ca2+,
392   beta0 (Na<+> Cm(CO3)2<->)
      Value in this parameterfile (chemapp) = -1,99548264 = R * -0,24; Reference:
      FZK-INE 002/04
      Remark:
393   beta1 (Na<+> Cm(CO3)2<->)
      Value in this parameterfile (chemapp) = 1,862450464 = R * 0,224, alpha1 = 2;
      Reference: FZK-INE 002/04
```

Remark:

394 cphi (Na<+> Cm(CO3)2<->)

Value in this parameterfile (chemapp) = 0,2361321124 = R * 0,0284; Reference: FZK-INE 002/04

Remark:

395 beta0 (Na<+> Cm(CO3)3<3->)

Value in this parameterfile (chemapp) = 1,039313875 = R * 0,125; Reference: FZK-INE 002/04

Remark:

396 beta1 (Na<+> Cm(CO3)3<3->)

Value in this parameterfile (chemapp) = 39,32763703 = R * 4,73, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

397 cphi (Na<+> Cm(CO3)3<3->)

Value in this parameterfile (chemapp) = 0,0058201577 = R * 0,0007; Reference: FZK-INE 002/04

Remark:

398 beta0 (Na<+> Cm(CO3)4<5->)

Value in this parameterfile (chemapp) = 16,811941242 = R * 2,022; Reference: FZK-INE 002/04

Remark:

399 beta1 (Na<+> Cm(CO3)4<5->)

Value in this parameterfile (chemapp) = 159,80490142 = R * 19,22, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

400 cphi (Na<+> Cm(CO3)4<5->)

Value in this parameterfile (chemapp) = -2,535925855 = R * -0,305; Reference: FZK-INE 002/04

Remark:

401 beta0 (Na<+> Cm(SO4)2<->)

Value in this parameterfile (chemapp) = -2,943336894 = R * -0,354; Reference: FZK-INE 002/04

Remark:

402 beta1 (Na<+> Cm(SO4)2<->)

Value in this parameterfile (chemapp) = -3,3258044 = R * -0,4, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

403 cphi (Na<+> Cm(SO4)2<->)

Value in this parameterfile (chemapp) = 0,424040061 = R * 0,051; Reference: FZK-INE 002/04

Remark:

404 beta1 (Ra<2+> (HSO4)<->)

Value in this parameterfile (chemapp) = 26,007790408 = R * 3,128, alpha1 = 2; Reference: SM4759

Remark: valid with logK of RaSO4, higher temp, Available

405 beta1 (Ra<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = 43,73432786 = R * 5,26, alpha1 = 2; Reference: SM4759

Remark: approximated using parameters for BaSO4, higher temp, Available

406 beta2 (Ra<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = -1272,120183 = R * -153, alpha2 = 12; Reference: SM4759

Remark: approximated using parameters for BaSO4, higher temp, Available

407 theta (Ra<2+> H<+>)

Value in this parameterfile (chemapp) = 0,407411039 = R * 0,049; Reference: SM4759

Remark: valid with logK of RaSO4

408 lambda ((CO2)<0> Ca<2+>)

Value in this parameterfile (chemapp) = 1,521555513 = R * 0,183; Reference: HMW

Remark:

409 lambda ((CO2)<0> Cl<->)

Value in this parameterfile (chemapp) = -0,041572555 = R * -0,005; Reference: HMW

Remark:

410 beta0 (Cl<-> Ca<2+>)

Value in this parameterfile (chemapp) = 2,6265540249 = R * 0,3159; Reference: HMW

Remark:

411 beta1 (Cl<-> Ca<2+>)

Value in this parameterfile (chemapp) = 13,419620754 = R * 1,614, alpha1 = 2; Reference: HMW

Remark:

412 cphi (Cl<-> Ca<2+>)

Value in this parameterfile (chemapp) = -0,00282693374 = R * -0,00034; Reference: HMW

Remark:

413 beta0 ((HCO3)<-> Ca<2+>)

Value in this parameterfile (chemapp) = 3,3258044 = R * 0,4; Reference: HMW

Remark:

414 beta1 ((HCO3)<-> Ca<2+>)

Value in this parameterfile (chemapp) = 24,752299247 = R * 2,977, alpha1 = 2; Reference: HMW

Remark:

415 beta0 ((HSO4)<-> Ca<2+>)

Value in this parameterfile (chemapp) = 1,7834626095 = R * 0,2145; Reference: HMW

Remark:

416 beta1 ((HSO4)<-> Ca<2+>)

Value in this parameterfile (chemapp) = 21,03571283 = R * 2,53, alpha1 = 2; Reference: HMW

Remark:

417 beta0 (OH<-> Ca<2+>)

Value in this parameterfile (chemapp) = -1,4525450717 = R * -0,1747; Reference: HMW

Remark:

418 beta1 (OH<-> Ca<2+>)

Value in this parameterfile (chemapp) = -1,9148318833 = R * -0,2303, alpha1 = 2; Reference: HMW

Remark:

419 beta2 (OH<-> Ca<2+>)

Value in this parameterfile (chemapp) = -47,55900292 = R * -5,72, alpha2 = 12; Reference: HMW

Remark:

420 beta0 ((SO4)<2-> Ca<2+>)

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      Value in this parameterfile (chemapp) = 1,6629022 = R * 0,2; Reference: HMW
      Remark:
421   beta1 ((SO4)<2-> Ca<2+>)
      Value in this parameterfile (chemapp) = 26,5839860203 = R * 3,1973, alpha1 =
      1,4; Reference: HMW
      Remark:
422   beta2 ((SO4)<2-> Ca<2+>)
      Value in this parameterfile (chemapp) = -450,97907664 = R * -54,24, alpha2 =
      12; Reference: HMW
      Remark:
423   lambda ((CO2)<0> (HSO4)<->)
      Value in this parameterfile (chemapp) = -0,024943533 = R * -0,003; Reference:
      HMW
      Remark:
424   lambda ((CO2)<0> K<+>)
      Value in this parameterfile (chemapp) = 0,424040061 = R * 0,051; Reference: HMW
      Remark:
425   lambda ((CO2)<0> Mg<2+>)
      Value in this parameterfile (chemapp) = 1,521555513 = R * 0,183; Reference: HMW
      Remark:
426   lambda ((CO2)<0> Na<+>)
      Value in this parameterfile (chemapp) = 0,8314511 = R * 0,1; Reference: HMW
      Remark:
427   lambda ((CO2)<0> (SO4)<2->)
      Value in this parameterfile (chemapp) = 0,806507567 = R * 0,097; Reference: HMW
      Remark:
428   beta0 (H<+> Cl<->)
      Value in this parameterfile (chemapp) = 1,4758257025 = R * 0,1775; Reference:
      HMW
      Remark:
429   beta1 (H<+> Cl<->)
      Value in this parameterfile (chemapp) = 2,4486234895 = R * 0,2945, alpha1 = 2;
      Reference: HMW
      Remark:
430   cphi (H<+> Cl<->)
      Value in this parameterfile (chemapp) = 0,0066516088 = R * 0,0008; Reference:
      HMW
      Remark:
431   beta0 (H<+> (HSO4)<->)
      Value in this parameterfile (chemapp) = 1,7169465215 = R * 0,2065; Reference:
      HMW
      Remark:
432   beta1 (H<+> (HSO4)<->)
      Value in this parameterfile (chemapp) = 4,6195423116 = R * 0,5556, alpha1 = 2;
      Reference: HMW
      Remark:
433   beta0 (H<+> (SO4)<2->)
      Value in this parameterfile (chemapp) = 0,2477724278 = R * 0,0298; Reference:
      HMW
      Remark:
434   cphi (H<+> (SO4)<2->)
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      Value in this parameterfile (chemapp) = 0,3641755818 = R * 0,0438; Reference:
      HMW
      Remark:
435   beta0 ((CO3)<2-> K<+>)
      Value in this parameterfile (chemapp) = 1,2371992368 = R * 0,1488; Reference:
      HMW
      Remark:
436   beta1 ((CO3)<2-> K<+>)
      Value in this parameterfile (chemapp) = 11,88975073 = R * 1,43, alpha1 = 2;
      Reference: HMW
      Remark:
437   cphi ((CO3)<2-> K<+>)
      Value in this parameterfile (chemapp) = -0,0124717665 = R * -0,0015; Reference:
      HMW
      Remark:
438   beta0 (Cl<-> K<+>)
      Value in this parameterfile (chemapp) = 0,40200660685 = R * 0,04835; Reference:
      HMW
      Remark:
439   beta1 (Cl<-> K<+>)
      Value in this parameterfile (chemapp) = 1,7643392342 = R * 0,2122, alpha1 = 2;
      Reference: HMW
      Remark:
440   cphi (Cl<-> K<+>)
      Value in this parameterfile (chemapp) = -0,00698418924 = R * -0,00084;
      Reference: HMW
      Remark:
441   beta0 ((HCO3)<-> K<+>)
      Value in this parameterfile (chemapp) = 0,2461095256 = R * 0,0296; Reference:
      HMW
      Remark:
442   beta1 ((HCO3)<-> K<+>)
      Value in this parameterfile (chemapp) = -0,108088643 = R * -0,013, alpha1 = 2;
      Reference: HMW
      Remark:
443   cphi ((HCO3)<-> K<+>)
      Value in this parameterfile (chemapp) = -0,066516088 = R * -0,008; Reference:
      HMW
      Remark:
444   beta0 (K<+> (HSO4)<->)
      Value in this parameterfile (chemapp) = -0,0024943533 = R * -0,0003; Reference:
      HMW
      Remark:
445   beta1 (K<+> (HSO4)<->)
      Value in this parameterfile (chemapp) = 1,4425676585 = R * 0,1735, alpha1 = 2;
      Reference: HMW
      Remark:
446   beta0 (OH<-> K<+>)
      Value in this parameterfile (chemapp) = 1,0792235278 = R * 0,1298; Reference:
      HMW
      Remark:
447   beta1 (OH<-> K<+>)
```

Value in this parameterfile (chemapp) = 2,66064352 = R * 0,32, alpha1 = 2; Reference: HMW

Remark:

448 cphi (OH<-> K<+>)

Value in this parameterfile (chemapp) = 0,0340894951 = R * 0,0041; Reference: HMW

Remark:

449 beta0 (K<+> (SO4)<2->)

Value in this parameterfile (chemapp) = 0,41530982445 = R * 0,04995; Reference: HMW

Remark:

450 beta1 (K<+> (SO4)<2->)

Value in this parameterfile (chemapp) = 6,4794984223 = R * 0,7793, alpha1 = 2; Reference: HMW

Remark:

451 beta0 (Cl<-> Mg<2+>)

Value in this parameterfile (chemapp) = 2,92961795085 = R * 0,35235; Reference: HMW

Remark:

452 beta1 (Cl<-> Mg<2+>)

Value in this parameterfile (chemapp) = 13,9808502465 = R * 1,6815, alpha1 = 2; Reference: HMW

Remark:

453 cphi (Cl<-> Mg<2+>)

Value in this parameterfile (chemapp) = 0,04315231209 = R * 0,00519; Reference: HMW

Remark:

454 beta0 ((HCO3)<-> Mg<2+>)

Value in this parameterfile (chemapp) = 2,735474119 = R * 0,329; Reference: HMW

Remark:

455 beta1 ((HCO3)<-> Mg<2+>)

Value in this parameterfile (chemapp) = 5,0485710792 = R * 0,6072, alpha1 = 2; Reference: HMW

Remark:

456 beta0 (Mg<2+> (HSO4)<->)

Value in this parameterfile (chemapp) = 3,9460669206 = R * 0,4746; Reference: HMW

Remark:

457 beta1 (Mg<2+> (HSO4)<->)

Value in this parameterfile (chemapp) = 14,375789519 = R * 1,729, alpha1 = 2; Reference: HMW

Remark:

458 beta0 (Mg<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = 1,837506931 = R * 0,221; Reference: HMW

Remark:

459 beta1 (Mg<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = 27,795410273 = R * 3,343, alpha1 = 1,4; Reference: HMW

Remark:

460 beta2 (Mg<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = -309,54924453 = R * -37,23, alpha2 = 12; Reference: HMW

Remark:

461 cphi (Mg<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = 0,207862775 = R * 0,025; Reference: HMW

Remark:

462 beta0 (Na<+> (CO3)<2->)

Value in this parameterfile (chemapp) = 0,3317489889 = R * 0,0399; Reference: SM 4191

Remark: This value instead of that from hmw was used to estimate Pitzer-parameters in SM 5325 (Np(V) with carbonate), It was therefore adopted for this database, (hmw=0,0399, SM4191=0,0362

463 beta1 (Na<+> (CO3)<2->)

Value in this parameterfile (chemapp) = 11,548855779 = R * 1,389, alpha1 = 2; Reference: SM 4191

Remark: This value instead of that from hmw was used to estimate Pitzer-parameters in SM 5325 (Np(V) with carbonate), It was therefore adopted for this database, (hmw=1,389, SM4191=1,51

464 cphi (Na<+> (CO3)<2->)

Value in this parameterfile (chemapp) = 0,0365838484 = R * 0,0044; Reference: SM 4191

Remark: This value instead of that from hmw was used to estimate Pitzer-parameters in SM 5325 (Np(V) with carbonate), It was therefore adopted for this database, Hmw=0,0044, SM4191=0,0052

465 beta0 (Na<+> Cl<->)

Value in this parameterfile (chemapp) = 0,6360600915 = R * 0,0765; Reference: HMW

Remark:

466 beta1 (Na<+> Cl<->)

Value in this parameterfile (chemapp) = 2,1983567084 = R * 0,2644, alpha1 = 2; Reference: HMW

Remark:

467 cphi (Na<+> Cl<->)

Value in this parameterfile (chemapp) = 0,01055942897 = R * 0,00127; Reference: HMW

Remark:

468 beta0 (Na<+> (HCO3)<->)

Value in this parameterfile (chemapp) = 0,2303119547 = R * 0,0277; Reference: SM 4191

Remark: This value instead of that from hmw was used to estimate Pitzer-parameters in SM 5325 (Np(V) with carbonate), It was therefore adopted for this database, Hmw=0,0277, SM4191=0,028

469 beta1 (Na<+> (HCO3)<->)

Value in this parameterfile (chemapp) = 0,3417264021 = R * 0,0411, alpha1 = 2; Reference: SM 4191

Remark: This value instead of that from hmw was used to estimate Pitzer-parameters in SM 5325 (Np(V) with carbonate), It was therefore adopted for this database, Hmw=0,0411, SM4191=0,044

470 beta0 (Na<+> (HSO4)<->)

Value in this parameterfile (chemapp) = 0,3774787994 = R * 0,0454; Reference: HMW

Remark:

471 beta1 (Na<+> (HSO4)<->)

Value in this parameterfile (chemapp) = 3,309175378 = R * 0,398, alpha1 = 2; Reference: HMW

Remark:

472 beta0 (Na<+> OH<->)
Value in this parameterfile (chemapp) = 0,7183737504 = R * 0,0864; Reference: HMW
Remark:

473 beta1 (Na<+> OH<->)
Value in this parameterfile (chemapp) = 2,103571283 = R * 0,253, alpha1 = 2; Reference: HMW
Remark:

474 cphi (Na<+> OH<->)
Value in this parameterfile (chemapp) = 0,0365838484 = R * 0,0044; Reference: HMW
Remark:

475 beta0 (Na<+> (SO4)<2->)
Value in this parameterfile (chemapp) = 0,16279812538 = R * 0,01958; Reference: HMW
Remark:

476 beta1 (Na<+> (SO4)<2->)
Value in this parameterfile (chemapp) = 9,254050743 = R * 1,113, alpha1 = 2; Reference: HMW
Remark:

477 cphi (Na<+> (SO4)<2->)
Value in this parameterfile (chemapp) = 0,04132311967 = R * 0,00497; Reference: HMW
Remark:

478 theta (H<+> Ca<2+>)
Value in this parameterfile (chemapp) = 0,764935012 = R * 0,092; Reference: HMW
Remark:

479 psi (H<+> Cl<-> Ca<2+>)
Value in this parameterfile (chemapp) = -0,124717665 = R * -0,015; Reference: HMW
Remark:

480 theta (Mg<2+> Ca<2+>)
Value in this parameterfile (chemapp) = 0,058201577 = R * 0,007; Reference: HMW
Remark:

481 psi (Mg<2+> Ca<2+> Cl<->)
Value in this parameterfile (chemapp) = -0,099774132 = R * -0,012; Reference: HMW
Remark:

482 psi (Mg<2+> Ca<2+> (SO4)<2->)
Value in this parameterfile (chemapp) = 0,199548264 = R * 0,024; Reference: HMW
Remark:

483 theta ((CO3)<2-> Cl<->)
Value in this parameterfile (chemapp) = -0,16629022 = R * -0,02; Reference: HMW
Remark:

484 psi ((CO3)<2-> Cl<-> K<+>)
Value in this parameterfile (chemapp) = 0,033258044 = R * 0,004; Reference: HMW
Remark:

485 psi ((CO3)<2-> Cl<-> Na<+>)
Value in this parameterfile (chemapp) = 0,0706733435 = R * 0,0085; Reference: HMW
Remark:

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486   theta ((HCO3)<-> Cl<->)
      Value in this parameterfile (chemapp) = 0,24943533 = R * 0,03; Reference: HMW
      Remark:
487   psi ((HCO3)<-> Cl<-> Mg<2+>)
      Value in this parameterfile (chemapp) = -0,798193056 = R * -0,096; Reference:
      HMW
      Remark:
488   psi ((HCO3)<-> Cl<-> Na<+>)
      Value in this parameterfile (chemapp) = -0,124717665 = R * -0,015; Reference:
      HMW
      Remark:
489   theta (Cl<-> (HSO4)<->)
      Value in this parameterfile (chemapp) = -0,049887066 = R * -0,006; Reference:
      HMW
      Remark:
490   psi (Cl<-> (HSO4)<-> H<+>)
      Value in this parameterfile (chemapp) = 0,108088643 = R * 0,013; Reference: HMW
      Remark:
491   psi (Cl<-> (HSO4)<-> Na<+>)
      Value in this parameterfile (chemapp) = -0,049887066 = R * -0,006; Reference:
      HMW
      Remark:
492   theta (OH<-> Cl<->)
      Value in this parameterfile (chemapp) = -0,41572555 = R * -0,05; Reference: HMW
      Remark:
493   psi (OH<-> Cl<-> Ca<2+>)
      Value in this parameterfile (chemapp) = -0,207862775 = R * -0,025; Reference:
      HMW
      Remark:
494   psi (OH<-> Cl<-> K<+>)
      Value in this parameterfile (chemapp) = -0,049887066 = R * -0,006; Reference:
      HMW
      Remark:
495   psi (OH<-> Cl<-> Na<+>)
      Value in this parameterfile (chemapp) = -0,049887066 = R * -0,006; Reference:
      HMW
      Remark:
496   theta (Cl<-> (SO4)<2->)
      Value in this parameterfile (chemapp) = 0,16629022 = R * 0,02; Reference: HMW
      Remark:
497   psi (Cl<-> (SO4)<2-> Ca<2+>)
      Value in this parameterfile (chemapp) = -0,149661198 = R * -0,018; Reference:
      HMW
      Remark:
498   psi (Cl<-> (SO4)<2-> Mg<2+>)
      Value in this parameterfile (chemapp) = -0,033258044 = R * -0,004; Reference:
      HMW
      Remark:
499   psi (Cl<-> (SO4)<2-> Na<+>)
      Value in this parameterfile (chemapp) = 0,0116403154 = R * 0,0014; Reference:
      HMW
      Remark:
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500 theta ((HCO3)<-> (CO3)<2->)
Value in this parameterfile (chemapp) = -0,33258044 = R * -0,04; Reference: HMW
Remark:
501 psi ((HCO3)<-> (CO3)<2-> K<+>)
Value in this parameterfile (chemapp) = 0,099774132 = R * 0,012; Reference: HMW
Remark:
502 psi ((HCO3)<-> (CO3)<2-> Na<+>)
Value in this parameterfile (chemapp) = 0,016629022 = R * 0,002; Reference: HMW
Remark:
503 theta (K<+> Ca<2+>)
Value in this parameterfile (chemapp) = 0,266064352 = R * 0,032; Reference: HMW
Remark:
504 psi (K<+> Ca<2+> Cl<->)
Value in this parameterfile (chemapp) = -0,207862775 = R * -0,025; Reference: HMW
Remark:
505 theta (H<+> K<+>)
Value in this parameterfile (chemapp) = 0,041572555 = R * 0,005; Reference: HMW
Remark:
506 psi (H<+> K<+> Cl<->)
Value in this parameterfile (chemapp) = -0,091459621 = R * -0,011; Reference: HMW
Remark:
507 psi (H<+> K<+> (HSO4)<->)
Value in this parameterfile (chemapp) = -0,2203345415 = R * -0,0265; Reference: HMW
Remark:
508 psi (H<+> K<+> (SO4)<2->)
Value in this parameterfile (chemapp) = 1,637958667 = R * 0,197; Reference: HMW
Remark:
509 psi (K<+> Mg<2+> Cl<->)
Value in this parameterfile (chemapp) = -0,182919242 = R * -0,022; Reference: HMW
Remark:
510 psi (K<+> Mg<2+> (SO4)<2->)
Value in this parameterfile (chemapp) = -0,399096528 = R * -0,048; Reference: HMW
Remark:
511 theta (H<+> Mg<2+>)
Value in this parameterfile (chemapp) = 0,8314511 = R * 0,1; Reference: HMW
Remark:
512 psi (H<+> Mg<2+> Cl<->)
Value in this parameterfile (chemapp) = -0,091459621 = R * -0,011; Reference: HMW
Remark:
513 psi (H<+> Mg<2+> (HSO4)<->)
Value in this parameterfile (chemapp) = -0,1479982958 = R * -0,0178; Reference: HMW
Remark:
514 theta (Na<+> Ca<2+>)
Value in this parameterfile (chemapp) = 0,58201577 = R * 0,07; Reference: HMW

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      Remark:
515   psi (Na<+> Ca<2+> Cl<->)
      Value in this parameterfile (chemapp) = -0,058201577 = R * -0,007; Reference:
      HMW
      Remark:
516   psi (Na<+> Ca<2+> (SO4)<2->)
      Value in this parameterfile (chemapp) = -0,457298105 = R * -0,055; Reference:
      HMW
      Remark:
517   theta (H<+> Na<+>)
      Value in this parameterfile (chemapp) = 0,299322396 = R * 0,036; Reference: HMW
      Remark:
518   psi (H<+> Na<+> Cl<->)
      Value in this parameterfile (chemapp) = -0,033258044 = R * -0,004; Reference:
      HMW
      Remark:
519   psi (H<+> Na<+> (HSO4)<->)
      Value in this parameterfile (chemapp) = -0,1072571919 = R * -0,0129; Reference:
      HMW
      Remark:
520   theta (Na<+> K<+>)
      Value in this parameterfile (chemapp) = -0,099774132 = R * -0,012; Reference:
      HMW
      Remark:
521   psi (Na<+> K<+> (CO3)<2->)
      Value in this parameterfile (chemapp) = 0,024943533 = R * 0,003; Reference: HMW
      Remark:
522   psi (Na<+> K<+> Cl<->)
      Value in this parameterfile (chemapp) = -0,0149661198 = R * -0,0018; Reference:
      HMW
      Remark:
523   psi (Na<+> K<+> (HCO3)<->)
      Value in this parameterfile (chemapp) = -0,024943533 = R * -0,003; Reference:
      HMW
      Remark:
524   psi (Na<+> K<+> (SO4)<2->)
      Value in this parameterfile (chemapp) = -0,08314511 = R * -0,01; Reference: HMW
      Remark:
525   theta (Na<+> Mg<2+>)
      Value in this parameterfile (chemapp) = 0,58201577 = R * 0,07; Reference: HMW
      Remark:
526   psi (Na<+> Mg<2+> Cl<->)
      Value in this parameterfile (chemapp) = -0,099774132 = R * -0,012; Reference:
      HMW
      Remark:
527   psi (Na<+> Mg<2+> (SO4)<2->)
      Value in this parameterfile (chemapp) = -0,124717665 = R * -0,015; Reference:
      HMW
      Remark:
528   theta (OH<-> (CO3)<2->)
      Value in this parameterfile (chemapp) = 0,8314511 = R * 0,1; Reference: HMW
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      Remark:
529   psi (OH<-> (CO3)<2-> K<+>)
      Value in this parameterfile (chemapp) = -0,08314511 = R * -0,01; Reference: HMW
      Remark:
530   psi (OH<-> (CO3)<2-> Na<+>)
      Value in this parameterfile (chemapp) = -0,141346687 = R * -0,017; Reference:
      HMW
      Remark:
531   theta ((CO3)<2-> (SO4)<2->)
      Value in this parameterfile (chemapp) = 0,16629022 = R * 0,02; Reference: HMW
      Remark:
532   psi ((CO3)<2-> (SO4)<2-> K<+>)
      Value in this parameterfile (chemapp) = -0,074830599 = R * -0,009; Reference:
      HMW
      Remark:
533   psi ((CO3)<2-> (SO4)<2-> Na<+>)
      Value in this parameterfile (chemapp) = -0,041572555 = R * -0,005; Reference:
      HMW
      Remark:
534   theta ((HCO3)<-> (SO4)<2->)
      Value in this parameterfile (chemapp) = 0,08314511 = R * 0,01; Reference: HMW
      Remark:
535   psi ((HCO3)<-> (SO4)<2-> Mg<2+>)
      Value in this parameterfile (chemapp) = -1,338636271 = R * -0,161; Reference:
      HMW
      Remark:
536   psi ((HCO3)<-> (SO4)<2-> Na<+>)
      Value in this parameterfile (chemapp) = -0,041572555 = R * -0,005; Reference:
      HMW
      Remark:
537   psi ((SO4)<2-> (HSO4)<-> K<+>)
      Value in this parameterfile (chemapp) = -0,5628923947 = R * -0,0677; Reference:
      HMW
      Remark:
538   psi ((SO4)<2-> (HSO4)<-> Mg<2+>)
      Value in this parameterfile (chemapp) = -0,3533667175 = R * -0,0425; Reference:
      HMW
      Remark:
539   psi ((SO4)<2-> (HSO4)<-> Na<+>)
      Value in this parameterfile (chemapp) = -0,0781564034 = R * -0,0094; Reference:
      HMW
      Remark:
540   theta (OH<-> (SO4)<2->)
      Value in this parameterfile (chemapp) = -0,108088643 = R * -0,013; Reference:
      HMW
      Remark:
541   psi (OH<-> (SO4)<2-> K<+>)
      Value in this parameterfile (chemapp) = -0,41572555 = R * -0,05; Reference: HMW
      Remark:
542   psi (OH<-> (SO4)<2-> Na<+>)
      Value in this parameterfile (chemapp) = -0,074830599 = R * -0,009; Reference:
      HMW
```

```
      Remark:
543   beta0 (Mg(OH)<+> Cl<->)
      Value in this parameterfile (chemapp) = -0,8314511 = R * -0,1; Reference: HMW
      Remark:
544   beta1 (Mg(OH)<+> Cl<->)
      Value in this parameterfile (chemapp) = 13,785459238 = R * 1,658, alpha1 = 2;
      Reference: HMW
      Remark:
545   psi (Mg<2+> Mg(OH)<+> Cl<->)
      Value in this parameterfile (chemapp) = 0,232806308 = R * 0,028; Reference: HMW
      Remark:
546   theta ((SO4)<2-> I<->)
      Value in this parameterfile (chemapp) = 0,86811809351 = R * 0,10441; Reference:
      I/Se-AB
      Remark:
547   theta ((SO4)<2-> SeO3<2->)
      Value in this parameterfile (chemapp) = 0,47326196612 = R * 0,05692; Reference:
      I/Se-AB
      Remark:
548   theta ((SO4)<2-> SeO4<2->)
      Value in this parameterfile (chemapp) = -0,49038985878 = R * -0,05898;
      Reference: I/Se-AB
      Remark:
549   beta0 (Ca<2+> I<->)
      Value in this parameterfile (chemapp) = 3,68191490613 = R * 0,44283; Reference:
      I/Se-AB
      Remark:
550   beta1 (Ca<2+> I<->)
      Value in this parameterfile (chemapp) = 15,03246959778 = R * 1,80798, alpha1 =
      2; Reference: I/Se-AB
      Remark:
551   cphi (Ca<2+> I<->)
      Value in this parameterfile (chemapp) = -0,0223411390193305 = R * -0,00269;
      Reference: I/Se-AB
      Remark: calculated from cphi = cgamma*2*WURZEL(2) where cgamma =-0,00095
552   theta (Cl<-> I<->)
      Value in this parameterfile (chemapp) = 0,14317587942 = R * 0,01722; Reference:
      I/Se-AB
      Remark:
553   theta (Cl<-> SeO3<2->)
      Value in this parameterfile (chemapp) = -0,06443746025 = R * -0,00775;
      Reference: I/Se-AB
      Remark:
554   theta (Cl<-> SeO4<2->)
      Value in this parameterfile (chemapp) = 0,02635699987 = R * 0,00317; Reference:
      I/Se-AB
      Remark:
555   psi (K<+> (SO4)<2-> SeO3<2->)
      Value in this parameterfile (chemapp) = -0,85448229547 = R * -0,10277;
      Reference: I/Se-AB
      Remark:
556   psi (K<+> (SO4)<2-> SeO4<2->)
```

Value in this parameterfile (chemapp) = 0,06052964008 = R * 0,00728; Reference: I/Se-AB

Remark:

557 psi (K<+> (SO4)<2-> I<->)

Value in this parameterfile (chemapp) = -0,05753641612 = R * -0,00692; Reference: I/Se-AB

Remark:

558 psi (K<+> Cl<-> SeO3<2->)

Value in this parameterfile (chemapp) = 0,02111885794 = R * 0,00254; Reference: I/Se-AB

Remark:

559 psi (K<+> Cl<-> I<->)

Value in this parameterfile (chemapp) = -0,02261546992 = R * -0,00272; Reference: I/Se-AB

Remark:

560 beta0 (K<+> HSeO3<->)

Value in this parameterfile (chemapp) = 0,22241316925 = R * 0,02675; Reference: I/Se-AB

Remark:

561 beta1 (K<+> HSeO3<->)

Value in this parameterfile (chemapp) = 11,84102769554 = R * 1,42414, alpha1 = 2; Reference: I/Se-AB

Remark:

562 beta0 (K<+> I<->)

Value in this parameterfile (chemapp) = 0,55399586793 = R * 0,06663; Reference: I/Se-AB

Remark:

563 beta1 (K<+> I<->)

Value in this parameterfile (chemapp) = 2,67777141266 = R * 0,32206, alpha1 = 2; Reference: I/Se-AB

Remark:

564 cphi (K<+> I<->)

Value in this parameterfile (chemapp) = -0,01962224596 = R * -0,00236; Reference: I/Se-AB

Remark: calculated from cgamma=-0,00118

565 psi (K<+> Mg<2+> SeO4<2->)

Value in this parameterfile (chemapp) = -0,37980686248 = R * -0,04568; Reference: I/Se-AB

Remark:

566 psi (K<+> Mg<2+> I<->)

Value in this parameterfile (chemapp) = -0,13353104666 = R * -0,01606; Reference: I/Se-AB

Remark:

567 beta0 (K<+> SeO3<2->)

Value in this parameterfile (chemapp) = 1,98592095235 = R * 0,23885; Reference: I/Se-AB

Remark:

568 beta1 (K<+> SeO3<2->)

Value in this parameterfile (chemapp) = 19,43508631739 = R * 2,33749, alpha1 = 2; Reference: I/Se-AB

Remark:

569 cphi (K<+> SeO3<2->)

Value in this parameterfile (chemapp) = -0,0475043166516292 = R * -0,00571; Reference: I/Se-AB

Remark: calculated from cphi =cgamma*2*WURZEL(2) where cgamma = 0,00202

570 beta0 (K<+> SeO4<2->)

Value in this parameterfile (chemapp) = 0,78829878791 = R * 0,09481; Reference: I/Se-AB

Remark:

571 beta1 (K<+> SeO4<2->)

Value in this parameterfile (chemapp) = 13,49736143185 = R * 1,62335, alpha1 = 2; Reference: I/Se-AB

Remark:

572 cphi (K<+> SeO4<2->)

Value in this parameterfile (chemapp) = 0,00493856757269412 = R * 0,00059; Reference: I/Se-AB

Remark: calculated from cphi =cgamma*2*WURZEL(2) with cgamma = 0,00021

573 psi (Mg<2+> (SO4)<2-> SeO4<2->)

Value in this parameterfile (chemapp) = 0,5030279155 = R * 0,0605; Reference: I/Se-AB

Remark:

574 psi (Mg<2+> (SO4)<2-> I<->)

Value in this parameterfile (chemapp) = -0,47259680524 = R * -0,05684; Reference: I/Se-AB

Remark:

575 psi (Mg<2+> Cl<-> SeO4<2->)

Value in this parameterfile (chemapp) = 0,07807325829 = R * 0,00939; Reference: I/Se-AB

Remark:

576 psi (Mg<2+> Cl<-> I<->)

Value in this parameterfile (chemapp) = -0,09436969985 = R * -0,01135; Reference: I/Se-AB

Remark:

577 beta0 (Mg<2+> I<->)

Value in this parameterfile (chemapp) = 4,1140200428 = R * 0,4948; Reference: I/Se-AB

Remark:

578 beta1 (Mg<2+> I<->)

Value in this parameterfile (chemapp) = 15,22337077034 = R * 1,83094, alpha1 = 2; Reference: I/Se-AB

Remark:

579 cphi (Mg<2+> I<->)

Value in this parameterfile (chemapp) = 0,0592628108723294 = R * 0,00713; Reference: I/Se-AB

Remark: calculated from cphi = cgamma*2*WURZEL(2) where cgamma = 0,00252

580 beta0 (Mg<2+> SeO4<2->)

Value in this parameterfile (chemapp) = 2,72391694871 = R * 0,32761; Reference: I/Se-AB

Remark:

581 beta1 (Mg<2+> SeO4<2->)

Value in this parameterfile (chemapp) = 32,46010037933 = R * 3,90403, alpha1 = 1,4; Reference: I/Se-AB

Remark:

582 cphi (Mg<2+> SeO4<2->)

```
      Value in this parameterfile (chemapp) = 0,07449801856 = R * 0,00896; Reference:
      I/Se-AB
      Remark: calculated from cphi =cgamma*2*WURZEL(4) with cgamma = 0,00224
583   psi (Na<+> (SO4)<2-> SeO3<2->)
      Value in this parameterfile (chemapp) = -0,16446102758 = R * -0,01978;
      Reference: I/Se-AB
      Remark:
584   psi (Na<+> (SO4)<2-> SeO4<2->)
      Value in this parameterfile (chemapp) = 0,21601099578 = R * 0,02598; Reference:
      I/Se-AB
      Remark:
585   psi (Na<+> (SO4)<2-> I<->)
      Value in this parameterfile (chemapp) = -0,15664538724 = R * -0,01884;
      Reference: I/Se-AB
      Remark:
586   psi (Na<+> Cl<-> I<->)
      Value in this parameterfile (chemapp) = -0,03334118911 = R * -0,00401;
      Reference: I/Se-AB
      Remark:
587   beta0 (Na<+> HSeO3<->)
      Value in this parameterfile (chemapp) = -0,93795998591 = R * -0,11281;
      Reference: I/Se-AB
      Remark:
588   beta1 (Na<+> HSeO3<->)
      Value in this parameterfile (chemapp) = 14,72840793051 = R * 1,77141, alpha1 =
      2; Reference: I/Se-AB
      Remark:
589   beta0 (Na<+> I<->)
      Value in this parameterfile (chemapp) = 1,04064419676 = R * 0,12516; Reference:
      I/Se-AB
      Remark:
590   beta1 (Na<+> I<->)
      Value in this parameterfile (chemapp) = 2,62123273786 = R * 0,31526, alpha1 =
      2; Reference: I/Se-AB
      Remark:
591   cphi (Na<+> I<->)
      Value in this parameterfile (chemapp) = 0,0016629022 = R * 0,0002; Reference:
      I/Se-AB
      Remark: calculated from cgamma=0,0001
592   psi (Na<+> K<+> SeO3<2->)
      Value in this parameterfile (chemapp) = 0,00706733435 = R * 0,00085; Reference:
      I/Se-AB
      Remark:
593   psi (Na<+> K<+> SeO4<2->)
      Value in this parameterfile (chemapp) = 0,16204981939 = R * 0,01949; Reference:
      I/Se-AB
      Remark:
594   psi (Na<+> K<+> I<->)
      Value in this parameterfile (chemapp) = -0,03051425537 = R * -0,00367;
      Reference: I/Se-AB
      Remark:
595   psi (Na<+> Mg<2+> SeO4<2->)
```

Value in this parameterfile (chemapp) = -0,12945693627 = R * -0,01557; Reference: I/Se-AB

Remark:

596 psi (Na<+> Mg<2+> I<->)

Value in this parameterfile (chemapp) = -0,15157353553 = R * -0,01823; Reference: I/Se-AB

Remark:

597 beta0 (Na<+> SeO3<2->)

Value in this parameterfile (chemapp) = 0,76460243156 = R * 0,09196; Reference: I/Se-AB

Remark:

598 beta1 (Na<+> SeO3<2->)

Value in this parameterfile (chemapp) = 13,30554566308 = R * 1,60028, alpha1 = 2; Reference: I/Se-AB

Remark:

599 cphi (Na<+> SeO3<2->)

Value in this parameterfile (chemapp) = 0,0277500463608527 = R * 0,00334; Reference: I/Se-AB

Remark: calculated from cphi =cgamma*2*WURZEL(2) where cgamma = 0,00118

600 beta0 (Na<+> SeO4<2->)

Value in this parameterfile (chemapp) = 0,81241086981 = R * 0,09771; Reference: I/Se-AB

Remark:

601 beta1 (Na<+> SeO4<2->)

Value in this parameterfile (chemapp) = 0,650735203415 = R * 0,07827, alpha1 = 2; Reference: I/Se-AB

Remark:

602 beta0 (Cs<+> (SO4)<2->)

Value in this parameterfile (chemapp) = 0,5936560854 = R * 0,0714; Reference: SM5322

Remark:

603 beta1 (Cs<+> (SO4)<2->)

Value in this parameterfile (chemapp) = 9,985727711 = R * 1,201, alpha1 = 2; Reference: SM5322

Remark:

604 cphi (Cs<+> (SO4)<2->)

Value in this parameterfile (chemapp) = 0,02419522701 = R * 0,00291; Reference: SM5322

Remark:

605 beta0 (Cs<+> Cl<->)

Value in this parameterfile (chemapp) = 0,28917869258 = R * 0,03478; Reference: SM5322

Remark:

606 beta1 (Cs<+> Cl<->)

Value in this parameterfile (chemapp) = 0,33041866714 = R * 0,03974, alpha1 = 2; Reference: SM5322

Remark:

607 cphi (Cs<+> Cl<->)

Value in this parameterfile (chemapp) = -0,004123997456 = R * -0,0005; Reference: SM5322

Remark:

608 psi (Cs<+> K<+> Cl<->)

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      Value in this parameterfile (chemapp) = -0,0108088643 = R * -0,0013; Reference:
      SM5322
      Remark:
609   psi (Cs<+> K<+> (SO4)<2->)
      Value in this parameterfile (chemapp) = -0,0349209462 = R * -0,0042; Reference:
      SM5322
      Remark:
610   psi (Cs<+> Mg<2+> Cl<->)
      Value in this parameterfile (chemapp) = -0,365838484 = R * -0,044; Reference:
      SM5322
      Remark:
611   psi (Cs<+> Mg<2+> (SO4)<2->)
      Value in this parameterfile (chemapp) = -0,66516088 = R * -0,08; Reference:
      SM5322
      Remark:
612   theta (Cs<+> Mg<2+>)
      Value in this parameterfile (chemapp) = -0,648531858 = R * -0,078; Reference:
      SM5322
      Remark:
613   psi (Cs<+> Na<+> Cl<->)
      Value in this parameterfile (chemapp) = -0,01122458985 = R * -0,00135;
      Reference: SM5322
      Remark:
614   psi (Cs<+> Na<+> (SO4)<2->)
      Value in this parameterfile (chemapp) = 0,0191233753 = R * 0,0023; Reference:
      SM5322
      Remark:
615   theta (Cs<+> Na<+>)
      Value in this parameterfile (chemapp) = -0,28152934246 = R * -0,03386;
      Reference: SM5322
      Remark:
616   beta0 (Li<+> Cl<->)
      Value in this parameterfile (chemapp) = 1,74371924692 = R * 0,20972; Reference:
      SM250
      Remark:
617   beta1 (Li<+> Cl<->)
      Value in this parameterfile (chemapp) = -2,8585288818 = R * -0,3438, alpha1 =
      2; Reference: SM250
      Remark:
618   cphi (Li<+> Cl<->)
      Value in this parameterfile (chemapp) = -0,03600183263 = R * -0,00433;
      Reference: SM250
      Remark:
619   psi (Li<+> Na<+> Cl<->)
      Value in this parameterfile (chemapp) = -0,0182919242 = R * -0,0022; Reference:
      SM251
      Remark:
620   theta (Li<+> Na<+>)
      Value in this parameterfile (chemapp) = 0,099774132 = R * 0,012; Reference:
      SM251
      Remark:
621   beta0 (Li<+> OH<->)
```

Value in this parameterfile (chemapp) = 0,42279288435 = R * 0,05085; Reference: SM250

Remark:

622 beta1 (Li<+> OH<->)

Value in this parameterfile (chemapp) = -0,60255261217 = R * -0,07247, alpha1 = 2; Reference: SM250

Remark:

623 cphi (Li<+> OH<->)

Value in this parameterfile (chemapp) = -0,02801990207 = R * -0,00337; Reference: SM250

Remark:

624 psi (Cd<2+> Ca<2+> Cl<->)

Value in this parameterfile (chemapp) = -0,48415397553 = R * -0,05823; Reference: ULT

Remark:

625 psi (Cd<2+> Ca<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = 0,60238632195 = R * 0,07245; Reference: ULT

Remark:

626 theta (Cd<2+> Ca<2+>)

Value in this parameterfile (chemapp) = -1,67994694755 = R * -0,20205; Reference: ULT

Remark:

627 psi (Cd<2+> Cl<-> (SO4)<2->)

Value in this parameterfile (chemapp) = -0,0440669083 = R * -0,0053; Reference: ULT

Remark:

628 psi (Cd<2+> K<+> Cl<->)

Value in this parameterfile (chemapp) = -0,46212052138 = R * -0,05558; Reference: ULT

Remark:

629 psi (Cd<2+> K<+> (SO4)<2->)

Value in this parameterfile (chemapp) = -0,29391796385 = R * -0,03535; Reference: ULT

Remark:

630 theta (Cd<2+> K<+>)

Value in this parameterfile (chemapp) = -0,45912729742 = R * -0,05522; Reference: ULT

Remark:

631 psi (Cd<2+> Mg<2+> Cl<->)

Value in this parameterfile (chemapp) = -0,77383153877 = R * -0,09307; Reference: ULT

Remark:

632 psi (Cd<2+> Mg<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = 0,16595763956 = R * 0,01996; Reference: ULT

Remark:

633 theta (Cd<2+> Mg<2+>)

Value in this parameterfile (chemapp) = -0,55017119287 = R * -0,06617; Reference: ULT

Remark:

634 psi (Cd<2+> Na<+> (SO4)<2->)

Value in this parameterfile (chemapp) = -0,1180660562 = R * -0,0142; Reference: ULT

Remark:

635 psi (Cd<2+> Na<+> Cl<->)

Value in this parameterfile (chemapp) = -0,48091131624 = R * -0,05784; Reference: ULT

Remark:

636 theta (Cd<2+> Na<+>)

Value in this parameterfile (chemapp) = 0,224491797 = R * 0,027; Reference: ULT

Remark:

637 psi (Cl<-> (SO4)<2-> Zn<2+>)

Value in this parameterfile (chemapp) = 0,226187957244 = R * 0,0272; Reference: ULT

Remark:

638 beta0 (Zn<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = 1,51382301777 = R * 0,18207; Reference: ULT

Remark:

639 beta1 (Zn<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = 24,469605873 = R * 2,943, alpha1 = 1,4; Reference: ULT

Remark:

640 beta2 (Zn<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = -1645,35858179 = R * -197,89, alpha2 = 20; Reference: ULT

Remark:

641 cphi (Zn<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = 0,27803724784 = R * 0,03344; Reference: ULT

Remark:

642 psi (Zn<2+> Ca<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = 0,291007885 = R * 0,035; Reference: ULT

Remark:

643 psi (Zn<2+> Ca<2+> Cl<->)

Value in this parameterfile (chemapp) = -0,2386264657 = R * -0,0287; Reference: ULT

Remark:

644 beta0 (Zn<2+> Cl<->)

Value in this parameterfile (chemapp) = 0,54227240742 = R * 0,06522; Reference: ULT

Remark:

645 beta1 (Zn<2+> Cl<->)

Value in this parameterfile (chemapp) = 45,8852918557 = R * 5,5187, alpha1 = 2; Reference: ULT

Remark:

646 beta2 (Zn<2+> Cl<->)

Value in this parameterfile (chemapp) = -36,2329760358 = R * -4,3578, alpha2 = 2,5; Reference: ULT

Remark:

647 cphi (Zn<2+> Cl<->)

Value in this parameterfile (chemapp) = 0,03101312603 = R * 0,00373; Reference: ULT

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      Remark:
648   beta0 (Zn<2+> H2SiO4<2->)
      Value in this parameterfile (chemapp) = 1,837506931 = R * 0,221; Reference: ULT
      Remark:
649   beta1 (Zn<2+> H2SiO4<2->)
      Value in this parameterfile (chemapp) = 27,795410273 = R * 3,343, alpha1 = 1,4;
      Reference: ULT
      Remark:
650   beta2 (Zn<2+> H2SiO4<2->)
      Value in this parameterfile (chemapp) = -309,54924453 = R * -37,23, alpha2 =
      12; Reference: ULT
      Remark:
651   cphi (Zn<2+> H2SiO4<2->)
      Value in this parameterfile (chemapp) = 0,207862775 = R * 0,025; Reference: ULT
      Remark:
652   beta0 (Zn<2+> H3SiO4<->)
      Value in this parameterfile (chemapp) = 3,9460669206 = R * 0,4746; Reference:
      ULT
      Remark:
653   beta1 (Zn<2+> H3SiO4<->)
      Value in this parameterfile (chemapp) = 14,375789519 = R * 1,729, alpha1 = 2;
      Reference: ULT
      Remark:
654   psi (Zn<2+> K<+> Cl<->)
      Value in this parameterfile (chemapp) = -0,2145143838 = R * -0,0258; Reference:
      ULT
      Remark:
655   psi (Zn<2+> K<+> (SO4)<2->)
      Value in this parameterfile (chemapp) = -0,1779305354 = R * -0,0214; Reference:
      ULT
      Remark:
656   theta (Zn<2+> K<+>)
      Value in this parameterfile (chemapp) = -0,814822078 = R * -0,098; Reference:
      ULT
      Remark:
657   psi (Zn<2+> Mg<2+> Cl<->)
      Value in this parameterfile (chemapp) = -0,19347867097 = R * -0,02327;
      Reference: ULT
      Remark:
658   psi (Zn<2+> Na<+> Cl<->)
      Value in this parameterfile (chemapp) = -0,21476381913 = R * -0,02583;
      Reference: ULT
      Remark:
659   psi (Zn<2+> Na<+> (SO4)<2->)
      Value in this parameterfile (chemapp) = 0,4373432786 = R * 0,0526; Reference:
      ULT
      Remark:
660   theta (Zn<2+> Na<+>)
      Value in this parameterfile (chemapp) = -1,06558772976 = R * -0,12816;
      Reference: ULT
      Remark:
661   lambda (Zn<2+> SiO2<0>)
```

Value in this parameterfile (chemapp) = 2,4319944675 = R * 0,2925; Reference: ULT

Remark:

662 beta0 (Cd<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = 1,86968408857 = R * 0,22487; Reference: ULT

Remark:

663 beta1 (Cd<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = 19,4434839735 = R * 2,3385, alpha1 = 1,4; Reference: ULT

Remark:

664 beta2 (Cd<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = -497,407306064 = R * -59,824, alpha2 = 12; Reference: ULT

Remark:

665 cphi (Cd<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = 0,04331860231 = R * 0,00521; Reference: ULT

Remark:

666 beta0 (Cd<2+> Cl<->)

Value in this parameterfile (chemapp) = -0,33324560088 = R * -0,04008; Reference: ULT

Remark:

667 beta1 (Cd<2+> Cl<->)

Value in this parameterfile (chemapp) = -26,40788467732 = R * -3,17612, alpha1 = 2,5; Reference: ULT

Remark:

668 beta2 (Cd<2+> Cl<->)

Value in this parameterfile (chemapp) = -373,5718106811 = R * -44,9301, alpha2 = 12; Reference: ULT

Remark:

669 cphi (Cd<2+> Cl<->)

Value in this parameterfile (chemapp) = 0,04431634363 = R * 0,00533; Reference: ULT

Remark:

670 beta0 (Ni<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = 1,41712525484 = R * 0,17044; Reference: Koda

Remark:

671 beta1 (Ni<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = 24,6425477018 = R * 2,9638, alpha1 = 1,4; Reference: Koda

Remark:

672 beta2 (Ni<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = -618,566360356 = R * -74,396, alpha2 = 12; Reference: Koda

Remark:

673 cphi (Ni<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = 0,0731984604907 = R * 0,0088; Reference: Koda

Remark:

674 beta0 (Ni<2+> Cl<->)

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      Value in this parameterfile (chemapp) = 3,35947816955 = R * 0,40405; Reference:
      Koda
      Remark:
675   beta1 (Ni<2+> Cl<->)
      Value in this parameterfile (chemapp) = 15,3760251923 = R * 1,8493, alpha1 =
      2,5; Reference: Koda
      Remark:
676   cphi (Ni<2+> Cl<->)
      Value in this parameterfile (chemapp) = -0,0533733404623 = R * -0,00642;
      Reference: Koda
      Remark:
677   psi (Ni<2+> Cl<-> (SO4)<2->)
      Value in this parameterfile (chemapp) = 0,0385344326806 = R * 0,00463;
      Reference: Koda
      Remark:
678   psi (Ni<2+> K<+> Cl<->)
      Value in this parameterfile (chemapp) = 0,124784181088 = R * 0,01501;
      Reference: Koda
      Remark:
679   psi (Ni<2+> K<+> (SO4)<2->)
      Value in this parameterfile (chemapp) = -0,86346196735 = R * -0,10385;
      Reference: Koda
      Remark:
680   theta (Ni<2+> K<+>)
      Value in this parameterfile (chemapp) = -2,03256535906 = R * -0,24446;
      Reference: Koda
      Remark:
681   psi (Ni<2+> Mg<2+> Cl<->)
      Value in this parameterfile (chemapp) = 0,185205732525 = R * 0,02228;
      Reference: Koda
      Remark:
682   psi (Ni<2+> Mg<2+> (SO4)<2->)
      Value in this parameterfile (chemapp) = 0,413971188179 = R * 0,04979;
      Reference: Koda
      Remark:
683   theta (Ni<2+> Mg<2+>)
      Value in this parameterfile (chemapp) = -1,24534745758 = R * -0,14978;
      Reference: Koda
      Remark:
684   psi (Ni<2+> Na<+> Cl<->)
      Value in this parameterfile (chemapp) = -0,0308202293748 = R * -0,00371;
      Reference: Koda
      Remark:
685   psi (Ni<2+> Na<+> (SO4)<2->)
      Value in this parameterfile (chemapp) = -0,15440046927 = R * -0,01857;
      Reference: Koda
      Remark:
686   theta (Ni<2+> Na<+>)
      Value in this parameterfile (chemapp) = 0,373920188692 = R * 0,04497;
      Reference: Koda
      Remark:
687   psi (Ni<2+> Ca<2+> (SO4)<2->)
```

Value in this parameterfile (chemapp) = 0,171387015243 = R * 0,02061; Reference: Koda

Remark:

688 theta (Ni<2+> Ca<2+>)

Value in this parameterfile (chemapp) = -0,509879072564 = R * -0,06132; Reference: Koda

Remark:

689 psi ((CO3)<2-> H2SiO4<2-> K<+>)

Value in this parameterfile (chemapp) = -0,074830599 = R * -0,009; Reference: R1990

Remark:

690 psi ((CO3)<2-> H2SiO4<2-> Na<+>)

Value in this parameterfile (chemapp) = -0,041572555 = R * -0,005; Reference: R1990

Remark:

691 psi ((HCO3)<-> H2SiO4<2-> Mg<2+>)

Value in this parameterfile (chemapp) = -1,338636271 = R * -0,161; Reference: R1990

Remark:

692 psi ((HCO3)<-> H2SiO4<2-> Na<+>)

Value in this parameterfile (chemapp) = -0,041572555 = R * -0,005; Reference: R1990

Remark:

693 psi ((SO4)<2-> Al(OH)4<-> K<+>)

Value in this parameterfile (chemapp) = -0,5628923947 = R * -0,0677; Reference: R1990

Remark:

694 psi ((SO4)<2-> Al(OH)4<-> Mg<2+>)

Value in this parameterfile (chemapp) = -0,3533667175 = R * -0,0425; Reference: R1990

Remark:

695 psi ((SO4)<2-> Al(OH)4<-> Na<+>)

Value in this parameterfile (chemapp) = -0,0781564034 = R * -0,0094; Reference: R1990

Remark:

696 psi ((SO4)<2-> H3SiO4<-> K<+>)

Value in this parameterfile (chemapp) = -0,5628923947 = R * -0,0677; Reference: R1990

Remark:

697 psi ((SO4)<2-> H3SiO4<-> Mg<2+>)

Value in this parameterfile (chemapp) = -0,3533667175 = R * -0,0425; Reference: R1990

Remark:

698 psi ((SO4)<2-> H3SiO4<-> Na<+>)

Value in this parameterfile (chemapp) = -0,0781564034 = R * -0,0094; Reference: R1990

Remark:

699 beta0 (Al<3+> Cl<->)

Value in this parameterfile (chemapp) = 5,81458697763 = R * 0,69933; Reference: R1990

Remark:

700 beta1 (Al<3+> Cl<->)

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      Value in this parameterfile (chemapp) = 48,59557300637 = R * 5,84467, alpha1 =
      2; Reference: R1990
      Remark:
701   cphi (Al<3+> Cl<->)
      Value in this parameterfile (chemapp) = 0,02269861503 = R * 0,00273; Reference:
      R1990
      Remark:
702   beta0 (Ca<2+> Al(OH)4<->)
      Value in this parameterfile (chemapp) = 1,7834626095 = R * 0,2145; Reference:
      R1990
      Remark:
703   beta1 (Ca<2+> Al(OH)4<->)
      Value in this parameterfile (chemapp) = 21,03571283 = R * 2,53, alpha1 = 2;
      Reference: R1990
      Remark:
704   beta0 (Ca<2+> H2SiO4<2->)
      Value in this parameterfile (chemapp) = 1,6629022 = R * 0,2; Reference: R1990
      Remark:
705   beta1 (Ca<2+> H2SiO4<2->)
      Value in this parameterfile (chemapp) = 26,5839860203 = R * 3,1973, alpha1 =
      1,4; Reference: R1990
      Remark:
706   beta2 (Ca<2+> H2SiO4<2->)
      Value in this parameterfile (chemapp) = -450,97907664 = R * -54,24, alpha2 =
      12; Reference: R1990
      Remark:
707   beta0 (Ca<2+> H3SiO4<->)
      Value in this parameterfile (chemapp) = 1,7834626095 = R * 0,2145; Reference:
      R1990
      Remark:
708   beta1 (Ca<2+> H3SiO4<->)
      Value in this parameterfile (chemapp) = 21,03571283 = R * 2,53, alpha1 = 2;
      Reference: R1990
      Remark:
709   psi (Ca<2+> Mg<2+> H2SiO4<2->)
      Value in this parameterfile (chemapp) = 0,199548264 = R * 0,024; Reference:
      R1990
      Remark:
710   psi (Cl<-> Al(OH)4<-> H<+>)
      Value in this parameterfile (chemapp) = 0,108088643 = R * 0,013; Reference:
      R1990
      Remark:
711   psi (Cl<-> Al(OH)4<-> Na<+>)
      Value in this parameterfile (chemapp) = -0,049887066 = R * -0,006; Reference:
      R1990
      Remark:
712   theta (Cl<-> Al(OH)4<->)
      Value in this parameterfile (chemapp) = -0,049887066 = R * -0,006; Reference:
      R1990
      Remark:
713   psi (Cl<-> H2SiO4<2-> Ca<2+>)
```

```
      Value in this parameterfile (chemapp) = -0,149661198 = R * -0,018; Reference:
      R1990
      Remark:
714   psi (Cl<-> H2SiO4<2-> Mg<2+>)
      Value in this parameterfile (chemapp) = -0,033258044 = R * -0,004; Reference:
      R1990
      Remark:
715   psi (Cl<-> H2SiO4<2-> Na<+>)
      Value in this parameterfile (chemapp) = 0,0116403154 = R * 0,0014; Reference:
      R1990
      Remark:
716   psi (Cl<-> H3SiO4<-> H<+>)
      Value in this parameterfile (chemapp) = 0,108088643 = R * 0,013; Reference:
      R1990
      Remark:
717   theta (Cl<-> H3SiO4<->)
      Value in this parameterfile (chemapp) = -0,049887066 = R * -0,006; Reference:
      R1990
      Remark:
718   beta0 (H<+> Al(OH)4<->)
      Value in this parameterfile (chemapp) = 1,7510360166 = R * 0,2106; Reference:
      R1990
      Remark:
719   beta1 (H<+> Al(OH)4<->)
      Value in this parameterfile (chemapp) = 4,423319852 = R * 0,532, alpha1 = 2;
      Reference: R1990
      Remark:
720   beta0 (H<+> H2SiO4<2->)
      Value in this parameterfile (chemapp) = 0,1804248887 = R * 0,0217; Reference:
      R1990
      Remark:
721   cphi (H<+> H2SiO4<2->)
      Value in this parameterfile (chemapp) = 0,3417264021 = R * 0,0411; Reference:
      R1990
      Remark:
722   beta0 (H<+> H3SiO4<->)
      Value in this parameterfile (chemapp) = 1,7510360166 = R * 0,2106; Reference:
      R1990
      Remark:
723   beta1 (H<+> H3SiO4<->)
      Value in this parameterfile (chemapp) = 4,423319852 = R * 0,532, alpha1 = 2;
      Reference: R1990
      Remark:
724   psi (H2SiO4<2-> Al(OH)4<-> K<+>)
      Value in this parameterfile (chemapp) = -0,5628923947 = R * -0,0677; Reference:
      R1990
      Remark:
725   psi (H2SiO4<2-> Al(OH)4<-> Mg<2+>)
      Value in this parameterfile (chemapp) = -0,3533667175 = R * -0,0425; Reference:
      R1990
      Remark:
726   psi (H2SiO4<2-> Al(OH)4<-> Na<+>)
```

```
      Value in this parameterfile (chemapp) = -0,0781564034 = R * -0,0094; Reference:
      R1990
      Remark:
727   psi (H3SiO4<-> H2SiO4<2-> K<+>)
      Value in this parameterfile (chemapp) = -0,5628923947 = R * -0,0677; Reference:
      R1990
      Remark:
728   psi (H3SiO4<-> H2SiO4<2-> Mg<2+>)
      Value in this parameterfile (chemapp) = -0,3533667175 = R * -0,0425; Reference:
      R1990
      Remark:
729   psi (H3SiO4<-> H2SiO4<2-> Na<+>)
      Value in this parameterfile (chemapp) = -0,0781564034 = R * -0,0094; Reference:
      R1990
      Remark:
730   beta0 (K<+> Al(OH)4<->)
      Value in this parameterfile (chemapp) = -0,0024943533 = R * -0,0003; Reference:
      R1990
      Remark:
731   beta1 (K<+> Al(OH)4<->)
      Value in this parameterfile (chemapp) = 1,4425676585 = R * 0,1735, alpha1 = 2;
      Reference: R1990
      Remark:
732   psi (K<+> H<+> H3SiO4<->)
      Value in this parameterfile (chemapp) = -0,2203345415 = R * -0,0265; Reference:
      R1990
      Remark:
733   psi (K<+> H<+> H2SiO4<2->)
      Value in this parameterfile (chemapp) = 1,637958667 = R * 0,197; Reference:
      R1990
      Remark:
734   psi (K<+> H<+> Al(OH)4<->)
      Value in this parameterfile (chemapp) = -0,2203345415 = R * -0,0265; Reference:
      R1990
      Remark:
735   beta0 (K<+> H2SiO4<2->)
      Value in this parameterfile (chemapp) = 0,4148940989 = R * 0,0499; Reference:
      R1990
      Remark:
736   beta1 (K<+> H2SiO4<2->)
      Value in this parameterfile (chemapp) = 6,4794984223 = R * 0,7793, alpha1 = 2;
      Reference: R1990
      Remark:
737   beta0 (K<+> H3SiO4<->)
      Value in this parameterfile (chemapp) = -0,0024943533 = R * -0,0003; Reference:
      R1990
      Remark:
738   beta1 (K<+> H3SiO4<->)
      Value in this parameterfile (chemapp) = 1,4425676585 = R * 0,1735, alpha1 = 2;
      Reference: R1990
      Remark:
739   psi (K<+> Mg<2+> H2SiO4<2->)
```

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      Value in this parameterfile (chemapp) = -0,698418924 = R * -0,084; Reference:
      R1990
      Remark:
740   beta0 (Mg<2+> Al(OH)4<->)
      Value in this parameterfile (chemapp) = 3,9460669206 = R * 0,4746; Reference:
      R1990
      Remark:
741   beta1 (Mg<2+> Al(OH)4<->)
      Value in this parameterfile (chemapp) = 14,375789519 = R * 1,729, alpha1 = 2;
      Reference: R1990
      Remark:
742   psi (Mg<2+> H<+> H3SiO4<->)
      Value in this parameterfile (chemapp) = -0,1479982958 = R * -0,0178; Reference:
      R1990
      Remark:
743   psi (Mg<2+> H<+> Al(OH)4<->)
      Value in this parameterfile (chemapp) = -0,1479982958 = R * -0,0178; Reference:
      R1990
      Remark:
744   beta0 (Mg<2+> H2SiO4<2->)
      Value in this parameterfile (chemapp) = 1,837506931 = R * 0,221; Reference:
      R1990
      Remark:
745   beta1 (Mg<2+> H2SiO4<2->)
      Value in this parameterfile (chemapp) = 27,795410273 = R * 3,343, alpha1 = 1,4;
      Reference: R1990
      Remark:
746   beta2 (Mg<2+> H2SiO4<2->)
      Value in this parameterfile (chemapp) = -309,54924453 = R * -37,23, alpha2 =
      12; Reference: R1990
      Remark:
747   cphi (Mg<2+> H2SiO4<2->)
      Value in this parameterfile (chemapp) = 0,207862775 = R * 0,025; Reference:
      R1990
      Remark:
748   beta0 (Mg<2+> H3SiO4<->)
      Value in this parameterfile (chemapp) = 3,9460669206 = R * 0,4746; Reference:
      R1990
      Remark:
749   beta1 (Mg<2+> H3SiO4<->)
      Value in this parameterfile (chemapp) = 14,375789519 = R * 1,729, alpha1 = 2;
      Reference: R1990
      Remark:
750   psi (Na<+> Ca<2+> H2SiO4<2->)
      Value in this parameterfile (chemapp) = -0,457298105 = R * -0,055; Reference:
      R1990
      Remark:
751   psi (Na<+> H<+> H3SiO4<->)
      Value in this parameterfile (chemapp) = -0,1072571919 = R * -0,0129; Reference:
      R1990
      Remark:
752   psi (Na<+> H<+> Al(OH)4<->)
```

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      Value in this parameterfile (chemapp) = -0,1072571919 = R * -0,0129; Reference:
      R1990
      Remark:
753   beta0 (Na<+> H2SiO4<2->)
      Value in this parameterfile (chemapp) = 0,1629644156 = R * 0,0196; Reference:
      R1990
      Remark:
754   beta1 (Na<+> H2SiO4<2->)
      Value in this parameterfile (chemapp) = 9,254050743 = R * 1,113, alpha1 = 2;
      Reference: R1990
      Remark:
755   cphi (Na<+> H2SiO4<2->)
      Value in this parameterfile (chemapp) = 0,041572555 = R * 0,005; Reference:
      R1990
      Remark:
756   beta0 (Na<+> H3SiO4<->)
      Value in this parameterfile (chemapp) = 0,3774787994 = R * 0,0454; Reference:
      R1990
      Remark:
757   beta1 (Na<+> H3SiO4<->)
      Value in this parameterfile (chemapp) = 3,309175378 = R * 0,398, alpha1 = 2;
      Reference: R1990
      Remark:
758   psi (Na<+> K<+> H2SiO4<2->)
      Value in this parameterfile (chemapp) = -0,08314511 = R * -0,01; Reference:
      R1990
      Remark:
759   psi (Na<+> Mg<2+> H2SiO4<2->)
      Value in this parameterfile (chemapp) = -0,124717665 = R * -0,015; Reference:
      R1990
      Remark:
760   psi (OH<-> H2SiO4<2-> K<+>)
      Value in this parameterfile (chemapp) = -0,41572555 = R * -0,05; Reference:
      R1990
      Remark:
761   psi (OH<-> H2SiO4<2-> Na<+>)
      Value in this parameterfile (chemapp) = -0,074830599 = R * -0,009; Reference:
      R1990
      Remark:
762   beta0 (Sr<2+> (SO4)<2->)
      Value in this parameterfile (chemapp) = 1,82919242 = R * 0,22; Reference: FZK-
      INE 002/04
      Remark:
763   beta1 (Sr<2+> (SO4)<2->)
      Value in this parameterfile (chemapp) = 23,94579168 = R * 2,88, alpha1 = 1,4;
      Reference: FZK-INE 002/04
      Remark:
764   beta2 (Sr<2+> (SO4)<2->)
      Value in this parameterfile (chemapp) = -347,5465598 = R * -41,8, alpha2 = 12;
      Reference: FZK-INE 002/04
      Remark:
765   cphi (Sr<2+> (SO4)<2->)
```

Value in this parameterfile (chemapp) = 1,57975709 = R * 0,19; Reference: FZK-INE 002/04

Remark:

766 beta0 (Sr<2+> Cl<->)

Value in this parameterfile (chemapp) = 2,37587151825 = R * 0,28575; Reference: FZK-INE 002/04

Remark:

767 beta1 (Sr<2+> Cl<->)

Value in this parameterfile (chemapp) = 13,86236846475 = R * 1,66725, alpha1 = 2; Reference: FZK-INE 002/04

Remark:

768 cphi (Sr<2+> Cl<->)

Value in this parameterfile (chemapp) = -0,0108088643 = R * -0,0013; Reference: FZK-INE 002/04

Remark:

769 psi (Sr<2+> K<+> Cl<->)

Value in this parameterfile (chemapp) = -0,207862775 = R * -0,025; Reference: FZK-INE 002/04

Remark:

770 theta (Sr<2+> K<+>)

Value in this parameterfile (chemapp) = 0,266064352 = R * 0,032; Reference: FZK-INE 002/04

Remark:

771 psi (Sr<2+> Mg<2+> Cl<->)

Value in this parameterfile (chemapp) = -0,099774132 = R * -0,012; Reference: FZK-INE 002/04

Remark:

772 psi (Sr<2+> Mg<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = 0,199548264 = R * 0,024; Reference: FZK-INE 002/04

Remark:

773 theta (Sr<2+> Mg<2+>)

Value in this parameterfile (chemapp) = 0,058201577 = R * 0,007; Reference: FZK-INE 002/04

Remark:

774 psi (Sr<2+> Na<+> Cl<->)

Value in this parameterfile (chemapp) = -0,058201577 = R * -0,007; Reference: FZK-INE 002/04

Remark:

775 psi (Sr<2+> Na<+> (SO4)<2->)

Value in this parameterfile (chemapp) = -0,457298105 = R * -0,055; Reference: FZK-INE 002/04

Remark:

776 theta (Sr<2+> Na<+>)

Value in this parameterfile (chemapp) = 0,58201577 = R * 0,07; Reference: FZK-INE 002/04

Remark:

777 beta0 (Ag<+> Cl<->)

Value in this parameterfile (chemapp) = 0,4980392089 = R * 0,0599; Reference: /FRI1985/

Remark:

778 beta1 (Ag<+> Cl<->)

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      Value in this parameterfile (chemapp) = 1,49661198 = R * 0,18, alpha1 = 2;
      Reference: /FRI1985/
      Remark:
779   cphi (Ag<+> Cl<->)
      Value in this parameterfile (chemapp) = 0,54593079226 = R * 0,06566; Reference:
      /FRI1985/
      Remark: calculated from cgamma = 0,03283
780   beta0 (H<+> AgCl2<->)
      Value in this parameterfile (chemapp) = 1,8483157953 = R * 0,2223; Reference:
      /FRI1985/
      Remark:
781   beta1 (H<+> AgCl2<->)
      Value in this parameterfile (chemapp) = 3,059740048 = R * 0,368, alpha1 = 2;
      Reference: /FRI1985/
      Remark:
782   cphi (H<+> AgCl2<->)
      Value in this parameterfile (chemapp) = 0,54593079226 = R * 0,06566; Reference:
      /FRI1985/
      Remark: calculated from cgamma = -0,01011
783   beta0 (H<+> AgCl3<2->)
      Value in this parameterfile (chemapp) = 2,9624602693 = R * 0,3563; Reference:
      /FRI1985/
      Remark:
784   beta1 (H<+> AgCl3<2->)
      Value in this parameterfile (chemapp) = 13,6565843175 = R * 1,6425, alpha1 = 2;
      Reference: /FRI1985/
      Remark:
785   cphi (H<+> AgCl3<2->)
      Value in this parameterfile (chemapp) = -0,00376271815062409 = R * -0,00045;
      Reference: /FRI1985/
      Remark: calculated from cgamma = -0,00016
786   beta0 (H<+> AgCl4<3->)
      Value in this parameterfile (chemapp) = 5,1782774508 = R * 0,6228; Reference:
      /FRI1985/
      Remark:
787   beta1 (H<+> AgCl4<3->)
      Value in this parameterfile (chemapp) = 42,90287676 = R * 5,16, alpha1 = 2;
      Reference: /FRI1985/
      Remark:
788   cphi (H<+> AgCl4<3->)
      Value in this parameterfile (chemapp) = 0,0198735945790846 = R * 0,00239;
      Reference: /FRI1985/
      Remark: calculated from cgamma = 0,00069
789   beta0 (Na<+> AgCl2<->)
      Value in this parameterfile (chemapp) = 1,230547628 = R * 0,148; Reference:
      /FRI1985/
      Remark:
790   beta1 (Na<+> AgCl2<->)
      Value in this parameterfile (chemapp) = 2,436151723 = R * 0,293, alpha1 = 2;
      Reference: /FRI1985/
      Remark:
791   cphi (Na<+> AgCl2<->)
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      Value in this parameterfile (chemapp) = 0,54593079226 = R * 0,06566; Reference:
      /FRI1985/
      Remark: calculated from cgamma = -0,0152
792   beta0 (Na<+> AgCl3<2->)
      Value in this parameterfile (chemapp) = 1,0709090168 = R * 0,1288; Reference:
      /FRI1985/
      Remark:
793   beta1 (Na<+> AgCl3<2->)
      Value in this parameterfile (chemapp) = 9,9774132 = R * 1,2, alpha1 = 2;
      Reference: /FRI1985/
      Remark:
794   cphi (Na<+> AgCl3<2->)
      Value in this parameterfile (chemapp) = -0,25304279562947 = R * -0,03043;
      Reference: /FRI1985/
      Remark: calculated from cgamma = -0,01076
795   beta0 (Na<+> AgCl4<3->)
      Value in this parameterfile (chemapp) = 2,8568659796 = R * 0,3436; Reference:
      /FRI1985/
      Remark:
796   beta1 (Na<+> AgCl4<3->)
      Value in this parameterfile (chemapp) = 33,258044 = R * 4, alpha1 = 2;
      Reference: /FRI1985/
      Remark:
797   cphi (Na<+> AgCl4<3->)
      Value in this parameterfile (chemapp) = -0,561933087301364 = R * -0,06758;
      Reference: /FRI1985/
      Remark: calculated from cgamma = -0,01951
798   beta0 (K<+> AgCl2<->)
      Value in this parameterfile (chemapp) = 1,8000916315 = R * 0,2165; Reference:
      /FRI1985/
      Remark:
799   beta1 (K<+> AgCl2<->)
      Value in this parameterfile (chemapp) = 3,009852982 = R * 0,362, alpha1 = 2;
      Reference: /FRI1985/
      Remark:
800   cphi (K<+> AgCl2<->)
      Value in this parameterfile (chemapp) = 0,54593079226 = R * 0,06566; Reference:
      /FRI1985/
      Remark: calculated from cgamma = -0,012
801   beta0 (K<+> AgCl3<2->)
      Value in this parameterfile (chemapp) = 0,16629022 = R * 0,02; Reference:
      /FRI1985/
      Remark:
802   beta1 (K<+> AgCl3<2->)
      Value in this parameterfile (chemapp) = 6,992503751 = R * 0,841, alpha1 = 2;
      Reference: /FRI1985/
      Remark:
803   cphi (K<+> AgCl3<2->)
      Value in this parameterfile (chemapp) = -0,572638668548104 = R * -0,06887;
      Reference: /FRI1985/
      Remark: calculated from cgamma = -0,02435
804   beta0 (K<+> AgCl4<3->)
```

```
      Value in this parameterfile (chemapp) = 1,8632819151 = R * 0,2241; Reference:
      /FRI1985/
      Remark:
805   beta1 (K<+> AgCl4<3->)
      Value in this parameterfile (chemapp) = 29,208877143 = R * 3,513, alpha1 = 2;
      Reference: /FRI1985/
      Remark:
806   cphi (K<+> AgCl4<3->)
      Value in this parameterfile (chemapp) = -12,6154122110711 = R * -1,51728;
      Reference: /FRI1985/
      Remark: calculated from cgamma = -0,438
807   beta0 (Na<+> MoO4<2->)
      Value in this parameterfile (chemapp) = 0,964483276 = R * 0,116; Reference:
      /GMR1992/
      Remark:
808   beta1 (Na<+> MoO4<2->)
      Value in this parameterfile (chemapp) = 19,015286657 = R * 2,287, alpha1 = 2;
      Reference: /GMR1992/
      Remark:
809   cphi (Na<+> MoO4<2->)
      Value in this parameterfile (chemapp) = 0,141101930648403 = R * 0,01697;
      Reference: /GMR1992/
      Remark: calculated from cgamma = 0,006
810   theta (Cl<-> MoO4<2->)
      Value in this parameterfile (chemapp) = 0,291007885 = R * 0,035; Reference:
      /GMR1992/
      Remark:
811   beta0 (Mg<2+> MoO4<2->)
      Value in this parameterfile (chemapp) = 4,115682945 = R * 0,495; Reference:
      /GMR1992/
      Remark:
812   beta1 (Mg<2+> MoO4<2->)
      Value in this parameterfile (chemapp) = 54,29375683 = R * 6,53, alpha1 = 2;
      Reference: /GMR1992/
      Remark:
813   cphi (Mg<2+> MoO4<2->)
      Value in this parameterfile (chemapp) = -2,760417652 = R * -0,332; Reference:
      /GMR1992/
      Remark: calculated from cgamma = -0,083
814   psi (Mg<2+> Na<+> MoO4<2->)
      Value in this parameterfile (chemapp) = 0,49887066 = R * 0,06; Reference:
      /GMR1992/
      Remark:
815   beta0 (Na<+> (AsO4)<3->)
      Value in this parameterfile (chemapp) = 1,98517264636 = R * 0,23876; Reference:
      Koda
      Remark:
816   beta1 (Na<+> (AsO4)<3->)
      Value in this parameterfile (chemapp) = 32,6361185772 = R * 3,9252, alpha1 = 2;
      Reference: Koda
      Remark:
817   cphi (Na<+> (AsO4)<3->)
```

```
      Value in this parameterfile (chemapp) = -0,114781824355 = R * -0,01381;
      Reference: Koda
      Remark:
818   beta0 (K<+> (AsO4)<3->)
      Value in this parameterfile (chemapp) = 2,07180985098 = R * 0,24918; Reference:
      Koda
      Remark:
819   beta1 (K<+> (AsO4)<3->)
      Value in this parameterfile (chemapp) = 61,2929121898 = R * 7,3718, alpha1 = 2;
      Reference: Koda
      Remark:
820   cphi (K<+> (AsO4)<3->)
      Value in this parameterfile (chemapp) = -0,0360957866043 = R * -0,00434;
      Reference: Koda
      Remark:
821   beta0 (Na<+> (HAsO4)<2->)
      Value in this parameterfile (chemapp) = 0,16163409384 = R * 0,01944; Reference:
      Koda
      Remark:
822   beta1 (Na<+> (HAsO4)<2->)
      Value in this parameterfile (chemapp) = 14,4830467109 = R * 1,7419, alpha1 = 2;
      Reference: Koda
      Remark:
823   cphi (Na<+> (HAsO4)<2->)
      Value in this parameterfile (chemapp) = 0,0131003435316 = R * 0,00158;
      Reference: Koda
      Remark:
824   beta0 (K<+> (HAsO4)<2->)
      Value in this parameterfile (chemapp) = 0,589698378164 = R * 0,07092;
      Reference: Koda
      Remark:
825   beta1 (K<+> (HAsO4)<2->)
      Value in this parameterfile (chemapp) = 17,5619101342 = R * 2,1122, alpha1 = 2;
      Reference: Koda
      Remark:
826   cphi (K<+> (HAsO4)<2->)
      Value in this parameterfile (chemapp) = 0,0026589806178 = R * 0,00032;
      Reference: Koda
      Remark:
827   beta0 (Na<+> (H2AsO4)<->)
      Value in this parameterfile (chemapp) = -0,766065785496 = R * -0,09214;
      Reference: Koda
      Remark:
828   beta1 (Na<+> (H2AsO4)<->)
      Value in this parameterfile (chemapp) = 3,32755044731 = R * 0,40021, alpha1 =
      2; Reference: Koda
      Remark:
829   cphi (Na<+> (H2AsO4)<->)
      Value in this parameterfile (chemapp) = 0,145138104016 = R * 0,01746;
      Reference: Koda
      Remark:
830   beta0 (K<+> (H2AsO4)<->)
```

```
      Value in this parameterfile (chemapp) = -2,0777962989 = R * -0,2499; Reference:
      Koda
      Remark:
831   beta1 (K<+> (H2AsO4)<->)
      Value in this parameterfile (chemapp) = 4,66626986342 = R * 0,56122, alpha1 =
      2; Reference: Koda
      Remark:
832   cphi (K<+> (H2AsO4)<->)
      Value in this parameterfile (chemapp) = 0,509962217674 = R * 0,06133;
      Reference: Koda
      Remark:
833   theta ((AsO4)<3-> Cl<->)
      Value in this parameterfile (chemapp) = 0,813117603245 = R * 0,0978; Reference:
      Koda
      Remark:
834   theta ((AsO4)<3-> (SO4)<2->)
      Value in this parameterfile (chemapp) = -2,16085826379 = R * -0,25989;
      Reference: Koda
      Remark:
835   theta ((HAsO4)<2-> Cl<->)
      Value in this parameterfile (chemapp) = -0,113734195969 = R * -0,01368;
      Reference: Koda
      Remark:
836   theta ((H2AsO4)<-> Cl<->)
      Value in this parameterfile (chemapp) = 3,69546755906 = R * 0,44446; Reference:
      Koda
      Remark:
837   psi (Na<+> (AsO4)<3-> (SO4)<2->)
      Value in this parameterfile (chemapp) = 0,62159284236 = R * 0,07476; Reference:
      Koda
      Remark:
838   psi (Na<+> (HAsO4)<2-> Cl<->)
      Value in this parameterfile (chemapp) = 0,207264130208 = R * 0,02493;
      Reference: Koda
      Remark:
839   psi (K<+> (HAsO4)<2-> Cl<->)
      Value in this parameterfile (chemapp) = 0,103923072989 = R * 0,0125; Reference:
      Koda
      Remark:
840   psi (Na<+> (H2AsO4)<-> Cl<->)
      Value in this parameterfile (chemapp) = -0,696656247668 = R * -0,08379;
      Reference: Koda
      Remark:
841   psi (K<+> (H2AsO4)<-> Cl<->)
      Value in this parameterfile (chemapp) = -1,48139642487 = R * -0,17817;
      Reference: Koda
      Remark:
842   beta0 (Cu<2+> Cl<->)
      Value in this parameterfile (chemapp) = 1,24476544181 = R * 0,14971; Reference:
      Koda
      Remark:
843   beta1 (Cu<2+> Cl<->)
```

Value in this parameterfile (chemapp) = 7,5138235907 = R * 0,9037, alpha1 = 1; Reference: Koda

Remark: 1 kein Tippfehler!

844 cphi (Cu<2+> Cl<->)

Value in this parameterfile (chemapp) = -0,02269861503 = R * -0,00273; Reference: Koda

Remark:

845 beta0 (Cu<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = 1,84191362183 = R * 0,22153; Reference: Koda

Remark:

846 beta1 (Cu<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = 20,64725887608 = R * 2,48328, alpha1 = 1,4; Reference: Koda

Remark:

847 beta2 (Cu<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = -325,3651073542 = R * -39,1322, alpha2 = 12; Reference: Koda

Remark:

848 cphi (Cu<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = 0,03167828691 = R * 0,00381; Reference: Koda

Remark:

849 theta (Cu<2+> Na<+>)

Value in this parameterfile (chemapp) = -0,8505744753 = R * -0,1023; Reference: Koda

Remark:

850 theta (Cu<2+> K<+>)

Value in this parameterfile (chemapp) = -1,3660741573 = R * -0,1643; Reference: Koda

Remark:

851 theta (Cu<2+> Mg<2+>)

Value in this parameterfile (chemapp) = 0,9137647589 = R * 0,1099; Reference: Koda

Remark:

852 theta (Cu<2+> Ca<2+>)

Value in this parameterfile (chemapp) = -1,0667517613 = R * -0,1283; Reference: Koda

Remark:

853 psi (Cu<2+> Na<+> Cl<->)

Value in this parameterfile (chemapp) = -0,025666895457 = R * -0,00309; Reference: Koda

Remark:

854 psi (Cu<2+> K<+> Cl<->)

Value in this parameterfile (chemapp) = -0,011947952307 = R * -0,00144; Reference: Koda

Remark:

855 psi (Cu<2+> Mg<2+> Cl<->)

Value in this parameterfile (chemapp) = -0,51816032552 = R * -0,06232; Reference: Koda

Remark:

856 psi (Cu<2+> Ca<2+> Cl<->)

Value in this parameterfile (chemapp) = -0,18774165838 = R * -0,02258; Reference: Koda

Remark:

857 psi (Cu<2+> Na<+> (SO4)<2->)

Value in this parameterfile (chemapp) = 0,46602834155 = R * 0,05605; Reference: Koda

Remark:

858 psi (Cu<2+> K<+> (SO4)<2->)

Value in this parameterfile (chemapp) = 0,15331958284 = R * 0,01844; Reference: Koda

Remark:

859 psi (Cu<2+> Mg<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = -0,52206814569 = R * -0,06279; Reference: Koda

Remark:

860 psi (Cu<2+> Ca<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = 0,7333398702 = R * 0,0882; Reference: Koda

Remark:

861 psi (Cu<2+> Cl<-> (SO4)<2->)

Value in this parameterfile (chemapp) = 0,15722740301 = R * 0,01891; Reference: Koda

Remark:

862 beta0 (Co<2+> Cl<->)

Value in this parameterfile (chemapp) = 3,15884901912 = R * 0,37992; Reference: Koda

Remark:

863 beta1 (Co<2+> Cl<->)

Value in this parameterfile (chemapp) = 10,55518856939 = R * 1,26949, alpha1 = 2; Reference: Koda

Remark:

864 cphi (Co<2+> Cl<->)

Value in this parameterfile (chemapp) = -0,05612294925 = R * -0,00675; Reference: Koda

Remark:

865 beta0 (Co<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = 1,58025596066 = R * 0,19006; Reference: Koda

Remark:

866 beta1 (Co<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = 23,5076169503 = R * 2,8273, alpha1 = 1,4; Reference: Koda

Remark:

867 beta2 (Co<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = -481,4243215687 = R * -57,9017, alpha2 = 12; Reference: Koda

Remark:

868 cphi (Co<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = 0,05786899656 = R * 0,00696; Reference: Koda

Remark:

869 theta (Co<2+> Na<+>)

Value in this parameterfile (chemapp) = 0,63747355837 = R * 0,07667; Reference: Koda

Remark:

870 theta (Co<2+> K<+>)

Value in this parameterfile (chemapp) = 0,36642049977 = R * 0,04407; Reference: Koda

Remark:

871 theta (Co<2+> Mg<2+>)

Value in this parameterfile (chemapp) = 4,1165143961 = R * 0,4951; Reference: Koda

Remark:

872 theta (Co<2+> Ca<2+>)

Value in this parameterfile (chemapp) = -0,43792529437 = R * -0,05267; Reference: Koda

Remark:

873 psi (Co<2+> Na<+> Cl<->)

Value in this parameterfile (chemapp) = -0,10326622662 = R * -0,01242; Reference: Koda

Remark:

874 psi (Co<2+> K<+> Cl<->)

Value in this parameterfile (chemapp) = -0,24103767389 = R * -0,02899; Reference: Koda

Remark:

875 psi (Co<2+> Mg<2+> Cl<->)

Value in this parameterfile (chemapp) = -0,75262953572 = R * -0,09052; Reference: Koda

Remark:

876 psi (Co<2+> Ca<2+> Cl<->)

Value in this parameterfile (chemapp) = 0,0057877311071 = R * 0,0007; Reference: Koda

Remark:

877 psi (Co<2+> Na<+> (SO4)<2->)

Value in this parameterfile (chemapp) = -0,17161150704 = R * -0,02064; Reference: Koda

Remark:

878 psi (Co<2+> K<+> (SO4)<2->)

Value in this parameterfile (chemapp) = -0,35103865442 = R * -0,04222; Reference: Koda

Remark:

879 psi (Co<2+> Mg<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = -2,1276833649 = R * -0,2559; Reference: Koda

Remark:

880 psi (Co<2+> Ca<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = -0,09362139386 = R * -0,01126; Reference: Koda

Remark:

881 psi (Co<2+> Cl<-> (SO4)<2->)

Value in this parameterfile (chemapp) = 0,133032176 = R * 0,016; Reference: Koda

Remark:

882 beta0 (Na<+> CrO4<2->)

Value in this parameterfile (chemapp) = 0,507318203176 = R * 0,06102; Reference: Koda

Remark:

883 beta1 (Na<+> CrO4<2->)

Value in this parameterfile (chemapp) = 13,7962681023 = R * 1,6593, alpha1 = 2; Reference: Koda

Remark:

884 cphi (Na<+> CrO4<2->)

Value in this parameterfile (chemapp) = 0,0289029031382 = R * 0,00348; Reference: Koda

Remark:

885 beta0 (K<+> CrO4<2->)

Value in this parameterfile (chemapp) = 0,604065853172 = R * 0,07265; Reference: Koda

Remark:

886 beta1 (K<+> CrO4<2->)

Value in this parameterfile (chemapp) = 10,592687014 = R * 1,274, alpha1 = 2; Reference: Koda

Remark:

887 beta0 (Mg<2+> CrO4<2->)

Value in this parameterfile (chemapp) = 0,87177647835 = R * 0,10485; Reference: Koda

Remark:

888 beta1 (Mg<2+> CrO4<2->)

Value in this parameterfile (chemapp) = 76,5691632501 = R * 9,2091, alpha1 = 1,4; Reference: Koda

Remark:

889 cphi (Mg<2+> CrO4<2->)

Value in this parameterfile (chemapp) = 0,122730496871 = R * 0,01476; Reference: Koda

Remark:

890 theta (CrO4<2-> Cl<->)

Value in this parameterfile (chemapp) = 0,669368022566 = R * 0,08051; Reference: Koda

Remark:

891 psi (Na<+> CrO4<2-> Cl<->)

Value in this parameterfile (chemapp) = -0,0700281374464 = R * -0,00842; Reference: Koda

Remark:

892 psi (K<+> CrO4<2-> Cl<->)

Value in this parameterfile (chemapp) = 0,195083371593 = R * 0,02346; Reference: Koda

Remark:

893 psi (Na<+> Ca<2+> CrO4<2->)

Value in this parameterfile (chemapp) = -12,7702574449 = R * -1,5359; Reference: Koda

Remark:

894 psi (K<+> Mg<2+> CrO4<2->)

Value in this parameterfile (chemapp) = -0,0157343806164 = R * -0,00189; Reference: Koda

Remark:

895 psi (Mg<2+> CrO4<2-> (SO4)<2->)

Value in this parameterfile (chemapp) = -1,06625289064 = R * -0,12824; Reference: Koda

Remark:

896 psi (Na<+> Mg<2+> CrO4<2->)

Value in this parameterfile (chemapp) = -0,197378176629 = R * -0,02374; Reference: Koda

Remark:

897 beta0 (Mn<2+> Cl<->)

Value in this parameterfile (chemapp) = 2,58772525853 = R * 0,31123; Reference: Koda

Remark:

898 beta1 (Mn<2+> Cl<->)

Value in this parameterfile (chemapp) = 16,6814034193 = R * 2,0063, alpha1 = 2; Reference: Koda

Remark: a-Wert geraten von MOO

899 cphi (Mn<2+> Cl<->)

Value in this parameterfile (chemapp) = -0,05288028996 = R * -0,00636; Reference: Koda

Remark:

900 beta0 (Mn<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = 1,81439259042 = R * 0,21822; Reference: Koda

Remark:

901 beta1 (Mn<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = 23,06104456449 = R * 2,77359, alpha1 = 1,4; Reference: Koda

Remark: a-Wert geraten von MOO

902 beta2 (Mn<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = -489,1368619723 = R * -58,8293, alpha2 = 12; Reference: Koda

Remark: a-Wert geraten von MOO

903 cphi (Mn<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = 0,03009852982 = R * 0,00362; Reference: Koda

Remark:

904 theta (Mn<2+> Na<+>)

Value in this parameterfile (chemapp) = 0,35128808975 = R * 0,04225; Reference: Koda

Remark:

905 theta (Mn<2+> K<+>)

Value in this parameterfile (chemapp) = -2,0736390434 = R * -0,2494; Reference: Koda

Remark:

906 theta (Mn<2+> Mg<2+>)

Value in this parameterfile (chemapp) = 2,6257225738 = R * 0,3158; Reference: Koda

Remark:

907 theta (Mn<2+> Ca<2+>)

Value in this parameterfile (chemapp) = -0,5288028996 = R * -0,0636; Reference: Koda

Remark:

908 psi (Mn<2+> Na<+> Cl<->)

Value in this parameterfile (chemapp) = -0,10900323921 = R * -0,01311; Reference: Koda

Remark:

909 psi (Mn<2+> K<+> Cl<->)

Value in this parameterfile (chemapp) = 0,066707321753 = R * 0,00802; Reference: Koda

Remark:

910 psi (Mn<2+> Mg<2+> Cl<->)

Value in this parameterfile (chemapp) = -0,51566597222 = R * -0,06202; Reference: Koda

Remark:

911 psi (Mn<2+> Ca<2+> Cl<->)

Value in this parameterfile (chemapp) = -0,040333692861 = R * -0,00485; Reference: Koda

Remark:

912 psi (Mn<2+> Na<+> (SO4)<2->)

Value in this parameterfile (chemapp) = -0,13278274067 = R * -0,01597; Reference: Koda

Remark:

913 psi (Mn<2+> K<+> (SO4)<2->)

Value in this parameterfile (chemapp) = 0,60180430618 = R * 0,07238; Reference: Koda

Remark:

914 psi (Mn<2+> Mg<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = -0,8788438127 = R * -0,1057; Reference: Koda

Remark:

915 psi (Mn<2+> Ca<2+> (SO4)<2->)

Value in this parameterfile (chemapp) = 0,13461193309 = R * 0,01619; Reference: Koda

Remark:

916 psi (Mn<2+> Cl<-> (SO4)<2->)

Value in this parameterfile (chemapp) = 0,15539821059 = R * 0,01869; Reference: Koda

Remark:

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/by convention/ by convention

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Anlage 2: Output-Datei der geochemischen Modellierung mit OPW

```
**************************************************************************
 This is NATHAN 2.7.1

 This program contains ChemApp
 Copyright GTT-Technologies, Kaiserstrasse 100,
 D-52134 Herzogenrath, Germany
 http://www.gtt-technologies.de

 No warranty is given for the correctness of
 calculations done with NATHAN. Propositions
 and error messages are welcome.

 Helge C. Moog
 Gesellschaft fuer Anlagen- und Reaktorsicherheit (GRS)
 Theodor-Heuss-Str. 4, 38122 Braunschweig,
 Germany
 http://www.grs.de/geochemie
 helge.moog@grs.de
**************************************************************************

 Used input file:
 Opa+3BSK3+3SF.ni



 Version of prepare.f:          236
 Active Chemapp-Version:          554
 Number of phases =          406
 Number of system components =           48
 Name of paramaterfile used:
 tdb-hmw-118#1-1-1.dat


 > 3*(BSK3+3SF) mit Opalinustonloesung

 > Es sollen ca. 1.5 m3 Lösung übrig bleiben

 > p = 40 bar, Gasphase aktiv aber unbestimmtes Volumen


**************************************************************************
 Step            1:
 Charge balance before calculation =     0.000000D+00
 Relative error of charge balance prior of calculation = 0.000000D+00

 Active CHEMAPP-stream:

 SYSTEM UNITS:
 Pressure     : Pa
```

```
Volume       :  m3
Temperature  : K
Energy       : J
Amount       : mol

TARGET LIMITS:
Pressure/bar : 2.00000E+01  6.00000E+01
Volume/dm3   : 1.00000E-07  1.00000E+50
Temperature/K:  298.15      6000.00

T = 298.15 K
P = 4.00000E+06 Pa

STREAM CONSTITUENT
OH<->/AQUEOUS/
AMOUNT/mol    =  2.59438350000000E+00
Na<+>/AQUEOUS/
AMOUNT/mol    =  2.59438350000000E+00
BSK3+3SF
AMOUNT/mol    =  3.00000000000000E+00
H
AMOUNT/mol    =  7.28928089466300E+05
O
AMOUNT/mol    =  3.64775198961700E+05
NA
AMOUNT/mol    =  8.43292552100000E+02
K
AMOUNT/mol    =  5.28434525000000E+00
MG
AMOUNT/mol    =  3.24120756000000E+01
CA
AMOUNT/mol    =  4.55539549000000E+01
CL
AMOUNT/mol    =  8.54050679100000E+02
S
AMOUNT/mol    =  7.53460921000000E+01
C
AMOUNT/mol    =  3.90794535000000E+00
SR
AMOUNT/mol    =  2.07092515000000E+00

ELIMINATED PHASES:
K2HAsO4:3H2O
K3AsO4:7H2O
KH2AsO4
Na2HAsO4:7H2O
Na3AsO4:12H2O
NaH2AsO4:H2O
```

T = 298.15 K
P = 4.00000E+06 Pa
V = 1.51472E+02 m3

STREAM CONSTITUENTS	AMOUNT/mol
OH<->/AQUEOUS/	2.5944E+00
Na<+>/AQUEOUS/	2.5944E+00
BSK3+3SF	3.0000E+00
H	7.2893E+05
O	3.6478E+05
NA	8.4329E+02
K	5.2843E+00
MG	3.2412E+01
CA	4.5554E+01
CL	8.5405E+02
S	7.5346E+01
C	3.9079E+00
SR	2.0709E+00

	EQUIL AMOUNT	MOLE FRACTION	FUGACITY
PHASE: GAS	mol		Pa
H2	2.3834E+05	9.9921E-01	3.9968E+06
H2O(g)	1.8931E+02	7.9363E-04	3.1745E+03
CO2(g)	9.4309E-02	3.9537E-07	1.5815E+00
H2S(g)	5.4748E-08	2.2952E-13	9.1808E-07
O2(g)	NOT CALCD.	NOT CALCD.	<1.0000E-75
TOTAL:	2.3853E+05	1.0000E+00	1.0000E+00
PHASE: AQUEOUS	mol	MOLALITY	ACTIVITY
H2O	8.2484E+04	5.5508E+01	9.7414E-01
H<+>	9.0851E-05	6.1139E-08	4.4975E-08
OH<->	5.8668E-04	3.9482E-07	2.2454E-07
O2(aq)	NOT CALCD.	NOT CALCD.	<1.0000E-75
(CO2)<0>	6.9683E-04	4.6894E-07	5.1406E-07
(CO3)<2->	8.2280E-05	5.5372E-08	5.3966E-09
(HCO3)<->	1.3142E-02	8.8441E-06	5.0694E-06
(HSO4)<->	3.6046E-47	2.4258E-50	1.5493E-50
(SO4)<2->	5.1332E-41	3.4545E-44	3.5390E-45
Ca(CO3)<0>	8.5964E-06	5.7851E-09	5.7851E-09
Ca<2+>	6.1909E+00	4.1662E-03	7.8341E-04
Cl<->	8.5405E+02	5.7474E-01	3.8455E-01
K<+>	5.2843E+00	3.5562E-03	2.0748E-03
Mg(CO3)<0>	2.8957E-05	1.9487E-08	1.9487E-08
Mg(OH)<+>	2.4649E-04	1.6588E-07	1.4818E-07
Mg<2+>	3.2412E+01	2.1812E-02	4.4324E-03
Na<+>	6.5199E+02	4.3877E-01	2.7762E-01
H2S<0>	1.3172E-09	8.8643E-13	8.8643E-13
HS<->	5.8105E-09	3.9103E-12	2.0235E-12
H2SiO4<2->	2.7283E-14	1.8360E-17	1.7347E-18
H3SiO4<->	2.2733E-09	1.5299E-12	9.7858E-13

SiO2<0>	4.2378E-07	2.8519E-10	2.8519E-10
Al(OH)4<->	7.0998E-06	4.7779E-09	2.5949E-09
Al<3+>	9.3246E-12	6.2751E-15	1.5095E-16
Fe<2+>	5.5272E+01	3.7196E-02	6.4619E-03
Fe<3+>	9.6498E-36	6.4940E-39	1.3324E-39
(AsO4)<3->	6.3678E-17	4.2853E-20	1.8321E-22
(H2AsO4)<->	3.0798E-16	2.0726E-19	1.8333E-19
(HAsO4)<2->	3.1333E-15	2.1086E-18	2.2769E-19
H2AsO3<->	4.5831E-01	3.0843E-04	1.5961E-04
HAsO2<0>	1.5725E+01	1.0582E-02	1.0582E-02
B(OH)3<0>	6.1072E+02	4.1099E-01	4.1099E-01
Cr<3+>	1.0828E-08	7.2870E-12	7.4630E-15
CrO4<2->	7.5213E-53	5.0616E-56	7.3779E-57
Cu<+>	8.7266E-10	5.8727E-13	3.0188E-13
Cu<2+>	5.0152E-20	3.3750E-23	4.3054E-24
Cu(CO3)2<2->	1.4782E-46	9.9475E-50	6.2041E-51
Cu(HCO3)<->	1.8599E-11	1.2517E-14	6.4772E-15
Cu(OH)<+>	3.1118E-21	2.0941E-24	1.0765E-24
Cu(OH)2(aq)	2.0045E-22	1.3490E-25	1.3490E-25
Cu(OH)3<->	3.4363E-25	2.3125E-28	1.1967E-28
Cu(OH)4<2->	4.6028E-30	3.0975E-33	1.9319E-34
Cu2(OH)<3+>	2.3859E-40	1.6056E-43	1.6444E-46
Cu2(OH)2<2+>	7.8932E-39	5.3118E-42	3.4199E-43
Cu3(OH)4<2+>	3.6079E-58	2.4280E-61	1.5632E-62
CuCO3<0>	1.9291E-22	1.2982E-25	1.2982E-25
Mn<2+>	2.3707E-08	1.5954E-11	3.4376E-12
MoO4<2->	1.3036E-01	8.7730E-05	1.4399E-05
(NH4)<+>	8.6564E+01	5.8255E-02	2.9946E-02
NO3<->	NOT CALCD.	NOT CALCD.	<1.0000E-75
Ni<2+>	4.1372E-05	2.7842E-08	5.2877E-09
HNi(P2O7)<->	2.1451E-07	1.4436E-10	7.4703E-11
Ni(HPO4)<0>	1.3102E-05	8.8169E-09	8.8169E-09
Ni(P2O7)<2->	6.1307E-05	4.1257E-08	2.5732E-09
(H2P2O7)<2->	4.8997E-04	3.2973E-07	2.0565E-08
(H2PO4)<->	3.1277E+00	2.1048E-03	1.0892E-03
(H3P2O7)<->	4.7227E-10	3.1782E-13	1.6447E-13
(HP2O7)<3->	1.6688E-01	1.1231E-04	1.0235E-07
(HPO4)<2->	3.5407E+01	2.3827E-02	1.4861E-03
(P2O7)<4->	1.6096E+00	1.0832E-03	9.0615E-10
(PO4)<3->	2.4070E-02	1.6198E-05	1.4761E-08
H3PO4<0>	1.0048E-05	6.7618E-09	6.7618E-09
H4P2O7<0>	1.0992E-16	7.3970E-20	7.3970E-20
Sn(OH)6<2->	2.7345E-11	1.8402E-14	1.1477E-15
Sn<2+>	1.2555E-12	8.4489E-16	5.4396E-17
Sn<4+>	2.1513E-29	1.4478E-32	1.5526E-38
SnO3<2->	1.6747E-13	1.1270E-16	7.0291E-18
Sr<2+>	2.0709E+00	1.3937E-03	2.5874E-04
SrSO4<0>	2.7130E-43	1.8257E-46	1.8257E-46
Ti(OH)4<0>	3.3787E-07	2.2737E-10	2.2737E-10

(UO2)(H2PO4)(H3PO4)<+>	1.8591E-28	1.2511E-31	6.4313E-32
(UO2)(H2PO4)<+>	8.1140E-21	5.4604E-24	2.8069E-24
(UO2)(H2PO4)2<0>	2.0765E-22	1.3974E-25	1.3974E-25
(UO2)(H3PO4)<2+>	1.2719E-27	8.5594E-31	5.5107E-32
(UO2)(HAsO4)<0>	9.9790E-32	6.7155E-35	6.7155E-35
(UO2)(HPO4)<0>	5.4350E-17	3.6576E-20	3.6576E-20
U|+III|<3+>	1.1257E-23	7.5752E-27	7.7582E-30
U|+IV|(CO3)4<4->	1.7739E-19	1.1938E-22	1.3557E-26
U|+IV|(CO3)5<6->	1.0400E-20	6.9988E-24	5.5145E-36
U|+IV|(OH)<3+>	5.4171E-17	3.6455E-20	7.9950E-22
U|+IV|(OH)2(CO3)2<2->	5.6770E-12	3.8204E-15	4.4268E-16
U|+IV|(OH)2<2+>	3.9987E-11	2.6910E-14	4.9069E-15
U|+IV|(OH)3<+>	6.1903E-08	4.1658E-11	2.7467E-11
U|+IV|(OH)4<0>	4.6990E-06	3.1623E-09	3.1623E-09
U|+IV|(SO4)<2+>	3.9503E-62	2.6584E-65	1.7115E-66
U|+IV|(SO4)2<0>	NOT CALCD.	NOT CALCD.	<1.0000E-75
U|+IV|<4+>	1.7499E-22	1.1776E-25	1.2440E-28
U|+IV|Cl<3+>	3.7462E-21	2.5211E-24	2.5820E-27
(U|+V|O2)(CO3)3<5->	4.9293E-19	3.3172E-22	8.3351E-33
(U|+V|O2)<+>	1.7535E-11	1.1800E-14	6.0660E-15
(U|+VI|O2)(CO3)<0>	9.8286E-20	6.6143E-23	6.6143E-23
(U|+VI|O2)(CO3)2<2->	2.0372E-20	1.3710E-23	1.6589E-24
(U|+VI|O2)(CO3)3<4->	3.3030E-20	2.2228E-23	1.5106E-27
(U|+VI|O2)(H2AsO4)<+>	1.3837E-35	9.3121E-39	4.7869E-39
(U|+VI|O2)(H2AsO4)2<0>	9.7941E-53	6.5911E-56	6.5911E-56
(U|+VI|O2)(OH)<+>	3.8267E-19	2.5753E-22	1.7748E-22
(U|+VI|O2)(OH)2<0>	7.3985E-19	4.9789E-22	4.9789E-22
(U|+VI|O2)(OH)3<->	2.7559E-19	1.8546E-22	8.8131E-23
(U|+VI|O2)(OH)4<2->	5.1696E-23	3.4790E-26	4.1988E-27
(U|+VI|O2)(PO4)<->	1.0195E-15	6.8608E-19	3.5504E-19
(U|+VI|O2)(SO4)<0>	1.0758E-62	7.2395E-66	7.2395E-66
(U|+VI|O2)(SO4)2<2->	NOT CALCD.	NOT CALCD.	<1.0000E-75
(U|+VI|O2)(SO4)3<4->	NOT CALCD.	NOT CALCD.	<1.0000E-75
(U|+VI|O2)<2+>	1.0210E-20	6.8708E-24	1.4163E-24
(U|+VI|O2)11(CO3)6(OH)12	NOT CALCD.	NOT CALCD.	<1.0000E-75
(U|+VI|O2)2(CO3)(OH)3<->	4.8805E-32	3.2844E-35	1.6997E-35
(U|+VI|O2)2(OH)<3+>	1.2940E-37	8.7080E-41	8.9184E-44
(U|+VI|O2)2(OH)2<2+>	1.6303E-35	1.0972E-38	2.3894E-39
(U|+VI|O2)3(CO3)6<6->	NOT CALCD.	NOT CALCD.	<1.0000E-75
(U|+VI|O2)3(OH)4<2+>	9.4411E-51	6.3535E-54	8.8189E-55
(U|+VI|O2)3(OH)5<+>	7.9006E-48	5.3168E-51	4.3996E-51
(U|+VI|O2)3(OH)7<->	1.5295E-49	1.0293E-52	4.8910E-53
(U|+VI|O2)3O(OH)2(HCO3)<	2.2517E-54	1.5153E-57	7.7895E-58
(U|+VI|O2)4(OH)7<+>	2.7183E-63	1.8293E-66	1.3821E-66
(U|+VI|O2)Cl<+>	2.3948E-21	1.6116E-24	8.2847E-25
(U|+VI|O2)Cl2<0>	2.6146E-23	1.7596E-26	1.7596E-26
(U|+VI|O2)SiO(OH)3<+>	3.7692E-25	2.5365E-28	1.3039E-28
V<2+>	1.2193E-03	8.2051E-07	5.2826E-08
V<3+>	3.7195E-04	2.5031E-07	2.5635E-10

VO<2+>	8.9986E-07	6.0557E-10	3.8988E-11
VO2<+>	NOT CALCD.	NOT CALCD.	<1.0000E-75
Zr(OH)<3+>	2.7517E-23	1.8518E-26	1.8965E-29
Zr(OH)2<2+>	4.4585E-17	3.0004E-20	1.9317E-21
Zr(OH)4<0>	9.6371E-07	6.4854E-10	6.4854E-10
Zr<4+>	5.6441E-28	3.7983E-31	4.0734E-37
TOTAL:	8.4845E+04		1.0000E+00
PHASE: BASRSO4-IDMIX	mol	MOLE FRACTION	ACTIVITY
SrSO4	0.0000E+00	1.0000E+00	4.0127E-42
TOTAL:	0.0000E+00	1.0000E+00	4.0127E-42
	mol		ACTIVITY
Fe3O4_Magnetite	4.7818E+04		1.0000E+00
U|+IV|(OH)4(am)	1.9453E+04		1.0000E+00
ZrO2(monoclinic)	1.5274E+04		1.0000E+00
Mn(OH)2	2.3728E+03		1.0000E+00
Eskolaite_Cr2O3	2.0938E+03		1.0000E+00
Ni(cr)	1.9371E+03		1.0000E+00
U|+IV|(SiO4)(c)_Coffinit	1.0690E+03		1.0000E+00
FeCO3_Siderite	1.0251E+03		1.0000E+00
Rutile-TiO2	1.8953E+02		1.0000E+00
Cassiterite_SnO2	1.8768E+02		1.0000E+00
FeAl2O4_Hercynite	1.2706E+02		1.0000E+00
Na2[B4O5(OH)4]:8H2O_Bora	9.6947E+01		1.0000E+00
Cu(OH)2(s)	8.3477E+01		1.0000E+00
Ni3S2(cr)	4.8564E+01		1.0000E+00
CaMoO4_Powellite	3.9363E+01		1.0000E+00
V2O4	1.4875E+01		1.0000E+00
SnO2(cr)_Cassiterite	0.0000E+00		1.0000E+00
Gibbsite_Al(OH)3	0.0000E+00		1.8040E-01
CuO(s)	0.0000E+00		9.3118E-02
Anatase_TiO2	0.0000E+00		8.1922E-02
Fe(OH)2(cr)	0.0000E+00		7.5090E-02
MnHPO4	0.0000E+00		4.5217E-02
Fe(OH)2_precipitated	0.0000E+00		1.6516E-02
FeS	0.0000E+00		4.1394E-03
AlOOH_Boehmite	0.0000E+00		4.0468E-03
NaCl_Halite	0.0000E+00		2.8242E-03
SrCO3(s)	0.0000E+00		2.6516E-03
Mg(CO3)_Magnesite	0.0000E+00		1.4997E-03
Ca(CO3)_Calcite	0.0000E+00		9.8191E-04
Ca(CO3)_Aragonite	0.0000E+00		6.4147E-04
Dawsonite_NaAlCO3(OH)2	0.0000E+00		5.3003E-04
Dolomite-ord_CaMg(CO3)2	0.0000E+00		1.3720E-04
KCl_Sylvite	0.0000E+00		9.8796E-05
Fe2(SiO4)_Fayalite	0.0000E+00		9.7681E-05
Ni(OH)2(cr)	0.0000E+00		8.3034E-05
Chamosite-7A_Fe2Al2SiO5(	0.0000E+00		1.6620E-05
Mg(OH)2_Brucite	0.0000E+00		1.5925E-05
Fe3Si2O5(OH)4_Greenalite	0.0000E+00		1.5395E-05

FeSiO3(cr)	0.0000E+00	1.1688E-05
SnS_Herzenbergite	0.0000E+00	1.0264E-05
CaMg(CO3)2_Dolomite	0.0000E+00	1.0254E-05
MgMoO4:5H2O(s)	0.0000E+00	4.4165E-06
Dolomite-dis_CaMg(CO3)2	0.0000E+00	3.9170E-06
Na(HCO3)_Nahcolite	0.0000E+00	3.4742E-06
Mg(CO3):3H2O_Nesquehonit	0.0000E+00	3.0210E-06
Ni(CO3)(cr)	0.0000E+00	2.8665E-06
Tridymite_SiO2	0.0000E+00	1.9184E-06
Chalcedony-SiO2	0.0000E+00	1.5249E-06
FeCl2:4H2O	0.0000E+00	9.8581E-07
NiO(cr)	0.0000E+00	8.6174E-07
Coesite_SiO2	0.0000E+00	4.4100E-07
Fe(OH)3(cr)	0.0000E+00	1.6288E-07
SiO2(am)-GWB	0.0000E+00	1.4748E-07
Al2O3_Corundum	0.0000E+00	1.0764E-07
MgCl2:6H2O_Bischoffite	0.0000E+00	1.9411E-08
CaCl2:6H2O_Antarcticite	0.0000E+00	7.0894E-09
K(HCO3)_Kalicinite	0.0000E+00	5.3930E-09
Na2(CO3):10H2O_Natron	0.0000E+00	2.0662E-09
Daphnite-7A_Fe5AlAlSi3O1	0.0000E+00	1.5001E-09
Ni(CO3):5.5H2O(cr)	0.0000E+00	9.8329E-10
Na2(CO3):7H2O	0.0000E+00	9.4745E-10
CaCl2:4H2O	0.0000E+00	2.3057E-10
Rhodochrosite_MnCO3	0.0000E+00	2.2798E-10
NiCO3	0.0000E+00	1.9059E-10
Na2(CO3):H2O_Thermonatri	0.0000E+00	1.2481E-10
KMgCl3:6H2O_Carnallite	0.0000E+00	2.0135E-11
FeS2	0.0000E+00	1.9940E-11
Ni2SiO4	0.0000E+00	8.9149E-12
Ca(OH)2_Portlandite	0.0000E+00	5.6438E-12
CSH(0.8)_Ca0.8SiO2.8_H2O	0.0000E+00	4.3397E-12
KNa(CO3):6H2O	0.0000E+00	4.1393E-12
CaNa2(CO3)2:5H2O_Gayluss	0.0000E+00	3.5500E-12
Na2Ca(CO3)2:2H2O_Pirsson	0.0000E+00	2.5168E-12
Mg2Al2SiO5(OH)4_Amesit-7	0.0000E+00	2.1908E-12
NiCl2:6H2O(cr)	0.0000E+00	6.8476E-13
Kaolinite_Al2Si2O5(OH)4	0.0000E+00	2.1531E-13
Na.96Al.96Si2.04O6:H2O_A	0.0000E+00	1.0347E-13
NiCl2:4H2O(cr)	0.0000E+00	8.5389E-14
Ripidolite-14A_Mg3Fe2Al2	0.0000E+00	3.0378E-14
CSH(1.1)_Ca(1.1)SiO(3.1)	0.0000E+00	2.9676E-14
Mg4Al2O7:10H2O_Hydrotalc	0.0000E+00	2.0901E-14
U|+VI|O3:2H2O(c)_Schoepi	0.0000E+00	1.0894E-14
NaOH	0.0000E+00	7.6846E-15
NiCl2:2H2O(cr)	0.0000E+00	6.7459E-15
Na3(CO3)(HCO3):2H2O_Tron	0.0000E+00	5.6595E-15
MnCl2:4H2O	0.0000E+00	6.9404E-16
NiS2(cr)	0.0000E+00	4.9978E-16

Delafossite_CuFeO2	0.0000E+00	2.5806E-16
Minnesotaite_Fe3Si4O10(O	0.0000E+00	1.7236E-16
Ni2(SiO4)(oliv)	0.0000E+00	4.2137E-17
Mg4Al4Si2O10(OH)8_Amesit	0.0000E+00	2.6812E-17
K2(CO3):1.5H2O	0.0000E+00	1.9459E-17
Ripidolite-7A_Mg3Fe2Al2S	0.0000E+00	1.2745E-17
Ni9S8(cr)	0.0000E+00	7.1021E-18
Mesolite_Na.676Ca.657Al1	0.0000E+00	5.0439E-18
(U|+VI|O2)(CO3)(c)_Ruthe	0.0000E+00	4.3700E-18
Goethite_FeOOH	0.0000E+00	4.2968E-18
Maximum-Microcline_KAlSi	0.0000E+00	2.3629E-18
NiCl2(cr)	0.0000E+00	1.7859E-18
Ca2Cl2(OH)2:H2O	0.0000E+00	1.3282E-19
MnCl2:KCl:2H2O	0.0000E+00	5.4041E-20
Na.96Al.96Si2.04O6_Analc	0.0000E+00	3.8918E-20
Ferroaluminoceladonite_K	0.0000E+00	3.4628E-20
Scolecite_CaAl2Si3O10:3H	0.0000E+00	1.2899E-20
alpha-NiS	0.0000E+00	9.3808E-21
beta-NiS	0.0000E+00	2.5249E-21
K2Na(HCO3)(CO3):2H2O_Tro	0.0000E+00	2.0203E-21
Saponite-Na_Na.33Mg3Al.3	0.0000E+00	1.2427E-21
Saponite-Mg_Mg3.165Al.33	0.0000E+00	9.6252E-22
Saponite-Ca_Ca.165Mg3Al.	0.0000E+00	6.6118E-22
Saponite-K_K.33Mg3Al.33S	0.0000E+00	5.3887E-22
CSH(1.8)_Ca(1.8)SiO(3.8)	0.0000E+00	4.9891E-22
Illite_K0.6Mg0.25Al1.8Al	0.0000E+00	2.0962E-22
Saponite-H_H.33Mg3Al.33S	0.0000E+00	7.3928E-23
KMgAlSi4O10(OH)2_Celadon	0.0000E+00	1.2472E-23
Beidellite-Na_Na.33Al2.3	0.0000E+00	4.2408E-24
Talc_Mg3Si4O10(OH)2	0.0000E+00	3.5044E-24
Beidellite-Mg_Mg.165Al2.	0.0000E+00	3.2811E-24
CaCl2:MnCl2:8H2O	0.0000E+00	2.5953E-24
C2ASH8_Ca2Al2SiO7:8H2O_G	0.0000E+00	2.4491E-24
Beidellite-Ca_Ca.165Al2.	0.0000E+00	2.2564E-24
Na4(U|+VI|O2)(CO3)3(c)	0.0000E+00	1.9484E-24
Beidellite-K_K.33Al2.33S	0.0000E+00	1.8390E-24
MgCl2:MnCl2:8H2O	0.0000E+00	1.7156E-24
C2AH8_Ca2Al2O5:8H2O_Dica	0.0000E+00	1.2413E-24
Montmorillonite-Na_Na0.3	0.0000E+00	9.3319E-25
Montmorillonite-Mg_Mg0.4	0.0000E+00	7.2199E-25
Smectite-high-Fe-Mg_Ca.0	0.0000E+00	6.0326E-25
Montmorillonite-Ca_Ca0.1	0.0000E+00	4.9652E-25
Montmorillonite-K_K0.33M	0.0000E+00	4.0467E-25
Beidellite-H_H.33Al2.33S	0.0000E+00	2.5229E-25
Smectite-low-Fe-Mg_Ca.02	0.0000E+00	8.8450E-26
Montmorillonite-H_H0.33M	0.0000E+00	5.5516E-26
Pyrophyllite_Al2Si4O10(O	0.0000E+00	1.2052E-26
Na2(U|+VI|2O7)(c)	0.0000E+00	4.7509E-28
Mg2CaCl6:12H2O_Tachyhydr	0.0000E+00	1.6473E-28

Ca4Al2Cl2O6:10H2O_Friede	0.0000E+00	1.6536E-29
C3AH6_Ca3Al2O6:6H2O_Hydr	0.0000E+00	3.3009E-32
C3AS(0.5)_Ca3Al2Si(0.5)O	0.0000E+00	1.9072E-32
C3ASH4_Ca3Al2SiO8:4H2O_S	0.0000E+00	1.8274E-32
Mordenite_Ca.2895Na.361A	0.0000E+00	7.9329E-33
2MgCl2:MnCl2:12H2O	0.0000E+00	3.4235E-33
Hematite_Fe2O3	0.0000E+00	1.6816E-34
(U|+VI|O2)2(SiO4):2H2O(c	0.0000E+00	8.9004E-35
Ferroceladonite_KFeFeSi4	0.0000E+00	1.2707E-35
Ca(U|+VI|O2)2(SiO3OH)2:5	0.0000E+00	5.8225E-36
Cronstedtite-7A_Fe2Fe2Si	0.0000E+00	2.2428E-36
Trevorite_NiFe2O4	0.0000E+00	9.2260E-38
(U|+VI|O2)3(PO4)2:4H2O(c	0.0000E+00	1.4441E-38
Ca4Cl2(OH)6:13H2O	0.0000E+00	6.9964E-39
Sepiolite_Mg4Si6O15(OH)2	0.0000E+00	2.5485E-39
MgCl2:2MnCl2:12H2O	0.0000E+00	1.5806E-39
Stilbite_Ca1.019Na.136K.	0.0000E+00	8.1294E-41
Laumontite_K0.2Na0.2Ca1.	0.0000E+00	1.3218E-43
Ca(SO4):2H2O_Gypsum	0.0000E+00	9.3679E-44
Ca(SO4)_Anhydrite	0.0000E+00	5.9013E-44
K2Si4O9	0.0000E+00	4.4469E-44
Chabazite_K0.6Na0.2Ca1.5	0.0000E+00	1.5699E-44
Bassanite_CaSO4:0.5H2O	0.0000E+00	1.2654E-44
CaSO4:0.5H2O(beta)	0.0000E+00	8.5925E-45
Fe(SO4):7H2O_Melanterite	0.0000E+00	4.1851E-45
Na2(SO4):10H2O_Mirabilit	0.0000E+00	3.3973E-45
Mg(SO4):7H2O_Epsomite	0.0000E+00	9.5072E-46
Mg(SO4):6H2O_Hexahydrite	0.0000E+00	5.5055E-46
Na2(SO4)_Thenardite	0.0000E+00	4.9532E-46
Mg(SO4):H2O_Kieserite	0.0000E+00	1.8857E-47
K2(SO4)_Arcanite	0.0000E+00	8.6379E-49
KMgCl(SO4):3H2O_Kainite	0.0000E+00	1.6871E-50
NiSO4:7H2O(cr)	0.0000E+00	4.0796E-51
alpha-NiSO4:6H2O	0.0000E+00	4.0705E-51
beta-NiSO4:6H2O	0.0000E+00	2.7679E-51
Morenosite_NiSO4:7H2O	0.0000E+00	2.0073E-51
NiSO4:6H2O(alpha)	0.0000E+00	1.9717E-51
Mg2Cl(OH)3:4H2O_Oxychlor	0.0000E+00	6.7613E-52
K2CrO4:MgCrO4	0.0000E+00	1.1593E-52
K(HSO4)_Mercallite	0.0000E+00	7.8732E-54
Nontronite-Na_Na.33Fe2Al	0.0000E+00	3.5495E-54
Nontronite-Mg_Mg.165Fe2A	0.0000E+00	2.7462E-54
Nontronite-Ca_Ca.165Fe2A	0.0000E+00	1.8886E-54
Nontronite-K_K.33Fe2Al.3	0.0000E+00	1.5392E-54
Nontronite-H_H.33Fe2Al.3	0.0000E+00	1.3331E-54
MnSO4:5H2O	0.0000E+00	6.0765E-55
MnSO4:4H2O	0.0000E+00	5.1724E-55
U|+IV|(OH)2(SO4)(c)	0.0000E+00	3.3572E-55
MnSO4:H2O	0.0000E+00	3.2047E-55

KAlCl4	0.0000E+00	2.5539E-55
UO2(OH)2:2H2O	0.0000E+00	1.6002E-56
U|+VI|O3:2H2O(c)_Metasch	0.0000E+00	9.1364E-57
Na(U|+VI|O2)(OH)3(c)_Cla	0.0000E+00	7.9940E-57
NiSO4(cr)	0.0000E+00	3.4361E-58
Na2CrO4:6H2O	0.0000E+00	1.3660E-58
K3AlCl6	0.0000E+00	1.3362E-58
Na2CrO4:4H2O	0.0000E+00	6.0357E-59
MgCrO4:5H2O	0.0000E+00	4.5646E-59
MgCrO4	0.0000E+00	1.6843E-59
K2CrO4	0.0000E+00	2.8835E-62
Na2(U|+VI|O2)2(Si2O5)3:4	0.0000E+00	3.2159E-64
K8(HCO3)4(CO3)2:3H2O	0.0000E+00	8.4024E-67
Phillipsite_K0.7Na0.7Ca1	0.0000E+00	1.4296E-69
Na2CrO4:MgCrO4:2H2O	0.0000E+00	4.5625E-71
K2Ca(SO4)2:H2O_Syngenite	0.0000E+00	<1.0000E-75
K2Mg(SO4)2:4H2O_Leonite	0.0000E+00	<1.0000E-75
K2Mg(SO4)2:6H2O_Picromer	0.0000E+00	<1.0000E-75
K2MgCa2(SO4)4:2H2O_Polyh	0.0000E+00	<1.0000E-75
K3(HSO4)(SO4)	0.0000E+00	<1.0000E-75
K8(HSO4)6(SO4)_Misenite	0.0000E+00	<1.0000E-75
Na2Ca(SO4)2_Glauberite	0.0000E+00	<1.0000E-75
Na2Mg(SO4)2:4H2O_Bloedit	0.0000E+00	<1.0000E-75
Na3(HSO4)(SO4)	0.0000E+00	<1.0000E-75
Na4Ca(SO4)3:2H2O	0.0000E+00	<1.0000E-75
Na6(CO3)(SO4)2_Burkeite	0.0000E+00	<1.0000E-75
NaK3(SO4)2_Glaserite	0.0000E+00	<1.0000E-75
FeK2(SO4)2:6H2O	0.0000E+00	<1.0000E-75
FeNa2(SO4)2:4H2O	0.0000E+00	<1.0000E-75
Fe2(SO4)3	0.0000E+00	<1.0000E-75
KFe3(SO4)2(OH)6_Jarosite	0.0000E+00	<1.0000E-75
NaFe3(SO4)2(OH)6_Jarosit	0.0000E+00	<1.0000E-75
Cu2CO3(OH)2(s)	0.0000E+00	<1.0000E-75
Cu3(CO3)2(OH)2(s)	0.0000E+00	<1.0000E-75
MnSO4:K2SO4:4H2O	0.0000E+00	<1.0000E-75
MnSO4:Na2SO4:2H2O	0.0000E+00	<1.0000E-75
beta-Ni(OH)2	0.0000E+00	<1.0000E-75
K2Ni(SO4)2:6H2O(cr)	0.0000E+00	<1.0000E-75
Na2Ni(SO4)2:4H2O(cr)	0.0000E+00	<1.0000E-75
Ca(U|+VI|6O19):11H2O(c)_	0.0000E+00	<1.0000E-75
K2(U|+VI|6O19):11H2O(c)_	0.0000E+00	<1.0000E-75
Clinoptilolite-Ca_Ca1.73	0.0000E+00	<1.0000E-75
Clinoptilolite-K_K3.467A	0.0000E+00	<1.0000E-75
Clinoptilolite-Na_Na3.46	0.0000E+00	<1.0000E-75
Clinoptilolite-NH4_(NH4)	0.0000E+00	<1.0000E-75
Erionite_K1.5Na0.9Ca0.9A	0.0000E+00	<1.0000E-75
KAl(SO4)2	0.0000E+00	<1.0000E-75
KAl(SO4)2:12H2O	0.0000E+00	<1.0000E-75
KAl(SO4)2:3H2O	0.0000E+00	<1.0000E-75

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KAl3(OH)6(SO4)2_Alunite    0.0000E+00                  <1.0000E-75
Stellerite_Ca2.0Al4.0Si1   0.0000E+00                  <1.0000E-75
C9S6H16_Ca9Si6O21:16H2O_   0.0000E+00                  <1.0000E-75
Ca6Al2(SO4)3(OH)12:26H2O   0.0000E+00                  <1.0000E-75
BSK3+3SF                   0.0000E+00                  <1.0000E-75
HAW-Kokille                0.0000E+00                  <1.0000E-75
*********************************************************************
  Cp_EQUIL       H_EQUIL       S_EQUIL       G_EQUIL       V_EQUIL
    J.K-1           J            J.K-1           J            m3
*********************************************************************
 4.28888E+04  -1.21067E+11  -7.25259E+06  -1.18904E+11   1.51472E+02

Properties for AQUEOUS:
pH =  7.3470
Eh/V = -0.4820
Total solute molality =  1.5890
Ionic strength =  0.7251
Osmotic coefficient =  0.9151
Debye-Hueckel slope =  0.3905

Mole fraction of system components:
              GAS          AQUEOUS
H              9.9960E-01   6.5807E-01
O              3.9705E-04   3.3263E-01
NA             0.0000E+00   2.5661E-03
K              0.0000E+00   2.0798E-05
MG             0.0000E+00   1.2756E-04
CA             0.0000E+00   2.4366E-05
CL             0.0000E+00   3.3613E-03
S              1.1471E-13   2.8053E-14
C              1.9761E-07   5.4937E-08
FE             0.0000E+00   2.1754E-04
SI             0.0000E+00   1.6768E-12
AL             0.0000E+00   2.7943E-11
U              0.0000E+00   1.8738E-11
P              0.0000E+00   1.6574E-04
AS             0.0000E+00   6.3693E-05
N              0.0000E+00   3.4069E-04
NI             0.0000E+00   4.5652E-10
B              0.0000E+00   2.4036E-03
ZR             0.0000E+00   3.7929E-12
MN             0.0000E+00   9.3303E-14
SR             0.0000E+00   8.1506E-06
MO             0.0000E+00   5.1307E-07
CU             0.0000E+00   3.5077E-15
CR             0.0000E+00   4.2617E-14
SN             0.0000E+00   1.1322E-16
Ti             0.0000E+00   1.3297E-12
V              0.0000E+00   6.2661E-09
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System density/g.cm-3 including gaseous phase = 0.146689
System density/g.cm-3 excluding gaseous phase =  5.97786

                Cp/J.K-1          H/J      S/J.K-1          G/J          V/m3
AQUEOUS       2.43061E+04 -2.05131E+10  5.06503E+04 -2.05282E+10  1.50690E+00
FeAl2O4_Hercy 0.00000E+00 -2.38834E+08  7.29037E-08 -2.38834E+08  1.27062E-07
Fe3O4_Magneti 0.00000E+00 -4.85375E+10  5.56182E-05 -4.85375E+10  2.12903E+00
Na2[B4O5(OH)4 0.00000E+00 -5.34949E+08 -5.23076E-07 -5.34949E+08  9.69470E-08
Cu(OH)2(s)    0.00000E+00 -3.82380E+07 -5.95742E-09 -3.82380E+07  8.34765E-08
FeCO3_Siderit 0.00000E+00 -6.95074E+08  1.72967E-07 -6.95074E+08  1.02513E-06
Cassiterite_S 0.00000E+00 -9.75238E+07 -8.78174E-09 -9.75238E+07  1.87685E-07
Eskolaite_Cr2 0.00000E+00 -2.20070E+09 -1.88218E-06 -2.20070E+09  2.09379E-06
Rutile-TiO2   0.00000E+00  7.94539E+07  3.74870E-08  7.94539E+07  1.89526E-07
V2O4          0.00000E+00 -1.96076E+07 -1.62260E-08 -1.96076E+07  1.48751E-08
Mn(OH)2       0.00000E+00 -1.62285E+09 -4.96806E-07 -1.62285E+09  2.37283E-06
CaMoO4_Powell 0.00000E+00 -5.71464E+07 -3.92172E-08 -5.71464E+07  3.93631E-08
Ni(cr)        0.00000E+00  7.55453E+00  4.31089E-15  7.55453E+00  1.93706E-06
Ni3S2(cr)     0.00000E+00 -1.02553E+07 -1.01508E-08 -1.02553E+07  4.85639E-08
U|+IV|(OH)4(a 0.00000E+00 -2.85945E+10 -1.27428E-05 -2.85945E+10  1.94529E-05
U|+IV|(SiO4)( 0.00000E+00 -2.01500E+09  7.44687E-07 -2.01500E+09  1.06896E-06
ZrO2(monoclin 0.00000E+00 -1.59274E+10 -6.87257E-06 -1.59274E+10  1.52744E-05

               Dens/g.cm-3  Thermal exp Bulk mod/bar     Cv/J.K-1   Grueneisen
AQUEOUS       1.04908E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
FeAl2O4_Hercy 1.73806E+05  0.00000E+00  1.41931E+08  0.00000E+00  0.00000E+00
Fe3O4_Magneti 5.20018E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
Na2[B4O5(OH)4 3.81372E+05  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
Cu(OH)2(s)    9.75607E+04  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
FeCO3_Siderit 1.15854E+05  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
Cassiterite_S 1.50709E+05  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
Eskolaite_Cr2 1.51990E+05  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
Rutile-TiO2   7.98788E+04  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
V2O4          1.65881E+05  0.00000E+00  1.41931E+08  0.00000E+00  0.00000E+00
Mn(OH)2       8.89527E+04  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
CaMoO4_Powell 2.00016E+05  0.00000E+00  1.41931E+08  0.00000E+00  0.00000E+00
Ni(cr)        5.86934E+04  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
Ni3S2(cr)     2.40212E+05  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
U|+IV|(OH)4(a 3.06058E+05  0.00000E+00  1.41931E+08  0.00000E+00  0.00000E+00
U|+IV|(SiO4)( 3.30112E+05  0.00000E+00  1.41931E+08  0.00000E+00  0.00000E+00
ZrO2(monoclin 1.23223E+05  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
System Volume : 1.51472129055100254D+02 m3

System composition in [mol]:
500 |   1|IA |-1.66777633992811499E-10<< EA
500 |   2|IA | 7.28930683849802241E+05<< H
500 |   3|IA | 4.06009593591355486E+05<< O
500 |   4|IA | 8.45886935600006609E+02<< NA
500 |   5|IA | 5.28434524999914679E+00<< K
```

```
500 |   6|IA | 3.24120756000014651E+01<< MG
500 |   7|IA | 4.55539549000069499E+01<< CA
500 |   8|IA | 8.54050679099954436E+02<< CL
500 |   9|IA | 9.71278323151877885E+01<< S
500 |  10|IA | 1.02523726004436094E+03<< C
500 |  11|IA | 1.44660489927476883E+05<< FE
500 |  12|IA | 1.06895515479519167E+03<< SI
500 |  13|IA | 2.54123094442883769E+02<< AL
500 |  16|IA | 2.05218938456352153E+04<< U
500 |  23|IA | 4.21126758835344646E+01<< P
500 |  27|IA | 1.61833169606606688E+01<< AS
500 |  29|IA | 8.65642870911732558E+01<< N
500 |  31|IA | 2.08275138260861968E+03<< NI
500 |  32|IA | 9.98510776061101183E+02<< B
500 |  33|IA | 1.52744485003947011E+04<< ZR
500 |  37|IA | 2.37282560746382023E+03<< MN
500 |  38|IA | 2.07092514996680954E+00<< SR
500 |  39|IA | 3.94934333958771902E+01<< MO
500 |  41|IA | 8.34765366820890051E+01<< CU
500 |  44|IA | 4.18758829989180049E+03<< CR
500 |  45|IA | 1.87684609552692024E+02<< SN
500 |  46|IA | 1.89525769319153994E+02<< Ti
500 |  47|IA | 2.97517740938135979E+01<< V

Aq. phase composition in [mol]:
500 |   1|IA |-1.66777633992811499E-10<< EA
500 |   2|IA | 1.67204112196569680E+05<< H
500 |   3|IA | 8.45158310510683950E+04<< O
500 |   4|IA | 6.51992993951642120E+02<< NA
500 |   5|IA | 5.28434524999914679E+00<< K
500 |   6|IA | 3.24120756000014651E+01<< MG
500 |   7|IA | 6.19088489366154260E+00<< CA
500 |   8|IA | 8.54050679099954436E+02<< CL
500 |   9|IA | 7.12771849521058518E-09<< S
500 |  10|IA | 1.39586128549676006E-02<< C
500 |  11|IA | 5.52722374065751012E+01<< FE
500 |  12|IA | 4.26056899013073178E-07<< SI
500 |  13|IA | 7.09985479598024753E-06<< AL
500 |  16|IA | 4.76099495212858821E-06<< U
500 |  23|IA | 4.21126758835344646E+01<< P
500 |  27|IA | 1.61833169606606688E+01<< AS
500 |  29|IA | 8.65642870911732558E+01<< N
500 |  31|IA | 1.15994827469500988E-04<< NI
500 |  32|IA | 6.10722892764372205E+02<< B
500 |  33|IA | 9.63706675097301375E-07<< ZR
500 |  37|IA | 2.37067573824971334E-08<< MN
500 |  38|IA | 2.07092514996680954E+00<< SR
500 |  39|IA | 1.30363389531777840E-01<< MO
500 |  41|IA | 8.91255339980191924E-10<< CU
```

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500 |  44|IA | 1.08282720390760685E-08<< CR
500 |  45|IA | 2.87683811558726258E-11<< SN
500 |  46|IA | 3.37865847864726265E-07<< Ti
500 |  47|IA | 1.59209961990387262E-03<< V
Gas Phase    : ********************************************************
 Total Volume : 1.47836149438553207D+02 m3
 Total Mass   : 4.83884102816370432D+05 g
 Pressure     : 3.99999999999999953D+06 Pa

Solution: ************************************************************
Total Volume :  1.50690141022926150D+00 m3
Total Mass   :  1.58085714617310581D+06 g
Density      :  1.04907801893462474D+06 g / m3

System component molalities:
   1 EA                          -1.12235804380722771E-13  mol/kg H2O
   2 H                            1.12522229536872885E+02  mol/kg H2O
   3 O                            5.68760517674815134E+01  mol/kg H2O
   4 NA                           4.38767350623597785E-01  mol/kg H2O
   5 K                            3.55617036782835154E-03  mol/kg H2O
   6 MG                           2.18121370492505469E-02  mol/kg H2O
   7 CA                           4.16623826943913339E-03  mol/kg H2O
   8 CL                           5.74744755301412003E-01  mol/kg H2O
   9 S                            4.79669289263302070E-12  mol/kg H2O
  10 C                            9.39363403835729646E-06  mol/kg H2O
  11 FE                           3.71961867610500832E-02  mol/kg H2O
  12 SI                           2.86720652720291514E-10  mol/kg H2O
  13 AL                           4.77794164591214729E-09  mol/kg H2O
  16 U                            3.20397482926437945E-09  mol/kg H2O
  23 P                            2.83402849363426981E-02  mol/kg H2O
  27 AS                           1.08907782338189853E-02  mol/kg H2O
  29 N                            5.82545874847723646E-02  mol/kg H2O
  31 NI                           7.80602607803621657E-08  mol/kg H2O
  32 B                            4.10994087527385310E-01  mol/kg H2O
  33 ZR                           6.48539215196047424E-10  mol/kg H2O
  37 MN                           1.59537774563359434E-11  mol/kg H2O
  38 SR                           1.39365660339918962E-03  mol/kg H2O
  39 MO                           8.77297755862276198E-05  mol/kg H2O
  41 CU                           5.99782126311079665E-13  mol/kg H2O
  44 CR                           7.28702958235986056E-12  mol/kg H2O
  45 SN                           1.93600644463800483E-14  mol/kg H2O
  46 Ti                           2.27371312742659162E-10  mol/kg H2O
  47 V                            1.07142459908989624E-06  mol/kg H2O

Solid Phases : *******************************************************
Total Volume :  2.12907820631774758D+00 m3
Total Mass   :  2.01545149215867023D+04 kg
                                mol                                    activity
     mole fraction
```

```
  79 FeAl2O4_Hercynite            1.27061543671514485D+02
  85 Fe3O4_Magnetite              4.78176757180016793D+04
 107 Na2[B4O5(OH)4]:8H2O_Bora     9.69469708241822445D+01
 140 Cu(OH)2(s)                   8.34765366811977430D+01
 144 FeCO3_Siderite               1.02512899239376793D+03
 166 Cassiterite_SnO2             1.87684609552663261D+02
 173 Eskolaite_Cr2O3              2.09379414994048602D+03
 183 Rutile-TiO2                  1.89525768981288138D+02
 187 V2O4                         1.48750909970968479D+01
 192 Mn(OH)2                      2.37282560744011334D+03
 200 CaMoO4_Powellite             3.93630700063454100D+01
 215 Ni(cr)                       1.93705951823382384D+03
 217 Ni3S2(cr)                    4.85639161266561956D+01
 283 U|+IV|(OH)4(am)              1.94529386865050874D+04
 284 U|+IV|(SiO4)(c)_Coffinit     1.06895515436913479D+03
 400 ZrO2(monoclinic)             1.52744484994309951D+04

Other information: ***************************************************
Total volume of solid phases      =  2.12907820631774758D+00 m3
Charge balance after calculation  = -1.66777633992811499D-10
Relative error of charge balance  = -8.91156296945682992D-14
 kw =      13.984  (Should be at current T:    13.9960)
 Eh =      -0.482
 pH =       7.347
pHCl=       3.881
phi =      0.0006
T   =    298.1500 K

CPU-Time:     3.530  s
************************************************************************
End of calculation
***************************************************
* Nathan:                                         *
* Kaum war der Vater tot, so kommt ein jeder mit  *
* seinem Ring, und jeder will der Fuerst des Hauses *
* sein. Man untersucht, man zankt, man klagt.     *
* Umsonst; der rechte Ring war nicht erweislich; -  *
*                                                 *
* Fast so unerweislich, als uns ist -             *
* der rechte Glaube.                              *
*                                                 *
* Aus: "Nathan, der Weise" von G. E. Lessing      *
***************************************************
```

Anlage 3: Output-Datei der geochemischen Modellierung mit NaCl-Lösung

```
**************************************************************************
 This is NATHAN 2.7.1

 This program contains ChemApp
 Copyright GTT-Technologies, Kaiserstrasse 100,
 D-52134 Herzogenrath, Germany
 http://www.gtt-technologies.de

 No warranty is given for the correctness of
 calculations done with NATHAN. Propositions
 and error messages are welcome.

 Helge C. Moog
 Gesellschaft fuer Anlagen- und Reaktorsicherheit (GRS)
 Theodor-Heuss-Str. 4, 38122 Braunschweig,
 Germany
 http://www.grs.de/geochemie
 helge.moog@grs.de
 **************************************************************************

 Used input file:
 NaCl+3BSK3+3SF.ni



 Version of prepare.f:          236
 Active Chemapp-Version:          554
 Number of phases =          406
 Number of system components =           48
 Name of paramaterfile used:
 tdb-hmw-118#1-1-1.dat


 > n*3.0684 m3 ges. NaCl-Loesung

 > reagiert mit 3BSK3+3SF

 >


 **************************************************************************
 Step            1:
 Charge balance before calculation =  (no charged constituents set for aq. phase)

 Active CHEMAPP-stream:

 SYSTEM UNITS:
 Pressure     : Pa
 Volume       :  m3
```

```
Temperature  : K
Energy       : J
Amount       : mol

TARGET LIMITS:
Pressure/bar : 2.00000E+01  6.00000E+01
Volume/dm3   : 1.00000E-07  1.00000E+50
Temperature/K:  298.15      6000.00

T = 298.15 K
P = 4.00000E+06 Pa

STREAM CONSTITUENT
BSK3+3SF
AMOUNT/mol    =  3.00000000000000E+00
H
AMOUNT/mol    =  7.12210450028760E+05
O
AMOUNT/mol    =  3.56105225014380E+05
NA
AMOUNT/mol    =  3.92619034774110E+04
CL
AMOUNT/mol    =  3.92619034774098E+04

ELIMINATED PHASES:
K2HAsO4:3H2O
K3AsO4:7H2O
KH2AsO4
Na2HAsO4:7H2O
Na3AsO4:12H2O
NaH2AsO4:H2O

T = 298.15 K
P = 4.00000E+06 Pa
V = 1.52377E+02 m3

STREAM CONSTITUENTS        AMOUNT/mol
BSK3+3SF                   3.0000E+00
H                          7.1221E+05
O                          3.5611E+05
NA                         3.9262E+04
CL                         3.9262E+04

                         EQUIL AMOUNT  MOLE FRACTION     FUGACITY
PHASE: GAS                    mol                          Pa
H2                         2.3852E+05     9.9939E-01     3.9976E+06
H2O(g)                     1.4517E+02     6.0826E-04     2.4330E+03
CO2(g)                     8.6349E-02     3.6180E-07     1.4472E+00
H2S(g)                     5.4788E-08     2.2956E-13     9.1825E-07
```

O2(g)	NOT CALCD.	NOT CALCD.	<1.0000E-75
TOTAL:	2.3866E+05	1.0000E+00	1.0000E+00
PHASE: AQUEOUS	mol	MOLALITY	ACTIVITY
H2O	7.3724E+04	5.5508E+01	7.4661E-01
H<+>	5.0774E-05	3.8229E-08	1.7570E-07
OH<->	1.1845E-04	8.9182E-08	4.4051E-08
O2(aq)	NOT CALCD.	NOT CALCD.	<1.0000E-75
(CO2)<0>	2.0059E-04	1.5103E-07	4.7041E-07
(CO3)<2->	1.5935E-05	1.1998E-08	2.4799E-10
(HCO3)<->	3.6225E-03	2.7275E-06	9.1008E-07
(HSO4)<->	3.6198E-48	2.7254E-51	1.3676E-51
(SO4)<2->	5.8526E-42	4.4066E-45	7.9965E-47
Cl<->	8.2977E+03	6.2476E+00	6.2600E+00
Na<+>	7.9598E+03	5.9931E+00	6.0385E+00
H2S<0>	1.1775E-09	8.8659E-13	8.8659E-13
HS<->	2.4708E-09	1.8603E-12	5.1806E-13
H2SiO4<2->	4.0800E-15	3.0720E-18	3.9219E-20
H3SiO4<->	1.8273E-10	1.3758E-13	8.6432E-14
SiO2<0>	2.2250E-07	1.6752E-10	1.6752E-10
Al(OH)4<->	2.1028E-06	1.5832E-09	3.2675E-10
Al<3+>	6.8966E-11	5.1926E-14	1.2832E-14
Fe<2+>	1.6280E+02	1.2258E-01	1.4062E-01
Fe<3+>	2.0505E-34	1.5438E-37	1.1326E-37
(AsO4)<3->	1.2178E-17	9.1691E-21	2.0561E-24
(H2AsO4)<->	1.4648E-17	1.1029E-20	3.1400E-20
(HAsO4)<2->	3.2564E-16	2.4518E-19	9.9823E-21
H2AsO3<->	1.7014E-01	1.2810E-04	3.5675E-05
HAsO2<0>	1.6013E+01	1.2057E-02	1.2057E-02
B(OH)3<0>	3.2260E+02	2.4289E-01	2.4289E-01
Cr<3+>	4.6059E-03	3.4679E-06	6.6318E-13
CrO4<2->	5.4004E-54	4.0661E-57	2.4853E-58
Cu<+>	9.5137E-09	7.1631E-12	2.0079E-12
Cu<2+>	2.4092E-18	1.8139E-21	1.1186E-22
Cu(CO3)2<2->	1.4150E-46	1.0654E-49	3.4040E-52
Cu(HCO3)<->	9.4428E-12	7.1097E-15	1.9800E-15
Cu(OH)<+>	2.5998E-20	1.9575E-23	5.4871E-24
Cu(OH)2(aq)	1.7916E-22	1.3490E-25	1.3490E-25
Cu(OH)3<->	1.1197E-25	8.4305E-29	2.3478E-29
Cu(OH)4<2->	3.0908E-30	2.3271E-33	7.4355E-36
Cu2(OH)<3+>	1.5125E-34	1.1388E-37	2.1778E-44
Cu2(OH)2<2+>	3.5395E-36	2.6650E-39	8.8855E-42
Cu3(OH)4<2+>	1.6179E-55	1.2181E-58	4.0614E-61
CuCO3<0>	2.0587E-22	1.5500E-25	1.5500E-25
Mn<2+>	1.4043E-07	1.0574E-10	8.9315E-11
MoO4<2->	3.9493E+01	2.9736E-02	6.7572E-03
(NH4)<+>	8.6564E+01	6.5176E-02	1.8270E-02
NO3<->	NOT CALCD.	NOT CALCD.	<1.0000E-75
Ni<2+>	5.5501E-05	4.1788E-08	8.0687E-08
HNi(P2O7)<->	1.8255E-12	1.3745E-15	3.8277E-16

Ni(HPO4)<0>	4.5863E-08	3.4531E-11	3.4531E-11
Ni(P2O7)<2->	1.4029E-09	1.0563E-12	3.3749E-15
(H2P2O7)<2->	1.1214E-08	8.4433E-12	2.6978E-14
(H2PO4)<->	5.2089E-03	3.9219E-06	1.0922E-06
(H3P2O7)<->	4.0199E-15	3.0267E-18	8.4289E-19
(HP2O7)<3->	2.6596E-04	2.0025E-07	3.4367E-14
(HPO4)<2->	1.5855E-01	1.1938E-04	3.8143E-07
(P2O7)<4->	2.0970E+01	1.5789E-02	7.7886E-17
(PO4)<3->	7.5053E-03	5.6509E-06	9.6981E-13
H3PO4<0>	3.5180E-08	2.6488E-11	2.6488E-11
H4P2O7<0>	1.9670E-21	1.4810E-24	1.4810E-24
Sn(OH)6<2->	1.0786E-11	8.1212E-15	2.5949E-17
Sn<2+>	5.6310E-10	4.2397E-13	1.4136E-15
Sn<4+>	1.3524E-18	1.0183E-21	6.1567E-36
SnO3<2->	1.4673E-13	1.1047E-16	3.5299E-19
Ti(OH)4<0>	1.7739E-07	1.3356E-10	1.3356E-10
(UO2)(H2PO4)(H3PO4)<+>	3.1092E-32	2.3410E-35	6.5621E-36
(UO2)(H2PO4)<+>	3.4642E-22	2.6083E-25	7.3114E-26
(UO2)(H2PO4)2<0>	4.8474E-27	3.6497E-30	3.6497E-30
(UO2)(H3PO4)<2+>	2.2338E-27	1.6819E-30	5.6076E-33
(UO2)(HAsO4)<0>	1.0158E-31	7.6483E-35	7.6483E-35
(UO2)(HPO4)<0>	3.2389E-19	2.4387E-22	2.4387E-22
U|+III|<3+>	9.3115E-18	7.0109E-21	1.3407E-27
U|+IV|(CO3)4<4->	8.9365E-22	6.7285E-25	4.0813E-29
U|+IV|(CO3)5<6->	2.5294E-13	1.9044E-16	7.6288E-40
U|+IV|(OH)<3+>	1.9942E-15	1.5015E-18	1.0588E-19
U|+IV|(OH)2(CO3)2<2->	1.7895E-12	1.3474E-15	2.4288E-17
U|+IV|(OH)2<2+>	5.0319E-10	3.7886E-13	1.2749E-13
U|+IV|(OH)3<+>	1.7174E-07	1.2931E-10	1.4000E-10
U|+IV|(OH)4<0>	4.2000E-06	3.1623E-09	3.1623E-09
U|+IV|(SO4)<2+>	1.0400E-59	7.8302E-63	2.6107E-65
U|+IV|(SO4)2<0>	NOT CALCD.	NOT CALCD.	<1.0000E-75
U|+IV|<4+>	1.2211E-20	9.1943E-24	8.3978E-26
U|+IV|Cl<3+>	1.9706E-13	1.4837E-16	2.8374E-23
(U|+V|O2)(CO3)3<5->	8.2058E-07	6.1783E-10	5.3790E-36
(U|+V|O2)<+>	1.9113E-10	1.4391E-13	4.0339E-14
(U|+VI|O2)(CO3)<0>	1.0487E-19	7.8958E-23	7.8958E-23
(U|+VI|O2)(CO3)2<2->	1.8332E-20	1.3802E-23	9.1003E-26
(U|+VI|O2)(CO3)3<4->	9.9220E-22	7.4705E-25	3.8081E-30
(U|+VI|O2)(H2AsO4)<+>	1.0091E-34	7.5980E-38	2.1298E-38
(U|+VI|O2)(H2AsO4)2<0>	6.6711E-53	5.0228E-56	5.0228E-56
(U|+VI|O2)(OH)<+>	5.0179E-19	3.7781E-22	9.0447E-22
(U|+VI|O2)(OH)2<0>	6.6115E-19	4.9780E-22	4.9780E-22
(U|+VI|O2)(OH)3<->	1.1292E-18	8.5021E-22	1.7287E-23
(U|+VI|O2)(OH)4<2->	2.4723E-24	1.8614E-27	1.6157E-28
(U|+VI|O2)(PO4)<->	2.8899E-18	2.1758E-21	6.0594E-22
(U|+VI|O2)(SO4)<0>	5.6439E-63	4.2494E-66	4.2494E-66
(U|+VI|O2)(SO4)2<2->	NOT CALCD.	NOT CALCD.	<1.0000E-75
(U|+VI|O2)(SO4)3<4->	NOT CALCD.	NOT CALCD.	<1.0000E-75

(U|+VI|O2)<2+>	3.4146E-20	2.5710E-23	3.6791E-23
(U|+VI|O2)11(CO3)6(OH)12	NOT CALCD.	NOT CALCD.	<1.0000E-75
(U|+VI|O2)2(CO3)(OH)3<->	1.8980E-32	1.4291E-35	3.9798E-36
(U|+VI|O2)2(OH)<3+>	8.2000E-32	6.1740E-35	1.1807E-41
(U|+VI|O2)2(OH)2<2+>	1.1301E-35	8.5088E-39	6.2057E-38
(U|+VI|O2)3(CO3)6<6->	NOT CALCD.	NOT CALCD.	<1.0000E-75
(U|+VI|O2)3(OH)4<2+>	4.9354E-49	3.7159E-52	2.2901E-53
(U|+VI|O2)3(OH)5<+>	1.6841E-48	1.2680E-51	2.2413E-50
(U|+VI|O2)3(OH)7<->	6.2645E-49	4.7167E-52	9.5900E-54
(U|+VI|O2)3O(OH)2(HCO3)<	2.2449E-53	1.6903E-56	4.7380E-57
(U|+VI|O2)4(OH)7<+>	1.4373E-63	1.0822E-66	7.0398E-66
(U|+VI|O2)Cl<+>	1.6599E-18	1.2498E-21	3.5034E-22
(U|+VI|O2)Cl2<0>	1.6087E-19	1.2112E-22	1.2112E-22
(U|+VI|O2)SiO(OH)3<+>	1.4175E-24	1.0673E-27	2.9917E-28
V<2+>	8.9749E-02	6.7574E-05	2.2530E-07
V<3+>	2.9662E+01	2.2333E-02	4.2709E-09
VO<2+>	5.0757E-05	3.8216E-08	1.2742E-10
VO2<+>	NOT CALCD.	NOT CALCD.	<1.0000E-75
Zr(OH)<3+>	1.0247E-17	7.7150E-21	1.4754E-27
Zr(OH)2<2+>	1.1744E-14	8.8426E-18	2.9482E-20
Zr(OH)4<0>	5.0597E-07	3.8096E-10	3.8096E-10
Zr<4+>	3.5483E-17	2.6716E-20	1.6153E-34
TOTAL:	9.0660E+04		1.0000E+00
	mol		ACTIVITY
Fe3O4_Magnetite	4.7783E+04		1.0000E+00
NaCl_Halite	3.0964E+04		1.0000E+00
U|+IV|(OH)4(am)	1.9453E+04		1.0000E+00
ZrO2(monoclinic)	1.5274E+04		1.0000E+00
Mn(OH)2	2.3728E+03		1.0000E+00
Eskolaite_Cr2O3	2.0938E+03		1.0000E+00
Ni(cr)	2.0501E+03		1.0000E+00
U|+IV|(SiO4)(c)_Coffinit	1.0690E+03		1.0000E+00
FeCO3_Siderite	1.0212E+03		1.0000E+00
Rutile-TiO2	1.8953E+02		1.0000E+00
Cassiterite_SnO2	1.8768E+02		1.0000E+00
Na2[B4O5(OH)4]:8H2O_Bora	1.6898E+02		1.0000E+00
FeAl2O4_Hercynite	1.2706E+02		1.0000E+00
Cu(OH)2(s)	8.3477E+01		1.0000E+00
Ni3S2(cr)	1.0891E+01		1.0000E+00
SnO2(cr)_Cassiterite	0.0000E+00		1.0000E+00
CuO(s)	0.0000E+00		1.2150E-01
Gibbsite_Al(OH)3	0.0000E+00		1.1579E-01
Anatase_TiO2	0.0000E+00		8.1922E-02
Fe(OH)2(cr)	0.0000E+00		6.2891E-02
V2O4	0.0000E+00		2.6935E-02
Fe(OH)2_precipitated	0.0000E+00		1.3833E-02
FeS	0.0000E+00		5.9032E-03
AlOOH_Boehmite	0.0000E+00		3.3891E-03
FeCl2:4H2O	0.0000E+00		1.9615E-03

Dawsonite_NaAlCO3(OH)2	0.0000E+00	1.7333E-03
MnHPO4	0.0000E+00	3.0154E-04
Fe2(SiO4)_Fayalite	0.0000E+00	6.8521E-05
Ni(OH)2(cr)	0.0000E+00	4.8766E-05
SnS_Herzenbergite	0.0000E+00	1.7479E-05
Na(HCO3)_Nahcolite	0.0000E+00	1.3566E-05
FeSiO3(cr)	0.0000E+00	7.5026E-06
Chamosite-7A_Fe2Al2SiO5(	0.0000E+00	6.2668E-06
Fe3Si2O5(OH)4_Greenalite	0.0000E+00	4.0721E-06
Ni(CO3)(cr)	0.0000E+00	2.0101E-06
Tridymite_SiO2	0.0000E+00	1.1269E-06
Chalcedony-SiO2	0.0000E+00	8.9573E-07
NiO(cr)	0.0000E+00	6.6034E-07
Coesite_SiO2	0.0000E+00	2.5905E-07
Fe(OH)3(cr)	0.0000E+00	1.0454E-07
Al2O3_Corundum	0.0000E+00	9.8501E-08
SiO2(am)-GWB	0.0000E+00	8.6632E-08
Na2(CO3):7H2O	0.0000E+00	3.1998E-09
Na2(CO3):10H2O_Natron	0.0000E+00	3.1417E-09
Na2(CO3):H2O_Thermonatri	0.0000E+00	2.0797E-09
NiCl2:6H2O(cr)	0.0000E+00	5.6122E-10
Rhodochrosite_MnCO3	0.0000E+00	2.7220E-10
Ni(CO3):5.5H2O(cr)	0.0000E+00	1.5963E-10
Daphnite-7A_Fe5AlAlSi3O1	0.0000E+00	1.4961E-10
NiCO3	0.0000E+00	1.3365E-10
NiCl2:4H2O(cr)	0.0000E+00	1.1914E-10
FeS2	0.0000E+00	2.8436E-11
NiCl2:2H2O(cr)	0.0000E+00	1.6023E-11
Ni2SiO4	0.0000E+00	3.0749E-12
MnCl2:4H2O	0.0000E+00	1.6488E-12
Na3(CO3)(HCO3):2H2O_Tron	0.0000E+00	2.8223E-13
Na.96Al.96Si2.04O6:H2O_A	0.0000E+00	1.1744E-13
Kaolinite_Al2Si2O5(OH)4	0.0000E+00	3.9935E-14
NaOH	0.0000E+00	3.2792E-14
U|+VI|O3:2H2O(c)_Schoepi	0.0000E+00	8.3476E-15
NiCl2(cr)	0.0000E+00	7.2216E-15
NiS2(cr)	0.0000E+00	4.9978E-16
Delafossite_CuFeO2	0.0000E+00	3.6794E-16
Minnesotaite_Fe3Si4O10(O	0.0000E+00	2.0525E-17
Ni2(SiO4)(oliv)	0.0000E+00	1.4534E-17
Ni9S8(cr)	0.0000E+00	7.1021E-18
(U|+VI|O2)(CO3)(c)_Ruthe	0.0000E+00	5.2167E-18
Goethite_FeOOH	0.0000E+00	3.5984E-18
Na.96Al.96Si2.04O6_Analc	0.0000E+00	5.7635E-20
alpha-NiS	0.0000E+00	9.3808E-21
beta-NiS	0.0000E+00	2.5249E-21
Na4(U|+VI|O2)(CO3)3(c)	0.0000E+00	1.0994E-21
Beidellite-Na_Na.33Al2.3	0.0000E+00	7.0154E-25
Beidellite-H_H.33Al2.33S	0.0000E+00	2.3683E-26

Na2(U|+VI|2O7)(c)	0.0000E+00	1.9208E-26
Pyrophyllite_Al2Si4O10(O	0.0000E+00	1.0064E-27
Hematite_Fe2O3	0.0000E+00	1.5388E-34
(U|+VI|O2)2(SiO4):2H2O(c	0.0000E+00	5.2262E-35
Cronstedtite-7A_Fe2Fe2Si	0.0000E+00	8.4569E-37
Trevorite_NiFe2O4	0.0000E+00	6.4695E-38
(U|+VI|O2)3(PO4)2:4H2O(c	0.0000E+00	3.7703E-43
Na2(SO4)_Thenardite	0.0000E+00	5.2951E-45
Na2(SO4):10H2O_Mirabilit	0.0000E+00	2.5399E-45
Fe(SO4):7H2O_Melanterite	0.0000E+00	3.1967E-46
alpha-NiSO4:6H2O	0.0000E+00	2.8446E-52
NiSO4:7H2O(cr)	0.0000E+00	2.1851E-52
beta-NiSO4:6H2O	0.0000E+00	1.9343E-52
NiSO4:6H2O(alpha)	0.0000E+00	1.3779E-52
Morenosite_NiSO4:7H2O	0.0000E+00	1.0751E-52
Nontronite-Na_Na.33Fe2Al	0.0000E+00	5.8718E-55
U|+IV|(OH)2(SO4)(c)	0.0000E+00	1.9709E-55
MnSO4:H2O	0.0000E+00	1.4420E-55
Nontronite-H_H.33Fe2Al.3	0.0000E+00	1.2514E-55
MnSO4:4H2O	0.0000E+00	1.0478E-55
MnSO4:5H2O	0.0000E+00	9.4343E-56
Na(U|+VI|O2)(OH)3(c)_Cla	0.0000E+00	3.4106E-56
UO2(OH)2:2H2O	0.0000E+00	9.3981E-57
U|+VI|O3:2H2O(c)_Metasch	0.0000E+00	5.3658E-57
Na2CrO4:6H2O	0.0000E+00	4.4123E-58
Na2CrO4:4H2O	0.0000E+00	3.3190E-58
NiSO4(cr)	0.0000E+00	1.1848E-58
Na2(U|+VI|O2)2(Si2O5)3:4	0.0000E+00	1.8431E-64
Na3(HSO4)(SO4)	0.0000E+00	<1.0000E-75
Na6(CO3)(SO4)2_Burkeite	0.0000E+00	<1.0000E-75
FeNa2(SO4)2:4H2O	0.0000E+00	<1.0000E-75
Fe2(SO4)3	0.0000E+00	<1.0000E-75
NaFe3(SO4)2(OH)6_Jarosit	0.0000E+00	<1.0000E-75
Cu2CO3(OH)2(s)	0.0000E+00	<1.0000E-75
Cu3(CO3)2(OH)2(s)	0.0000E+00	<1.0000E-75
MnSO4:Na2SO4:2H2O	0.0000E+00	<1.0000E-75
beta-Ni(OH)2	0.0000E+00	<1.0000E-75
Na2Ni(SO4)2:4H2O(cr)	0.0000E+00	<1.0000E-75
Clinoptilolite-Na_Na3.46	0.0000E+00	<1.0000E-75
Clinoptilolite-NH4_(NH4)	0.0000E+00	<1.0000E-75
BSK3+3SF	0.0000E+00	<1.0000E-75
HAW-Kokille	0.0000E+00	<1.0000E-75

Cp_EQUIL	H_EQUIL	S_EQUIL	G_EQUIL	V_EQUIL
J.K-1	J	J.K-1	J	m3
4.77220E+05	-1.33764E+11	-7.28220E+06	-1.31593E+11	1.52377E+02

Properties for AQUEOUS:

pH = 6.7552
Eh/V = -0.4470
Total solute molality = 12.7516
Ionic strength = 6.6848
Osmotic coefficient = 1.2720
Debye-Hueckel slope = 0.3905

Mole fraction of system components:

	GAS	AQUEOUS
H	9.9970E-01	6.1794E-01
O	3.0440E-04	3.1163E-01
NA	0.0000E+00	3.3060E-02
CL	0.0000E+00	3.4464E-02
S	1.1475E-13	1.5153E-14
C	1.8085E-07	1.5955E-08
FE	0.0000E+00	6.7618E-04
SI	0.0000E+00	9.2489E-13
AL	0.0000E+00	8.7340E-12
U	0.0000E+00	2.1569E-11
P	0.0000E+00	1.7491E-04
AS	0.0000E+00	6.7216E-05
N	0.0000E+00	3.5954E-04
NI	0.0000E+00	2.3072E-10
B	0.0000E+00	1.3399E-03
ZR	0.0000E+00	2.1015E-12
MN	0.0000E+00	5.8328E-13
MO	0.0000E+00	1.6403E-04
CU	0.0000E+00	3.9554E-14
CR	0.0000E+00	1.9130E-08
SN	0.0000E+00	2.3842E-15
Ti	0.0000E+00	7.3677E-13
V	0.0000E+00	1.2357E-04

System density/g.cm-3 including gaseous phase = 0.159492
System density/g.cm-3 excluding gaseous phase = 5.33978

	Cp/J.K-1	H/J	S/J.K-1	G/J	V/m3
AQUEOUS	4.60394E+05	-2.10526E+10	2.77702E+04	-2.10608E+10	1.49674E+00
NaCl_Halite	0.00000E+00	-1.18934E+10	-8.59042E-06	-1.18934E+10	8.36497E-01
FeAl2O4_Hercy	0.00000E+00	-2.38834E+08	7.29037E-08	-2.38834E+08	1.27062E-07
Fe3O4_Magneti	0.00000E+00	-4.85024E+10	5.55780E-05	-4.85024E+10	2.12750E+00
Na2[B4O5(OH)4	0.00000E+00	-9.32415E+08	-9.11721E-07	-9.32415E+08	1.68978E-07
Cu(OH)2(s)	0.00000E+00	-3.82380E+07	-5.95742E-09	-3.82380E+07	8.34765E-08
FeCO3_Siderit	0.00000E+00	-6.92437E+08	1.72311E-07	-6.92437E+08	1.02124E-06
Cassiterite_S	0.00000E+00	-9.75238E+07	-8.78174E-09	-9.75238E+07	1.87685E-07
Eskolaite_Cr2	0.00000E+00	-2.20069E+09	-1.88218E-06	-2.20069E+09	2.09379E-06
Rutile-TiO2	0.00000E+00	7.94539E+07	3.74870E-08	7.94539E+07	1.89526E-07
Mn(OH)2	0.00000E+00	-1.62285E+09	-4.96806E-07	-1.62285E+09	2.37283E-06
Ni(cr)	0.00000E+00	7.99531E+00	4.56241E-15	7.99531E+00	2.05008E-06

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Ni3S2(cr)     0.00000E+00 -2.29985E+06 -2.27639E-09 -2.29985E+06  1.08909E-08
U|+IV|(OH)4(a 0.00000E+00 -2.85945E+10 -1.27428E-05 -2.85945E+10  1.94529E-05
U|+IV|(SiO4)( 0.00000E+00 -2.01500E+09  7.44687E-07 -2.01500E+09  1.06896E-06
ZrO2(monoclin 0.00000E+00 -1.59274E+10 -6.87257E-06 -1.59274E+10  1.52744E-05

              Dens/g.cm-3  Thermal exp Bulk mod/bar     Cv/J.K-1   Grueneisen
AQUEOUS       1.23546E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
NaCl_Halite   2.16333E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
FeAl2O4_Hercy 1.73806E+05  0.00000E+00  1.41931E+08  0.00000E+00  0.00000E+00
Fe3O4_Magneti 5.20018E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
Na2[B4O5(OH)4 3.81372E+05  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
Cu(OH)2(s)    9.75607E+04  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
FeCO3_Siderit 1.15854E+05  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
Cassiterite_S 1.50709E+05  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
Eskolaite_Cr2 1.51990E+05  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
Rutile-TiO2   7.98788E+04  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
Mn(OH)2       8.89527E+04  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
Ni(cr)        5.86934E+04  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
Ni3S2(cr)     2.40212E+05  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
U|+IV|(OH)4(a 3.06058E+05  0.00000E+00  1.41931E+08  0.00000E+00  0.00000E+00
U|+IV|(SiO4)( 3.30112E+05  0.00000E+00  1.41931E+08  0.00000E+00  0.00000E+00
ZrO2(monoclin 1.23223E+05  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
System Volume : 1.52377208410995337D+02 m3

System composition in [mol]:
500 |   1|IA |-9.62561369952013816E-11<< EA
500 |   2|IA | 7.12210450028764899E+05<< H
500 |   3|IA | 3.97337025260537572E+05<< O
500 |   4|IA | 3.92619034774110987E+04<< NA
500 |   8|IA | 3.92619034774098473E+04<< CL
500 |   9|IA | 2.17817402151881048E+01<< S
500 |  10|IA | 1.02132931469438972E+03<< C
500 |  11|IA | 1.44660489927476912E+05<< FE
500 |  12|IA | 1.06895515479519031E+03<< SI
500 |  13|IA | 2.54123094443164774E+02<< AL
500 |  16|IA | 2.05218938456351898E+04<< U
500 |  23|IA | 4.21126758834627282E+01<< P
500 |  27|IA | 1.61833169606625802E+01<< AS
500 |  29|IA | 8.65642870911205478E+01<< N
500 |  31|IA | 2.08275138260861968E+03<< NI
500 |  32|IA | 9.98510776061260344E+02<< B
500 |  33|IA | 1.52744485003946957E+04<< ZR
500 |  37|IA | 2.37282560746371837E+03<< MN
500 |  39|IA | 3.94934333959687578E+01<< MO
500 |  41|IA | 8.34765366820889909E+01<< CU
500 |  44|IA | 4.18758829989179867E+03<< CR
500 |  45|IA | 1.87684609552659538E+02<< SN
500 |  46|IA | 1.89525769319153994E+02<< Ti
500 |  47|IA | 2.97517740938127453E+01<< V
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Aq. phase composition in [mol]:
500 |   1|IA |-9.62561369952013816E-11<< EA
500 |   2|IA | 1.48778377768739301E+05<< H
500 |   3|IA | 7.50296950019459036E+04<< O
500 |   4|IA | 7.95978555196814705E+03<< NA
500 |   8|IA | 8.29774230112769510E+03<< CL
500 |   9|IA | 3.64830097396324719E-09<< S
500 |  10|IA | 3.84151106640733073E-03<< C
500 |  11|IA | 1.62800565483434553E+02<< FE
500 |  12|IA | 2.22680766817209320E-07<< SI
500 |  13|IA | 2.10285089800944589E-06<< AL
500 |  16|IA | 5.19301023383186877E-06<< U
500 |  23|IA | 4.21126758834627282E+01<< P
500 |  27|IA | 1.61833169606625802E+01<< AS
500 |  29|IA | 8.65642870911205478E+01<< N
500 |  31|IA | 5.55483564376417895E-05<< NI
500 |  32|IA | 3.22597277739663241E+02<< B
500 |  33|IA | 5.05972565919156119E-07<< ZR
500 |  37|IA | 1.40434439986077670E-07<< MN
500 |  39|IA | 3.94934333959687578E+01<< MO
500 |  41|IA | 9.52319272117555123E-09<< CU
500 |  44|IA | 4.60587602073415578E-03<< CR
500 |  45|IA | 5.74031613244723557E-10<< SN
500 |  46|IA | 1.77388878195528909E-07<< Ti
500 |  47|IA | 2.97517740938127453E+01<< V
Gas Phase    : ********************************************************
 Total Volume : 1.47916427764369075D+02 m3
 Total Mass   : 4.83444571231442678D+05 g
 Pressure     : 3.99999999999999953D+06 Pa

Solution: ************************************************************
Total Volume :  1.49674366984964458D+00 m3
Total Mass   :  1.84917421025139256D+06 g
Density      :  1.23546486115231179D+06 g / m3

System component molalities:
   1 EA                         -7.21865029397567103E-14  mol/kg H2O
   2 H                           1.12018691274988186E+02  mol/kg H2O
   3 O                           5.64915975488305833E+01  mol/kg H2O
   4 NA                          5.99310715530855553E+00  mol/kg H2O
   8 CL                          6.24756263006341328E+00  mol/kg H2O
   9 S                           2.74689041922392306E-12  mol/kg H2O
  10 C                           2.89236277899348400E-06  mol/kg H2O
  11 FE                          1.22576321625373755E-01  mol/kg H2O
  12 SI                          1.67661514025567016E-10  mol/kg H2O
  13 AL                          1.58328521304085840E-09  mol/kg H2O
  16 U                           3.90993784779453050E-09  mol/kg H2O
  23 P                           3.17076104021376953E-02  mol/kg H2O
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```
  27 AS                          1.21847946832677866E-02  mol/kg H2O
  29 N                           6.51762594573546267E-02  mol/kg H2O
  31 NI                          4.18236459083682181E-08  mol/kg H2O
  32 B                           2.42890972486889706E-01  mol/kg H2O
  33 ZR                          3.80958480024646102E-10  mol/kg H2O
  37 MN                          1.05736346995454842E-10  mol/kg H2O
  39 MO                          2.97355219845788880E-02  mol/kg H2O
  41 CU                          7.17023267348546679E-12  mol/kg H2O
  44 CR                          3.46787088120743245E-06  mol/kg H2O
  45 SN                          4.32201715266013658E-13  mol/kg H2O
  46 Ti                          1.33560200616575169E-10  mol/kg H2O
  47 V                           2.24008007553249747E-02  mol/kg H2O

Solid Phases : *********************************************************
Total Volume :  2.96403697677661837D+00 m3
Total Mass   :  2.19704013611463743D+04 kg
                                mol                                    activity
     mole fraction
  53 NaCl_Halite                 3.09641611762821522D+04
  79 FeAl2O4_Hercynite           1.27061546170156944D+02
  85 Fe3O4_Magnetite             4.77831295639078235D+04
 107 Na2[B4O5(OH)4]:8H2O_Bora    1.68978374580399276D+02
 140 Cu(OH)2(s)                  8.34765366725657998D+01
 144 FeCO3_Siderite              1.02123912409987997D+03
 166 Cassiterite_SnO2            1.87684609552085504D+02
 173 Eskolaite_Cr2O3             2.09379184700788892D+03
 183 Rutile-TiO2                 1.89525769141765124D+02
 192 Mn(OH)2                     2.37282560732328375D+03
 215 Ni(cr)                      2.05007871682513587D+03
 217 Ni3S2(cr)                   1.08908700783757801D+01
 283 U|+IV|(OH)4(am)             1.94529386858696707D+04
 284 U|+IV|(SiO4)(c)_Coffinit    1.06895515457250963D+03
 400 ZrO2(monoclinic)            1.52744484998887237D+04

Other information: *****************************************************
Total volume of solid phases      =  2.96403697677661837D+00 m3
Charge balance after calculation  = -9.62561369952013816D-11
Relative error of charge balance  = -5.68813690485893110D-15
 kw =      13.984  (Should be at current T:    13.9960)
 Eh =      -0.447
 pH =       6.755
pHCl=       2.979
phi =      0.0010
T   =    298.1500 K

CPU-Time:    11.220  s
************************************************************************
End of calculation
************************************************
```

```
* Nathan:                                              *
* Kaum war der Vater tot, so kommt ein jeder mit      *
* seinem Ring, und jeder will der Fuerst des Hauses   *
* sein. Man untersucht, man zankt, man klagt.         *
* Umsonst; der rechte Ring war nicht erweislich; -    *
*                                                     *
* Fast so unerweislich, als uns ist -                 *
* der rechte Glaube.                                  *
*                                                     *
* Aus: "Nathan, der Weise" von G. E. Lessing          *
*******************************************************
```

Anlage 4: Output-Datei der geochemischen Modellierung mit IP21-Lösung

```
**************************************************************************
 This is NATHAN 2.7.1

 This program contains ChemApp
 Copyright GTT-Technologies, Kaiserstrasse 100,
 D-52134 Herzogenrath, Germany
 http://www.gtt-technologies.de

 No warranty is given for the correctness of
 calculations done with NATHAN. Propositions
 and error messages are welcome.

 Helge C. Moog
 Gesellschaft fuer Anlagen- und Reaktorsicherheit (GRS)
 Theodor-Heuss-Str. 4, 38122 Braunschweig,
 Germany
 http://www.grs.de/geochemie
 helge.moog@grs.de
**************************************************************************

 Used input file:
 IP21+3BSK3+3SF.ni



 Version of prepare.f:          236
 Active Chemapp-Version:          554
 Number of phases =          406
 Number of system components =           48
 Name of paramaterfile used:
 tdb-hmw-118#1-1-1.dat


 > Berechnung von n*3.0684 m3 IP21-Loesung

 > mit BSK3+3SF

 >


**************************************************************************
 Step            1:
 Charge balance before calculation =  (no charged constituents set for aq. phase)

 Active CHEMAPP-stream:

 SYSTEM UNITS:
 Pressure     : Pa
 Volume       :  m3
```

```
Temperature  : K
Energy       : J
Amount       : mol

TARGET LIMITS:
Pressure/bar : 2.00000E+01  6.00000E+01
Volume/dm3   : 1.00000E-07  1.00000E+50
Temperature/K:  298.15      6000.00

T = 298.15 K
P = 4.00000E+06 Pa

STREAM CONSTITUENT
BSK3+3SF
AMOUNT/mol    =  3.00000000000000E+00
H
AMOUNT/mol    =  1.02045272143284E+06
O
AMOUNT/mol    =  5.21747746144681E+05
NA
AMOUNT/mol    =  4.42624462838430E+03
K
AMOUNT/mol    =  5.21997303213620E+03
MG
AMOUNT/mol    =  3.86432443059239E+04
CA
AMOUNT/mol    =  5.82853342308084E+00
CL
AMOUNT/mol    =  8.11836706250860E+04
S
AMOUNT/mol    =  2.88034635706537E+03

ELIMINATED PHASES:
K2HAsO4:3H2O
K3AsO4:7H2O
KH2AsO4
Na2HAsO4:7H2O
Na3AsO4:12H2O
NaH2AsO4:H2O

T = 298.15 K
P = 4.00000E+06 Pa
V = 1.49299E+02 m3

STREAM CONSTITUENTS        AMOUNT/mol
BSK3+3SF                   3.0000E+00
H                          1.0205E+06
O                          5.2175E+05
NA                         4.4262E+03
```

K	5.2200E+03
MG	3.8643E+04
CA	5.8285E+00
CL	8.1184E+04
S	2.8803E+03

	EQUIL AMOUNT	MOLE FRACTION	FUGACITY
PHASE: GAS	mol		Pa
H2	2.2831E+05	9.9975E-01	3.9990E+06
H2O(g)	5.7235E+01	2.5063E-04	1.0025E+03
CO2(g)	7.4869E-05	3.2785E-10	1.3114E-03
H2S(g)	2.7226E-06	1.1922E-11	4.7688E-05
O2(g)	NOT CALCD.	NOT CALCD.	<1.0000E-75
TOTAL:	2.2837E+05	1.0000E+00	1.0000E+00
PHASE: AQUEOUS	mol	MOLALITY	ACTIVITY
H2O	6.2018E+04	5.5508E+01	3.0763E-01
H<+>	7.6401E-07	6.8382E-10	1.6939E-08
OH<->	6.8004E-03	6.0866E-06	1.8827E-07
O2(aq)	NOT CALCD.	NOT CALCD.	<1.0000E-75
(CO2)<0>	4.7750E-08	4.2738E-11	4.2626E-10
(CO3)<2->	4.0121E-05	3.5910E-08	9.9618E-12
(HCO3)<->	4.2912E-04	3.8407E-07	3.5245E-09
(HSO4)<->	3.1040E-49	2.7782E-52	2.1205E-50
(SO4)<2->	9.5258E-41	8.5259E-44	1.2860E-44
Ca(CO3)<0>	4.3796E-07	3.9199E-10	3.9199E-10
Ca<2+>	5.8285E+00	5.2167E-03	2.8756E-02
Cl<->	1.3526E+04	1.2106E+01	2.9324E+02
K<+>	1.4866E+01	1.3306E-02	2.6232E-03
Mg(CO3)<0>	3.5900E-03	3.2131E-06	3.2131E-06
Mg(OH)<+>	3.8141E+01	3.4137E-02	1.1098E-02
Mg<2+>	7.3565E+03	6.5843E+00	3.9592E+02
Na<+>	4.4249E+01	3.9605E-02	1.2891E-01
H2S<0>	5.1444E-08	4.6044E-11	4.6044E-11
HS<->	3.0241E-06	2.7067E-09	2.7907E-10
H2SiO4<2->	1.4718E-15	1.3173E-18	1.2162E-19
H3SiO4<->	3.7718E-13	3.3759E-16	2.5841E-14
SiO2<0>	3.1777E-08	2.8442E-11	2.8442E-11
Al(OH)4<->	3.1616E-10	2.8297E-13	2.1506E-11
Al<3+>	1.0640E-17	9.5230E-21	2.5313E-18
Fe<2+>	3.4557E+00	3.0929E-03	4.2633E-03
Fe<3+>	3.7642E-34	3.3691E-37	3.3100E-40
(AsO4)<3->	6.2548E-12	5.5982E-15	4.1671E-22
(H2AsO4)<->	1.4456E-20	1.2939E-23	5.9152E-20
(HAsO4)<2->	6.7023E-13	5.9988E-16	1.9505E-19
H2AsO3<->	1.7681E+00	1.5825E-03	1.6316E-04
HAsO2<0>	1.4415E+01	1.2902E-02	1.2902E-02
B(OH)3<0>	9.9851E+02	8.9370E-01	8.9370E-01
Cr<3+>	6.0826E-06	5.4441E-09	2.2469E-15
CrO4<2->	6.3852E-55	5.7150E-58	2.9124E-57

Cu<+>	7.8061E-09	6.9867E-12	1.1404E-12
Cu<2+>	5.0088E-19	4.4830E-22	6.1241E-24
Cu(CO3)2<2->	7.5870E-50	6.7906E-53	3.0071E-56
Cu(HCO3)<->	4.8959E-13	4.3820E-16	4.5180E-17
Cu(OH)<+>	8.7880E-21	7.8655E-24	1.2839E-24
Cu(OH)2(aq)	1.5072E-22	1.3490E-25	1.3490E-25
Cu(OH)3<->	1.0873E-24	9.7319E-28	1.0034E-28
Cu(OH)4<2->	3.4266E-28	3.0669E-31	1.3582E-34
Cu2(OH)<3+>	7.5521E-37	6.7594E-40	2.7897E-46
Cu2(OH)2<2+>	1.9683E-37	1.7617E-40	4.8645E-43
Cu3(OH)4<2+>	8.9970E-57	8.0526E-60	2.2235E-62
CuCO3<0>	3.8086E-25	3.4088E-28	3.4088E-28
Mn<2+>	1.6700E-09	1.4947E-12	4.8897E-12
MoO4<2->	3.9493E+01	3.5348E-02	7.7375E-08
(NH4)<+>	8.6564E+01	7.7478E-02	1.2646E-02
NO3<->	NOT CALCD.	NOT CALCD.	<1.0000E-75
Ni<2+>	1.6698E-09	1.4945E-12	5.3871E-11
HNi(P2O7)<->	2.0193E-18	1.8074E-21	1.8635E-22
Ni(HPO4)<0>	1.4380E-12	1.2870E-15	1.2870E-15
Ni(P2O7)<2->	4.2998E-14	3.8484E-17	1.7042E-20
(H2P2O7)<2->	4.7849E-12	4.2826E-15	1.8965E-18
(H2PO4)<->	6.3698E-05	5.7012E-08	5.8782E-09
(H3P2O7)<->	6.1905E-20	5.5407E-23	5.7127E-24
(HP2O7)<3->	4.1454E-06	3.7103E-09	2.5059E-17
(HPO4)<2->	5.3722E-02	4.8083E-05	2.1293E-08
(P2O7)<4->	2.0983E+01	1.8780E-02	5.8908E-19
(PO4)<3->	9.2895E-02	8.3144E-05	5.6156E-13
H3PO4<0>	1.5356E-11	1.3744E-14	1.3744E-14
H4P2O7<0>	1.0812E-27	9.6769E-31	9.6769E-31
Sn(OH)6<2->	2.0302E-10	1.8171E-13	8.0469E-17
Sn<2+>	3.1325E-11	2.8037E-14	7.7416E-17
Sn<4+>	7.4970E-23	6.7100E-26	3.1329E-39
SnO3<2->	3.9479E-11	3.5335E-14	1.5648E-17
Ti(OH)4<0>	2.5335E-08	2.2675E-11	2.2675E-11
(UO2)(H2PO4)(H3PO4)<+>	6.8648E-39	6.1442E-42	1.0029E-42
(UO2)(H2PO4)<+>	1.4741E-25	1.3193E-28	2.1535E-29
(UO2)(H2PO4)2<0>	6.4643E-33	5.7857E-36	5.7857E-36
(UO2)(H3PO4)<2+>	6.4433E-32	5.7669E-35	1.5924E-37
(UO2)(HAsO4)<0>	9.1379E-32	8.1787E-35	8.1787E-35
(UO2)(HPO4)<0>	8.3242E-22	7.4504E-25	7.4504E-25
U|+III|<3+>	1.1286E-19	1.0101E-22	4.1689E-29
U|+IV|(CO3)4<4->	9.9033E-18	8.8638E-21	3.1850E-37
U|+IV|(CO3)5<6->	2.0427E+02	1.8282E-01	2.3915E-49
U|+IV|(OH)<3+>	7.9130E-20	7.0824E-23	1.3563E-21
U|+IV|(OH)2(CO3)2<2->	5.3884E-15	4.8228E-18	2.1456E-21
U|+IV|(OH)2<2+>	3.8759E-12	3.4690E-15	6.9798E-15
U|+IV|(OH)3<+>	2.6287E-08	2.3528E-11	3.2758E-11
U|+IV|(OH)4<0>	3.5331E-06	3.1623E-09	3.1623E-09
U|+IV|(SO4)<2+>	5.0919E-60	4.5574E-63	1.2584E-65

U|+IV|(SO4)2<0>	NOT CALCD.	NOT CALCD.	<1.0000E-75
U|+IV|<4+>	2.0873E-28	1.8682E-31	2.5170E-28
U|+IV|Cl<3+>	1.0784E-14	9.6522E-18	3.9837E-24
(U|+V|O2)(CO3)3<5->	5.8070E-08	5.1974E-11	1.9795E-40
(U|+V|O2)<+>	1.5677E-10	1.4031E-13	2.2903E-14
(U|+VI|O2)(CO3)<0>	1.9394E-22	1.7358E-25	1.7358E-25
(U|+VI|O2)(CO3)2<2->	2.0381E-23	1.8241E-26	8.0363E-30
(U|+VI|O2)(CO3)3<4->	4.3970E-16	3.9354E-19	1.3509E-35
(U|+VI|O2)(H2AsO4)<+>	1.5030E-35	1.3452E-38	2.1958E-39
(U|+VI|O2)(H2AsO4)2<0>	1.0899E-53	9.7549E-57	9.7549E-57
(U|+VI|O2)(OH)<+>	3.2696E-20	2.9264E-23	2.1155E-22
(U|+VI|O2)(OH)2<0>	5.5598E-19	4.9762E-22	4.9762E-22
(U|+VI|O2)(OH)3<->	3.6921E-20	3.3045E-23	7.3854E-23
(U|+VI|O2)(OH)4<2->	1.7573E-21	1.5728E-24	2.9502E-27
(U|+VI|O2)(PO4)<->	2.0808E-19	1.8624E-22	1.9202E-23
(U|+VI|O2)(SO4)<0>	4.1787E-62	3.7400E-65	3.7400E-65
(U|+VI|O2)(SO4)2<2->	NOT CALCD.	NOT CALCD.	<1.0000E-75
(U|+VI|O2)(SO4)3<4->	NOT CALCD.	NOT CALCD.	<1.0000E-75
(U|+VI|O2)<2+>	7.3758E-22	6.6015E-25	2.0135E-24
(U|+VI|O2)11(CO3)6(OH)12	NOT CALCD.	NOT CALCD.	<1.0000E-75
(U|+VI|O2)2(CO3)(OH)3<->	4.0505E-34	3.6253E-37	3.7379E-38
(U|+VI|O2)2(OH)<3+>	4.0914E-34	3.6619E-37	1.5113E-43
(U|+VI|O2)2(OH)2<2+>	3.2523E-39	2.9109E-42	3.3950E-39
(U|+VI|O2)3(CO3)6<6->	NOT CALCD.	NOT CALCD.	<1.0000E-75
(U|+VI|O2)3(OH)4<2+>	3.9710E-50	3.5542E-53	1.2524E-54
(U|+VI|O2)3(OH)5<+>	9.8914E-48	8.8531E-51	5.2387E-51
(U|+VI|O2)3(OH)7<->	2.0468E-50	1.8319E-53	4.0942E-53
(U|+VI|O2)3O(OH)2(HCO3)<	1.6670E-56	1.4920E-59	2.4354E-60
(U|+VI|O2)4(OH)7<+>	3.6641E-65	3.2795E-68	1.6448E-66
(U|+VI|O2)Cl<+>	6.1476E-18	5.5023E-21	8.9813E-22
(U|+VI|O2)Cl2<0>	1.6251E-17	1.4546E-20	1.4546E-20
(U|+VI|O2)SiO(OH)3<+>	3.3506E-26	2.9989E-29	4.8950E-30
V<2+>	3.0421E-02	2.7228E-05	7.5183E-08
V<3+>	3.7190E-01	3.3286E-04	1.3738E-10
VO<2+>	7.0865E-06	6.3426E-09	1.7513E-11
VO2<+>	NOT CALCD.	NOT CALCD.	<1.0000E-75
Zr(OH)<3+>	8.6861E-21	7.7744E-24	3.2086E-30
Zr(OH)2<2+>	1.1088E-16	9.9242E-20	2.7403E-22
Zr(OH)4<0>	7.2263E-08	6.4678E-11	6.4678E-11
Zr<4+>	1.9669E-21	1.7604E-24	8.2194E-38
TOTAL:	8.4374E+04		1.0000E+00
	mol		ACTIVITY
Fe3O4_Magnetite	4.7714E+04		1.0000E+00
MgCl2:6H2O_Bischoffite	2.3830E+04		1.0000E+00
U|+IV|(OH)4(am)	1.9249E+04		1.0000E+00
ZrO2(monoclinic)	1.5274E+04		1.0000E+00
KMgCl3:6H2O_Carnallite	5.2051E+03		1.0000E+00
NaCl_Halite	4.3820E+03		1.0000E+00
Mn(OH)2	2.3728E+03		1.0000E+00

Eskolaite_Cr2O3	2.0938E+03	1.0000E+00
Mg(OH)2_Brucite	1.7050E+03	1.0000E+00
FeS	1.5136E+03	1.0000E+00
U|+IV|(SiO4)(c)_Coffinit	1.0690E+03	1.0000E+00
Ni3S2(cr)	6.9425E+02	1.0000E+00
Rutile-TiO2	1.8953E+02	1.0000E+00
Cassiterite_SnO2	1.8768E+02	1.0000E+00
Mg4Al2O7:10H2O_Hydrotalc	1.2706E+02	1.0000E+00
Cu(OH)2(s)	8.3477E+01	1.0000E+00
V2O4	1.4675E+01	1.0000E+00
SnO2(cr)_Cassiterite	0.0000E+00	1.0000E+00
CuO(s)	0.0000E+00	2.9486E-01
Mg(CO3)_Magnesite	0.0000E+00	2.4728E-01
CaMoO4_Powellite	0.0000E+00	1.9725E-01
Na2[B4O5(OH)4]:8H2O_Bora	0.0000E+00	1.0673E-01
KCl_Sylvite	0.0000E+00	9.5247E-02
Anatase_TiO2	0.0000E+00	8.1922E-02
Ni(cr)	0.0000E+00	7.1857E-02
Fe(OH)2(cr)	0.0000E+00	3.4828E-02
Fe(OH)2_precipitated	0.0000E+00	7.6604E-03
SnS_Herzenbergite	0.0000E+00	5.3487E-03
FeAl2O4_Hercynite	0.0000E+00	4.5563E-03
FeCl2:4H2O	0.0000E+00	3.7614E-03
Gibbsite_Al(OH)3	0.0000E+00	1.7831E-03
Dolomite-ord_CaMg(CO3)2	0.0000E+00	1.5329E-03
FeCO3_Siderite	0.0000E+00	1.2179E-03
CaCl2:6H2O_Antarcticite	0.0000E+00	1.5008E-04
AlOOH_Boehmite	0.0000E+00	1.2666E-04
CaMg(CO3)2_Dolomite	0.0000E+00	1.1456E-04
Ca(CO3)_Calcite	0.0000E+00	6.6533E-05
CaCl2:4H2O	0.0000E+00	4.8945E-05
Dolomite-dis_CaMg(CO3)2	0.0000E+00	4.3762E-05
Ca(CO3)_Aragonite	0.0000E+00	4.3465E-05
Mg4Al4Si2O10(OH)8_Amesit	0.0000E+00	3.9905E-05
Fe2(SiO4)_Fayalite	0.0000E+00	2.1014E-05
Ripidolite-14A_Mg3Fe2Al2	0.0000E+00	1.5768E-05
Mg(CO3):3H2O_Nesquehonit	0.0000E+00	1.5688E-05
Mg2CaCl6:12H2O_Tachyhydr	0.0000E+00	9.3309E-06
MgMoO4:5H2O(s)	0.0000E+00	6.6583E-06
Mg2Al2SiO5(OH)4_Amesit-7	0.0000E+00	2.6728E-06
FeSiO3(cr)	0.0000E+00	1.7120E-06
MnHPO4	0.0000E+00	9.2156E-07
Ni(OH)2(cr)	0.0000E+00	5.9472E-07
FeS2	0.0000E+00	2.5008E-07
Tridymite_SiO2	0.0000E+00	1.9132E-07
Chalcedony-SiO2	0.0000E+00	1.5207E-07
Fe3Si2O5(OH)4_Greenalite	0.0000E+00	4.8380E-08
Coesite_SiO2	0.0000E+00	4.3980E-08
Fe(OH)3(cr)	0.0000E+00	2.3850E-08

NiO(cr)	0.0000E+00	1.9544E-08
SiO2(am)-GWB	0.0000E+00	1.4708E-08
Ripidolite-7A_Mg3Fe2Al2S	0.0000E+00	6.6152E-09
Dawsonite_NaAlCO3(OH)2	0.0000E+00	5.3557E-09
Saponite-Mg_Mg3.165Al.33	0.0000E+00	1.4602E-09
Na(HCO3)_Nahcolite	0.0000E+00	1.1216E-09
Chamosite-7A_Fe2Al2SiO5(	0.0000E+00	1.1062E-09
Al2O3_Corundum	0.0000E+00	3.3392E-10
Saponite-Ca_Ca.165Mg3Al.	0.0000E+00	2.7708E-10
Saponite-Na_Na.33Mg3Al.3	0.0000E+00	2.2311E-10
Ca(OH)2_Portlandite	0.0000E+00	1.4564E-10
Saponite-K_K.33Mg3Al.33S	0.0000E+00	1.3465E-10
Ni(CO3)(cr)	0.0000E+00	5.3909E-11
Ca2Cl2(OH)2:H2O	0.0000E+00	2.3102E-11
Saponite-H_H.33Mg3Al.33S	0.0000E+00	1.2387E-11
2MgCl2:MnCl2:12H2O	0.0000E+00	7.5150E-12
MgCl2:MnCl2:8H2O	0.0000E+00	7.2905E-12
MnCl2:4H2O	0.0000E+00	5.7093E-12
NiCl2:4H2O(cr)	0.0000E+00	5.0310E-12
K(HCO3)_Kalicinite	0.0000E+00	4.7405E-12
CSH(0.8)_Ca0.8SiO2.8_H2O	0.0000E+00	4.6294E-12
MnCl2:KCl:2H2O	0.0000E+00	4.2975E-12
NiCl2:6H2O(cr)	0.0000E+00	4.0236E-12
NiCl2:2H2O(cr)	0.0000E+00	3.9854E-12
Talc_Mg3Si4O10(OH)2	0.0000E+00	8.6072E-13
Rhodochrosite_MnCO3	0.0000E+00	5.9861E-13
NiS2(cr)	0.0000E+00	9.6792E-14
Ni9S8(cr)	0.0000E+00	1.9141E-14
Na2(CO3):H2O_Thermonatri	0.0000E+00	1.5687E-14
CSH(1.1)_Ca(1.1)SiO(3.1)	0.0000E+00	1.1830E-14
NiCl2(cr)	0.0000E+00	1.0580E-14
Ni2SiO4	0.0000E+00	6.3643E-15
CaCl2:MnCl2:8H2O	0.0000E+00	4.5321E-15
NiCO3	0.0000E+00	3.5844E-15
U|+VI|O3:2H2O(c)_Schoepi	0.0000E+00	3.4383E-15
NaOH	0.0000E+00	2.9918E-15
Delafossite_CuFeO2	0.0000E+00	1.2002E-15
Daphnite-7A_Fe5AlAlSi3O1	0.0000E+00	3.1375E-16
Na2(CO3):7H2O	0.0000E+00	1.1812E-16
Ni(CO3):5.5H2O(cr)	0.0000E+00	3.2639E-17
Na.96Al.96Si2.04O6:H2O_A	0.0000E+00	1.3025E-17
Na2(CO3):10H2O_Natron	0.0000E+00	8.1124E-18
Na2Ca(CO3)2:2H2O_Pirsson	0.0000E+00	6.7689E-18
KNa(CO3):6H2O	0.0000E+00	4.4492E-18
Goethite_FeOOH	0.0000E+00	1.9924E-18
Kaolinite_Al2Si2O5(OH)4	0.0000E+00	6.6250E-19
CaNa2(CO3)2:5H2O_Gayluss	0.0000E+00	3.0069E-19
alpha-NiS	0.0000E+00	3.4995E-20
Minnesotaite_Fe3Si4O10(O	0.0000E+00	1.7059E-20

(U|+VI|O2)(CO3)(c)_Ruthe	0.0000E+00	1.1468E-20
K2(CO3):1.5H2O	0.0000E+00	1.0189E-20
beta-NiS	0.0000E+00	9.4189E-21
Ni2(SiO4)(oliv)	0.0000E+00	2.1616E-21
CSH(1.8)_Ca(1.8)SiO(3.8)	0.0000E+00	4.3254E-22
Maximum-Microcline_KAlSi	0.0000E+00	2.4624E-22
Na3(CO3)(HCO3):2H2O_Tron	0.0000E+00	7.2520E-23
MgCl2:2MnCl2:12H2O	0.0000E+00	5.5251E-23
Na.96Al.96Si2.04O6_Analc	0.0000E+00	1.5514E-23
Mesolite_Na.676Ca.657Al1	0.0000E+00	1.0399E-23
KMgAlSi4O10(OH)2_Celadon	0.0000E+00	8.1396E-24
Ca4Al2Cl2O6:10H2O_Friede	0.0000E+00	5.8935E-24
Smectite-high-Fe-Mg_Ca.0	0.0000E+00	2.8519E-24
Ferroaluminoceladonite_K	0.0000E+00	1.6692E-25
Scolecite_CaAl2Si3O10:3H	0.0000E+00	1.0214E-25
Smectite-low-Fe-Mg_Ca.02	0.0000E+00	9.9348E-27
C2AH8_Ca2Al2O5:8H2O_Dica	0.0000E+00	2.5434E-27
Na2(U|+VI|2O7)(c)	0.0000E+00	2.2841E-27
Sepiolite_Mg4Si6O15(OH)2	0.0000E+00	1.2278E-27
Illite_K0.6Mg0.25Al1.8Al	0.0000E+00	8.3585E-28
C2ASH8_Ca2Al2SiO7:8H2O_G	0.0000E+00	5.0047E-28
K2Na(HCO3)(CO3):2H2O_Tro	0.0000E+00	1.9192E-28
Montmorillonite-Mg_Mg0.4	0.0000E+00	7.6125E-29
Montmorillonite-Ca_Ca0.1	0.0000E+00	1.4461E-29
Montmorillonite-Na_Na0.3	0.0000E+00	1.1644E-29
C3AS(0.5)_Ca3Al2Si(0.5)O	0.0000E+00	1.0195E-29
Montmorillonite-K_K0.33M	0.0000E+00	7.0274E-30
Beidellite-Mg_Mg.165Al2.	0.0000E+00	1.9640E-30
Montmorillonite-H_H0.33M	0.0000E+00	6.4649E-31
Beidellite-Ca_Ca.165Al2.	0.0000E+00	3.7309E-31
Beidellite-Na_Na.33Al2.3	0.0000E+00	3.0041E-31
Beidellite-K_K.33Al2.33S	0.0000E+00	1.8130E-31
C3AH6_Ca3Al2O6:6H2O_Hydr	0.0000E+00	5.5419E-32
C3ASH4_Ca3Al2SiO8:4H2O_S	0.0000E+00	3.0680E-32
Beidellite-H_H.33Al2.33S	0.0000E+00	1.6679E-32
Pyrophyllite_Al2Si4O10(O	0.0000E+00	1.1679E-33
Na4(U|+VI|O2)(CO3)3(c)	0.0000E+00	8.0997E-34
Ca4Cl2(OH)6:13H2O	0.0000E+00	7.9725E-34
Hematite_Fe2O3	0.0000E+00	1.1449E-34
(U|+VI|O2)2(SiO4):2H2O(c	0.0000E+00	8.8665E-36
Ca(U|+VI|O2)2(SiO3OH)2:5	0.0000E+00	4.7012E-38
Cronstedtite-7A_Fe2Fe2Si	0.0000E+00	3.2762E-38
Trevorite_NiFe2O4	0.0000E+00	1.4247E-39
Ferroceladonite_KFeFeSi4	0.0000E+00	9.0744E-40
Mordenite_Ca.2895Na.361A	0.0000E+00	2.5975E-40
Mg2Cl(OH)3:4H2O_Oxychlor	0.0000E+00	2.4116E-41
Ca(SO4)_Anhydrite	0.0000E+00	7.8715E-42
Mg(SO4):H2O_Kieserite	0.0000E+00	1.9329E-42
Ca(SO4):2H2O_Gypsum	0.0000E+00	1.2462E-42

Bassanite_CaSO4:0.5H2O	0.0000E+00	9.4850E-43
K3AlCl6	0.0000E+00	8.9019E-43
CaSO4:0.5H2O(beta)	0.0000E+00	6.4408E-43
Mg(SO4):6H2O_Hexahydrite	0.0000E+00	1.7725E-43
KMgCl(SO4):3H2O_Kainite	0.0000E+00	1.6627E-43
Mg(SO4):7H2O_Epsomite	0.0000E+00	9.6661E-44
KAlCl4	0.0000E+00	1.8307E-45
Na2(SO4)_Thenardite	0.0000E+00	3.8808E-46
K2Si4O9	0.0000E+00	1.5652E-47
K2(SO4)_Arcanite	0.0000E+00	5.0173E-48
Fe(SO4):7H2O_Melanterite	0.0000E+00	3.1428E-48
(U|+VI|O2)3(PO4)2:4H2O(c	0.0000E+00	5.9725E-49
Na2(SO4):10H2O_Mirabilit	0.0000E+00	2.6258E-50
Stilbite_Ca1.019Na.136K.	0.0000E+00	4.0477E-52
K(HSO4)_Mercallite	0.0000E+00	1.3624E-53
K2CrO4:MgCrO4	0.0000E+00	4.0939E-54
U|+IV|(OH)2(SO4)(c)	0.0000E+00	1.7353E-54
MgCrO4	0.0000E+00	5.9388E-55
MnSO4:H2O	0.0000E+00	5.2311E-55
alpha-NiSO4:6H2O	0.0000E+00	1.4947E-55
beta-NiSO4:6H2O	0.0000E+00	1.0164E-55
NiSO4:6H2O(alpha)	0.0000E+00	7.2403E-56
NiSO4:7H2O(cr)	0.0000E+00	4.7308E-56
MnSO4:4H2O	0.0000E+00	2.6591E-56
Morenosite_NiSO4:7H2O	0.0000E+00	2.3277E-56
MnSO4:5H2O	0.0000E+00	9.8652E-57
MgCrO4:5H2O	0.0000E+00	5.0550E-57
Laumontite_K0.2Na0.2Ca1.	0.0000E+00	3.5953E-57
Na(U|+VI|O2)(OH)3(c)_Cla	0.0000E+00	3.1106E-57
UO2(OH)2:2H2O	0.0000E+00	1.5950E-57
U|+VI|O3:2H2O(c)_Metasch	0.0000E+00	9.1067E-58
Nontronite-Mg_Mg.165Fe2A	0.0000E+00	3.6078E-58
Nontronite-Ca_Ca.165Fe2A	0.0000E+00	6.8536E-59
Nontronite-Na_Na.33Fe2Al	0.0000E+00	5.5186E-59
Nontronite-K_K.33Fe2Al.3	0.0000E+00	3.3305E-59
Nontronite-H_H.33Fe2Al.3	0.0000E+00	1.9343E-59
Chabazite_K0.6Na0.2Ca1.5	0.0000E+00	1.6459E-59
NiSO4(cr)	0.0000E+00	1.2721E-59
Na2CrO4:4H2O	0.0000E+00	5.1092E-62
K2CrO4	0.0000E+00	1.8194E-62
Na2CrO4:6H2O	0.0000E+00	1.1531E-62
Na2CrO4:MgCrO4:2H2O	0.0000E+00	1.1073E-68
Na2(U|+VI|O2)2(Si2O5)3:4	0.0000E+00	1.5128E-71
K2Ca(SO4)2:H2O_Syngenite	0.0000E+00	<1.0000E-75
K2Mg(SO4)2:4H2O_Leonite	0.0000E+00	<1.0000E-75
K2Mg(SO4)2:6H2O_Picromer	0.0000E+00	<1.0000E-75
K2MgCa2(SO4)4:2H2O_Polyh	0.0000E+00	<1.0000E-75
K3(HSO4)(SO4)	0.0000E+00	<1.0000E-75
K8(HCO3)4(CO3)2:3H2O	0.0000E+00	<1.0000E-75

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K8(HSO4)6(SO4)_Misenite    0.0000E+00                  <1.0000E-75
Na2Ca(SO4)2_Glauberite     0.0000E+00                  <1.0000E-75
Na2Mg(SO4)2:4H2O_Bloedit   0.0000E+00                  <1.0000E-75
Na3(HSO4)(SO4)             0.0000E+00                  <1.0000E-75
Na4Ca(SO4)3:2H2O           0.0000E+00                  <1.0000E-75
Na6(CO3)(SO4)2_Burkeite    0.0000E+00                  <1.0000E-75
NaK3(SO4)2_Glaserite       0.0000E+00                  <1.0000E-75
FeK2(SO4)2:6H2O            0.0000E+00                  <1.0000E-75
FeNa2(SO4)2:4H2O           0.0000E+00                  <1.0000E-75
Fe2(SO4)3                  0.0000E+00                  <1.0000E-75
KFe3(SO4)2(OH)6_Jarosite   0.0000E+00                  <1.0000E-75
NaFe3(SO4)2(OH)6_Jarosit   0.0000E+00                  <1.0000E-75
Cu2CO3(OH)2(s)             0.0000E+00                  <1.0000E-75
Cu3(CO3)2(OH)2(s)          0.0000E+00                  <1.0000E-75
MnSO4:K2SO4:4H2O           0.0000E+00                  <1.0000E-75
MnSO4:Na2SO4:2H2O          0.0000E+00                  <1.0000E-75
beta-Ni(OH)2               0.0000E+00                  <1.0000E-75
K2Ni(SO4)2:6H2O(cr)        0.0000E+00                  <1.0000E-75
Na2Ni(SO4)2:4H2O(cr)       0.0000E+00                  <1.0000E-75
Ca(U|+VI|6O19):11H2O(c)_   0.0000E+00                  <1.0000E-75
K2(U|+VI|6O19):11H2O(c)_   0.0000E+00                  <1.0000E-75
Clinoptilolite-Ca_Ca1.73   0.0000E+00                  <1.0000E-75
Clinoptilolite-K_K3.467A   0.0000E+00                  <1.0000E-75
Clinoptilolite-Na_Na3.46   0.0000E+00                  <1.0000E-75
Clinoptilolite-NH4_(NH4)   0.0000E+00                  <1.0000E-75
Erionite_K1.5Na0.9Ca0.9A   0.0000E+00                  <1.0000E-75
KAl(SO4)2                  0.0000E+00                  <1.0000E-75
KAl(SO4)2:12H2O            0.0000E+00                  <1.0000E-75
KAl(SO4)2:3H2O             0.0000E+00                  <1.0000E-75
KAl3(OH)6(SO4)2_Alunite    0.0000E+00                  <1.0000E-75
Phillipsite_K0.7Na0.7Ca1   0.0000E+00                  <1.0000E-75
Stellerite_Ca2.0Al4.0Si1   0.0000E+00                  <1.0000E-75
C9S6H16_Ca9Si6O21:16H2O_   0.0000E+00                  <1.0000E-75
Ca6Al2(SO4)3(OH)12:26H2O   0.0000E+00                  <1.0000E-75
BSK3+3SF                   0.0000E+00                  <1.0000E-75
HAW-Kokille                0.0000E+00                  <1.0000E-75
*********************************************************************
  Cp_EQUIL       H_EQUIL       S_EQUIL       G_EQUIL       V_EQUIL
    J.K-1           J           J.K-1           J            m3
*********************************************************************
 2.24676E+06  -1.87874E+11  -6.86749E+06  -1.85827E+11   1.49299E+02

Properties for AQUEOUS:
pH =  7.7711
Eh/V = -0.5071
Total solute molality = 20.0088
Ionic strength = 22.8350
Osmotic coefficient =  3.2704
Debye-Hueckel slope =  0.3905
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Mole fraction of system components:

	GAS	AQUEOUS
H	9.9987E-01	5.8113E-01
O	1.2530E-04	3.1217E-01
NA	0.0000E+00	2.0179E-04
K	0.0000E+00	6.7793E-05
MG	0.0000E+00	3.3721E-02
CA	0.0000E+00	2.6579E-05
CL	0.0000E+00	6.1681E-02
S	5.9603E-12	1.4025E-11
C	1.6390E-10	4.6575E-03
FE	0.0000E+00	1.5759E-05
SI	0.0000E+00	1.4491E-13
AL	0.0000E+00	1.4418E-15
U	0.0000E+00	9.3149E-04
P	0.0000E+00	1.9204E-04
AS	0.0000E+00	7.3799E-05
N	0.0000E+00	3.9475E-04
NI	0.0000E+00	7.6212E-15
B	0.0000E+00	4.5534E-03
ZR	0.0000E+00	3.2953E-13
MN	0.0000E+00	7.6153E-15
MO	0.0000E+00	1.8010E-04
CU	0.0000E+00	3.5600E-14
CR	0.0000E+00	2.7738E-11
SN	0.0000E+00	1.2487E-15
Ti	0.0000E+00	1.1553E-13
V	0.0000E+00	1.8347E-06

System density/g.cm-3 including gaseous phase = 0.195482
System density/g.cm-3 excluding gaseous phase = 3.69814

	Cp/J.K-1	H/J	S/J.K-1	G/J	V/m3
AQUEOUS	2.23393E+06	-2.15185E+10	1.32399E+05	-2.15580E+10	1.49629E+00
KMgCl3:6H2O_C	0.00000E+00	-1.31636E+10	1.98773E-06	-1.31636E+10	8.98297E-01
Mg(OH)2_Bruci	0.00000E+00	-1.41840E+09	-1.61167E-09	-1.41840E+09	4.19946E-02
MgCl2:6H2O_Bi	0.00000E+00	-5.03941E+10	6.55493E-06	-5.03941E+10	3.08768E+00
NaCl_Halite	0.00000E+00	-1.68313E+09	-1.21570E-06	-1.68313E+09	1.18380E-01
FeS	0.00000E+00	-1.54337E+08	-3.63949E-08	-1.54337E+08	1.51363E-06
Fe3O4_Magneti	0.00000E+00	-4.84327E+10	5.54982E-05	-4.84327E+10	2.12444E+00
Cu(OH)2(s)	0.00000E+00	-3.82380E+07	-5.95742E-09	-3.82380E+07	8.34765E-08
Cassiterite_S	0.00000E+00	-9.75238E+07	-8.78174E-09	-9.75238E+07	1.87685E-07
Eskolaite_Cr2	0.00000E+00	-2.20070E+09	-1.88218E-06	-2.20070E+09	2.09379E-06
Rutile-TiO2	0.00000E+00	7.94539E+07	3.74870E-08	7.94539E+07	1.89526E-07
V2O4	0.00000E+00	-1.93435E+07	-1.60075E-08	-1.93435E+07	1.46747E-08
Mn(OH)2	0.00000E+00	-1.62285E+09	-4.96806E-07	-1.62285E+09	2.37283E-06
Ni3S2(cr)	0.00000E+00	-1.46606E+08	-1.45111E-07	-1.46606E+08	6.94250E-07
U|+IV|(OH)4(a	0.00000E+00	-2.82943E+10	-1.26090E-05	-2.82943E+10	1.92487E-05

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U|+IV|(SiO4)( 0.00000E+00 -2.01500E+09  7.44687E-07 -2.01500E+09  1.06896E-06
Mg4Al2O7:10H2 0.00000E+00 -8.13865E+08 -5.47679E-07 -8.13865E+08  1.27062E-07
ZrO2(monoclin 0.00000E+00 -1.59274E+10 -6.87257E-06 -1.59274E+10  1.52744E-05

              Dens/g.cm-3  Thermal exp Bulk mod/bar     Cv/J.K-1   Grueneisen
AQUEOUS       1.31271E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
KMgCl3:6H2O_C 1.61000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
Mg(OH)2_Bruci 2.36783E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
MgCl2:6H2O_Bi 1.56905E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
NaCl_Halite   2.16333E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
FeS           8.79110E+04  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
Fe3O4_Magneti 5.20018E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
Cu(OH)2(s)    9.75607E+04  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
Cassiterite_S 1.50709E+05  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
Eskolaite_Cr2 1.51990E+05  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
Rutile-TiO2   7.98788E+04  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
V2O4          1.65881E+05  0.00000E+00  1.41931E+08  0.00000E+00  0.00000E+00
Mn(OH)2       8.89527E+04  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
Ni3S2(cr)     2.40212E+05  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
U|+IV|(OH)4(a 3.06058E+05  0.00000E+00  1.41931E+08  0.00000E+00  0.00000E+00
U|+IV|(SiO4)( 3.30112E+05  0.00000E+00  1.41931E+08  0.00000E+00  0.00000E+00
Mg4Al2O7:10H2 4.43332E+05  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
ZrO2(monoclin 1.23223E+05  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
System Volume : 1.49298686869624248D+02 m3

System composition in [mol]:
500 |   1|IA | 1.94165253718742746E-09<< EA
500 |   2|IA | 1.02045272143285570E+06<< H
500 |   3|IA | 5.62979546390846954E+05<< O
500 |   4|IA | 4.42624462838427826E+03<< NA
500 |   5|IA | 5.21997303213619853E+03<< K
500 |   6|IA | 3.86432443059244906E+04<< MG
500 |   7|IA | 5.82853342308118982E+00<< CA
500 |   8|IA | 8.11836706250888528E+04<< CL
500 |   9|IA | 2.90212809728055436E+03<< S
500 |  10|IA | 1.02132931469436824E+03<< C
500 |  11|IA | 1.44660489927478979E+05<< FE
500 |  12|IA | 1.06895515479518963E+03<< SI
500 |  13|IA | 2.54123094442875271E+02<< AL
500 |  16|IA | 2.05218938456352407E+04<< U
500 |  23|IA | 4.21126758835316437E+01<< P
500 |  27|IA | 1.61833169606622072E+01<< AS
500 |  29|IA | 8.65642870911768370E+01<< N
500 |  31|IA | 2.08275138260861968E+03<< NI
500 |  32|IA | 9.98510776061514093E+02<< B
500 |  33|IA | 1.52744485003946138E+04<< ZR
500 |  37|IA | 2.37282560746382160E+03<< MN
500 |  39|IA | 3.94934333958794284E+01<< MO
500 |  41|IA | 8.34765366820889909E+01<< CU
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500 |  44|IA | 4.18758829989179867E+03<< CR
500 |  45|IA | 1.87684609552691967E+02<< SN
500 |  46|IA | 1.89525769319154023E+02<< Ti
500 |  47|IA | 2.97517740938139355E+01<< V

Aq. phase composition in [mol]:
500 |   1|IA | 1.94165253718742746E-09<< EA
500 |   2|IA | 1.27434903943133788E+05<< H
500 |   3|IA | 6.84557245287656406E+04<< O
500 |   4|IA | 4.42494242725455891E+01<< NA
500 |   5|IA | 1.48663170557705033E+01<< K
500 |   6|IA | 7.39462934255757500E+03<< MG
500 |   7|IA | 5.82853342308118982E+00<< CA
500 |   8|IA | 1.35258647871565263E+04<< CL
500 |   9|IA | 3.07555423013874318E-06<< S
500 |  10|IA | 1.02132923982514910E+03<< C
500 |  11|IA | 3.45565861587647838E+00<< FE
500 |  12|IA | 3.17776108520413768E-08<< SI
500 |  13|IA | 3.16161025989136205E-10<< AL
500 |  16|IA | 2.04265039607543997E+02<< U
500 |  23|IA | 4.21126758835316437E+01<< P
500 |  27|IA | 1.61833169606622072E+01<< AS
500 |  29|IA | 8.65642870911768370E+01<< N
500 |  31|IA | 1.67124217305270618E-09<< NI
500 |  32|IA | 9.98510776061514093E+02<< B
500 |  33|IA | 7.22631447005471318E-08<< ZR
500 |  37|IA | 1.66995770552764042E-09<< MN
500 |  39|IA | 3.94934333958794284E+01<< MO
500 |  41|IA | 7.80662549768159283E-09<< CU
500 |  44|IA | 6.08256423901209180E-06<< CR
500 |  45|IA | 2.73826872733568198E-10<< SN
500 |  46|IA | 2.53347302121996252E-08<< Ti
500 |  47|IA | 4.02325709988830604E-01<< V
Gas Phase    : ************************************************************
 Total Volume : 1.41531560489057028D+02 m3
 Total Mass   : 4.61277240217084240D+05 g
 Pressure     : 3.99999999999999953D+06 Pa

Solution: ****************************************************************
Total Volume :  1.49628813455203247D+00 m3
Total Mass   :  1.96419917478533578D+06 g
Density      :  1.31271452966068545D+06 g / m3

System component molalities:
   1 EA                          1.73610344726753064E-12  mol/kg H2O
   2 H                           1.14058132952689959E+02  mol/kg H2O
   3 O                           6.12699651985366813E+01  mol/kg H2O
   4 NA                          3.96045868172047594E-02  mol/kg H2O
   5 K                           1.33058080227420692E-02  mol/kg H2O
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   6 MG                          6.61841921319812609E+00  mol/kg H2O
   7 CA                          5.21671551136136408E-03  mol/kg H2O
   8 CL                          1.21060622832346816E+01  mol/kg H2O
   9 S                           2.75271501315612322E-09  mol/kg H2O
  10 C                           9.14120877561372169E-01  mol/kg H2O
  11 FE                          3.09292005292859627E-03  mol/kg H2O
  12 SI                          2.84419327149048852E-11  mol/kg H2O
  13 AL                          2.82973778932806456E-13  mol/kg H2O
  16 U                           1.82823452007624315E-01  mol/kg H2O
  23 P                           3.76921317181735521E-02  mol/kg H2O
  27 AS                          1.44845631801034241E-02  mol/kg H2O
  29 N                           7.74776820203523925E-02  mol/kg H2O
  31 NI                          1.49581281165519017E-12  mol/kg H2O
  32 B                           8.93697655247882583E-01  mol/kg H2O
  33 ZR                          6.46777225924889030E-11  mol/kg H2O
  37 MN                          1.49466317397183836E-12  mol/kg H2O
  39 MO                          3.53478296576856116E-02  mol/kg H2O
  41 CU                          6.98716836106189790E-12  mol/kg H2O
  44 CR                          5.44408085383030444E-09  mol/kg H2O
  45 SN                          2.45083418199158353E-13  mol/kg H2O
  46 Ti                          2.26753576724400237E-11  mol/kg H2O
  47 V                           3.60093803975938907E-04  mol/kg H2O

Solid Phases : *******************************************************
Total Volume :  6.27083824601520767D+00 m3
Total Mass   :  2.67597014210345114D+04 kg
                                mol                                    activity
     mole fraction
  29 KMgCl3:6H2O_Carnallite       5.20510671508042833D+03
  33 Mg(OH)2_Brucite              1.70501681511172137D+03
  39 MgCl2:6H2O_Bischoffite       2.38302452442896501D+04
  53 NaCl_Halite                  4.38199520411173307D+03
  83 FeS                          1.51362716974443674D+03
  85 Fe3O4_Magnetite              4.77144690330395533D+04
 140 Cu(OH)2(s)                   8.34765366742823716D+01
 166 Cassiterite_SnO2             1.87684609552418152D+02
 173 Eskolaite_Cr2O3              2.09379414690461726D+03
 183 Rutile-TiO2                  1.89525769293819280D+02
 187 V2O4                         1.46747241919125528D+01
 192 Mn(OH)2                      2.37282560746215177D+03
 217 Ni3S2(cr)                    6.94250460868982827D+02
 283 U|+IV|(OH)4(am)              1.92486736512642856D+04
 284 U|+IV|(SiO4)(c)_Coffinit     1.06895515476341211D+03
 373 Mg4Al2O7:10H2O_Hydrotalc     1.27061547221279554D+02
 400 ZrO2(monoclinic)             1.52744485003223508D+04

Other information: ***************************************************
Total volume of solid phases      =  6.27083824601520767D+00 m3
Charge balance after calculation  =  1.94165253718742746D-09
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Relative error of charge balance  =  6.50838978115876322D-14
 kw =      13.984  (Should be at current T:    13.9960)
 Eh =      -0.507
 pH =       7.771
pHCl=       2.652
phi =      0.0029
T   =    298.1500 K

CPU-Time:     9.510  s
*******************************************************************************
End of calculation
*************************************************
* Nathan:                                       *
* Kaum war der Vater tot, so kommt ein jeder mit    *
* seinem Ring, und jeder will der Fuerst des Hauses *
* sein. Man untersucht, man zankt, man klagt.       *
* Umsonst; der rechte Ring war nicht erweislich; -  *
*                                               *
* Fast so unerweislich, als uns ist -               *
* der rechte Glaube.                            *
*                                               *
* Aus: "Nathan, der Weise" von G. E. Lessing        *
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