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Titel	**Nagra/PSI Chemical Thermodynamic Data Base 01/01 for the GEM-Selektor (V.2-PSI) Geochemical Modeling Code: Release 28-02-03**	Ersetzt TM-44-02-09
Autoren	**Tres Thoenen and Dmitrii Kulik**	Erstellt 28.2.2003/TT44

Abstract:

This report documents how the Nagra/PSI Chemical Thermodynamic Data Base 01/01 (Nagra/PSI TDB 01/01) was adjusted in order to use it with the GEM-Selektor (V.2-PSI) geochemical modeling code. The resulting version of the Nagra/PSI TDB 01/01 is called Nagra/PSI TDB 01/01 GEMS.

The original Nagra/PSI TDB 01/01 was designed to be used with geochemical modeling codes that apply the law of mass action algorithm. The essential thermodynamic data at standard conditions (1 bar, 25°C) are equilibrium constants ($\log_{10}K^\circ$) for the formation reactions of product species from master species. GEM-Selektor is a geochemical modeling code based on a Gibbs energy minimization algorithm. The essential thermodynamic data are molar Gibbs energies of formation from the elements ($\Delta_f G^\circ$) for all chemical species.

The main task in porting the Nagra/PSI TDB 01/01 to GEMS was to derive $\Delta_f G^\circ$ of each aqueous species, solid, and gas from the equilibrium constant of its formation reaction and $\Delta_f G^\circ$ of all master species taking part in that reaction.

Thus, any $\log_{10}K^\circ$ contained in the Nagra/PSI TDB 01/01 is perfectly reproducible at 1 bar and 25°C by using the appropriate values of $\Delta_f G^\circ$ derived in this report.

Additional data given in order to extend calculation of chemical equilibria to elevated temperatures should not be considered as part of the official Nagra/PSI TDB 01/01 GEMS. The official data are restricted to the minimal set required for the calculation of chemical equilibria at standard conditions (25°C and 1 bar). These are the $\Delta_f G^\circ$ values for DComp records and the $\log_{10}K^\circ$ and $\Delta_f G^\circ$ values for ReacDC records.

Web-Version

http://les.web.psi.ch/Software/GEMS-PSI

1 Introduction

This report documents how the Nagra/PSI Chemical Thermodynamic Data Base 01/01 (Nagra/PSI TDB 01/01, [2002HUM/BER]) was adjusted in order to use it as a built-in default database for the GEM-Selektor (V.2-PSI) geochemical modeling code (both database and modeling code are available for download at http://les.web.psi.ch/Software/GEMS-PSI), referred to as GEMS below. The resulting version of the database is called Nagra/PSI TDB 01/01 GEMS.

The original Nagra/PSI TDB 01/01 was designed to be used with geochemical modeling codes that apply the **law of mass action (LMA) algorithm**. The essential thermodynamic data at 1 bar and 25˚C are equilibrium constants ($\log_{10}K^\circ$) for the formation reactions of product species, which comprise aqueous product species, solids, and gases. Each formation reaction involves a single product species which is related to at least one of the aqueous master species. Two types of such master species can be distinguished: The *primary master species* are the basic building blocks for setting up reactions, while the *secondary master species* themselves are related to *primary master species* by means of formation reactions. In addition, the Nagra/PSI TDB 01/01 also contains data for chemical elements.

With this database structure, the minimal dataset required to calculate geochemical equilibria at 1 bar and 25˚C consists of a $\log_{10}K^\circ$ for the formation reaction of each secondary master species and of each product species, whereas no thermodynamic data are required for the primary master species.

GEMS is a geochemical modeling code based on a **Gibbs energy minimization (GEM) algorithm**. The essential thermodynamic data are Gibbs energies of formation from the elements ($\Delta_f G^\circ$) for each chemical entity (aqueous species, solid, and gas) available in the GEMS database. There are two kinds of record formats for chemical entities: DComp format contains "directly provided" standard-state molar thermodynamic properties such as $\Delta_f G^\circ$, S° C_p°, and V° (at $P_\circ$, $T_\circ$), plus necessary parameters for temperature/pressure corrections. ReacDC format defines $\Delta_f G^\circ$, S°, etc. of a chemical entity through $\log_{10}K^\circ$ (or $\Delta_r G^\circ$), $\Delta_r S^\circ$, $\Delta_r C_p^\circ$, and $\Delta_r V^\circ$ of a reaction and standard molar properties of other entities involved in the reaction.

The main task in porting the Nagra/PSI TDB 01/01 to GEMS was to derive $\Delta_f G^\circ$ of each aqueous species, solid, and gas from its formation constant and from $\Delta_f G^\circ$ of the master species taking part in the corresponding formation reaction. Thus, any $\log_{10}K^\circ$ contained in the Nagra/PSI TDB 01/01 is perfectly reproducible at 1 bar and 25˚C by using the appropriate values of $\Delta_f G^\circ$ derived in this report and listed in Table A1 in the Appendix.

In addition to these $\Delta_f G^\circ$ and $\log_{10}K^\circ$ data, the Nagra/PSI TDB 01/01 GEMS also includes some data for the extrapolation of $\Delta_f G^\circ$ and $\log_{10}K^\circ$ to temperatures above 25˚C. The revised HKF (Helgeson-Kirkham-Flowers) equation of state [1988TAN/HEL] is used for calculating the change in the partial molal Gibbs energy of aqueous species as a function of pressure and temperature. [1988TAN/HEL], [1995HAA/SHO], [1995POK/HEL], [1997SHO/SAS], [1997SHO/SAS2], [1997SVE/SHO], [1998SAS/SHO] and [1999MUR/SHO] published HKF parameters for numerous aqueous species. We decided to adopt these parameters, if available, for aqueous species in the Nagra/PSI TDB 01/01 GEMS. Thus, the corresponding DComp records contain $\Delta_f G^\circ$, as derived from the Nagra/PSI TDB 01/01, and the HKF parameters taken from the sources listed above. Note that these parameters were adopted without a critical evaluation.

If HKF parameters were not available, reaction properties allowing temperature extrapolations like $\Delta_r H^\circ$, $\Delta_r S^\circ$, or $\Delta_r C_p^\circ$ were taken form the Nagra/PSI TDB 01/01, together with $\log_{10} K^\circ$, and stored in ReacDC records.

Note: The Nagra/PSI TDB 01/01 GEMS contains numerous thermodynamic data that were taken from the literature without being critically reviewed. The only data that have gone through a thorough review and evaluation process (as described in [2002HUM/BER]) are (1) the $\log_{10} K^\circ$ values directly taken from the Nagra/PSI TDB 01/01 for ReacDC records and (2) the $\Delta_f G^\circ$ values for DComp records of secondary master species and product species, which were all derived from reviewed $\log_{10} K^\circ$ values taken from the Nagra/PSI TDB 01/01. Note, however, that the derived values for $\Delta_f G^\circ$ depend upon the choice of $\Delta_f G^\circ$ for the primary master species (which have not been reviewed by us).

2 Basic Procedure

The Nagra/PSI TDB 01/01 was ported to GEMS in five steps.

1. **Atomic weights, S° and C_p° for the elements**: The Nagra/PSI TDB 01/01 contains atomic weights, standard molar third-law entropies S° and standard molar heat capacities C_p° for the elements. All values for S° and C_p° were adopted for GEMS. Some of the atomic weights were slightly adjusted to conform to the IUPAC recommendations [1999IUPAC]. In addition, values for C_p° that are missing in the Nagra/PSI TDB 01/01 were added.

2. **$\Delta_f G^\circ$ and S° for the *primary master species***[1]: For most of the *primary master species* data for $\Delta_f G^\circ$ and S° were selected not from the Nagra/PSI TDB 01/01 but from other sources. This is perfectly permissible, since the primary purpose of the Nagra/PSI TDB 01/01 GEMS is to reproduce the $\log_{10} K^\circ$ from the Nagra/PSI TDB 01/01.

3. **$\Delta_f G^\circ$ and S° for the *secondary master species***: Values of $\Delta_f G^\circ$ for the *secondary master species* were calculated from the $\log_{10} K^\circ$ values of the Nagra/PSI TDB 01/01 and the values derived in step 2 for $\Delta_f G^\circ$ of the corresponding *primary master species*. Thus the values of $\log_{10} K^\circ$ listed in the Nagra/PSI TDB 01/01 for the *secondary master species* can be faithfully reproduced with the appropriate $\Delta_f G^\circ$ values given in this report. Values for S° were selected from other sources, as they are relevant for temperature corrections only.

4. **$\Delta_f G^\circ$ for *product species***: Values of $\Delta_f G^\circ$ for the *product species* were calculated from the $\log_{10} K^\circ$ values of the Nagra/PSI TDB 01/01 and from the values derived in step 2 and step 3 for $\Delta_f G^\circ$ of the corresponding *primary* and *secondary master species*. These calculations, as well as those in step 3, were carried out with the database management program PMATCHC [2001PEA/THO].

5. **Additional thermodynamic data**: For the charged aqueous species, extended Debye-Hückel or WATEQ a parameters and WATEQ b parameters were adopted from the Nagra/PSI TDB 01/01. These data, together with the $\Delta_f G^\circ$ values derived in steps 2 to 4

[1] The GEMS database structure does not distinguish between master species and product species, only between independent components (IC) and dependent components (DC). IC are the chemical elements and DC comprise aqueous species, solids, and gases. In the following, *primary master species*, *secondary master species*, and (*aqueous*) *product species* are written in italics, as a reminder that they refer to the Nagra/PSI TDB 01/01 database structure.

are sufficient to calculate thermodynamic equilibria at standard pressure and temperature. Additional data are needed for calculations at elevated pressures and temperatures. These were added, if available, in the last step. However, the quality of these data was not reviewed.

The data records of Nagra/PSI TDB 01/01 GEMS are distributed among several GEMS database files. Their organization is shown in Table 1.

2.1 Thermodynamic Data for the Elements

The selected values for the atomic weights, S°, and C_p° of the elements are listed in Table 2. S° and C_p° were adopted from the Nagra/PSI TDB 01/01. The atomic weights were also taken from the Nagra/PSI TDB 01/01, but some of them were slightly adjusted to conform to the IUPAC recommendations [1999IUPAC]. In addition, values for C_p° that are missing in the Nagra/PSI TDB 01/01 were selected. This concerns Am(cr), Ba(cr), Eu(cr), Ni(cr), Ra(cr), Sn(cr), Sr(cr), Th(cr), and Zr(cr).

2.2 Thermodynamic Data for *Primary Master Species*

The values for $\Delta_f G^\circ$ and S° were selected independently from the Nagra/PSI TDB 01/01. They are listed in Table 3. Most of the values were taken from [1997SHO/SAS], the sources are indicated in Table A2 (see Appendix).

$\Delta_f G^\circ$ values were found for all *primary master species*, except for $Sn(OH)_4(aq)$.

For further calculations with the database management program PMATCHC, the database backup file AUG20_GEMS.BAC was prepared, which is identical with AUG20.BAC, the backup file representing the Nagra/PSI TDB 01/01, except for the values of $\Delta_f G^\circ$ and S° of the *primary master species*, which are replaced by those given in Table 3.

In Nagra/PSI TDB 01/01 GEMS the *primary master species* $Si(OH)_4(aq)$ and $Sn(OH)_4(aq)$ are formulated in non-conventional form as $SiO_2(aq)$ and $SnO_2(aq)$, resp., see the discussion in Chapter 3.

All *primary master species* are kept in GEMS DComp records. Note that GEMS calculations do not require the electron as a separate species, which is therefore not included in Nagra/PSI TDB 01/01 GEMS.

Table 1: Organization of Nagra/PSI TDB 01/01 GEMS database files. * stands for pdb or ndx.

	GEMS Record Type	Filename
Elements	IComp	.../icomp.kernel.nagra_psi.*
Primary Master Species	DComp	.../dcomp.kernel.nagra_psi.ions.*
Secondary Master Species	DComp	.../dcomp.kernel.nagra_psi.secms.*
Aqueous Product Species	DComp	.../dcomp.kernel.nagra_psi.prods.*
	ReacDC	.../reacdc.kernel.nagra_psi.prods.*
Solids	DComp	.../dcomp.kernel.nagra_psi.solids.*
	ReacDC	.../reacdc.kernel.nagra_psi.solids.*
Gases	DComp	.../dcomp.kernel.nagra_psi.gases.*

Table 2: Thermodynamic data for the elements at 25°C and 1 bar. The thermodynamic properties refer to one mole of atoms.

NBS/NIST: [1982WAG/EVA] IUPAC: [1999IUPAC]
CODATA: [1989COX/WAG] NEA: [1999RAR/RAN]
slop98.dat: Datafile slop98.dat (version 30. Oct. 1998) for SUPCRT92 [1992JOH/OEL]

Stable Phase at 25°C	Atomic Number	Default Valence	Atomic Weight	Reference	S° [J/mol/K]	Reference	C_p° [J/mol/K]	Reference
Al(cr)	13	3	26.9815	IUPAC	28.3	NEA(CODATA)	24.2	NEA(CODATA)
Am(cr)	95	3	243.061*	IUPAC	55.4	NEA	25.5	NEA
As(cr)	33	2	74.9216	IUPAC	35.69	[1995ROB/HEM]	24.54	[1995ROB/HEM]
B(cr)	5	3	10.812	IUPAC	5.90	NEA(CODATA)	11.087	NEA(CODATA)
Ba(cr)	56	2	137.328	IUPAC	62.42	NEA	28.07	NBS/NIST
Br_2(l)	35	-1	79.904	IUPAC	76.105	NEA(CODATA)	37.845	NBS/NIST
C(cr)	6	4	12.0108	IUPAC	5.74	[1978HEL/DEL]	8.682	[1978HEL/DEL]
Ca(cr)	20	2	40.078	IUPAC	41.590	NEA(CODATA)	25.929	NEA(CODATA)
Cl_2(g)	17	-1	35.453	IUPAC	111.54	NEA(CODATA)	16.9745	NEA(CODATA)
Cs(cr)	55	1	132.905	IUPAC	85.230	NEA(CODATA)	32.210	NEA(CODATA)
Eu(cr)	63	3	151.964	IUPAC	77.78	NBS/NIST	27.66	NBS/NIST
F_2(g)	9	-1	18.9984	IUPAC	101.396	NEA(CODATA)	15.652	NEA(CODATA)
Fe(cr)	26	2	55.845	IUPAC	27.28	NBS/NIST	24.961	[1963KUB/ALC]
H_2(g)	1	1	1.00795	IUPAC	65.34	slop98.dat	14.409	slop98.dat
I_2(cr)	53	-1	126.904	IUPAC	58.07	NEA(CODATA)	27.219	NBS/NIST
K(cr)	19	1	39.0983	IUPAC	64.68	NEA(CODATA)	29.6	NEA(CODATA)
Li(cr)	3	1	6.941	IUPAC	29.12	NEA(CODATA)	24.86	NEA(CODATA)
Mg(cr)	12	2	24.305	IUPAC	32.67	NEA(CODATA)	24.869	NEA(CODATA)
Mn(cr)	25	2	54.938	IUPAC	32.01	NBS/NIST	26.32	NBS/NIST
Mo(cr)	42	4	95.94	IUPAC	28.66	[1995ROB//HEM]	23.900	[1995ROB//HEM]
N_2(g)***	7	5	14.0067	IUPAC	95.8045	slop98.dat	14.567	slop98.dat
Na(cr)	11	1	22.9898	IUPAC	51.3	NEA(CODATA)	28.23	NEA(CODATA)
Nb(cr)	41	5	92.906	IUPAC	36.40	NBS/NIST	24.60	NBS/NIST
Ni(cr)	28	2	58.693	IUPAC	29.87	NBS/NIST	26.07	NBS/NIST
Np(cr)	93	5	237.048*	IUPAC	50.46	NEA	29.62	NEA
O_2(g)	8	-2	15.9994	IUPAC	102.569	slop98.dat	14.661	slop98.dat
P(cr)	15	5	30.9738	IUPAC	41.09	NEA(CODATA)	23.824	NEA(CODATA)
Pd(cr)	46	2	106.42	IUPAC	37.82	[1998SAS/SHO]	25.34	[1998SAS/SHO]
Pu(cr)	94	5	244.064*	IUPAC	54.46	NEA	31.49	NEA
Ra(cr)	88	2	226.025*	IUPAC	71	NBS/NIST	28.7	[1985LAN/RIE]
S(cr)	16	6	32.067	IUPAC	31.798	[1997MCC/SHO]	22.763	[1997MCC/SHO]
Se(cr)	34	6	78.96	IUPAC	42.27	NEA	25.03	NEA
Si(cr)	14	4	28.0855	IUPAC	18.81	NEA(CODATA)	19.789	NEA(CODATA)
Sn(cr)	50	4	118.711	IUPAC	51.212	[1985JAC/HEL]	26.352	[1985JAC/HEL]
Sr(cr)	38	2	87.62	IUPAC	55.7	NEA	26.4	NBS/NIST
Tc(cr)	43	4	97.907*	IUPAC	32.5	NEA	24.9	NEA
Th(cr)	90	4	232.038**	IUPAC	51.8	CODATA	26.23	CODATA
U(cr)	92	6	238.029**	IUPAC	50.2	NEA(CODATA)	27.66	NEA
Zr(cr)	40	4	91.224	IUPAC	39.0	NBS/NIST	25.36	NBS/NIST

* Atomic weight of longest-lived radionuclide ** Atomic weight of characteristic terrestrial isotopic composition
*** Nagra/PSI TDB 01/01 GEMS has two entries for elemental nitrogen (thermodynamically identical), see Chapter 8

2.3 Thermodynamic Data for *Secondary Master Species*

The values for S° were selected independently from the Nagra/PSI TDB 01/01. They are listed in Table 3. Most of the values were taken from [1997SHO/SAS], the sources are indicated in Table A2 (see Appendix). No values could be found for $H_2Se(aq)$, $I_2(aq)$, and for $TcO(OH)_2(aq)$.

Values for $\Delta_f G^\circ$ were calculated with PMATCHC from AUG20_GEMS.BAC. Data used were $\log_{10}K^\circ$ for the formation reactions of *secondary master species* (from Nagra/PSI TDB 01/01) and $\Delta_f G^\circ$ of the corresponding *primary master species* (from Table 3).

The *secondary master species* $Al(OH)_4^-$, $SiO(OH)_3^-$, and $SiO_2(OH)_2^{2-}$ are given in non-conventional form as AlO_2^-, $HSiO_3^-$, and SiO_3^{2-}, resp., see the discussion in Chapter 3. The derivation of thermodynamic data for these species is described in Chapter 5.

All *secondary master species* are kept in GEMS DComp records, with the exception of $SiO_2(OH)_2^{2-}$ (equivalent to SiO_3^{2-}), which is kept in a ReacDC record.

2.4 Thermodynamic Data for *Product Species*

Thermodynamic data for *product species* in Nagra/PSI TDB 01/01 GEMS are stored in ReacDC and DComp records.

For ReacDC records, $\log_{10}K^\circ$ values were taken directly from Nagra/PSI TDB 01/01. For DComp records, $\Delta_f G^\circ$ values were calculated with PMATCHC from AUG20_GEMS.BAC as described above for *secondary master species*.

For a small number of *product species* in Nagra/PSI TDB 01/01 the original data given were values of $\Delta_f G^\circ$ instead of $\log_{10}K^\circ$. These data had to be treated separately, as described in Chapter 4.

The derivation of thermodynamic data for silica *product species* is described in Chapter 5.

2.5 Additional Thermodynamic Data

For ReacDC records, $\log_{10}K^\circ$ (or $\Delta_r G^\circ$) values are sufficient for GEMS calculations of chemical equilibrium at 1 bar and 25°C. Additional data are needed for temperature extrapolations of $\log_{10}K^\circ$ or $\Delta_r G^\circ$. Based on the data available from Nagra/PSI TDB 01/01, four types of datasets can be distinguished in Nagra/PSI TDB 01/01 GEMS:

1.) $\Delta_r H^\circ$ and $\Delta_r C_p^\circ$ are given: This is sufficient for the 3-term extrapolation.

2.) $\Delta_r H^\circ$ is given and it is assumed that $\Delta_r C_p^\circ = 0$: This is sufficient for the 2-term extrapolation.

3.) No data are given and it is assumed that $\Delta_r S^\circ = \Delta_r C_p^\circ = 0$: This is sufficient for the 1-term extrapolation ($\Delta_r G^\circ$ = const.).

4.) No data are given and it is assumed that $\Delta_r H^\circ = \Delta_r C_p^\circ = 0$. This is sufficient for the 1-term extrapolation ($\log_{10}K^\circ$ = const.).

These temperature extrapolations (and their limitations) are discussed by [2002KUL]. The 2-term and the 1-term extrapolations can be applied with confidence only to isocoulombic and isoelectric reactions and possibly to reactions between solids and neutral species (see also Chapter 7). These extrapolations are not warranted for all other reactions and the user of the

Nagra/PSI TDB 01/01 GEMS must be aware of this when interpreting calculation results. Note that all datasets not sufficient for temperature extrapolations are marked with braces {} in Table A2 (see Appendix).

$\Delta_f G^\circ$ values from DComp records are sufficient for GEMS calculations of chemical equilibrium at 1 bar and 25°C. Additional data are needed for temperature corrections of $\Delta_f G^\circ$. Four types of datasets can be distinguished in Nagra/PSI TDB 01/01 GEMS:

1.) HKF-parameters for calculation of C_p°(P,T), S°, and other partial molal properties

2.) C_p°(T)-functions, S°

3.) C_p°, S°

4.) S°

Only the first two datasets allow rigorous temperature corrections for $\Delta_f G^\circ$. Therefore, all datasets of type 3 and 4 are marked with braces {} in Table A2.

The additional datasets for DComp records were included into Nagra/PSI TDB 01/01 GEMS without review and are usually not compatible with the corresponding data in the Nagra/PSI TDB 01/01. The sources are given in Table A2 (see also Chapter 1). Some of the HKF-parameters were estimated using the PRONSPREP algorithm (see Chapter 6).

Note: The additional datasets given for the calculation of chemical equilibria at elevated temperatures should not be considered as part of the official Nagra/PSI TDB 01/01 GEMS. The reason for this is that only the ReacDC data were taken from Nagra/PSI TDB 01/01 GEMS while the datasets chosen for DComp records do not necessarily reproduce the corresponding data in the Nagra/PSI TDB 01/01.

The official data are restricted to the minimal set required for the calculation of chemical equilibria at 1 bar and 25°C. These are the $\Delta_f G^\circ$ values for DComp records and the $\Delta_f G^\circ$ values calculated from the $\log_{10} K^\circ$ values of ReacDC records.

Table 3: Thermodynamic data selected for *primary master species* at 25°C and 1 bar. For references see Table A2.

Name in Nagra/PSI TDB 01/01	Non-conventional Stoich.	Record Type in GEMS	$\Delta_f G^\circ$ [kJ/mol]	S° [J/mol/K]
Primary Master Species				
Al+3		DComp	-483.708	-325.097
Am+3		DComp	-598.698	-204.600
B(OH)3		DComp	-968.763	154.808
Ba+2		DComp	-560.782	9.623
Br-		DComp	-104.056	82.843
Ca+2		DComp	-552.790	-56.484
Cl-		DComp	-131.290	56.735
Cs+		DComp	-291.667	132.842
e-		-	0	0
Eu+3		DComp	-574.463	-221.752
F-		DComp	-281.751	-13.180
Fe+2		DComp	-91.504	-105.855
H+		DComp	0	0
H2O		DComp	-237.183	69.923
HAsO4-2		DComp	-714.585	-1.674
HCO3-		DComp	-586.940	98.450
HPO4-2		DComp	-1089.140	-33.472
I-		DComp	-51.923	106.692
K+		DComp	-282.462	101.044
Li+		DComp	-292.600	11.297
Mg+2		DComp	-453.985	-138.072
Mn+2		DComp	-230.538	-67.781
MoO4-2		DComp	-838.474	37.656
Na+		DComp	-261.881	58.409
NbO3-		DComp	-950.186	13.390
Ni+2		DComp	-45.606	-128.867
NO3-		DComp	-110.905	146.942
NpO2+2		DComp	-795.900	-92.400
Pd+2		DComp	176.565	-88.282
PuO2+2		DComp	-762.400	-71.200
Ra+2		DComp	-561.493	53.974
SeO3-2		DComp	-369.866	12.970
Si(OH)4	SiO2	DComp	-833.411*	75.312*
Sn(OH)4	SnO2	DComp	-479.637*	-
Sn+2		DComp	-27.489	-16.736
SO4-2		DComp	-744.459	18.828
Sr+2		DComp	-563.836	-31.506
TcO4-		DComp	-632.202	198.700
Th+4		DComp	-705.004	-422.600
UO2+2		DComp	-952.613	-98.324
Zr+4		DComp	-557.602	-461.500

* Data refer to the non-conventional stoichiometry

Table 4: Thermodynamic data for *secondary master species* at 25˚C and 1 bar. For references see Table A2.

Name in Nagra/PSI TDB 01/01	Non-conventional Stoich.	Record Type in GEMS	$\Delta_f G^\circ$ [kJ/mol]	$\log_{10} K^\circ$	S° [J/mol/K]
Secondary Master Species					
Al(OH)4-	AlO2-	DComp	-827.479*		-30.209
As(OH)3	HAsO2	DComp	-456.561*		125.938*
CH4		DComp	-34.354		87.822
CO2		DComp	-386.015		117.570
CO3-2		DComp	-527.982		-49.999
Eu+2		DComp	-540.672		-10.042
Fe+3		DComp	-17.185		-277.399
H2		DComp	17.729		57.739
H2PO4-		DComp	-1130.306		90.374
H2Se		DComp	14.098		-
H3PO4		DComp	-1142.522		158.992
HS-		DComp	11.969		68.199
HSeO4-		DComp	-461.037		149.37
I2		DComp	-223.429		-
N2**		DComp	18.194		95.814
NH3		DComp	-26.670		107.822
NH4+		DComp	-79.395		111.169
Np+3		DComp	-512.753		-193.600
Np+4		DComp	-491.634		-426.400
NpO2+		DComp	-907.721		-45.900
O2		DComp	16.446		108.951
OH-		DComp	-157.270		-10.711
PO4-3		DComp	-1018.646		-221.752
Pu+3		DComp	-578.973		-184.500
Pu+4		DComp	-477.998		-414.500
PuO2+		DComp	-852.701		1.000
S2O3-2		DComp	-519.989		66.944
SiO(OH)3-	HSiO3-	DComp	-1014.598*		20.92*
SiO2(OH)2-2	SiO3-2	ReacDC	(-938.510*)	-23.14	(-46.226*)
SO3-2		DComp	-487.886		-29.288
TcO(OH)2		DComp	-562.835		-
U+4		DComp	-529.836		-416.726
UO2+		DComp	-961.084		-25.104

* Data refer to the non-conventional stoichiometry

** Nagra/PSI TDB 01/01 GEMS has two entries for N_2(aq) (thermodynamically identical), see Chapter 8

3 Non-Conventional Stoichiometry for Hydroxo Complexes

Thermodynamic data for hydroxo complexes based on the HKF equation of state (e.g., [1995HAA/SHO], [1997SHO/SAS], [1997SHO/SAS2], [1997SVE/SHO], [1998SAS/SHO], [1999MUR/SHO], and the database slop98.dat, see http://levee.wustl.edu/geopig) refer to a non-conventional stoichiometry of the complexes, which is obtained by subtracting the maximal number of H_2O from the conventional stoichiometry. Thus, e.g., $Fe(OH)_2^+$ can be written as FeO^+, and $Fe(OH)_3(aq)$ as $FeO_2H(aq)$, see Table 5. In order to retain temperature corrections provided by the HKF equation of state, we also adopted the non-conventional stoichiometry.

By definition, the standard molar thermodynamic properties of a non-conventional hydroxo complex are calculated from those of a conventional hydroxo complex by subtracting from the latter the corresponding standard molar thermodynamic properties of $H_2O(l)$ [1997SHO/SAS].

Therefore, $\Delta_r G^\circ$ of a reaction relating the conventional to the non-conventional hydroxo complex is always equal to zero as, e.g., in

$$Sn(OH)_4(aq) \rightleftharpoons SnO_2(aq) + 2H_2O(l) \; . \qquad (1)$$

This is obvious from

$$\Delta_f G^\circ(SnO_2, aq) = \Delta_f G^\circ(Sn(OH)_4, aq) - 2\Delta_f G^\circ(H_2O, l) \; .$$

As a consequence, $\log_{10} K^\circ$ is also equal to zero

$$\Delta_r G^\circ(1) = \log_{10} K^\circ(1) = 0 \; ,$$

which implies that for any reaction involving a hydroxo complex, $\log_{10} K^\circ$ is unaffected by the choice between conventional or non-conventional stoichiometry. For example, the formation of $CaSn(OH)_6(s)$ can be expressed in terms of $Sn(OH)_4(aq)$ as

$$Sn(OH)_4(aq) + 2H_2O(l) + Ca^{2+} \rightleftharpoons CaSn(OH)_6(s) + 2H^+ \qquad (2)$$

or in terms of $SnO_2(aq)$ as

$$SnO_2(aq) + 4H_2O(l) + Ca^{2+} \rightleftharpoons CaSn(OH)_6(s) + 2H^+ \; . \qquad (3)$$

Reaction (3) is obtained from reaction (2) by subtraction of reaction (1). Therefore,

$$\log_{10} K^\circ(2) = \log_{10} K^\circ(3) \; .$$

Non-conventional hydroxo complexes appear in the Nagra/PSI TDB 01/01 GEMS either as ReacDC or as DComp records. ReacDC records (see Table 6 for a list) were prepared by entering the formation reaction of the non-conventional complex and taking as $\log_{10} K^\circ$ the unchanged value of the corresponding formation reaction of the conventional complex from the Nagra/PSI TDB 01/01. $\Delta_f G^\circ$ of DComp records were calculated from $\Delta_f G^\circ$ of conventional hydroxo complexes by subtracting $\Delta_f G^\circ(H_2O, l)$, multiplied by an appropriate factor (see Table 7).

In the present version of the Nagra/PSI TDB 01/01 GEMS several hydroxo complexes still appear in their conventional form (see Table 8).

Table 5: Comparison of conventional and non-conventional compositions for hydroxo complexes. The superscript n± designates the charge of a complex.

Conventional Stoichiometry	Non-conventional Stoichiometry	Difference in H_2O
$Me(OH)^{n\pm}$	$Me(OH)^{n\pm}$	0
$Me(OH)_2^{n\pm}$	$MeO^{n\pm}$	1
$Me(OH)_3^{n\pm}$	$MeO_2H^{n\pm}$	1
$Me(OH)_4^{n\pm}$	$MeO_2^{n\pm}$	2
$Me(OH)_5^{n\pm}$	$MeO_3H^{n\pm}$	2
$Me(OH)_6^{n\pm}$	$MeO_3^{n\pm}$	3

Table 6: Non-conventional hydroxo complexes contained in Nagra/PSI TDB 01/01 GEMS as ReacDC records.

Conventional Stoichiometry	Non-conventional Stoichiometry
Secondary Master Species	
SiO2(OH)2-2	SiO3-2
Aqueous Product Species	
Al(OH)6SiO-	AlSiO4-
AlSiO(OH)3+2	AlHSiO3+2
AmSiO(OH)3+2	AmHSiO3+2
CaSiO2(OH)2	CaSiO3
Eu(SiO(OH)3)2+	EuSi2O5+
EuSiO(OH)3+2	EuHSiO3+2
FeSiO(OH)3+2	FeHSiO3+2
MgSiO2(OH)2	MgSiO3
Nb(OH)4+	NbO2+
Pd(OH)3-	PdO2H-
Pu(OH)4	PuO2
Sn(OH)5-	SnO3H-
Sn(OH)6-2	SnO3-2
Th(OH)4	ThO2

Table 7: Standard partial molal Gibbs energies for non-conventional hydroxo complexes contained in Nagra/PSI TDB 01/01 GEMS as DComp records.

Conventional Stoichiometry	$\Delta_f G^\circ$ [kJ/mol]	Non-conventional Stoichiometry	$\Delta_f G^\circ$ [kJ/mol]	Difference in H_2O
Primary Master Species				
Si(OH)4	-1307.777	SiO2	-833.411	2
Sn(OH)4	-954.003	SnO2	-479.637	2
Secondary Master Species				
Al(OH)4-	-1301.845	AlO2-	-827.479	2
As(OH)3	-693.744	HAsO2	-456.561	1
SiO(OH)3-	-1251.781	HSiO3-	-1014.598	1
Aqueous Product Species				
Al(OH)2+	-897.603	AlO+	-660.420	1
Al(OH)3	-1101.46	AlO2H	-864.277	1
Am(OH)2+	-986.302	AmO+	-749.119	1
Am(OH)3	-1163.550	AmO2H	-926.367	1
As(OH)4-	-823.957	AsO2-	-349.591	2
B(OH)4-	-1153.232	BO2-	-678.866	2
CaSiO(OH)3+	-1811.421	CaHSiO3+	-1574.238	1
Eu(OH)2+	-962.638	EuO+	-725.455	1
Eu(OH)3	-1150.732	EuO2H	-913.549	1
Eu(OH)4-	-1316.564	EuO2-	-842.198	2
Fe(OH)2+	-459.187	FeO+	-222.004	1
Fe(OH)3	-657.041	FeO2H	-419.858	1
Fe(OH)4-	-842.624	FeO2-	-368.258	2
MgSiO(OH)3+	-1714.328	MgHSiO3+	-1477.145	1
Nb(OH)5	-1466.472	NbO3H	-992.106	2
Ni(OH)2	-417.227	NiO	-180.044	1
Ni(OH)3-	-587.626	NiO2H-	-350.443	1
Ni(OH)4-2	-738.047	NiO2-2	-263.681	2
Pd(OH)2	-274.969	PdO	-37.786	1
Sn(OH)2	-457.903	SnO	-220.720	1
Sn(OH)3-	-639.147	SnO2H-	-401.964	1
U(OH)4	-1427.196	UO2	-952.830	2
UO2(OH)2	-1358.483	UO3	-1121.300	1
UO2(OH)3-	-1554.568	UO4H-	-1317.385	1
UO2(OH)4-2	-1712.980	UO4-2	-1238.614	2
Zr(OH)4	-1213.783	ZrO2	-976.600	1
Zr(OH)5-	-1652.188	ZrO3H-	-1177.822	2

Table 8: Hydroxo complexes in Nagra/PSI TDB 01/01 GEMS retaining the conventional stoichiometry. Non-conventional stoichiometries are indicated for a future update.

Conventional Stoichiometry	Non-conventional Stoichiometry	Difference in H_2O
Primary Master Species		
B(OH)3	HBO2	1
Secondary Master Species		
TcO(OH)2	TcO2	1
Aqueous Product Species		
(NpO2)2(OH)2+2	(NpO2)2O+2	1
(NpO2)2CO3(OH)3-	(NpO2)2O2HCO3-	1
(NpO2)3(OH)5+	(NpO2)3O2OH+	2
(PuO2)2(OH)2+2	(PuO2)2O+2	1
(UO2)2(OH)2+2	(UO2)2O+2	1
(UO2)2CO3(OH)3-	(UO2)2O2HCO3-	1
(UO2)3(OH)4+2	(UO2)3O2+2	2
(UO2)3(OH)5+	(UO2)3O2OH+	2
(UO2)3(OH)7-	(UO2)3O3OH-	3
(UO2)3O(OH)2HCO3+	(UO2)3O2HCO3+	1
(UO2)4(OH)7+	(UO2)4O3OH+	3
Fe2(OH)2+4	Fe2O+4	1
Fe3(OH)4+5	Fe3O2+5	2
Ni4(OH)4+4	Ni4O2+4	2
Np(OH)4	NpO2	2
NpO2(OH)2-	NpO3-	1
NpO2(OH)3-	NpO3OH-	1
NpO2(OH)4-2	NpO4-2	2
PdCl2(OH)2-2	PdOCl2-2	1
PuO2(OH)2	PuO3	1
Sn3(OH)4+2	Sn3O2+2	2
TcCO3(OH)2	TcCO4	1
TcCO3(OH)3-	TcCO4OH-	1
TcO(OH)3-	TcO2OH-	1
ThCO3(OH)3-	ThCO4OH-	1

4 $\Delta_f G^\circ$ vs. $\log_{10} K^\circ$ as Original Data

The original data for most of the *product species* in the Nagra/PSI TDB 01/01 are their formation constants. For a small number of *products species* (see Table 9 for a list), however, the original data are $\Delta_f G^\circ$ values from which the formation constants were derived by means of the $\Delta_f G^\circ$ values of the corresponding *master species*.

The $\Delta_f G^\circ$ values of these *product species* were recalculated for inclusion into DComp records of the Nagra/PSI TDB 01/01 GEMS by taking the formation constants from the Nagra/PSI TDB 01/01 and the $\Delta_f G^\circ$ of the *master species* from this report. In this way, the values of the formation constants from the Nagra/PSI TDB 01/01 are preserved even though the $\Delta_f G^\circ$ values of the participating species may all be different from those given in the Nagra/PSI TDB 01/01.

For ReacDC records the formation constants were directly taken from the Nagra/PSI TDB 01/01.

5 Silica Species

The Nagra/PSI TDB 01/01 contains the *primary master species* $Si(OH)_4(aq)$ and the *secondary master species* $SiO(OH)_3^-$ and $SiO_2(OH)_2^{2-}$ for use in formation reactions of silica *product species*. In Nagra/PSI TDB 01/01 GEMS they are included in their non-conventional form as $SiO_2(aq)$, $HSiO_3^-$, and SiO_3^{2-}, respectively.

Thermodynamic data for the *secondary master species* were derived as follows:

$SiO(OH)_3^-$ or $HSiO_3^-$: The formation reaction of $SiO(OH)_3^-$ is given in the Nagra/PSI TDB 01/01 as

$$Si(OH)_4(aq) \rightleftharpoons SiO(OH)_3^- + H^+ . \quad (4)$$

Table 9: Product species whose original data in the Nagra/PSI TDB 01/01 are values for $\Delta_f G^\circ$.

Name	Non-conventional Stoichiometry	Record Type in GEMS
Aqueous Product Species		
As(OH)4-	AsO2-	DComp
AsO4-3		DComp
H2AsO4-		DComp
H3AsO4		DComp
HF2-		DComp
HSO3-		DComp
Nb(OH)4+	NbO2+	ReacDC
Nb(OH)5	NbO3H	DComp
Solids		
Molybdite (MoO3)		DComp
Nb2O5(cr)		ReacDC
NbO2(cr)		DComp
Tugarinovite (MoO2)		DComp
USiO4(s)		ReacDC

$SiO_2(aq)$ is obtained from $Si(OH)_4(aq)$ by

$$Si(OH)_4(aq) \rightleftharpoons SiO_2(aq) + 2H_2O(l). \quad (5)$$

with

$$\log_{10}K^\circ(5) = 0 ,$$

see Chapter 4, and $HSiO_3^-$ is obtained from $SiO(OH)_3^-$ by

$$SiO(OH)_3^- \rightleftharpoons HSiO_3^- + H_2O(l) , \quad (6)$$

again with

$$\log_{10}K^\circ(6) = 0 .$$

Combining reactions (4), (5), and (6) results in

$$SiO_2(aq) + H_2O(l) \rightleftharpoons HSiO_3^- + H^+ , \quad (7)$$

with

$$\log_{10}K^\circ(7) = \log_{10}K^\circ(4) .$$

$\Delta_f G^\circ$ for the DComp record $HSiO_3^-$ was therefore calculated from $\log_{10}K^\circ(4)$ given by the Nagra/PSI TDB 01/01 and from the $\Delta_f G^\circ$ values of the *primary master species* $SiO_2(aq)$, $H_2O(l)$, and H^+ given in Table 3.

$SiO_2(OH)_2^{2-}$ or SiO_3^{2-}: The formation reaction of $SiO_2(OH)_2^{2-}$ is given in the Nagra/PSI TDB 01/01 as

$$Si(OH)_4(aq) \rightleftharpoons SiO_2(OH)_2^{2-} + 2H^+ . \quad (8)$$

This reaction is written with non-conventional stoichiometries as

$$SiO_2(aq) + H_2O(l) \rightleftharpoons SiO_3^{2-} + 2H^+ , \quad (9)$$

with

$$\log_{10}K^\circ(9) = \log_{10}K^\circ(8) .$$

SiO_3^{2-} is a ReacDC record with the reaction stoichiometry given by reaction (9) and the value for $\log_{10}K^\circ(8)$ taken from the Nagra/PSI TDB 01/01.

The silica *product species* in Nagra/PSI TDB 01/01 GEMS are listed in Table 10. All aqueous *product species* are contained in ReacDC records with their non-conventional stoichiometries. Take for example $CaSiO(OH)_3^+$ (non-conventional: $CaHSiO_3^+$): The formation reaction in the Nagra/PSI TDB 01/01 is

$$Ca^{2+} + SiO(OH)_3^- \rightleftharpoons CaSiO(OH)_3^+, \quad (10)$$

and in Nagra/PSI TDB 01/01 GEMS

$$Ca^{2+} + HSiO_3^- \rightleftharpoons CaHSiO_3^+ . \quad (11)$$

As it has become clear by know, $\log_{10}K^\circ$ is the same for both reactions. Thus, the values of $\log_{10}K^\circ$ for all silica *product species* in ReacDC records can be directly taken from the corresponding reactions in the Nagra/PSI TDB 01/01.

Table 10: Silica Species in Nagra/PSI TDB 01/01 GEMS.

Name	Non-conventional Stoichiometry	Record Type in GEMS
Primary Master Species		
Si(OH)4	SiO2	DComp
Secondary Master Species		
SiO(OH)3-	HSiO3-	DComp
SiO2(OH)2-2	SiO3-2	ReacDC
Aqueous Product Species		
Al(OH)6SiO-	AlSiO4-	ReacDC
AlSiO(OH)3+2	AlHSiO3+2	ReacDC
AmSiO(OH)3+2	AmHSiO3+2	ReacDC
CaSiO(OH)3+	CaHSiO3+	DComp
CaSiO2(OH)2	CaSiO3	ReacDC
Eu(SiO(OH)3)2+	EuSi2O5+	ReacDC
EuSiO(OH)3+2	EuHSiO3+2	ReacDC
FeSiO(OH)3+2	FeHSiO3+2	ReacDC
MgSiO(OH)3+	MgHSiO3+	DComp
MgSiO2(OH)2	MgSiO3	ReacDC
Solids		
Kaolinite (Al2Si2O5(OH)4)		DComp
Quartz (SiO2)		DComp
SiO2(am)		DComp
USiO4(s)		ReacDC

6 Data Estimates with PRONSPREP

Numerous DComp records in the Nagra/PSI TDB 01/01 GEMS contain parameters of the revised HKF equation of state [1988TAN/HEL] for the calculation of C_P°(P,T) and V°(P,T) using SUPCRT92 subroutines [1992JOH/OEL] incorporated into the GEMS code. The sources of these parameters are listed in Table A2 (see Appendix).

Missing HKF-parameters for aqueous 1-1 to 1-4 complexes with monovalent ligands or with SO_4^{2-} and CO_3^{2-} were estimated with PRONSPREP, a program by [1997SVE/SHO] that is incorporated into the GEMS code and extended with correlations for SO_4^{2-} and CO_3^{2-} from [1997SVE/SHO]. The estimation method is based on linear correlations among HKF-parameters and standard partial molal properties at 25°C and 1 bar.

7 Temperature Extrapolations for Isocoulombic Reactions

In order to apply the 1-term temperature extrapolation, [2002THO/BER] derived isocoulombic reactions (as well as reactions of solids with neutral aqueous species) for various actinides and Tc by linear combination of reactions listed in the Nagra/PSI TDB 01/01. The corresponding equilibrium constants were calculated in a similar way from those in the Nagra/PSI TDB 01/01. Some of these reactions (listed in Table 11) were adopted for the Nagra/PSI TDB 01/01 GEMS.

Table 11: Isocoulombic reactions and reactions involving solids and neutral species taken from [2002THO/BER]. Note that non-conventional stoichiometries are used for AmSiO(OH)3+2 and Pu(OH)4.

Name in Nagra/PSI TDB 01/01	Formation Reaction	T-Extrapolation	$\log_{10}K°$
Am(CO3)1.5(cr)	$AmCO_3^+ + 0.5CO_2(aq) + 0.5H_2O(l) \rightleftharpoons Am(CO_3)_{1.5}(cr) + H^+$	1-term isocoul. ($\Delta_rG° = const.$)	0.5595
AmCO3OH(cr)	$AmCO_3^+ + H_2O(l) \rightleftharpoons AmCO_3OH(cr) + H^+$	1-term isocoul. ($\Delta_rG° = const.$)	-0.60
AmSiO(OH)3+2	$AmF^{2+} + HSiO_3^- \rightleftharpoons AmHSiO_3^{2+} + F^-$	1-term isocoul. $\Delta_rG° = const.$	4.70
Pu(OH)4	$Pu^{4+} + UO_2(aq) \rightleftharpoons PuO_2(aq) + U^{4+}$	1-term isocoul. ($\Delta_rG° = const.$)	0.60
PuO2(hyd,ag)	$PuO_2(aq) \rightleftharpoons PuO_2(hyd,ag)$	1-term ($\log_{10}K° = const.$)	10.4*
TcCO3(OH)2	$TcO(OH)_2(aq) + HCO_3^- \rightleftharpoons TcCO_3(OH)_2(aq) + OH^-$	1-term isocoul. ($\Delta_rG° = const.$)	-5.029
ThCO3(OH)3-	$ThO_2(aq) + HCO_3^- + H_2O(l) \rightleftharpoons ThCO_3(OH)_3^-$	1-term isocoul. ($\Delta_rG° = const.$)	4.971

* Note that in [2002THO/BER] $\log_{10}K°$ of this reaction is erroneously given as 6.4.

8 Species and Data not Contained in Nagra/PSI TDB 01/01

Nagra/PSI TDB 01/01 does not include the aqueous species Sn^{4+} and ClO_4^-. The reason for their inclusion into Nagra/PSI TDB 01/01 GEMS is given in the following sections, together with a discussion of their thermodynamic data.

Nitrogen is treated specially in Nagra/PSI TDB 01/01 GEMS. It is observed that nitrogen gas in the atmosphere is not in equilibrium with aqueous nitrogen in streams, lakes, or oceans [1996STU/MOR]. In order to decouple atmospheric nitrogen from aqueous nitrogen in GEMS modeling, element "Nit" (with record key Nit:a:nitrogen_atm) was created in addition to the ordinary element "N" (N:e:nitrogen). Note that both of these have identical thermodynamic properties. "Nit" is used to define $N_2(g)$ (g:N0:N2:add) and $N_2(aq)$ (a:wN0:N2@:atm:), which are decoupled from all other nitrogen-bearing species that are defined through "N".

If for specific modeling purposes $N_2(g)$ and $N_2(aq)$ are assumed to be coupled with the other nitrogen-bearing species, they have to be defined through "N", which is the case for $N_2(g)$ with the record key (g:N0:N2:enp:) and $N_2(aq)$ with the record key (a:wN0:N2@:bnp:). Note that decoupled $N_2(g)$ is thermodynamically identical with coupled $N_2(g)$, and decoupled $N_2(aq)$ with coupled $N_2(aq)$.

8.1 Sn(IV)

Sn(II) and Sn(IV) are not redox coupled in the Nagra/PSI TDB 01/01 due to the lack of a reliable equilibrium constant for the reaction that links Sn^{2+} with Sn^{4+} (see the discussion in [2002HUM/BER]). Therefore, Sn^{4+} is not included in the Nagra/PSI TDB 01/01 and no $\Delta_fG°$ values are given for $Sn(OH)_4(aq)$, the *primary master species* for Sn(IV), and for the remaining Sn(IV) species and solids, $Sn(OH)_5^-$, $Sn(OH)_6^{2-}$, $CaSn(OH)_6(s)$, cassiterite, and $SnO_2(am)$.

Table 12: Thermodynamic data for Sn(IV) species and solids at 25°C and 1 bar.

Name in Nagra/PSI TDB 01/01	$\Delta_f G^\circ$ [kJ/mol]	Non-conventional Stoichiometry	$\Delta_f G^\circ$ [kJ/mol]	Record Type in GEMS
Primary Master Species				
Sn(OH)4	-954.003	SnO2	-479.637	DComp
Aqueous Product Species				
Sn(OH)5-	1145.52	SnO3H-	-671.156	ReacDC
Sn(OH)6-2	-1323.341	SnO3-2	-611.793	ReacDC
Solids				
CaSn(OH)6(s)	-1931.499			ReacDC
Cassiterite (SnO2)	-525.302			DComp
SnO2(am)	-521.306			ReacDC

Use of the Nagra/PSI TDB 01/01 with GEMS requires that a value be given for $\Delta_f G^\circ(Sn(OH)_4, aq, 298.15)$, otherwise it would not be possible to calculate $\Delta_f G^\circ$ of Sn(IV) species and solids from their equilibrium constants in Nagra/PSI TDB 01/01, and they would have to be excluded from GEMS calculations.

[2002HUM/BER] provided an estimate of

$$\log_{10} K^\circ(14, 298.15) = -1.4$$

for

$$Sn(OH)_4(aq) + 4H^+ \rightleftharpoons Sn^{4+} + 4H_2O(l) \qquad (14)$$

(note that this reaction is not part of the Nagra/PSI TDB 01/01). With this estimate, $\Delta_f G^\circ(Sn(OH)_4, aq, 298.15)$ can be calculated from $\Delta_f G^\circ(H^+, 298.15) = 0$, $\Delta_f G^\circ(H_2O, l, 298.15)$ given in Table 1, and from $\Delta_f G^\circ(Sn^{4+}, 298.15)$.

For the latter, we adopted the value given by [1985BAR/PAR] without critical review

$$\Delta_f G^\circ(Sn^{4+}, 298.15) = 2.72 \text{ kJ/mol}$$

Therefore,

$$\Delta_f G^\circ(Sn(OH)_4, aq, 298.15) = -954 \text{ kJ/mol}$$

This value – based on an estimate for $\log_{10} K^\circ(14, 298.15)$ and on an unreviewed value for $\Delta_f G^\circ(Sn^{4+}, 298.15)$ – should be interpreted as an **arbitrary reference value**. It is only provided for the calculation of $\Delta_f G^\circ$ (see Table 12) for Sn(IV) species and solids from their equilibrium constants listed in the Nagra/PSI TDB 01/01 and from the $\Delta_f G^\circ$ values of the appropriate *master species* in Tables 3 and 4.

Thus, the Nagra/PSI TDB 01/01 GEMS does couple Sn^{4+} with Sn^{2+} (in contrast to the Nagra/PSI TDB 01/01). Since this coupling rests on shaky ground, calculations involving Sn must be interpreted with extreme caution, especially with respect to the redox state of Sn.

8.2 Perchlorate

The perchlorate ion ClO_4^- is not considered in the Nagra/PSI TDB 01/01. In order to allow the retrieval of thermodynamic data by GEMS modeling of experiments in perchlorate media, thermodynamic data by [1997SHO/SAS] for ClO_4^- are included in the Nagra/PSI TDB 01/01 GEMS.

9 Acknowledgments

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Appendix

Table A1: $\Delta_f G^\circ$ values from the Nagra/PSI TDB 01/01 GEMS. Legend to phase state in GEMS record keys: a - aqueous species, s - solid, g - gas. Syntax of chemical formulae: The formal valence of an element (if different from the default valence, see Table 2) is enclosed in vertical bars, as in Am|3|+3. Neutral aqueous species are designated by @, as in B(OH)3@. Aqueous species, solids, or gases also contained in slop98.dat (version 30. Oct. 1998) for SUPCRT 92 [1992JOH/OEL] are marked with a #-sign.

Nagra/PSI TDB 01/01	GEMS Record Keys				Stoichiometry	$\Delta_f G^\circ$
Name	Phase State	Group	Name	TDB Set		[J/mol]
Primary Master Species						
# Al+3	a	Al	Al+3	anp	Al+3	-483708
Am+3	a	Am	Am+3	anp	Am|3|+3	-598698
# B(OH)3	a	B	B(OH)3@	anp	B(OH)3@	-968763
# Ba+2	a	Ba	Ba+2	anp	Ba+2	-560782
# Br-	a	wBr-1	Br-	anp	Br-	-104056
# Ca+2	a	Ca	Ca+2	anp	Ca+2	-552790
# Cl-	a	wCl-1	Cl-	anp	Cl-	-131290
# Cs+	a	Cs	Cs+	anp	Cs+	-291667
e-	-	-	-	-	-	0
# Eu+3	a	Eu+3	Eu+3	anp	Eu+3	-574463
# F-	a	wF	F-	anp	F-	-281751
# Fe+2	a	Fe+2	Fe+2	anp	Fe+2	-91504
# H+	a	w_	H+	anp	H+	0
# H2O	a	w_	H2O@	anp	H2O@	-237183
# HAsO4-2	a	As+5	HAsO4-2	anp	HAs|5|O4-2	-714585
# HCO3-	a	wC+4	HCO3-	anp	HCO3-	-586940
# HPO4-2	a	wP+5	HPO4-2	anp	HPO4-2	-1089140
# I-	a	wI-1	I-	anp	I-	-51923
# K+	a	K	K+	anp	K+	-282462
# Li+	a	Li	Li+	anp	Li+	-292600
# Mg+2	a	Mg	Mg+2	anp	Mg+2	-453985
# Mn+2	a	Mn+2	Mn+2	anp	Mn+2	-230538
# MoO4-2	a	Mo+6	MoO4-2	anp	Mo|6|O4-2	-838474
# Na+	a	Na	Na+	anp	Na+	-261881
# NbO3-	a	Nb+5	NbO3-	anp	NbO3-	-950186
# Ni+2	a	Ni	Ni+2	anp	Ni+2	-45606
# NO3-	a	wN+5	NO3-	anp	NO3-	-110905
NpO2+2	a	Np+6	NpO2+2	anp	Np|6|O2+2	-795900
# Pd+2	a	Pd	Pd+2	anp	Pd|2|+2	176565
PuO2+2	a	Pu+6	PuO2+2	anp	Pu|6|O2+2	-762400
# Ra+2	a	Ra	Ra+2	anp	Ra+2	-561493
# SeO3-2	a	Se+4	SeO3-2	anp	Se|4|O3-2	-369866
# Si(OH)4	a	Si	SiO2@	anp	SiO2@	-833411
Sn(OH)4	a	Sn+4	SnO2@	anp	Sn|4|O|-2|2@	-479637
# Sn+2	a	Sn+2	Sn+2	anp	Sn|2|+2	-27489
# SO4-2	a	wS+6	SO4-2	anp	S|6|O4-2	-744459
# Sr+2	a	Sr	Sr+2	anp	Sr+2	-563836
# TcO4-	a	Tc+7	TcO4-	anp	Tc|7|O4-	-632202
# Th+4	a	Th	Th+4	anp	Th+4	-705004
# UO2+2	a	U+6	UO2+2	anp	U|6|O2+2	-952613
# Zr+4	a	Zr	Zr+4	anp	Zr+4	-557602

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Table A1: Continued

Nagra/PSI TDB 01/01 Name	GEMS Record Keys Phase State	Group	Name	TDB Set	Stoichiometry	$\Delta_f G^\circ$ [J/mol]
Secondary Master Species						
# Al(OH)4-	a	Al	AlO2-	bnp	AlO2-	-827479
# As(OH)3	a	As+3	HAsO2@	bnp	HAs|3|O2@	-456561
# CH4	a	wC-4	CH4@	bnp	C|0|H|0|4@	-34354
# CO2	a	wC+4	CO2@	bnp	CO2@	-386015
# CO3-2	a	wC+4	CO3-2	bnp	CO3-2	-527982
# Eu+2	a	Eu+2	Eu+2	bnp	Eu|2|+2	-540672
# Fe+3	a	Fe+3	Fe+3	bnp	Fe|3|+3	-17185
# H2	a	wH0	H2@	bnp	H|0|2@	17729
# H2PO4-	a	wP+5	H2PO4-	bnp	H2PO4-	-1130306
H2Se	a	Se-2	H2Se@	bnp	H2Se|-2|@	14098
# H3PO4	a	wP+5	H3PO4@	bnp	H3PO4@	-1142522
# HS-	a	wS-2	HS-	bnp	HS|-2|-	11969
# HSeO4-	a	Se+6	HSeO4-	bnp	HSe|6|O4-	-461037
I2	a	wI0	I2@	bnp	I|0|2@	-223429
# N2	a	wN0	N2@	bnp	N|0|2@	18194
# NH3	a	wN-3	NH3@	bnp	N|-3|H3@	-26670
# NH4+	a	wN-3	NH4+	bnp	N|-3|H4+	-79395
Np+3	a	Np+3	Np+3	bnp	Np|3|+3	-512753
Np+4	a	Np+4	Np+4	bnp	Np|4|+4	-491634
NpO2+	a	Np+5	NpO2+	bnp	NpO2+	-907721
# O2	a	wO0	O2@	bnp	O|0|2@	16446
# OH-	a	wX	OH-	bnp	OH-	-157270
# PO4-3	a	wP+5	PO4-3	bnp	PO4-3	-1018646
Pu+3	a	Pu+3	Pu+3	bnp	Pu|3|+3	-578973
Pu+4	a	Pu+4	Pu+4	bnp	Pu|4|+4	-477998
PuO2+	a	Pu+5	PuO2+	bnp	PuO2+	-852701
# S2O3-2	a	wS+2	S2O3-2	bnp	S|0|S|4|O3-2	-519989
# SiO(OH)3-	a	Si	HSiO3-	bnp	HSiO3-	-1014598
SiO2(OH)2-2	a	Si	SiO3-2	bnp	SiO3-2	-938510
# SO3-2	a	wS+4	SO3-2	bnp	S|4|O3-2	-487886
TcO(OH)2	a	Tc+4	TcO(OH)2@	bnp	TcO(OH)2@	-562835
# U+4	a	U+4	U+4	bnp	U|4|+4	-529836
# UO2+	a	U+5	UO2+	bnp	U|5|O2+	-961084
Aqueous Product Species						
(NpO2)2(OH)2+2	a	Np+6	(NpO2)2(OH)2+2	cnp	(Np|6|O2)2(OH)2+2	-2030377
(NpO2)2CO3(OH)3-	a	Np+6	(NpO2)2CO3(OH)3-	cnp	(Np|6|O2)2CO3(OH)3-	-2814949
(NpO2)3(CO3)6-6	a	Np+6	(NpO2)3(CO3)6-6	cnp	(Np|6|O2)3(CO3)6-6	-5840079
(NpO2)3(OH)5+	a	Np+6	(NpO2)3(OH)5+	cnp	(Np|6|O2)3(OH)5+	-3475893
(PuO2)2(OH)2+2	a	Pu+6	(PuO2)2(OH)2+2	cnp	(Pu|6|O2)2(OH)2+2	-1956356
(UO2)2(OH)2+2	a	U+6	(UO2)2(OH)2+2	cnp	(U|6|O2)2(OH)2+2	-2347513
(UO2)2CO3(OH)3-	a	U+6	(UO2)2CO3(OH)3-	cnp	(U|6|O2)2CO3(OH)3-	-3139848
(UO2)2NpO2(CO3)6-6	a	UNp+6	(UO2)2NpO2(CO3)6	cnp	(U|6|O2)2Np|6|O2(CO3)6-6	-6174910
(UO2)2OH+3	a	U+6	(UO2)2(OH)+3	cnp	(U|6|O2)2(OH)+3	-2126997
(UO2)2PuO2(CO3)6-6	a	UPu+6	(UO2)2PuO2(CO3)6	cnp	(U|6|O2)2Pu|6|O2(CO3)6-6	-6136330
(UO2)3(CO3)6-6	a	U+6	(UO2)3(CO3)6-6	cnp	(U|6|O2)3(CO3)6-6	-6333963
(UO2)3(OH)4+2	a	U+6	(UO2)3(OH)4+2	cnp	(U|6|O2)3(OH)4+2	-3738645

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Table A1: Continued

Nagra/PSI TDB 01/01	GEMS Record Keys				Stoichiometry	$\Delta_f G^\circ$
Name	Phase State	Group	Name	TDB Set		[J/mol]
(UO2)3(OH)5+	a	U+6	(UO2)3(OH)5+	cnp	(U|6|O2)3(OH)5+	-3954994
(UO2)3(OH)7-	a	U+6	(UO2)3(OH)7-	cnp	(U|6|O2)3(OH)7-	-4341171
(UO2)3O(OH)2HCO3+	a	U+6	(UO2)3CO3(OH)3+	cnp	(U|6|O2)3CO3(OH)3+	-4101137
(UO2)4(OH)7+	a	U+6	(UO2)4(OH)7+	cnp	(U|6|O2)4(OH)7+	-5345727
# Al(OH)2+	a	Al	AlO+	cnp	AlO+	-660420
# Al(OH)3	a	Al	AlO2H@	cnp	AlO2H@	-864277
Al(OH)6SiO-	a	AlSi	AlSiO4-	cnp	AlSiO4-	-1681439
Al(SO4)2-	a	Al	Al(SO4)2-	cnp	Al(SO4)2-	-2006304
AlF+2	a	Al	AlF+2	cnp	AlF+2	-805871
AlF2+	a	Al	AlF2+	cnp	AlF2+	-1119872
AlF3	a	Al	AlF3@	cnp	AlF3@	-1424740
AlF4-	a	Al	AlF4-	cnp	AlF4-	-1720818
AlF5-2	a	Al	AlF5-2	cnp	AlF5-2	-2008334
AlF6-3	a	Al	AlF6-3	cnp	AlF6-3	-2290084
# AlOH+2	a	Al	AlOH+2	cnp	Al(OH)+2	-692595
AlSiO(OH)3+2	a	AlSi	AlHSiO3+2	cnp	AlHSiO3+2	-1540546
AlSO4+	a	Al	Al(SO4)+	cnp	Al(SO4)+	-1250429
Am(CO3)2-	a	Am	Am(CO3)2-	cnp	Am|3|(CO3)2-	-1724870
Am(CO3)3-3	a	Am	Am(CO3)3-3	cnp	Am(CO3)3-3	-2269405
Am(OH)2+	a	Am	AmO+	cnp	Am|3|O+	-749119
Am(OH)3	a	Am	AmO2H@	cnp	Am|3|O2H@	-926367
Am(SO4)2-	a	Am	Am(SO4)2-	cnp	Am|3|(SO4)2-	-2118440
AmCl+2	a	Am	AmCl+2	cnp	Am|3|Cl+2	-735981
AmCO3+	a	Am	Am(CO3)+	cnp	Am|3|(CO3)+	-1171202
AmF+2	a	Am	AmF+2	cnp	Am|3|F+2	-899856
AmF2+	a	Am	AmF2+	cnp	Am|3|F2+	-1195306
AmH2PO4+2	a	Am	Am(H2PO4)+2	cnp	Am|3|(H2PO4)+2	-1746129
AmNO3+2	a	Am	Am(NO3)+2	cnp	Am|3|(NO3)+2	-717195
AmOH+2	a	Am	Am(OH)+2	cnp	Am|3|(OH)+2	-794212
AmSiO(OH)3+2	a	AmSi	AmHSiO3+2	cnp	AmHSiO3+2	-1659531
AmSO4+	a	Am	Am(SO4)+	cnp	Am|3|(SO4)+	-1365133
# As(OH)4-	a	As+3	AsO2-	cnp	As|3|O2-	-349591
# AsO4-3	a	As+5	AsO4-3	cnp	As|5|O4-3	-648355
# B(OH)4-	a	B	BO2-	cnp	BO2-	-678866
# BaCO3	a	Ba	Ba(CO3)@	cnp	BaCO3@	-1104251
# BaHCO3+	a	Ba	Ba(HCO3)+	cnp	BaHCO3+	-1153325
# BaOH+	a	Ba	BaOH+	cnp	BaOH+	-721077
BaSO4	a	Ba	Ba(SO4)@	cnp	Ba(SO4)@	-1320652
# CaCO3	a	Ca	Ca(CO3)@	cnp	CaCO3@	-1099176
# CaF+	a	Ca	CaF+	cnp	CaF+	-839906
# CaHCO3+	a	Ca	Ca(HCO3)+	cnp	CaHCO3+	-1146041
# CaOH+	a	Ca	CaOH+	cnp	Ca(OH)+	-717024
# CaSiO(OH)3+	a	CaSi	Ca(HSiO3)+	cnp	CaHSiO3+	-1574238
CaSiO2(OH)2	a	CaSi	CaSiO3@	cnp	CaSiO3@	-1517557
# CaSO4	a	Ca	Ca(SO4)@	cnp	CaSO4@	-1310378
Eu(CO3)2-	a	Eu+3	Eu(CO3)2-	cnp	Eu(CO3)2-	-1699494
# Eu(OH)2+	a	Eu+3	EuO+	cnp	Eu|3|O+	-725455

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Table A1: Continued

Nagra/PSI TDB 01/01	GEMS Record Keys				Stoichiometry	$\Delta_f G^\circ$
Name	Phase State	Group	Name	TDB Set		[J/mol]
# Eu(OH)3	a	Eu+3	EuO2H@	cnp	Eu|3|O2H@	-913549
# Eu(OH)4-	a	Eu+3	EuO2-	cnp	Eu|3|O2-	-842198
Eu(SiO(OH)3)2+	a	Eu+3Si	EuSi2O5+	cnp	EuSi2O5+	-2439539
Eu(SO4)2-	a	Eu+3	Eu(SO4)2-	cnp	Eu(SO4)2-	-2095917
# EuCl+2	a	Eu+3	EuCl+2	cnp	Eu|3|Cl+2	-712032
# EuCl2+	a	Eu+3	EuCl2+	cnp	Eu|3|Cl2+	-845605
# EuCO3+	a	Eu+3	Eu(CO3)+	cnp	Eu|3|(CO3)+	-1148680
# EuF+2	a	Eu+3	EuF+2	cnp	Eu|3|F+2	-877904
# EuF2+	a	Eu+3	EuF2+	cnp	Eu|3|F2+	-1175067
EuOH+2	a	Eu+3	Eu(OH)+2	cnp	Eu|3|(OH)+2	-768037
EuSiO(OH)3+2	a	Eu+3Si	EuHSiO3+2	cnp	EuHSiO3+2	-1634155
# EuSO4+	a	Eu+3	Eu(SO4)+	cnp	Eu|3|(SO4)+	-1341469
# Fe(OH)2+	a	Fe+3	FeO+	cnp	Fe|3|O+	-222004
# Fe(OH)3	a	Fe+3	FeO2H@	cnp	Fe|3|O2H@	-419858
# Fe(OH)4-	a	Fe+3	FeO2-	cnp	Fe|3|O2-	-368258
Fe(SO4)2-	a	Fe+3	Fe(SO4)2-	cnp	Fe|3|(SO4)2-	-1536813
Fe2(OH)2+4	a	Fe+3	Fe2(OH)2+4	cnp	Fe|3|2(OH)2+4	-491898
Fe3(OH)4+5	a	Fe+3	Fe3(OH)4+5	cnp	Fe|3|3(OH)4+5	-964328
# FeCl+	a	Fe+2	FeCl+	cnp	FeCl+	-223593
# FeCl+2	a	Fe+3	FeCl+2	cnp	Fe|3|Cl+2	-156923
FeCl2+	a	Fe+3	FeCl2+	cnp	Fe|3|Cl2+	-291923
FeCl3	a	Fe+3	FeCl3@	cnp	Fe|3|Cl3@	-417505
FeCO3	a	Fe+2	Fe(CO3)@	cnp	FeCO3@	-644487
# FeF+	a	Fe+2	FeF+	cnp	Fe|2|F+	-378963
# FeF+2	a	Fe+3	FeF+2	cnp	Fe|3|F+2	-334326
FeF2+	a	Fe+3	FeF2+	cnp	Fe|3|F2+	-642333
FeF3	a	Fe+3	FeF3@	cnp	Fe|3|F3@	-942349
FeHCO3+	a	Fe+2	Fe(HCO3)+	cnp	FeHCO3+	-689860
FeHSO4+	a	Fe+2	Fe(HSO4)+	cnp	FeHSO4+	-853475
FeHSO4+2	a	Fe+3	Fe(HSO4)+2	cnp	Fe|3|HSO4+2	-787148
# FeOH+	a	Fe+2	FeOH+	cnp	FeOH+	-274461
# FeOH+2	a	Fe+3	FeOH+2	cnp	Fe|3|(OH)+2	-241868
FeSiO(OH)3+2	a	Fe+3Si	FeHSiO3+2	cnp	Fe|3|HSiO3+2	-1087151
FeSO4	a	Fe+2	Fe(SO4)@	cnp	Fe(SO4)@	-848806
FeSO4+	a	Fe+3	Fe(SO4)+	cnp	Fe|3|(SO4)+	-784705
# H2AsO4-	a	As+5	H2AsO4-	cnp	H2As|5|O4-	-753194
# H2S	a	wS-2	H2S@	cnp	H2S|-2|@	-27930
# H2SeO3	a	Se+4	H2SeO3@	cnp	H2Se|4|O3@	-433796
# H3AsO4	a	As+5	H3AsO4@	cnp	H3As|5|O4@	-766112
# HF	a	wF	HF@	cnp	HF@	-299879
# HF2-	a	wF	HF2-	cnp	HF2-	-584164
# HSe-	a	Se-2	HSe-	cnp	HSe|-2|-	35789
# HSeO3-	a	Se+4	HSeO3-	cnp	HSe|4|O3-	-417814
# HSO3-	a	wS+4	HSO3-	cnp	HS|4|O3-	-529098
# HSO4-	a	wS+6	HSO4-	cnp	HS|6|O4-	-755805
# I3-	a	wI0-1	I3-	cnp	I|1|I|-1|2-	-291735
# KOH	a	K	KOH@	cnp	KOH@	-437107

continued on next page

Table A1: Continued

Nagra/PSI TDB 01/01	GEMS Record Keys				Stoichiometry	$\Delta_f G^\circ$
Name	Phase State	Group	Name	TDB Set		[J/mol]
# KSO4-	a	K	K(SO4)-	cnp	KSO4-	-1031773
# LiOH	a	Li	LiOH@	cnp	LiOH@	-451925
LiSO4-	a	Li	Li(SO4)-	cnp	Li(SO4)-	-1040712
# MgCO3	a	Mg	Mg(CO3)@	cnp	MgCO3@	-998975
# MgF+	a	Mg	MgF+	cnp	MgF+	-746124
# MgHCO3+	a	Mg	Mg(HCO3)+	cnp	MgHCO3+	-1047022
# MgOH+	a	Mg	MgOH+	cnp	Mg(OH)+	-625868
# MgSiO(OH)3+	a	MgSi	Mg(HSiO3)+	cnp	MgHSiO3+	-1477145
MgSiO2(OH)2	a	MgSi	MgSiO3@	cnp	MgSiO3@	-1425031
# MgSO4	a	Mg	MgSO4@	cnp	Mg(SO4)@	-1211972
# MnCl+	a	Mn+2	MnCl+	cnp	MnCl+	-365310
MnCl2	a	Mn+2	MnCl2@	cnp	MnCl2@	-494544
MnCl3-	a	Mn+2	MnCl3-	cnp	MnCl3-	-622638
MnCO3	a	Mn+2	Mn(CO3)@	cnp	MnCO3@	-786489
# MnF+	a	Mn+2	MnF+	cnp	MnF+	-517083
MnHCO3+	a	Mn+2	Mn(HCO3)+	cnp	MnHCO3+	-828609
# MnOH+	a	Mn+2	MnOH+	cnp	Mn(OH)+	-407273
# MnSO4	a	Mn+2	Mn(SO4)@	cnp	MnSO4@	-987840
NaCO3-	a	Na	Na(CO3)-	cnp	NaCO3-	-797112
# NaF	a	Na	NaF@	cnp	NaF@	-542262
NaHCO3	a	Na	Na(HCO3)@	cnp	NaHCO3@	-847394
# NaOH	a	Na	NaOH@	cnp	NaOH@	-418124
# NaSO4-	a	Na	Na(SO4)-	cnp	Na(SO4)-	-1010336
Nb(OH)4+	a	Nb+5	NbO2+	cnp	Nb|5|O2+	-752366
# Nb(OH)5	a	Nb+5	NbO3H@	cnp	Nb|5|O3H@	-992106
Ni(CO3)2-2	a	Ni	Ni(CO3)2-2	cnp	Ni(CO3)2-2	-1135817
Ni(HS)2	a	Ni	Ni(HS)2@	cnp	Ni(HS|-2|)2@	-85027
Ni(NH3)2+2	a	Ni	Ni(NH3)2+2	cnp	Ni(N|-3|H3)2+2	-126915
Ni(NH3)3+2	a	Ni	Ni(NH3)3+2	cnp	Ni(N|-3|H3)3+2	-162717
Ni(NH3)4+2	a	Ni	Ni(NH3)4+2	cnp	Ni(N|-3|H3)4+2	-195666
Ni(NH3)5+2	a	Ni	Ni(NH3)5+2	cnp	Ni(N|-3|H3)5+2	-226331
Ni(NH3)6+2	a	Ni	Ni(NH3)6+2	cnp	Ni(N|-3|H3)6+2	-252430
Ni(NO3)2	a	Ni	Ni(NO3)2@	cnp	Ni(NO3)2@	-263991
# Ni(OH)2	a	Ni	NiO@	cnp	NiO@	-180044
# Ni(OH)3-	a	Ni	NiO2H-	cnp	NiO2H-	-350443
# Ni(OH)4-2	a	Ni	NiO2-2	cnp	NiO2-2	-263681
Ni(SO4)2-2	a	Ni	Ni(SO4)2-2	cnp	Ni(SO4)2-2	-1552790
Ni2OH+3	a	Ni	Ni2(OH)+3	cnp	Ni2OH+3	-272455
Ni4(OH)4+4	a	Ni	Ni4(OH)4+4	cnp	Ni4(OH)4+4	-971900
# NiCl+	a	Ni	NiCl+	cnp	NiCl+	-179179
NiCl2	a	Ni	NiCl2@	cnp	NiCl2@	-313665
NiCO3	a	Ni	Ni(CO3)@	cnp	NiCO3@	-596419
# NiF+	a	Ni	NiF+	cnp	NiF+	-334777
NiH2PO4+	a	Ni	Ni(H2PO4)+	cnp	NiH2PO4+	-1184725
NiHCO3+	a	Ni	Ni(HCO3)+	cnp	NiHCO3+	-638254
NiHP2O7-	a	Ni	Ni(HP2O7)-	cnp	NiHP2O7-	-2039548
NiHPO4	a	Ni	Ni(HPO4)@	cnp	Ni(HPO4)@	-1151493

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Table A1: Continued

	Nagra/PSI TDB 01/01	GEMS Record Keys				Stoichiometry	$\Delta_f G^\circ$
	Name	Phase State	Group	Name	TDB Set		[J/mol]
	NiHS+	a	Ni	Ni(HS)+	cnp	Ni(HS|-2|)+	-65031
	NiNH3+2	a	Ni	Ni(NH3)+2	cnp	Ni(N|-3|H3)+2	-87687
	NiNO3+	a	Ni	Ni(NO3)+	cnp	NiNO3+	-158794
#	NiOH+	a	Ni	NiOH+	cnp	NiOH+	-228562
	NiP2O7-2	a	Ni	Ni(P2O7)-2	cnp	NiP2O7-2	-2004329
	NiPO4-	a	Ni	Ni(PO4)-	cnp	NiPO4-	-1112050
	NiSO4	a	Ni	Ni(SO4)@	cnp	Ni(SO4)@	-803250
	Np(CO3)4-4	a	Np+4	Np(CO3)4-4	cnp	Np|4|(CO3)4-4	-2812988
	Np(CO3)5-6	a	Np+4	Np(CO3)5-6	cnp	Np|4|(CO3)5-6	-3334862
	Np(OH)4	a	Np+4	Np(OH)4@	cnp	Np|4|(OH)4@	-1384427
	Np(SO4)2	a	Np+4	Np(SO4)2@	cnp	Np|4|(SO4)2@	-2043626
	NpCl+3	a	Np+4	NpCl+3	cnp	Np|4|Cl+3	-631485
	NpF+3	a	Np+4	NpF+3	cnp	Np|4|F+3	-824528
	NpF2+2	a	Np+4	NpF2+2	cnp	Np|4|F2+2	-1144751
	NpNO3+3	a	Np+4	Np(NO3)+3	cnp	Np|4|NO3+3	-613384
	NpO2(CO3)2-2	a	Np+6	NpO2(CO3)2-2	cnp	Np|6|O2(CO3)2-2	-1946160
	NpO2(CO3)2-3	a	Np+5	NpO2(CO3)2-3	cnp	Np|5|O2(CO3)2-3	-2000957
	NpO2(CO3)2OH-4	a	Np+5	NpO2(CO3)2OH-4	cnp	Np|5|O2(CO3)2OH-4	-2170614
	NpO2(CO3)3-4	a	Np+6	NpO2(CO3)3-4	cnp	Np|6|O2(CO3)3-4	-2490410
	NpO2(CO3)3-5	a	Np+5	NpO2(CO3)3-5	cnp	Np|5|O2(CO3)3-5	-2523060
	NpO2(HPO4)2-2	a	Np+6	NpO2(HPO4)2-2	cnp	Np|6|O2(HPO4)2-2	-3028406
	NpO2(OH)	a	Np+5	NpO2(OH)@	cnp	Np|5|O2(OH)@	-1080403
	NpO2(OH)2-	a	Np+5	NpO2(OH)2-	cnp	Np|5|O2(OH)2-	-1247377
	NpO2(OH)3-	a	Np+6	NpO2(OH)3-	cnp	Np|6|O2(OH)3-	-1398996
	NpO2(OH)4-2	a	Np+6	NpO2(OH)4-2	cnp	Np|6|O2(OH)4-2	-1556267
	NpO2(SO4)2-2	a	Np+6	NpO2(SO4)2-2	cnp	Np|6|O2(SO4)2-2	-2311646
	NpO2Cl+	a	Np+6	NpO2Cl+	cnp	Np|6|O2Cl+	-929473
	NpO2CO3	a	Np+6	NpO2(CO3)@	cnp	Np|6|O2CO3@	-1377081
	NpO2CO3-	a	Np+5	NpO2(CO3)-	cnp	Np|5|O2CO3-	-1464014
	NpO2F	a	Np+5	NpO2F@	cnp	Np|5|O2F@	-1196321
	NpO2F+	a	Np+6	NpO2F+	cnp	Np|6|O2F+	-1103736
	NpO2F2	a	Np+6	NpO2F2@	cnp	Np|6|O2F2@	-1402782
	NpO2H2PO4+	a	Np+6	NpO2(H2PO4)+	cnp	Np|6|O2H2PO4+	-1945157
	NpO2HPO4	a	Np+6	NpO2(HPO4)@	cnp	Np|6|O2HPO4@	-1920430
	NpO2HPO4-	a	Np+5	NpO2(HPO4)-	cnp	Np|5|O2HPO4-	-2013699
	NpO2OH+	a	Np+6	NpO2(OH)+	cnp	Np|6|O2OH+	-1003972
	NpO2SO4	a	Np+6	NpO2(SO4)@	cnp	Np|6|O2S|6|O4@	-1559081
	NpO2SO4-	a	Np+5	NpO2(SO4)-	cnp	Np|5|O2S|6|O4-	-1654691
	NpOH+2	a	Np+3	Np(OH)+2	cnp	Np|3|OH+2	-711122
	NpOH+3	a	Np+4	Np(OH)+3	cnp	Np|4|OH+3	-727161
	NpSO4+2	a	Np+4	Np(SO4)+2	cnp	Np|4|S|6|O4+2	-1275193
	Pd(NH3)2+2	a	Pd	Pd(NH3)2+2	cnp	Pd|2|(N|-3|H3)2+2	17626
	Pd(NH3)3+2	a	Pd	Pd(NH3)3+2	cnp	Pd|2|(N|-3|H3)3+2	-51854
	Pd(NH3)4+2	a	Pd	Pd(NH3)4+2	cnp	Pd|2|(N|-3|H3)4+2	-117338
#	Pd(OH)2	a	Pd	PdO@	cnp	Pd|2|O@	-37786
	Pd(OH)3-	a	Pd	PdO2H-	cnp	Pd|2|O2H-	-209327
#	PdCl+	a	Pd	PdCl+	cnp	Pd|2|Cl+	16164

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Table A1: Continued

Nagra/PSI TDB 01/01 Name	GEMS Record Keys Phase State	Group	Name	TDB Set	Stoichiometry	$\Delta_f G^\circ$ [J/mol]
# PdCl2	a	Pd	PdCl2@	cnp	Pd|2|Cl2@	-133391
PdCl2(OH)2-2	a	Pd	PdCl2(OH)2-2	cnp	Pd|2|Cl2(OH)2-2	-520424
# PdCl3-	a	Pd	PdCl3-	cnp	Pd|2|Cl3-	-279522
PdCl3OH-2	a	Pd	PdCl3(OH)-2	cnp	Pd|2|Cl3OH-2	-468757
# PdCl4-2	a	Pd	PdCl4-2	cnp	Pd|2|Cl4-2	-415378
PdNH3+2	a	Pd	Pd(NH3)+2	cnp	Pd|2|N|-3|H3+2	95098
Pu(CO3)4-4	a	Pu+4	Pu(CO3)4-4	cnp	Pu|4|(CO3)4-4	-2794843
Pu(CO3)5-6	a	Pu+4	Pu(CO3)5-6	cnp	Pu|4|(CO3)5-6	-3314833
Pu(OH)4	a	Pu+4	PuO2@	cnp	Pu|4|O2@	-904416
Pu(SO4)2	a	Pu+4	Pu(SO4)2@	cnp	Pu|4|(S|6|O4)2@	-2030503
Pu(SO4)2-	a	Pu+3	Pu(SO4)2-	cnp	Pu|3|(S|6|O4)2-	-2100427
PuCl+2	a	Pu+3	PuCl+2	cnp	Pu|3|Cl+2	-717112
PuCl+3	a	Pu+4	PuCl+3	cnp	Pu|4|Cl+3	-619562
PuF+3	a	Pu+4	PuF+3	cnp	Pu|4|F+3	-810207
PuF2+2	a	Pu+4	PuF2+2	cnp	Pu|4|F2+2	-1131115
PuH3PO4+4	a	Pu+4	Pu(H3PO4)+4	cnp	Pu|4|H3P|5|O4+4	-1634219
PuNO3+3	a	Pu+4	Pu(NO3)+3	cnp	Pu|4|N|5|O3+3	-600033
PuO2(CO3)2-2	a	Pu+6	PuO2(CO3)2-2	cnp	Pu|6|O2(CO3)2-2	-1901701
PuO2(CO3)3-4	a	Pu+6	PuO2(CO3)3-4	cnp	Pu|6|O2(CO3)3-4	-2447377
PuO2(CO3)3-5	a	Pu+5	PuO2(CO3)3-5	cnp	Pu|5|O2(CO3)3-5	-2465186
PuO2(OH)2	a	Pu+6	PuO2(OH)2@	cnp	Pu|6|O2(OH)2@	-1161420
PuO2(SO4)2-2	a	Pu+6	PuO2(SO4)2-2	cnp	Pu|6|O2(S|6|O4)2-2	-2276434
PuO2Cl+	a	Pu+6	PuO2Cl+	cnp	Pu|6|O2Cl+	-897685
PuO2Cl2	a	Pu+6	PuO2Cl2@	cnp	Pu|6|O2Cl2@	-1021555
PuO2CO3	a	Pu+6	PuO2(CO3)@	cnp	Pu|6|O2CO3@	-1343466
PuO2CO3-	a	Pu+5	PuO2(CO3)-	cnp	Pu|5|O2CO3-	-1409908
PuO2F+	a	Pu+6	PuO2F+	cnp	Pu|6|O2F+	-1070179
PuO2F2	a	Pu+6	PuO2F2@	cnp	Pu|6|O2F2@	-1367284
PuO2OH	a	Pu+5	PuO2(OH)@	cnp	Pu|5|O2OH@	-1034345
PuO2OH+	a	Pu+6	PuO2(OH)+	cnp	Pu|6|O2OH+	-968189
PuO2SO4	a	Pu+6	PuO2(SO4)@	cnp	Pu|6|O2S|6|O4@	-1526152
PuOH+2	a	Pu+3	Pu(OH)+2	cnp	Pu|3|OH+2	-776770
PuOH+3	a	Pu+4	Pu(OH)+3	cnp	Pu|4|OH+3	-710728
PuSO4+	a	Pu+3	Pu(SO4)+	cnp	Pu|3|S|6|O4+	-1345693
PuSO4+2	a	Pu+4	Pu(SO4)+2	cnp	Pu|4|S|6|O4+2	-1261785
RaCl+	a	Ra	RaCl+	cnp	RaCl+	-692212
RaCO3	a	Ra	Ra(CO3)@	cnp	RaCO3@	-1103745
RaOH+	a	Ra	Ra(OH)+	cnp	RaOH+	-721617
RaSO4	a	Ra	Ra(SO4)@	cnp	RaSO4@	-1321649
S-2	a	wS-2	S-2	cnp	S|-2|-2	120422
# SeO4-2	a	Se+6	SeO4-2	cnp	Se|6|O4-2	-450763
# Sn(OH)2	a	Sn+2	SnO@	cnp	Sn|2|O@	-220720
Sn(OH)3-	a	Sn+2	SnO2H-	cnp	Sn|2|O2H-	-401964
Sn(OH)5-	a	Sn+4	SnO3H-	cnp	Sn|4|O3H-	-671156
Sn(OH)6-2	a	Sn+4	SnO3-2	cnp	Sn|4|O3-2	-611793
Sn3(OH)4+2	a	Sn+2	Sn3(OH)4+2	cnp	Sn|2|3(OH)4+2	-999234
SnCl+	a	Sn+2	SnCl+	cnp	Sn|2|Cl+	-168482

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Table A1: Continued

Nagra/PSI TDB 01/01	GEMS Record Keys				Stoichiometry	$\Delta_f G^\circ$
Name	Phase State	Group	Name	TDB Set		[J/mol]
SnCl2	a	Sn+2	SnCl2@	cnp	Sn|2|Cl2@	-303539
SnCl3-	a	Sn+2	SnCl3-	cnp	Sn|2|Cl3-	-433345
SnF+	a	Sn+2	SnF+	cnp	Sn|2|F+	-337780
# SnOH+	a	Sn+2	SnOH+	cnp	Sn|2|(OH)+	-242981
SnOHCl	a	Sn+2	Sn(OH)Cl@	cnp	Sn|2|OHCl@	-378267
SnSO4	a	Sn+2	Sn(SO4)@	cnp	Sn|2|SO4@	-786789
# SrCO3	a	Sr	Sr(CO3)@	cnp	Sr(CO3)@	-1107830
# SrHCO3+	a	Sr	Sr(HCO3)+	cnp	SrHCO3+	-1157538
# SrOH+	a	Sr	SrOH+	cnp	Sr(OH)+	-725159
SrSO4	a	Sr	Sr(SO4)@	cnp	Sr(SO4)@	-1321366
TcCO3(OH)2	a	Tc+4	TcCO3(OH)2@	cnp	Tc|4|CO3(OH)2@	-963799
TcCO3(OH)3-	a	Tc+4	TcCO3(OH)3-	cnp	Tc|4|CO3(OH)3-	-1153605
TcO(OH)+	a	Tc+4	TcO(OH)+	cnp	Tc|4|O(OH)+	-339922
TcO(OH)3-	a	Tc+4	TcO(OH)3-	cnp	Tc|4|O(OH)3-	-737800
TcO+2	a	Tc+4	TcO+2	cnp	Tc|4|O+2	-111301
Th(CO3)5-6	a	Th	Th(CO3)5-6	cnp	Th|4|(CO3)5-6	-3515012
Th(OH)4	a	Th	ThO2@	cnp	Th|4|O2@	-1074342
Th(SO4)2	a	Th	Th(SO4)2@	cnp	Th|4|(SO4)2@	-2260135
Th(SO4)3-2	a	Th	Th(SO4)3-2	cnp	Th|4|(SO4)3-2	-3009161
ThCO3(OH)3-	a	Th	Th(CO3)(OH)3-	cnp	Th|4|CO3(OH)3-	-1926840
ThF+3	a	Th	ThF+3	cnp	Th|4|F+3	-1032419
ThF2+2	a	Th	ThF2+2	cnp	Th|4|F2+2	-1349559
ThF3+	a	Th	ThF3+	cnp	Th|4|F3+	-1658137
ThF4	a	Th	ThF4@	cnp	Th|4|F4@	-1959295
ThHPO4+2	a	Th	Th(HPO4)+2	cnp	Th|4|HPO4+2	-1868349
ThOH+3	a	Th	Th(OH)+3	cnp	Th|4|OH+3	-928488
ThSO4+2	a	Th	Th(SO4)+2	cnp	Th|4|SO4+2	-1492844
U(CO3)4-4	a	U+4	U(CO3)4-4	cnp	U|4|(CO3)4-4	-2842800
U(CO3)5-6	a	U+4	U(CO3)5-6	cnp	U|4|(CO3)5-6	-3364389
U(NO3)2+2	a	U+4	U(NO3)2+2	cnp	U|4|(NO3)2+2	-764775
# U(OH)4	a	U+4	UO2@	cnp	U|4|O2@	-952830
U(SO4)2	a	U+4	U(SO4)2@	cnp	U|4|(SO4)2@	-2078746
UCl+3	a	U+4	UCl+3	cnp	U|4|Cl+3	-670944
UF+3	a	U+4	UF+3	cnp	U|4|F+3	-864557
UF2+2	a	U+4	UF2+2	cnp	U|4|F2+2	-1185979
UF3+	a	U+4	UF3+	cnp	U|4|F3+	-1498381
UF4	a	U+4	UF4@	cnp	U|4|F4@	-1802964
UF5-	a	U+4	UF5-	cnp	U|4|F5-	-2092763
UF6-2	a	U+4	UF6-2	cnp	U|4|F6-2	-2386329
UNO3+3	a	U+4	U(NO3)+3	cnp	U|4|(NO3)+3	-649132
UO2(CO3)2-2	a	U+6	UO2(CO3)2-2	cnp	U|6|O2(CO3)2-2	-2105271
UO2(CO3)3-4	a	U+6	UO2(CO3)3-4	cnp	(U|6|O2)(CO3)3-4	-2659852
UO2(CO3)3-5	a	U+5	UO2(CO3)3-5	cnp	(U|5|O2)(CO3)3-5	-2587325
UO2(H2PO4)2	a	U+6	UO2(H2PO4)2@	cnp	U|6|O2(H2PO4)2@	-3241309
# UO2(OH)2	a	U+6	UO3@	cnp	U|6|O3@	-1121300
UO2(OH)3-	a	U+6	UO4H-	cnp	U|6|O4H-	-1317385
# UO2(OH)4-2	a	U+6	UO4-2	cnp	U|6|O4-2	-1238614

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Table A1: Continued

Nagra/PSI TDB 01/01	GEMS Record Keys				Stoichiometry	$\Delta_f G^\circ$
Name	Phase State	Group	Name	TDB Set		[J/mol]
UO2(SO4)2-2	a	U+6	UO2(SO4)2-2	cnp	Ul6lO2(SO4)2-2	-2465162
UO2Cl+	a	U+6	UO2Cl+	cnp	Ul6lO2Cl+	-1084873
UO2Cl2	a	U+6	UO2Cl2@	cnp	Ul6lO2Cl2@	-1208914
UO2CO3	a	U+6	UO2(CO3)@	cnp	Ul6lO2(CO3)@	-1535791
UO2F+	a	U+6	UO2F+	cnp	Ul6lO2F+	-1263417
UO2F2	a	U+6	UO2F2@	cnp	Ul6lO2F2@	-1565317
UO2F3-	a	U+6	UO2F3-	cnp	Ul6lO2F3-	-1860082
UO2F4-2	a	U+6	UO2F4-2	cnp	Ul6lO2F4-2	-2146399
UO2H2PO4+	a	U+6	UO2(H2PO4)+	cnp	Ul6lO2(H2PO4)+	-2101528
UO2H2PO4H3PO4+	a	U+6	UO2H5(PO4)2+	cnp	Ul6lO2H5(PO4)2+	-3247074
UO2H3PO4+2	a	U+6	UO2(H3PO4)+2	cnp	Ul6lO2(H3PO4)+2	-2099473
UO2HPO4	a	U+6	UO2(HPO4)@	cnp	Ul6lO2(HPO4)@	-2083079
UO2NO3+	a	U+6	UO2(NO3)+	cnp	Ul6lO2(NO3)+	-1065230
# UO2OH+	a	U+6	UO2OH+	cnp	Ul6lO2(OH)+	-1160114
UO2PO4-	a	U+6	UO2(PO4)-	cnp	Ul6lO2(PO4)-	-2046776
UO2SO4	a	U+6	UO2(SO4)@	cnp	Ul6lO2(SO4)@	-1715052
# UOH+3	a	U+4	U(OH)+3	cnp	Ul4l(OH)+3	-763937
USO4+2	a	U+4	U(SO4)+2	cnp	Ul4l(SO4)+2	-1311854
# Zr(OH)4	a	Zr	ZrO2@	cnp	Zrl4lO2@	-976600
# Zr(OH)5-	a	Zr	ZrO3H-	cnp	Zrl4lO3H-	-1177822
ZrCl+3	a	Zr	ZrCl+3	cnp	ZrCl+3	-697453
ZrF+3	a	Zr	ZrF+3	cnp	ZrF+3	-897574
ZrF2+2	a	Zr	ZrF2+2	cnp	ZrF2+2	-1226701
ZrF3+	a	Zr	ZrF3+	cnp	ZrF3+	-1543842
ZrF4	a	Zr	ZrF4@	cnp	ZrF4@	-1856416
ZrF5-	a	Zr	ZrF5-	cnp	Zrl4lF5-	-2164423
ZrF6-2	a	Zr	ZrF6-2	cnp	Zrl4lF6-2	-2467294
# ZrOH+3	a	Zr	Zr(OH)+3	cnp	Zrl4lOH+3	-796497
ZrSO4+2	a	Zr	Zr(SO4)+2	cnp	Zrl4lSO4+2	-1342017
Solids						
(NH4)4NpO2(CO3)3(s)	s	NpCNHO	AM4NpO2(CO3)3	dnp	(Nl-3lH4)4Npl6lO2(CO3)3	-2850458
(UO2)3(PO4)2:4H2O(cr)	s	UPOH	(UO2)3(PO4)2w4	dnp	(Ul6lO2)3(PO4)2(H2O)4	-6125634
Am(CO3)1.5(cr)	s	AmCO	Am(CO3)1.5	dnp	Am(CO3)1.5	-1485995
Am(OH)3(am)	s	AmOH	Am(OH)3(am)	dnp	Am(OH)3	-1213210
Am(OH)3(cr)	s	AmOH	Am(OH)3(cr)	dnp	Am(OH)3	-1223485
AmCO3OH(cr)	s	AmCOH	AmCO3OH(cr)	dnp	AmCO3OH	-1404961
# Anhydrite	s	CaSO	Anh	dnp	CaSO4	-1322122
# Aragonite	s	CaCO	Arg	dnp	CaCO3	-1128355
As(cr)	s	As0	As	dnp	Asl0l	0
Baddeleyite	s	ZrO	Baddeleyite	dnp	Zrl4lO2	-1042813
# Barite	s	BaSO	Brt	dnp	BaSO4	-1362152
# Brucite	s	MgOH	Brc	dnp	Mg(OH)2	-832227
# Calcite	s	CaCO	Cal	dnp	CaCO3	-1129176
CaSn(OH)6(s)	s	SnCaOH	CaSn(OH)6(s)	dnp	CaSnl4l(OH)6	-1931499
# Cassiterite	s	SnO	Cst	dnp	Snl4lO2	-525302
# Celestite	s	SrSO	Cls	dnp	SrSO4	-1346150
Chernikovite	s	UPOH	chernikovite	dnp	Ul6lO2HPO4(H2O)4	-3058137

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Table A1: Continued

Nagra/PSI TDB 01/01	GEMS Record Keys				Stoichiometry	$\Delta_f G^\circ$
Name	Phase State	Group	Name	TDB Set		[J/mol]
# Dolomite(dis)	s	CaMgCO	Dis-Dol	dnp	CaMg(CO3)2	-2157149
# Dolomite(ord)	s	CaMgCO	Ord-Dol	dnp	CaMg(CO3)2	-2160289
Eu(OH)3(am)	s	EuOH	Eu(OH)3(am)	dnp	Eu|3|(OH)3	-1185551
Eu(OH)3(cr)	s	EuOH	Eu(OH)3(cr)	dnp	Eu|3|(OH)3	-1200962
Eu2(CO3)3(cr)	s	EuCO	Eu2(CO3)3	dnp	Eu|3|2(CO3)3	-2932653
EuF3(cr)	s	EuF	EuF3	dnp	Eu|3|F3	-1519035
EuOHCO3(cr)	s	EuCOH	EuCO3OH(cr)	dnp	EuOHCO3	-1383580
Fe(cr)	s	Fe0	Fe	dnp	Fe|0|	0
Fe(OH)3(am)	s	FeOH	Fe(OH)3(am)	dnp	Fe|3|(OH)3	-700194
Fe(OH)3(mic)	s	FeOH	Fe(OH)3(mic)	dnp	Fe|3|(OH)3	-711610
FeCO3(pr)	s	FeCO	FeCO3(pr)	dnp	FeCO3	-679136
# Fluorite	s	CaF	Fl	dnp	Ca|2|F2	-1176794
# Gibbsite	s	AlOH	Gbs	dnp	Al(OH)3	-1150986
# Goethite	s	FeOH	Gt	dnp	Fe|3|O(OH)	-497259
# Graphite	s	C0	Gr	dnp	C|0|	0
Gypsum	s	CaSO	Gp	dnp	CaSO4(H2O)2	-1797763
Hausmannite	s	MnO	Hausmannite	dnp	Mn|3|2Mn|2|O4	-1291984
# Hematite	s	FeO	Hem	dnp	Fe|3|2O3	-739527
K4NpO2(CO3)3(s)	s	NpKCO	K4NpO2(CO3)3	dnp	K4Np|6|O2(CO3)3	-3660384
# Kaolinite	s	AlSiOH	Kln	dnp	Al2Si2O5(OH)4	-3777714
# Magnesite	s	MgCO	Mgs	dnp	MgCO3	-1029275
# Magnetite	s	FeO	Mag	dnp	FeFe|3|2O|-2|4	-1017412
Manganite	s	MnOH	Manganite	dnp	Mn|3|OOH	-560262
Melanterite	s	FeSO	Melanterite	dnp	FeSO4(H2O)7	-2508855
Mo(cr)	s	Mo0	Mo	dnp	Mo|0|	0
Molybdite	s	MoO	Molybdite	dnp	Mo|6|O3	-670101
Na3NpO2(CO3)2(s)	s	NpNaCO	Na3NpO2(CO3)2	dnp	Na3Np|5|O2(CO3)2	-2833235
NaNpO2CO3(s,ag)	s	NpNaCO	NaNpO2CO3	dnp	NaNp|5|O2CO3	-1764139
NaNpO2CO3:3.5H2O(s,fr)	s	NpNaCOH	NaNpO2CO3w3.5	dnp	NaNp|5|O2CO3(H2O)3.5	-2591425
Nb2O5(cr)	s	NbO	Nb2O5(cr)	dnp	Nb|5|2O5	-1564952
NbO2(cr)	s	NbO	NbO2(cr)	dnp	Nb|4|O2	-757515
NiCO3(cr)	s	NiCO	NiCO3(cr)	dnp	NiCO3	-637517
NpO2(am,hyd)	s	NpO	NpO2(am)	dnp	Np|4|O2	-957438
NpO2CO3(s)	s	NpCO	NpO2CO3	dnp	Np|6|O2CO3	-1407219
NpO2OH(am,ag)	s	NpOH	NpO2OH(am,ag)	dnp	Np|5|O2OH	-1118076
NpO2OH(am,fr)	s	NpOH	NpO2OH(am,fr)	dnp	Np|5|O2OH	-1114651
NpO3:H2O(cr)	s	NpOH	NpO3w1	dnp	Np|6|O3H2O	-1239043
# Pd(cr)	s	Pd0	Pd	dnp	Pd|0|	0
# Pd(OH)2(s)	s	PdOH	Pd(OH)2(s)	dnp	Pd|2|(OH)2	-316338
Portlandite	s	CaOH	Portlandite	dnp	Ca(OH)2	-897013
Pu(HPO4)2(am,hyd)	s	PuPOH	Pu(HPO4)2	dnp	Pu|4|(HPO4)2	-2830088
Pu(OH)3(cr)	s	PuOH	Pu(OH)3(cr)	dnp	Pu|3|(OH)3	-1200335
PuO2(hyd,ag)	s	PuO	PuO2(hyd)	dnp	Pu|4|O2	-963780
PuO2(OH)2:H2O(cr)	s	PuOH	PuO2(OH)2w1	dnp	Pu|6|O2(OH)2H2O	-1442555
PuO2CO3(s)	s	PuCO	PuO2CO3	dnp	Pu|6|O2CO3	-1371436
PuO2OH(am)	s	PuOH	PuO2OH(am)	dnp	Pu|5|O2OH	-1061344

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Table A1: Continued

Nagra/PSI TDB 01/01 Name	GEMS Record Keys Phase State	Group	Name	TDB Set	Stoichiometry	$\Delta_f G^\circ$ [J/mol]
PuPO4(s,hyd)	s	PuPO	PuPO4	dnp	Pu|3|P|5|O4	-1738036
# Pyrite	s	FeS	Py	dnp	FeS|0|S|-2|	-173165
Pyrochroite	s	MnOH	pyrochroite	dnp	Mn(OH)2	-618142
Pyrolusite	s	MnO	Pyrolusite	dnp	Mn|4|O2	-468705
# Quartz	s	SiO	Qtz	dnp	SiO2	-854793
RaCO3(cr)	s	RaCO	RaCO3	dnp	RaCO3	-1136851
RaSO4(cr)	s	RaSO	RaSO4	dnp	RaS|6|O4	-1364516
# Rhodochrosite	s	MnCO	Rds	dnp	MnCO3	-822051
Rhodochrosite(syn)	s	MnCO	Rds-Syn	dnp	MnCO3	-817827
Rutherfordine	s	UCO	rutherfordine	dnp	U|6|O2CO3	-1563304
# S(rhomb)	s	S0	Sulfur	dnp	S|0|	0
Schoepite	s	UOH	Schoepite	dnp	U|6|O3(H2O)2	-1630142
Se(cr)	s	Se0	Se	dnp	Se|0|	0
# Siderite	s	FeCO	Sd	dnp	FeCO3	-681647
# SiO2(am)	s	SiO	Amor-Sl	dnp	SiO2	-848903
# Sn(cr)	s	Sn0	Sn	dnp	Sn|0|	0
# SnO(s)	s	SnO	Sn-Ox	dnp	Sn|2|O	-250402
SnO2(am)	s	SnO	SnO2(am)	dnp	Sn|4|O2	-521306
SnS(pr)	s	SnS	SnS	dnp	Sn|2|S|-2|	-99428
# Strontianite	s	SrCO	Str	dnp	SrCO3	-1144735
TcO2:1.6H2O(s)	s	TcOH	TcO2w1.6	dnp	Tc|4|O2(H2O)1.6	-753092
Theophrastite	s	NiOH	theophrastite	dnp	Ni(OH)2	-460037
ThF4(cr)	s	ThF	ThF4	dnp	Th|4|F4	-2004389
ThO2(s)	s	ThO	ThO2(s)	dnp	Th|4|O|-2|2	-1122860
Troilite	s	FeS	Tro	dnp	Fe|2|S|-2|	-109845
Tugarinovite	s	MoO	Tugarinovite	dnp	Mo|4|O2	-535098
U(OH)2SO4(cr)	s	USOH	U(OH)2SO4(cr)	dnp	U|4|(OH)2S|6|O4	-1766756
UF4:2.5H2O(cr)	s	UFOH	UF4w2.5	dnp	U|4|F4(H2O)2.5	-2417498
# UO2(s)	s	UO	UO2	dnp	U|4|O2	-1004202
USiO4(s)	s	USiO	USiO4	dnp	U|4|SiO4	-1854670
Witherite	s	BaCO	witherite	dnp	BaCO3	-1137634
Gases						
# CH4(g)	g	C-4	CH4	enp	C|-4|H4	-50659
# CO2(g)	g	C+4	CO2	enp	CO2	-394393
# H2(g)	g	H0	H2	enp	H|0|2	0
# H2S(g)	g	S-2	H2S	enp	H2S|-2|	-33752
# N2(g)	g	N0	N2	enp	N|0|2	0
# O2(g)	g	O0	O2	enp	O|0|2	0
Not in original Nagra/PSI TDB 01/01						
# -	a	wCl+7	ClO4-	add	Cl|7|O4-	-8535
# -	a	WN0	N2@	atm	Nit|0|2	18194
# -	g	N0	N2	add	Nit|0|2	0

Table A2 Sources of thermodynamic data for aqueous species, solids, and gases. Braces around thermodynamic parameters indicate that they are not sufficient for the reliable calculation of the temperature dependence of $\log_{10}K^\circ$ or $\Delta_f G^\circ$.

Nagra/PSI: Nagra/PSI TDB 01/01 [2002HUM/BER]
Nagra/PSI*: This work, calculated from $\log_{10}K^\circ$ in Nagra/PSI TDB 01/01, see text for discussion
Nagra/PSI**: [2002THO/BER], calculated from $\log_{10}K^\circ$ in Nagra/PSI TDB 01/01, see text for discussion
PRONSPREP: This work, estimated with PRONSPREP according to [1997SVE/SHO]
slop98.dat: Datafile slop98.dat (version 30. Oct 1998) for SUPCRT92 [1992JOH/OEL]
SUPCRT92: Datafile sprons92.dat (version 15. Feb. 1991) for SUPCRT92 [1992JOH/OEL]
SUPCRT92 code: Coded into SUPCRT92
#: Aqueous species, solid, or gas also contained in slop98.dat (version 30. Oct 1998)

Nagra/PSI TDB 01/01 Name	Non-conventional Stoich.	Record Type in GEMS	Source for $\Delta_f G^\circ$ or $\log_{10}K^\circ$	Assumptions	Data for Calculation of T-Dependence	Source
Primary Master Species						
# Al+3		DComp	[1997SHO/SAS]		HKF, S°	[1997SHO/SAS]
Am+3		DComp	[1995SIL/BID]		HKF, S°	[1999MUR/SHO]
# B(OH)3		DComp	[1989SHO/HEL]		HKF, S°	[1989SHO/HEL]
# Ba+2		DComp	[1997SHO/SAS]		HKF, S°	[1997SHO/SAS]
# Br-		DComp	[1997SHO/SAS]		HKF, S°	[1997SHO/SAS]
# Ca+2		DComp	[1997SHO/SAS]		HKF, S°	[1997SHO/SAS]
# Cl-		DComp	[1997SHO/SAS]		HKF, S°	[1997SHO/SAS]
# Cs+		DComp	[1997SHO/SAS]		HKF, S°	[1997SHO/SAS]
e-						
# Eu+3		DComp	[1997SHO/SAS]		HKF, S°	[1997SHO/SAS]
# F-		DComp	[1997SHO/SAS]		HKF, S°	[1997SHO/SAS]
# Fe+2		DComp	[1997SHO/SAS]		HKF, S°	[1997SHO/SAS]
# H+		DComp	$\Delta fG^\circ = 0$		standard hydrogen scale convention	[1997SHO/SAS]
# H2O		DComp	SUPCRT92		equation of state	SUPCRT 92 code
# HAsO4-2		DComp	[1997SHO/SAS]		HKF, S°	[1997SHO/SAS]
# HCO3-		DComp	[1997SHO/SAS]		HKF, S°	[1997SHO/SAS]
# HPO4-2		DComp	[1997SHO/SAS]		HKF, S°	[1997SHO/SAS]
# I-		DComp	[1997SHO/SAS]		HKF, S°	[1997SHO/SAS]
# K+		DComp	[1997SHO/SAS]		HKF, S°	[1997SHO/SAS]
# Li+		DComp	[1997SHO/SAS]		HKF, S°	[1997SHO/SAS]
# Mg+2		DComp	[1997SHO/SAS]		HKF, S°	[1997SHO/SAS]
# Mn+2		DComp	[1997SHO/SAS]		HKF, S°	[1997SHO/SAS]
# MoO4-2		DComp	[1997SHO/SAS]		HKF, S°	[1997SHO/SAS]
# Na+		DComp	[1997SHO/SAS]		HKF, S°	[1997SHO/SAS]
# NbO3-		DComp	[1997SHO/SAS]		HKF, S°	[1997SHO/SAS]
# Ni+2		DComp	[1997SHO/SAS]		HKF, S°	[1997SHO/SAS]
# NO3-		DComp	[1997SHO/SAS]		HKF, S°	[1997SHO/SAS]
NpO2+2		DComp	Nagra/PSI		$\{S^\circ\}$	Nagra/PSI
# Pd+2		DComp	[1998SAS/SHO]		HKF, S°	[1998SAS/SHO]
PuO2+2		DComp	Nagra/PSI		$\{S^\circ\}$	Nagra/PSI
# Ra+2		DComp	[1997SHO/SAS]		HKF, S°	[1997SHO/SAS]
# SeO3-2		DComp	[1997SHO/SAS]		HKF, S°	[1997SHO/SAS]
# Si(OH)4	SiO2	DComp	[1989SHO/HEL]		HKF, S°	[1989SHO/HEL]
Sn(OH)4	SnO2	DComp	this work			
# Sn+2		DComp	[1997SHO/SAS]		HKF, S°	[1997SHO/SAS]
# SO4-2		DComp	[1997SHO/SAS]		HKF, S°	[1997SHO/SAS]
# Sr+2		DComp	[1997SHO/SAS]		HKF, S°	[1997SHO/SAS]
# TcO4-		DComp	[1997SHO/SAS]		HKF, S°	[1997SHO/SAS]
# Th+4		DComp	[1997SHO/SAS]		HKF, S°	[1997SHO/SAS]
# UO2+2		DComp	[1997SHO/SAS2]		HKF, S°	[1997SHO/SAS2]
# Zr+4		DComp	[1997SHO/SAS]		HKF, S°	[1997SHO/SAS]

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Table A2: Continued

Nagra/PSI TDB 01/01 Name	Non-conventional Stoich.	Record Type in GEMS	Source for $\Delta_f G^\circ$ or $\log_{10} K^\circ$	Assumptions	Data for Calculation of T-Dependence	Source
Secondary Master Species						
# Al(OH)4-	AlO2-	DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
# As(OH)3	HAsO2	DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
# CH4		DComp	Nagra/PSI*		HKF, S°	[1990SHO/HEL]
# CO2		DComp	Nagra/PSI*		HKF, S°	[1989SHO/HEL]
# CO3-2		DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
# Eu+2		DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
# Fe+3		DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
# H2		DComp	Nagra/PSI*		HKF, S°	[1989SHO/HEL]
# H2PO4-		DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
H2Se		DComp	Nagra/PSI*			
# H3PO4		DComp	Nagra/PSI*		HKF, S°	[1989SHO/HEL]
# HS-		DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
# HSeO4-		DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
I2		DComp	Nagra/PSI*			
# N2		DComp	Nagra/PSI*		HKF, S°	[1989SHO/HEL]
# NH3		DComp	Nagra/PSI*		HKF, S°	[1989SHO/HEL]
# NH4+		DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
Np+3		DComp	Nagra/PSI*		{S°}	Nagra/PSI
Np+4		DComp	Nagra/PSI*		{S°}	Nagra/PSI
NpO2+		DComp	Nagra/PSI*		{S°}	Nagra/PSI
# O2		DComp	Nagra/PSI*		HKF, S°	[1989SHO/HEL]
# OH-		DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
# PO4-3		DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
Pu+3		DComp	Nagra/PSI*		{S°}	Nagra/PSI
Pu+4		DComp	Nagra/PSI*		{S°}	Nagra/PSI
PuO2+		DComp	Nagra/PSI*		{S°}	Nagra/PSI
# S2O3-2		DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
# SiO(OH)3-	HSiO3-	DComp	Nagra/PSI*		HKF, S°	[1997SVE/SHO]
SiO2(OH)2-2	SiO3-2	ReacDC	Nagra/PSI	{$\Delta_r C_p^\circ = 0$}	{$\Delta_r H^\circ$}	Nagra/PSI
# SO3-2		DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
TcO(OH)2		DComp	Nagra/PSI*			
# U+4		DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
# UO2+		DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS2]
Aqueous Product Species						
(NpO2)2(OH)2+2		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isoel. 1-Term	Nagra/PSI
(NpO2)2CO3(OH)3-		ReacDC	Nagra/PSI	{$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$}		
(NpO2)3(CO3)6-6		ReacDC	Nagra/PSI	{$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$}		
(NpO2)3(OH)5+		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isoel. 1-Term	Nagra/PSI
(PuO2)2(OH)2+2		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isoel. 1-Term	Nagra/PSI
(UO2)2(OH)2+2		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isoel. 1-Term	Nagra/PSI
(UO2)2CO3(OH)3-		ReacDC	Nagra/PSI	{$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$}		
(UO2)2NpO2(CO3)6-6		ReacDC	Nagra/PSI	{$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$}		
(UO2)2OH+3		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isoel. 1-Term	Nagra/PSI
(UO2)2PuO2(CO3)6-6		ReacDC	Nagra/PSI	{$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$}		
(UO2)3(CO3)6-6		ReacDC	Nagra/PSI	{$\Delta_r C_p^\circ = 0$}	{$\Delta_r H^\circ$}	Nagra/PSI
(UO2)3(OH)4+2		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isoel. 1-Term	Nagra/PSI

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Table A2: Continued

Nagra/PSI TDB 01/01 Name	Non-conventional Stoich.	Record Type in GEMS	Source for $\Delta_f G^\circ$ or $\log_{10} K^\circ$	Assumptions	Data for Calculation of T-Dependence	Source
(UO2)3(OH)5+		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isoel. 1-Term	Nagra/PSI
(UO2)3(OH)7-		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
(UO2)3O(OH)2HCO3+		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
(UO2)4(OH)7+		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isoel. 1-Term	Nagra/PSI
# Al(OH)2+	AlO+	DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
# Al(OH)3	AlO2H	DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
Al(OH)6SiO-	AlSiO4-	ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isocoul. 1-Term	Nagra/PSI
Al(SO4)2-		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
AlF+2		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
AlF2+		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
AlF3		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
AlF4-		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
AlF5-2		ReacDC	Nagra/PSI	$\{\Delta_r C_p^\circ = 0\}$	$\{\Delta_r H^\circ\}$	Nagra/PSI
AlF6-3		ReacDC	Nagra/PSI	$\{\Delta_r C_p^\circ = 0\}$	$\{\Delta_r H^\circ\}$	Nagra/PSI
# AlOH+2		DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
AlSiO(OH)3+2	AlHSiO3+2	ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
AlSO4+		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
Am(CO3)2-		DComp	Nagra/PSI*		HKF, S°	[1999MUR/SHO]
Am(CO3)3-3		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
Am(OH)2+	AmO+	DComp	Nagra/PSI*		HKF, S°	[1999MUR/SHO]
Am(OH)3	AmO2H	DComp	Nagra/PSI*		HKF, S°	[1999MUR/SHO]
Am(SO4)2-		DComp	Nagra/PSI*		HKF, S°	[1999MUR/SHO]
AmCl+2		DComp	Nagra/PSI*		HKF, S°	[1999MUR/SHO]
AmCO3+		DComp	Nagra/PSI*		HKF, S°	[1999MUR/SHO]
AmF+2		DComp	Nagra/PSI*		HKF, S°	[1999MUR/SHO]
AmF2+		DComp	Nagra/PSI*		HKF, S°	[1999MUR/SHO]
AmH2PO4+2		DComp	Nagra/PSI*		HKF, S°	[1999MUR/SHO]
AmNO3+2		DComp	Nagra/PSI*		HKF, S°	[1999MUR/SHO]
AmOH+2		DComp	Nagra/PSI*		HKF, S°	[1999MUR/SHO]
AmSiO(OH)3+2	AmHSiO3+2	ReacDC	Nagra/PSI**	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isocoul. 1-Term	Nagra/PSI**
AmSO4+		DComp	Nagra/PSI*		HKF, S°	[1999MUR/SHO]
# As(OH)4-	AsO2-	DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
# AsO4-3		DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
# B(OH)4-	BO2-	DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
# BaCO3		DComp	Nagra/PSI*		HKF, S°	[1997SVE/SHO]
# BaHCO3+		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
# BaOH+		DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
BaSO4		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
# CaCO3		DComp	Nagra/PSI*		HKF, S°	[1997SVE/SHO]
# CaF+		DComp	Nagra/PSI*		HKF, S°	[1997SVE/SHO]
# CaHCO3+		DComp	Nagra/PSI*		HKF, S°	slop98.dat
# CaOH+		DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
# CaSiO(OH)3+	CaHSiO3+	DComp	Nagra/PSI*		HKF, S°	[1997SVE/SHO]
CaSiO2(OH)2	CaSiO3	ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
# CaSO4		DComp	Nagra/PSI*		HKF, S°	[1997SVE/SHO]
Eu(CO3)2-		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
# Eu(OH)2+	EuO+	DComp	Nagra/PSI*		HKF, S°	[1995HAA/SHO]

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Table A2: Continued

Nagra/PSI TDB 01/01 Name	Non-conventional Stoich.	Record Type in GEMS	Source for $\Delta_f G^\circ$ or $\log_{10} K^\circ$	Assumptions	Data for Calculation of T-Dependence	Source
# Eu(OH)3	EuO2H	DComp	Nagra/PSI*		HKF, S°	[1995HAA/SHO]
# Eu(OH)4-	EuO2-	DComp	Nagra/PSI*		HKF, S°	[1995HAA/SHO]
Eu(SiO(OH)3)2+	EuSi2O5+	ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
Eu(SO4)2-		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
# EuCl+2		DComp	Nagra/PSI*		HKF, S°	[1995HAA/SHO]
# EuCl2+		DComp	Nagra/PSI*		HKF, S°	[1995HAA/SHO]
# EuCO3+		DComp	Nagra/PSI*		HKF, S°	slop98.dat
# EuF+2		DComp	Nagra/PSI*		HKF, S°	[1995HAA/SHO]
# EuF2+		DComp	Nagra/PSI*		HKF, S°	[1995HAA/SHO]
EuOH+2		DComp	Nagra/PSI*		HKF, S°	[1995HAA/SHO]
EuSiO(OH)3+2	EuHSiO3+2	ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
# EuSO4+		DComp	Nagra/PSI*		HKF, S°	[1995HAA/SHO]
# Fe(OH)2+	FeO+	DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
# Fe(OH)3	FeO2H	DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
# Fe(OH)4-	FeO2-	DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
Fe(SO4)2-		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
Fe2(OH)2+4		ReacDC	Nagra/PSI	$\Delta_r C_p^\circ = 0$	isoel. 2-Term	Nagra/PSI
Fe3(OH)4+5		ReacDC	Nagra/PSI	$\Delta_r C_p^\circ = 0$	isoel. 2-Term	Nagra/PSI
# FeCl+		DComp	Nagra/PSI*		HKF, S°	[1997SVE/SHO]
# FeCl+2		DComp	Nagra/PSI*		HKF, S°	[1997SVE/SHO]
FeCl2+		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
FeCl3		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
FeCO3		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
# FeF+		DComp	Nagra/PSI*		HKF, S°	[1997SVE/SHO]
# FeF+2		DComp	Nagra/PSI*		HKF, S°	[1997SVE/SHO]
FeF2+		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
FeF3		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
FeHCO3+		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
FeHSO4+		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
FeHSO4+2		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
# FeOH+		DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
# FeOH+2		DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
FeSiO(OH)3+2	FeHSiO3+2	ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
FeSO4		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
FeSO4+		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
# H2AsO4-		DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
# H2S		DComp	Nagra/PSI*		HKF, S°	[1989SHO/HEL]
# H2SeO3		DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
# H3AsO4		DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
# HF		DComp	Nagra/PSI*		HKF, S°	[1989SHO/HEL]
# HF2-		DComp	Nagra/PSI*		HKF, S°	[1988SHO/HEL]
# HSe-		DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
# HSeO3-		DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
# HSO3-		DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
# HSO4-		DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
# I3-		DComp	Nagra/PSI*		HKF, S°	[1988SHO/HEL]
# KOH		DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]

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Table A2: Continued

Nagra/PSI TDB 01/01 Name	Non-conventional Stoich.	Record Type in GEMS	Source for $\Delta_r G^\circ$ or $\log_{10} K^\circ$	Assumptions	Data for Calculation of T-Dependence	Source
# KSO4-		DComp	Nagra/PSI*		HKF, S°	[1997SVE/SHO]
# LiOH		DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
LiSO4-		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
# MgCO3		DComp	Nagra/PSI*		HKF, S°	[1997SVE/SHO]
# MgF+		DComp	Nagra/PSI*		HKF, S°	[1997SVE/SHO]
# MgHCO3+		DComp	Nagra/PSI*		HKF, S°	slop98.dat
# MgOH+		DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
# MgSiO(OH)3+	MgHSiO3+	DComp	Nagra/PSI*		HKF, S°	[1997SVE/SHO]
MgSiO2(OH)2	MgSiO3	ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
# MgSO4		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
# MnCl+		DComp	Nagra/PSI*		HKF, S°	[1997SVE/SHO]
MnCl2		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
MnCl3-		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
MnCO3		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
# MnF+		DComp	Nagra/PSI*		HKF, S°	[1997SVE/SHO]
MnHCO3+		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
# MnOH+		DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
# MnSO4		DComp	Nagra/PSI*		HKF, S°	[1997SVE/SHO]
NaCO3-		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
# NaF		DComp	Nagra/PSI*		HKF, S°	[1997SVE/SHO]
NaHCO3		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
# NaOH		DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
# NaSO4-		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
Nb(OH)4+	NbO2+	ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
# Nb(OH)5	NbO3H	DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
Ni(CO3)2-2		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
Ni(HS)2		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
Ni(NH3)2+2		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isocoul. 1-Term	Nagra/PSI
Ni(NH3)3+2		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isocoul. 1-Term	Nagra/PSI
Ni(NH3)4+2		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isocoul. 1-Term	Nagra/PSI
Ni(NH3)5+2		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isocoul. 1-Term	Nagra/PSI
Ni(NH3)6+2		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isocoul. 1-Term	Nagra/PSI
Ni(NO3)2		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
# Ni(OH)2	NiO	DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
# Ni(OH)3-	NiO2H-	DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
# Ni(OH)4-2	NiO2-2	DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
Ni(SO4)2-2		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
Ni2OH+3		ReacDC	Nagra/PSI	$\Delta_r C_p^\circ = 0$	isoel. 2-Term	Nagra/PSI
Ni4(OH)4+4		ReacDC	Nagra/PSI	$\Delta_r C_p^\circ = 0$	isoel. 2-Term	Nagra/PSI
# NiCl+		DComp	Nagra/PSI*		HKF, S°	[1997SVE/SHO]
NiCl2		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
NiCO3		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
# NiF+		DComp	Nagra/PSI*		HKF, S°	[1997SVE/SHO]
NiH2PO4+		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
NiHCO3+		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
NiHP2O7-		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
NiHPO4		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		

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Table A2: Continued

	Nagra/PSI TDB 01/01 Name	Non-conventional Stoich.	Record Type in GEMS	Source for $\Delta_f G^\circ$ or $\log_{10} K^\circ$	Assumptions	Data for Calculation of T-Dependence	Source
	NiHS+		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
	NiNH3+2		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isocoul. 1-Term	Nagra/PSI
	NiNO3+		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
#	NiOH+		DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
	NiP2O7-2		ReacDC	Nagra/PSI	$\{\Delta_r C_p^\circ = 0\}$	$\{\Delta_r H^\circ\}$	Nagra/PSI
	NiPO4-		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
	NiSO4		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
	Np(CO3)4-4		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
	Np(CO3)5-6		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
	Np(OH)4		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isoel. 1-Term	Nagra/PSI
	Np(SO4)2		ReacDC	Nagra/PSI	$\{\Delta_r C_p^\circ = 0\}$	$\{\Delta_r H^\circ\}$	Nagra/PSI
	NpCl+3		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
	NpF+3		ReacDC	Nagra/PSI	$\{\Delta_r C_p^\circ = 0\}$	$\{\Delta_r H^\circ\}$	Nagra/PSI
	NpF2+2		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
	NpNO3+3		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
	NpO2(CO3)2-2		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
	NpO2(CO3)2-3		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
	NpO2(CO3)2OH-4		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isoel. 1-Term	Nagra/PSI
	NpO2(CO3)3-4		ReacDC	Nagra/PSI	$\{\Delta_r C_p^\circ = 0\}$	$\{\Delta_r H^\circ\}$	Nagra/PSI
	NpO2(CO3)3-5		ReacDC	Nagra/PSI	$\{\Delta_r C_p^\circ = 0\}$	$\{\Delta_r H^\circ\}$	Nagra/PSI
	NpO2(HPO4)2-2		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
	NpO2(OH)		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isocoul. 1-Term	Nagra/PSI
	NpO2(OH)2-		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
	NpO2(OH)3-		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
	NpO2(OH)4-2		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
	NpO2(SO4)2-2		ReacDC	Nagra/PSI	$\{\Delta_r C_p^\circ = 0\}$	$\{\Delta_r H^\circ\}$	Nagra/PSI
	NpO2Cl+		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
	NpO2CO3		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
	NpO2CO3-		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
	NpO2F		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
	NpO2F+		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
	NpO2F2		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
	NpO2H2PO4+		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
	NpO2HPO4		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
	NpO2HPO4-		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
	NpO2OH+		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isoel. 1-Term	Nagra/PSI
	NpO2SO4		ReacDC	Nagra/PSI	$\{\Delta_r C_p^\circ = 0\}$	$\{\Delta_r H^\circ\}$	Nagra/PSI
	NpO2SO4-		ReacDC	Nagra/PSI	$\{\Delta_r C_p^\circ = 0\}$	$\{\Delta_r H^\circ\}$	Nagra/PSI
	NpOH+2		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isoel. 1-Term	Nagra/PSI
	NpOH+3		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isoel. 1-Term	Nagra/PSI
	NpSO4+2		ReacDC	Nagra/PSI	$\{\Delta_r C_p^\circ = 0\}$	$\{\Delta_r H^\circ\}$	Nagra/PSI
	Pd(NH3)2+2		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isocoul. 1-Term	Nagra/PSI
	Pd(NH3)3+2		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isocoul. 1-Term	Nagra/PSI
	Pd(NH3)4+2		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isocoul. 1-Term	Nagra/PSI
#	Pd(OH)2	PdO	DComp	Nagra/PSI*		HKF, S°	[1998SAS/SHO]
	Pd(OH)3-	PdO2H-	ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
#	PdCl+		DComp	Nagra/PSI*		HKF, S°	[1998SAS/SHO]

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Table A2: Continued

Nagra/PSI TDB 01/01 Name	Non-conventional Stoich.	Record Type in GEMS	Source for $\Delta_f G^\circ$ or $\log_{10} K^\circ$	Assumptions	Data for Calculation of T-Dependence	Source
# PdCl2		DComp	Nagra/PSI*		HKF, S°	[1998SAS/SHO]
PdCl2(OH)2-2		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isoel. 1-Term	Nagra/PSI
# PdCl3-		DComp	Nagra/PSI*		HKF, S°	[1998SAS/SHO]
PdCl3OH-2		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
# PdCl4-2		DComp	Nagra/PSI*		HKF, S°	[1998SAS/SHO]
PdNH3+2		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isocoul. 1-Term	Nagra/PSI
Pu(CO3)4-4		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
Pu(CO3)5-6		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
Pu(OH)4	PuO2	ReacDC	Nagra/PSI**	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isocoul. 1-Term	Nagra/PSI**
Pu(SO4)2		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
Pu(SO4)2-		ReacDC	Nagra/PSI	$\{\Delta_r C_p^\circ = 0\}$	$\{\Delta_r H^\circ\}$	Nagra/PSI
PuCl+2		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
PuCl+3		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
PuF+3		ReacDC	Nagra/PSI	$\{\Delta_r C_p^\circ = 0\}$	$\{\Delta_r H^\circ\}$	Nagra/PSI
PuF2+2		ReacDC	Nagra/PSI	$\{\Delta_r C_p^\circ = 0\}$	$\{\Delta_r H^\circ\}$	Nagra/PSI
PuH3PO4+4		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isocoul. 1-Term	Nagra/PSI
PuNO3+3		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
PuO2(CO3)2-2		ReacDC	Nagra/PSI	$\{\Delta_r C_p^\circ = 0\}$	$\{\Delta_r H^\circ\}$	Nagra/PSI
PuO2(CO3)3-4		ReacDC	Nagra/PSI	$\{\Delta_r C_p^\circ = 0\}$	$\{\Delta_r H^\circ\}$	Nagra/PSI
PuO2(CO3)3-5		ReacDC	Nagra/PSI	$\{\Delta_r C_p^\circ = 0\}$	$\{\Delta_r H^\circ\}$	Nagra/PSI
PuO2(OH)2		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isoel. 1-Term	Nagra/PSI
PuO2(SO4)2-2		ReacDC	Nagra/PSI	$\{\Delta_r C_p^\circ = 0\}$	$\{\Delta_r H^\circ\}$	Nagra/PSI
PuO2Cl+		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
PuO2Cl2		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
PuO2CO3		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
PuO2CO3-		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
PuO2F+		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
PuO2F2		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
PuO2OH		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isocoul. 1-Term	Nagra/PSI
PuO2OH+		ReacDC	Nagra/PSI	$\Delta_r C_p^\circ = 0$	isoel. 2-Term	Nagra/PSI
PuO2SO4		ReacDC	Nagra/PSI	$\{\Delta_r C_p^\circ = 0\}$	$\{\Delta_r H^\circ\}$	Nagra/PSI
PuOH+2		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isoel. 1-Term	Nagra/PSI
PuOH+3		ReacDC	Nagra/PSI	$\Delta_r C_p^\circ = 0$	isoel. 2-Term	Nagra/PSI
PuSO4+		ReacDC	Nagra/PSI	$\{\Delta_r C_p^\circ = 0\}$	$\{\Delta_r H^\circ\}$	Nagra/PSI
PuSO4+2		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
RaCl+		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
RaCO3		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
RaOH+		ReacDC	Nagra/PSI	$\{\Delta_r C_p^\circ = 0\}$	$\{\Delta_r H^\circ\}$	Nagra/PSI
RaSO4		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
S-2		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
# SeO4-2		DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
# Sn(OH)2	SnO	DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
Sn(OH)3-	SnO2H-	DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
Sn(OH)5-	SnO3H-	ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
Sn(OH)6-2	SnO3-2	ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
Sn3(OH)4+2		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isoel. 1-Term	Nagra/PSI
SnCl+		DComp	Nagra/PSI*		HKF, S°	PRONSPREP

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Table A2: Continued

	Nagra/PSI TDB 01/01 Name	Non-conventional Stoich.	Record Type in GEMS	Source for $\Delta_f G^\circ$ or $\log_{10} K^\circ$	Assumptions	Data for Calculation of T-Dependence	Source
	SnCl2		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
	SnCl3-		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
	SnF+		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
#	SnOH+		DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
	SnOHCl		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
	SnSO4		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
#	SrCO3		DComp	Nagra/PSI*		HKF, S°	[1997SVE/SHO]
#	SrHCO3+		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
#	SrOH+		DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
	SrSO4		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
	TcCO3(OH)2		ReacDC	Nagra/PSI**	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isocoul. 1-Term	Nagra/PSI**
	TcCO3(OH)3-		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
	TcO(OH)+		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isocoul. 1-Term	Nagra/PSI
	TcO(OH)3-		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
	TcO+2		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isoel. 1-Term	Nagra/PSI
	Th(CO3)5-6		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
	Th(OH)4	ThO2	ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isoel. 1-Term	Nagra/PSI
	Th(SO4)2		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
	Th(SO4)3-2		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
	ThCO3(OH)3-		ReacDC	Nagra/PSI**	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isocoul. 1-Term	Nagra/PSI**
	ThF+3		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
	ThF2+2		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
	ThF3+		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
	ThF4		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
	ThHPO4+2		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
	ThOH+3		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isoel. 1-Term	Nagra/PSI
	ThSO4+2		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
	U(CO3)4-4		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
	U(CO3)5-6		ReacDC	Nagra/PSI	$\{\Delta_r C_p^\circ = 0\}$	$\{\Delta_r H^\circ\}$	Nagra/PSI
	U(NO3)2+2		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
#	U(OH)4	UO2	DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS2]
	U(SO4)2		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
	UCl+3		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
	UF+3		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
	UF2+2		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
	UF3+		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
	UF4		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
	UF5-		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
	UF6-2		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
	UNO3+3		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
	UO2(CO3)2-2		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
	UO2(CO3)3-4		ReacDC	Nagra/PSI	$\{\Delta_r C_p^\circ = 0\}$	$\{\Delta_r H^\circ\}$	Nagra/PSI
	UO2(CO3)3-5		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
	UO2(H2PO4)2		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isoel. 1-Term	Nagra/PSI
#	UO2(OH)2	UO3	DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS2]
	UO2(OH)3-	UO4H-	DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS2]
#	UO2(OH)4-2	UO4-2	DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS2]

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Table A2: Continued

Nagra/PSI TDB 01/01 Name	Non-conventional Stoich.	Record Type in GEMS	Source for $\Delta_f G^\circ$ or $\log_{10} K^\circ$	Assumptions	Data for Calculation of T-Dependence	Source
UO2(SO4)2-2		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
UO2Cl+		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
UO2Cl2		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
UO2CO3		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
UO2F+		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
UO2F2		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
UO2F3-		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
UO2F4-2		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
UO2H2PO4+		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isoel. 1-Term	Nagra/PSI
UO2H2PO4H3PO4+		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isoel. 1-Term	Nagra/PSI
UO2H3PO4+2		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isocoul. 1-Term	Nagra/PSI
UO2HPO4		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
UO2NO3+		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
# UO2OH+		DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS2]
UO2PO4-		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
UO2SO4		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
# UOH+3		DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS2]
USO4+2		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
# Zr(OH)4	ZrO2	DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
# Zr(OH)5-	ZrO3H-	DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
ZrCl+3		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
ZrF+3		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
ZrF2+2		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
ZrF3+		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
ZrF4		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
ZrF5-		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
ZrF6-2		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
# ZrOH+3		DComp	Nagra/PSI*		HKF, S°	[1997SHO/SAS]
ZrSO4+2		DComp	Nagra/PSI*		HKF, S°	PRONSPREP
Solids						
(NH4)4NpO2(CO3)3(s)		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
(UO2)3(PO4)2:4H2O(cr)		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isoel. 1-Term	Nagra/PSI
Am(CO3)1.5(cr)		ReacDC	Nagra/PSI**	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isocoul. 1-Term	Nagra/PSI**
Am(OH)3(am)		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isoel. 1-Term	Nagra/PSI
Am(OH)3(cr)		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isoel. 1-Term	Nagra/PSI
AmCO3OH(cr)		ReacDC	Nagra/PSI**	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isocoul. 1-Term	Nagra/PSI**
# Anhydrite		DComp	Nagra/PSI*		$C_p^\circ(T)$, S°	[1978HEL/DEL]
# Aragonite		DComp	Nagra/PSI*		$C_p^\circ(T)$, S°	[1978HEL/DEL]
As(cr)		DComp	$\Delta_f G^\circ = 0$		$C_p^\circ(T)$, S°	[1995ROB/HEM]
Baddeleyite		DComp	Nagra/PSI*		$C_p^\circ(T)$, S°	[1995ROB/HEM]
# Barite		DComp	Nagra/PSI*		$C_p^\circ(T)$, S°	[1978HEL/DEL]
# Brucite		DComp	Nagra/PSI*		$C_p^\circ(T)$, S°	[1978HEL/DEL]
# Calcite		DComp	Nagra/PSI*		$C_p^\circ(T)$, S°	[1978HEL/DEL]
CaSn(OH)6(s)		ReacDC	this work	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isoel. 1-Term	Nagra/PSI
# Cassiterite		DComp	this work		$C_p^\circ(T)$, S°	[1985JAC/HEL]
# Celestite		DComp	Nagra/PSI*		$\{S^\circ\}$	[1978HEL/DEL]
Chernikovite		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isoel. 1-Term	Nagra/PSI

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Table A2: Continued

Nagra/PSI TDB 01/01 Name	Non-conventional Stoich.	Record Type in GEMS	Source for $\Delta_f G^\circ$ or $\log_{10} K^\circ$	Assumptions	Data for Calculation of T-Dependence	Source
# Dolomite(dis)		DComp	Nagra/PSI*		$C_p^\circ(T)$, S°	[1978HEL/DEL]
# Dolomite(ord)		DComp	Nagra/PSI*		$C_p^\circ(T)$, S°	[1978HEL/DEL]
Eu(OH)3(am)		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isoel. 1-Term	Nagra/PSI
Eu(OH)3(cr)		ReacDC	Nagra/PSI	$\Delta_r C_p^\circ = 0$	isoel. 2-Term	Nagra/PSI
Eu2(CO3)3(cr)		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
EuF3(cr)		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
EuOHCO3(cr)		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
Fe(cr)		DComp	$\Delta_f G^\circ = 0$		$C_p^\circ(T)$ S°	[1993KUB/ALC] [1982WAG/EVA]
Fe(OH)3(am)		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isoel. 1-Term	Nagra/PSI
Fe(OH)3(mic)		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isoel. 1-Term	Nagra/PSI
FeCO3(pr)		ReacDC	Nagra/PSI		$\Delta_r H^\circ$, $\Delta_r C_p^\circ$	Nagra/PSI
# Fluorite		DComp	Nagra/PSI*		$C_p^\circ(T)$, S°	[1978HEL/DEL]
# Gibbsite		DComp	Nagra/PSI*		$C_p^\circ(T)$, S°	[1978HEL/DEL]
# Goethite		DComp	Nagra/PSI*		$\{S^\circ\}$	[1995ROB/HEM]
# Graphite		DComp	$\Delta_f G^\circ = 0$		$C_p^\circ(T)$, S°	[1978HEL/DEL]
Gypsum		DComp	Nagra/PSI*		$C_p^\circ(T)$ S°	[1960KEL] [1995ROB/HEM]
Hausmannite		DComp	Nagra/PSI*		$C_p^\circ(T)$, S°	[1995ROB/HEM]
# Hematite		DComp	Nagra/PSI*		$C_p^\circ(T)$, S°	[1978HEL/DEL]
K4NpO2(CO3)3(s)		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
# Kaolinite		DComp	Nagra/PSI*		$C_p^\circ(T)$, S°	[1978HEL/DEL]
# Magnesite		DComp	Nagra/PSI*		$C_p^\circ(T)$, S°	[1978HEL/DEL]
# Magnetite		DComp	Nagra/PSI*		$C_p^\circ(T)$, S°	[1978HEL/DEL]
Manganite		DComp	Nagra/PSI*		$C_p^\circ(T)$, $S^\circ = 0$	not known
Melanterite		DComp	Nagra/PSI*		$\{S^\circ\}$	[1995ROB/HEM]
Mo(cr)		DComp	$\Delta_f G^\circ = 0$		$C_p^\circ(T)$, S°	[1995ROB/HEM]
Molybdite		DComp	Nagra/PSI*		$C_p^\circ(T)$, S°	[1995ROB/HEM]
Na3NpO2(CO3)2(s)		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
NaNpO2CO3(s,ag)		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
NaNpO2CO3:3.5H2O(s,fr)		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
Nb2O5(cr)		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
NbO2(cr)		DComp	Nagra/PSI*		$C_p^\circ(T)$ S°	[1961KIN/CHR] [1958KIN]
NiCO3(cr)		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
NpO2(am,hyd)		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isoel. 1-Term	Nagra/PSI
NpO2CO3(s)		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
NpO2OH(am,ag)		ReacDC	Nagra/PSI	$\Delta_r C_p^\circ = 0$	isocoul. 2-Term	Nagra/PSI
NpO2OH(am,fr)		ReacDC	Nagra/PSI	$\Delta_r C_p^\circ = 0$	isocoul. 2-Term	Nagra/PSI
NpO3:H2O(cr)		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isoel. 1-Term	Nagra/PSI
# Pd(cr)		DComp	$\Delta_f G^\circ = 0$		$C_p^\circ(T)$, S°	[1998SAS/SHO]
# Pd(OH)2(s)		DComp	Nagra/PSI*		$C_p^\circ(T)$, S°	[1998SAS/SHO]
Portlandite		DComp	Nagra/PSI*		$C_p^\circ(T)$, S°	[1995ROB/HEM]
Pu(HPO4)2(am,hyd)		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
Pu(OH)3(cr)		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isoel. 1-Term	Nagra/PSI
PuO2(hyd,ag)		ReacDC	Nagra/PSI**	$\Delta_r H^\circ = \Delta_r C_p^\circ = 0$	1-Term	Nagra/PSI**
PuO2(OH)2:H2O(cr)		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isoel. 1-Term	Nagra/PSI
PuO2CO3(s)		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
PuO2OH(am)		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isocoul. 1-Term	Nagra/PSI

continued on next page

Table A2: Continued

Nagra/PSI TDB 01/01 Name	Non-conventional Stoich.	Record Type in GEMS	Source for $\Delta_f G^\circ$ or $\log_{10} K^\circ$	Assumptions	Data for Calculation of T-Dependence	Source
PuPO4(s,hyd)		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
# Pyrite		DComp	Nagra/PSI*		$C_p^\circ(T)$, S°	[1978HEL/DEL]
Pyrochroite		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$	isoel. 1-Term	Nagra/PSI
Pyrolusite		DComp	Nagra/PSI*		$C_p^\circ(T)$, S°	[1995ROB/HEM]
# Quartz		DComp	Nagra/PSI*		$C_p^\circ(T)$, S°	[1978HEL/DEL]
RaCO3(cr)		ReacDC	Nagra/PSI	$\{\Delta_r C_p^\circ = 0\}$	$\{\Delta_r H^\circ\}$	Nagra/PSI
RaSO4(cr)		ReacDC	Nagra/PSI	$\{\Delta_r C_p^\circ = 0\}$	$\{\Delta_r H^\circ\}$	Nagra/PSI
# Rhodochrosite		DComp	Nagra/PSI*		$C_p^\circ(T)$, S°	[1978HEL/DEL]
Rhodochrosite(syn)		ReacDC	Nagra/PSI		$\Delta_r H^\circ$, $\Delta_r C_p^\circ$	Nagra/PSI
Rutherfordine		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
# S(rhomb)		DComp	$\Delta_f G^\circ = 0$		$C_p^\circ(T)$, S°	[1997MCC/SHO]
Schoepite		DComp	Nagra/PSI*		$\{C_p^\circ, S^\circ\}$	Nagra/PSI
Se(cr)		DComp	$\Delta_f G^\circ = 0$		$\{C_p^\circ, S^\circ\}$	[1999RAR/RAN]
# Siderite		DComp	Nagra/PSI*		$C_p^\circ(T)$, S°	[1978HEL/DEL] [1985HEL]
# SiO2(am)		DComp	Nagra/PSI*		$C_p^\circ(T)$, S°	[1978HEL/DEL]
# Sn(cr)		DComp	$\Delta_f G^\circ = 0$		$C_p^\circ(T)$, S°	[1985JAC/HEL]
# SnO(s)		DComp	Nagra/PSI*		$C_p^\circ(T)$, S°	[1985JAC/HEL]
SnO2(am)		ReacDC	this work	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
SnS(pr)		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
# Strontianite		DComp	Nagra/PSI*		$C_p^\circ(T)$, S°	[1978HEL/DEL]
TcO2:1.6H2O(s)		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	1-Term	Nagra/PSI
Theophrastite		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isoel. 1-Term	Nagra/PSI
ThF4(cr)		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
ThO2(s)		DComp	Nagra/PSI*		$C_p^\circ(T)$, S°	[1995ROB/HEM]
Troilite		DComp	Nagra/PSI*		$\{S^\circ\}$	[1995ROB/HEM]
Tugarinovite		DComp	Nagra/PSI*		$C_p^\circ(T)$ S°	[1960KIN/WEL] [1958KIN]
U(OH)2SO4(cr)		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
UF4:2.5H2O(cr)		ReacDC	Nagra/PSI	$\{\Delta_r S^\circ = \Delta_r C_p^\circ = 0\}$		
# UO2(s)		DComp	Nagra/PSI*		$C_p^\circ(T)$, S°	[1997SHO/SAS2]
USiO4(s)		ReacDC	Nagra/PSI	$\Delta_r S^\circ = \Delta_r C_p^\circ = 0$	isoel. 1-Term	Nagra/PSI
Witherite		ReacDC	Nagra/PSI		$\Delta_r H^\circ$, $\Delta_r C_p^\circ$	Nagra/PSI
Gases						
# CH4(g)		DComp	Nagra/PSI*		$C_p^\circ(T)$, S°	[1960KEL] [1982WAG/EVA]
# CO2(g)		DComp	Nagra/PSI*		$C_p^\circ(T)$, S°	[1960KEL] [1982WAG/EVA]
# H2(g)		DComp	Nagra/PSI*		$C_p^\circ(T)$, S°	[1960KEL] [1982WAG/EVA]
# H2S(g)		DComp	Nagra/PSI*		$C_p^\circ(T)$, S°	[1960KEL] [1982WAG/EVA]
# N2(g)		DComp	Nagra/PSI*		$C_p^\circ(T)$, S°	[1960KEL] [1982WAG/EVA]
# O2(g)		DComp	Nagra/PSI*		$C_p^\circ(T)$, S°	[1960KEL] [1982WAG/EVA]
Not in original Nagra/PSI TDB 01/01; for identification, GEMS record keys are indicated (see Table A1, p. 32)						
# a:wCl+7:ClO4-:add:		DComp	[1997SHO/SAS]		HKF, S°	[1997SHO/SAS]
# a:WN0:N2@:atm:		DComp	Nagra/PSI*		HKF, S°	[1989SHO/HEL]
# g:N0:N2:add:		DComp	Nagra/PSI*		$C_p^\circ(T)$, S°	[1960KEL] [1982WAG/EVA]