

# Chapter III

## Selected thorium data

This chapter presents the chemical thermodynamic data set for thorium species that has been selected in this review. Table III-1 contains the recommended thermodynamic data of the thorium compounds and species, Table III-2 the recommended thermodynamic data of chemical equilibrium reactions by which the thorium compounds and complexes are formed, and Table II-3 the temperature coefficients of the heat capacity data of Table III-1 where available.

The species and reactions in the tables appear in standard order of arrangement. Table III-2 contains information only on those reactions for which primary data selections are made in Chapter V of this review. These selected reaction data are used, together with data for key thorium species and auxiliary data selected in this review, to derive the corresponding formation data in Table III-1. The uncertainties associated with values for key thorium species and the auxiliary data are in some cases substantial, leading to comparatively large uncertainties in the formation quantities derived in this manner.

The values of  $\Delta_f G_m^\circ$  for many reactions are known more accurately than would be calculated directly from the uncertainties of the  $\Delta_f G_m^\circ$  values in Table III-1 and auxiliary data. The inclusion of a table for reaction data (Table III-2) in this report allows the use of equilibrium constants with total uncertainties that are based directly on the experimental accuracies. This is the main reason for including both Table III-1 and Table III-2.

The selected thermal functions of the heat capacities, listed in Table II-3 refer to the relation

$$C_{p,m}^\circ(T) = a + b \times T + c \times T^2 + d \times T^{-1} + e \times T^{-1/2}$$

A detailed discussion of the selection procedure is presented in Chapter V. It may be noted that this chapter contains data on more species or compounds than are present in the tables of Chapter III. The main reasons for this situation are the lack of information for a proper extrapolation of the primary data to standard conditions in some systems and lack of solid primary data in others.

A warning: The addition of any aqueous species and their data to this internally consistent data base can result in a modified data set, which is no longer rigorous and can lead to erroneous results. The situation is similar when gases or solids are added.

Table III-1: Selected thermodynamic data for thorium compounds and complexes. All ionic species listed in this table are aqueous species. Unless noted otherwise, all data refer to the reference temperature of 298.15 K and to the standard state, *i.e.*, a pressure of 0.1 MPa and, for aqueous species, infinite dilution ( $I = 0$ ). The uncertainties listed below each value represent total uncertainties and correspond in principle to the statistically defined 95% confidence interval. Values obtained from internal calculation, *cf.* footnotes (a) and (b), are rounded at the third digit after the decimal point and may therefore not be exactly identical to those given in Chapters V to XII. Systematically, all the values are presented with three digits after the decimal point, regardless of the significance of these digits. The data presented in this table are available on computer media from the OECD Nuclear Energy Agency.

Compound	$\Delta_f G_m^\circ$ (kJ·mol <sup>-1</sup> )	$\Delta_f H_m^\circ$ (kJ·mol <sup>-1</sup> )	$S_m^\circ$ (J·K <sup>-1</sup> ·mol <sup>-1</sup> )	$C_{p,m}^\circ$ (J·K <sup>-1</sup> ·mol <sup>-1</sup> )
Th(cr, $\alpha$ ) (fcc)	0.000	0.000	52.640 ±0.500	26.230 ±0.500
Th(g)	560.995 <sup>(a)</sup> ±6.002	602.000 ±6.000	190.170 ±0.010	20.790 ±0.005
Th <sup>4+</sup>	– 704.783 <sup>(a)</sup> ±5.298	– 768.700 ±2.300	– 423.100 ±16.000	– 224.000 ±15.000
ThO(g)	– 51.299 <sup>(a)</sup> ±6.002	– 26.000 ±6.000	240.070 ±0.050	31.270 ±0.100
ThO <sub>2</sub> (cr)	– 1168.988 <sup>(a)</sup> ±3.504	– 1226.400 ±3.500	65.230 ±0.200	61.740 ±0.150
ThO <sub>2</sub> (g)	– 462.128 <sup>(a)</sup> ±15.430	– 455.000 <sup>(b)</sup> ±15.403	281.700 ±3.000	46.840 ±0.500
ThH(g)			233.500 ±5.000	29.600 ±4.000
ThH <sub>2</sub> (cr)	– 105.468 <sup>(a)</sup> ±2.006	– 145.000 ±2.000	50.730 ±0.100	36.710 ±0.070
ThD <sub>2</sub> (cr)			55.720 ±0.560	47.670 ±0.470
ThT <sub>2</sub> (cr)			60.460 ±0.600	54.300 ±0.540
ThH <sub>3.75</sub> (cr)	– 142.877 <sup>(a)</sup> ±8.001	– 215.400 ±8.000	54.420 ±0.110	51.320 ±0.100
ThD <sub>3.75</sub> (cr)			63.970 ±0.640	69.710 ±0.700
ThT <sub>3.75</sub> (cr)			72.650 ±0.730	81.490 ±0.810

(Continued on next page)

Table III-1 (Continued)

Compound	$\Delta_f G_m^\circ$ (kJ·mol <sup>-1</sup> )	$\Delta_f H_m^\circ$ (kJ·mol <sup>-1</sup> )	$S_m^\circ$ (J·K <sup>-1</sup> ·mol <sup>-1</sup> )	$C_{p,m}^\circ$ (J·K <sup>-1</sup> ·mol <sup>-1</sup> )
Th(OH) <sup>3+</sup>	– 927.653 <sup>(b)</sup> ± 6.018	– 1010.330 <sup>(b)</sup> ± 6.707	– 252.765 <sup>(b)</sup> ± 28.180	
Th(OH) <sub>2</sub> <sup>2+</sup>	– 1143.673 <sup>(b)</sup> ± 6.018	– 1254.660 <sup>(b)</sup> ± 41.464	– 114.459 <sup>(b)</sup> ± 140.102	
Th(OH) <sub>4</sub> (aq)	– 1554.024 <sup>(b)</sup> ± 6.638			
Th <sub>2</sub> (OH) <sub>2</sub> <sup>6+</sup>	– 1850.168 <sup>(b)</sup> ± 10.974	– 2050.760 <sup>(b)</sup> ± 7.325	– 623.716 <sup>(b)</sup> ± 38.485	
Th <sub>2</sub> (OH) <sub>3</sub> <sup>5+</sup>	– 2082.171 <sup>(b)</sup> ± 10.658			
Th <sub>4</sub> (OH) <sub>8</sub> <sup>8+</sup>	– 4599.809 <sup>(b)</sup> ± 21.317	– 5118.440 <sup>(b)</sup> ± 23.204	– 708.329 <sup>(b)</sup> ± 96.221	
Th <sub>4</sub> (OH) <sub>12</sub> <sup>4+</sup>	– 5512.980 <sup>(b)</sup> ± 21.228			
Th <sub>6</sub> (OH) <sub>14</sub> <sup>10+</sup>	– 7338.604 <sup>(b)</sup> ± 32.523			
Th <sub>6</sub> (OH) <sub>15</sub> <sup>9+</sup>	– 7575.744 <sup>(b)</sup> ± 32.927	– 8426.850 <sup>(b)</sup> ± 25.977	– 608.102 <sup>(b)</sup> ± 124.441	
ThF(g)	– 0.788 <sup>(a)</sup> ± 15.422	30.000 ± 15.000	257.300 ± 12.000	34.700 ± 6.000
ThF <sup>3+</sup>	– 1036.936 <sup>(b)</sup> ± 5.411	– 1104.450 <sup>(b)</sup> ± 3.116	– 268.427 <sup>(b)</sup> ± 17.604	
ThF <sub>2</sub> (g)	– 601.857 <sup>(a)</sup> ± 20.222	– 590.000 ± 20.000	295.200 ± 10.000	52.400 ± 5.000
ThF <sub>2</sub> <sup>2+</sup>	– 1357.046 <sup>(b)</sup> ± 5.631	– 1442.700 <sup>(b)</sup> ± 2.672	– 162.534 <sup>(b)</sup> ± 16.726	
ThF <sub>3</sub> (g)	– 1159.774 <sup>(a)</sup> ± 15.294	– 1165.000 ± 15.000	339.300 ± 10.000	73.300 ± 5.000
ThF <sub>3</sub> <sup>+</sup>	– 1667.337 <sup>(b)</sup> ± 5.763			
ThF <sub>4</sub> (cr)	– 2005.736 <sup>(a)</sup> ± 10.001	– 2100.000 ± 10.000	142.060 ± 0.170	110.710 ± 0.130
ThF <sub>4</sub> (g)	– 1719.328 <sup>(a)</sup> ± 10.217	– 1750.700 <sup>(b)</sup> ± 10.198	353.000 ± 2.000	93.400 ± 2.000
ThF <sub>4</sub> (aq)	– 1976.887 <sup>(b)</sup> ± 6.066			

(Continued on next page)

Table III-1 (Continued)

Compound	$\Delta_f G_m^o$ (kJ·mol <sup>-1</sup> )	$\Delta_f H_m^o$ (kJ·mol <sup>-1</sup> )	$S_m^o$ (J·K <sup>-1</sup> ·mol <sup>-1</sup> )	$C_{p,m}^o$ (J·K <sup>-1</sup> ·mol <sup>-1</sup> )
ThOF(g)	– 566.186 <sup>(a)</sup> ±12.366	– 550.000 ±12.000	310.900 ±10.000	49.500 ±5.000
ThOF <sub>2</sub> (cr)	– 1589.171 <sup>(a)</sup> ±7.948	– 1663.800 ±7.800	107.700 ±5.100	
ThCl(g)	215.688 <sup>(a)</sup> ±20.318	247.000 ±20.000	269.200 ±12.000	36.400 ±6.000
ThCl <sup>3+</sup>	– 845.704 <sup>(b)</sup> ±5.330			
ThCl <sub>2</sub> (g)	– 191.337 <sup>(a)</sup> ±22.202	– 179.000 ±22.000	317.100 ±10.000	55.300 ±5.000
ThCl <sub>3</sub> (g)	– 563.764 <sup>(a)</sup> ±25.178	– 569.000 ±25.000	369.700 ±10.000	78.000 ±5.000
$\beta$ -ThCl <sub>4</sub>	– 1092.293 <sup>(a)</sup> ±1.984	– 1186.300 ±1.300	183.500 ±5.000	120.300 ±6.000
ThCl <sub>4</sub> · 2 H <sub>2</sub> O(cr)		– 1822.400 ±12.000		
ThCl <sub>4</sub> · 4 H <sub>2</sub> O(cr)		– 2456.200 ±12.000		
ThCl <sub>4</sub> · 7 H <sub>2</sub> O(cr)		– 3361.900 ±12.000		
ThCl <sub>4</sub> · 8 H <sub>2</sub> O(cr)		– 3661.300 ±12.000		
ThCl <sub>4</sub> (g)	– 922.956 <sup>(a)</sup> ±5.304	– 951.400 <sup>(b)</sup> ±5.166	403.400 ±4.000	101.400 ±3.000
ThOCl <sub>2</sub> (cr)	– 1153.564 <sup>(a)</sup> ±2.276	– 1231.500 ±2.100	116.900 ±2.900	
ThClO <sub>3</sub> <sup>3+</sup>	– 721.534 <sup>(b)</sup> ±5.515			
ThBr(g)	319.575 <sup>(a)</sup> ±20.318	365.000 ±20.000	281.100 ±12.000	37.400 ±6.000
ThBr <sup>3+</sup>	– 816.510 <sup>(b)</sup> ±5.352			
ThBr <sub>2</sub> (g)	– 0.027 <sup>(a)</sup> ±20.222	40.000 ±20.000	339.100 ±10.000	56.700 ±5.000
ThBr <sub>3</sub> (g)	– 371.073 <sup>(a)</sup> ±15.295	– 334.000 ±15.000	405.300 ±10.000	80.800 ±5.000

(Continued on next page)

Table III-1 (Continued)

Compound	$\Delta_f G_m^{\circ}$ (kJ·mol <sup>-1</sup> )	$\Delta_f H_m^{\circ}$ (kJ·mol <sup>-1</sup> )	$S_m^{\circ}$ (J·K <sup>-1</sup> ·mol <sup>-1</sup> )	$C_{p,m}^{\circ}$ (J·K <sup>-1</sup> ·mol <sup>-1</sup> )
$\beta$ -ThBr <sub>4</sub>	-925.023 <sup>(a)</sup> ±2.505	-963.800 ±2.000	227.000 ±5.000	125.200 ±6.000
ThBr <sub>4</sub> ·7 H <sub>2</sub> O(cr)		-3163.900 ±12.000		
ThBr <sub>4</sub> ·10 H <sub>2</sub> O(cr)		-4074.600 ±12.000		
ThBr <sub>4</sub> ·12 H <sub>2</sub> O(cr)		-4677.800 ±12.000		
ThBr <sub>4</sub> (g)	-769.026 <sup>(a)</sup> ±5.593	-742.300 <sup>(b)</sup> ±5.385	446.700 ±5.000	104.900 ±3.000
ThOBr <sub>2</sub> (cr)		-1129.800 ±5.400		
ThBrO <sub>3</sub> <sup>3+</sup>	-696.558 <sup>(b)</sup> ±5.366			
ThI(g)			288.600 ±12.000	37.500 ±6.000
ThI <sub>2</sub> (g)			355.600 ±10.000	57.400 ±5.000
ThI <sub>3</sub> (g)			430.000 ±10.000	81.800 ±5.000
ThI <sub>4</sub> (cr)	-659.487 <sup>(a)</sup> ±2.668	-669.600 ±2.200	251.000 ±5.000	137.100 ±10.000
ThI <sub>4</sub> (g)	-518.316 <sup>(a)</sup> ±5.753	-460.600 <sup>(b)</sup> ±5.463	478.500 ±6.000	106.200 ±4.000
ThOL <sub>2</sub> (cr)		-996.600 ±2.300		
ThIO <sub>3</sub> <sup>3+</sup>	-854.752 <sup>(b)</sup> ±5.385			
Th(IO <sub>3</sub> ) <sub>2</sub> <sup>2+</sup>	-997.243 <sup>(b)</sup> ±5.565			
Th(IO <sub>3</sub> ) <sub>3</sub> <sup>+</sup>	-1140.134 <sup>(b)</sup> ±5.825			
ThS(cr)	-391.862 <sup>(a)</sup> ±6.205	-396.300 ±6.200	69.810 ±0.700	47.720 ±0.500
ThS <sub>2</sub> (cr)			96.230 ±1.700	70.290 ±0.500

(Continued on next page)

Table III-1 (Continued)

Compound	$\Delta_f G_m^o$ (kJ·mol <sup>-1</sup> )	$\Delta_f H_m^o$ (kJ·mol <sup>-1</sup> )	$S_m^o$ (J·K <sup>-1</sup> ·mol <sup>-1</sup> )	$C_{p,m}^o$ (J·K <sup>-1</sup> ·mol <sup>-1</sup> )
Th <sub>2</sub> S <sub>3</sub> (cr)		– 1079.000 ±5.500		
ThOS(cr)			76.300 ±1.500	67.250 ±1.350
ThSO <sub>4</sub> <sup>2+</sup>	– 1484.006 <sup>(b)</sup> ±5.620	– 1657.120 <sup>(b)</sup> ±2.449	– 216.308 <sup>(b)</sup> ±17.316	
Th(SO <sub>4</sub> ) <sub>2</sub> (cr)				173.500 ±5.000
Th(SO <sub>4</sub> ) <sub>2</sub> · 9 H <sub>2</sub> O(cr)	– 4391.269 <sup>(b)</sup> ±5.404			
Th(SO <sub>4</sub> ) <sub>2</sub> (aq)	– 2248.102 <sup>(b)</sup> ±5.580	– 2547.000 <sup>(b)</sup> ±2.664	– 65.151 <sup>(b)</sup> ±17.219	
Th(SO <sub>4</sub> ) <sub>3</sub> <sup>2-</sup>	– 2998.147 <sup>(b)</sup> ±5.461			
ThOSe(cr)			93.500 ±1.900	72.650 ±1.500
ThN(cr)	– 353.638 <sup>(a)</sup> ±10.011	– 381.200 <sup>(b)</sup> ±10.000	56.000 ±1.500	45.000 ±1.100
ThN <sub>3</sub> <sup>3+</sup>	– 381.926 <sup>(b)</sup> ±6.739			
Th(N <sub>3</sub> ) <sub>2</sub> <sup>2+</sup>	– 57.415 <sup>(b)</sup> ±7.577			
Th <sub>3</sub> N <sub>4</sub> (cr)	– 1200.051 <sup>(a)</sup> ±15.659	– 1306.800 ±15.000	183.100 ±15.000	147.700 ±8.000
Th(NO <sub>3</sub> ) <sub>4</sub> · 4 H <sub>2</sub> O(cr)		– 2702.400 ±3.800		
Th(NO <sub>3</sub> ) <sub>4</sub> · 5 H <sub>2</sub> O(cr)	– 2322.651 <sup>(a)</sup> ±2.814	– 3005.400 ±2.800	543.100 ±0.800	480.700 ±0.800
ThNO <sub>3</sub> <sup>3+</sup>	– 822.997 <sup>(b)</sup> ±5.436			
Th(NO <sub>3</sub> ) <sub>2</sub> <sup>2+</sup>	– 939.499 <sup>(b)</sup> ±5.829			
Th <sub>4</sub> (PO <sub>4</sub> ) <sub>4</sub> P <sub>2</sub> O <sub>7</sub> (cr)			569.000 ±15.000	
ThH <sub>2</sub> PO <sub>4</sub> <sup>3+</sup>	– 1873.843 <sup>(b)</sup> ±5.822			

(Continued on next page)

Table III-1 (Continued)

Compound	$\Delta_f G_m^o$ (kJ·mol <sup>-1</sup> )	$\Delta_f H_m^o$ (kJ·mol <sup>-1</sup> )	$S_m^o$ (J·K <sup>-1</sup> ·mol <sup>-1</sup> )	$C_{p,m}^o$ (J·K <sup>-1</sup> ·mol <sup>-1</sup> )
ThH <sub>3</sub> PO <sub>4</sub> <sup>4+</sup>	– 1864.938 <sup>(b)</sup> ±5.804			
Th(H <sub>2</sub> PO <sub>4</sub> ) <sub>2</sub> <sup>2+</sup>	– 3038.907 <sup>(b)</sup> ±6.430			
Th(H <sub>3</sub> PO <sub>4</sub> )(H <sub>2</sub> PO <sub>4</sub> ) <sup>3+</sup>	– 3034.455 <sup>(b)</sup> ±6.430			
ThAs(cr)			79.800 ±0.500	50.500 ±0.500
Th <sub>3</sub> As <sub>4</sub> (cr)			274.600 ±1.500	183.300 ±1.500
ThBi(cr)	– 162.300 ±4.200			
ThBi <sub>2</sub> (cr)	– 207.100 ±6.300			
Th <sub>3</sub> Bi <sub>4</sub> (cr)	– 597.500 ±14.600			
Th <sub>5</sub> Bi <sub>3</sub> (cr)	– 532.200 ±16.700			
Th <sub>5</sub> Sn <sub>3</sub> (cr)	– 510.400 ±32.000			
ThC <sub>0.97</sub> (cr)	– 124.466 <sup>(a)</sup> ±6.308	– 124.200 ±6.300	59.100 ±0.900	45.200 ±0.400
ThC <sub>1.94</sub> (s)	– 126.705 <sup>(a)</sup> ±7.503	– 124.700 ±7.500	70.500 ±0.400	56.800 ±0.200
Th(CO <sub>3</sub> ) <sub>5</sub> <sup>6-</sup>	– 3521.231 <sup>(b)</sup> ±6.917			
Th(OH) <sub>2</sub> (CO <sub>3</sub> ) <sub>2</sub> <sup>2-</sup>	– 2285.078 <sup>(b)</sup> ±6.070			
ThOH(CO <sub>3</sub> ) <sub>4</sub> <sup>5-</sup>	– 3176.808 <sup>(b)</sup> ±6.217			
Th(OH) <sub>4</sub> (CO <sub>3</sub> ) <sup>2-</sup>	– 2092.167 <sup>(b)</sup> ±6.327			
ThSCN <sup>3+</sup>	– 623.499 <sup>(b)</sup> ±7.226			
Th(SCN) <sub>2</sub> <sup>2+</sup>	– 538.790 <sup>(b)</sup> ±10.626			

(Continued on next page)

Table III-1 (Continued)

Compound	$\Delta_f G_m^o$ (kJ·mol <sup>-1</sup> )	$\Delta_f H_m^o$ (kJ·mol <sup>-1</sup> )	$S_m^o$ (J·K <sup>-1</sup> ·mol <sup>-1</sup> )	$C_{p,m}^o$ (J·K <sup>-1</sup> ·mol <sup>-1</sup> )
ThSi <sub>2</sub> (cr)		– 169.500 ±9.600		
ThSiO <sub>4</sub> (huttonite)		– 2110.800 ±4.700		
ThSiO <sub>4</sub> (Thorite)		– 2117.500 ±4.200		
Na <sub>6</sub> Th(CO <sub>3</sub> ) <sub>5</sub> ·12 H <sub>2</sub> O(cr)	– 8002.562 <sup>(b)</sup> ±7.301			
ThTi <sub>2</sub> O <sub>6</sub> (cr)		– 3095.000 ±4.300		

(a) Value calculated internally using  $\Delta_f G_m^o = \Delta_f H_m^o - T \sum S_{m,i}^o$ .

(b) Value calculated internally from reaction data (see Table III-2).

Table III-2: Selected thermodynamic data for reactions involving thorium compounds and complexes. All ionic species listed in this table are aqueous species. Unless noted otherwise, all data refer to the reference temperature of 298.15 K and to the standard state, *i.e.*, a pressure of 0.1 MPa and, for aqueous species, infinite dilution ( $I = 0$ ). The uncertainties listed below each value represent total uncertainties and correspond in principal to the statistically defined 95% confidence interval. Values obtained from internal calculation, *cf.* footnote (a), are rounded at the third digit after the decimal point and may therefore not be exactly identical to those given in Chapters V to XII. Systematically, all the values are presented with three digits after the decimal point, regardless of the significance of these digits. The data presented in this table are available on computer media from the OECD Nuclear Energy Agency.

Species	Reaction			
	$\log_{10} K^\circ$	$\Delta_f G_m^\circ$ (kJ·mol $^{-1}$ )	$\Delta_f H_m^\circ$ (kJ·mol $^{-1}$ )	$\Delta_f S_m^\circ$ (J·K $^{-1}$ ·mol $^{-1}$ )
Th(g)	$\text{Th}(\text{cr}) \rightleftharpoons \text{Th}(\text{g})$		602.000 ±6.000	
ThO <sub>2</sub> (g)	$\text{ThO}_2(\text{cr}) \rightleftharpoons \text{ThO}_2(\text{g})$		771.400 ±15.000	
ThO <sub>2</sub> (am, hyd, fresh)	$4\text{OH}^- + \text{Th}^{4+} \rightleftharpoons 2\text{H}_2\text{O(l)} + \text{ThO}_2(\text{am, hyd, fresh})$	46.700 ±0.900	-266.566 ±5.137	
ThO <sub>2</sub> (am, hyd, aged)	$4\text{OH}^- + \text{Th}^{4+} \rightleftharpoons 2\text{H}_2\text{O(l)} + \text{ThO}_2(\text{am, hyd, aged})$	47.500 ±0.900	-271.132 ±5.137	
Th(OH) <sup>3+</sup>	$\text{H}_2\text{O(l)} + \text{Th}^{4+} \rightleftharpoons \text{H}^+ + \text{Th(OH)}^{3+}$	-2.500 ±0.500	14.270 ±2.854	44.200 ±6.300
Th(OH) <sup>2+</sup>	$2\text{H}_2\text{O(l)} + \text{Th}^{4+} \rightleftharpoons 2\text{H}^+ + \text{Th(OH)}_2^{2+}$	-6.200 ±0.500	35.390 ±2.854	85.700 ±41.400
Th(OH) <sub>4</sub> (aq)	$4\text{H}_2\text{O(l)} + \text{Th}^{4+} \rightleftharpoons 4\text{H}^+ + \text{Th(OH)}_4(\text{aq})$	-17.400 ±0.700	99.320 ±3.996	168.741 <sup>(a)</sup> ±139.186
Th <sub>2</sub> (OH) <sub>2</sub> <sup>6+</sup>	$2\text{H}_2\text{O(l)} + 2\text{Th}^{4+} \rightleftharpoons 2\text{H}^+ + \text{Th}_2(\text{OH})_2^{6+}$	-5.900 ±0.500	33.677 ±2.854	58.300 ±5.700
				82.584 <sup>(a)</sup> ±21.380

(Continued on next page)

Table III-2 (Continued)

Species	Reaction			
	$\log_{10} K^\circ$	$\Delta_f G_m^\circ$ (kJ·mol <sup>-1</sup> )	$\Delta_f H_m^\circ$ (kJ·mol <sup>-1</sup> )	$\Delta_f S_m^\circ$ (J·K <sup>-1</sup> ·mol <sup>-1</sup> )
Th <sub>2</sub> (OH) <sub>3</sub> <sup>5+</sup>	3H <sub>2</sub> O(l) + 2Th <sup>4+</sup> ⇌ 3H <sup>+</sup> + Th <sub>2</sub> (OH) <sub>3</sub> <sup>5+</sup>	-6.800 ±0.200	38.815 ±1.142	
Th <sub>4</sub> (OH) <sub>8</sub> <sup>8+</sup>	8H <sub>2</sub> O(l) + 4Th <sup>4+</sup> ⇌ 8H <sup>+</sup> + Th <sub>4</sub> (OH) <sub>8</sub> <sup>8+</sup>	-20.400 ±0.400	116.444 ±2.283	243.000 ±21.300
Th <sub>4</sub> (OH) <sub>12</sub> <sup>4+</sup>	12H <sub>2</sub> O(l) + 4Th <sup>4+</sup> ⇌ 12H <sup>+</sup> + Th <sub>4</sub> (OH) <sub>12</sub> <sup>4+</sup>	-26.600 ±0.200	151.834 ±1.142	
Th <sub>6</sub> (OH) <sub>14</sub> <sup>10+</sup>	14H <sub>2</sub> O(l) + 6Th <sup>4+</sup> ⇌ 14H <sup>+</sup> + Th <sub>6</sub> (OH) <sub>14</sub> <sup>10+</sup>	-36.800 ±1.200	210.056 ±6.850	
Th <sub>6</sub> (OH) <sub>15</sub> <sup>9+</sup>	15H <sub>2</sub> O(l) + 6Th <sup>4+</sup> ⇌ 15H <sup>+</sup> + Th <sub>6</sub> (OH) <sub>15</sub> <sup>9+</sup>	-36.800 ±1.500	210.056 ±8.562	472.800 ±22.000
ThF <sup>3+</sup>	F <sup>-</sup> + Th <sup>4+</sup> ⇌ ThF <sup>3+</sup>	8.870 ±0.150	-50.630 ±0.856	-0.400 ±2.000
ThF <sub>2</sub> <sup>2+</sup>	2F <sup>-</sup> + Th <sup>4+</sup> ⇌ ThF <sub>2</sub> <sup>2+</sup>	15.630 ±0.230	-89.217 ±1.313	-3.300 ±0.400
ThF <sub>3</sub> <sup>+</sup>	3F <sup>-</sup> + Th <sup>4+</sup> ⇌ ThF <sub>3</sub> <sup>+</sup>	20.670 ±0.160	-117.985 ±0.913	
ThF <sub>4</sub> (cr, hyd)	4HF(aq) + Th <sup>4+</sup> ⇌ 4H <sup>+</sup> + ThF <sub>4</sub> (cr, hyd)	19.110 ±0.400	-109.081 ±2.283	
ThF <sub>4</sub> (g)	ThF <sub>4</sub> (cr) ⇌ ThF <sub>4</sub> (g)		349.300 ±2.000	
ThF <sub>4</sub> (aq)	4F <sup>-</sup> + Th <sup>4+</sup> ⇌ ThF <sub>4</sub> (aq)	25.580 ±0.180	-146.012 ±1.027	

(Continued on next page)

Table III-2 (Continued)

Species	Reaction			
	$\log_{10} K^\circ$	$\Delta_f G_m^\circ$ (kJ·mol <sup>-1</sup> )	$\Delta_f H_m^\circ$ (kJ·mol <sup>-1</sup> )	$\Delta_f S_m^\circ$ (J·K <sup>-1</sup> ·mol <sup>-1</sup> )
ThCl <sup>3+</sup>	$\text{Cl}^- + \text{Th}^{4+} \rightleftharpoons \text{ThCl}^{3+}$			
	1.700 ±0.100	-9.704 ±0.571		
ThCl <sub>4</sub> (g)	$\beta\text{-ThCl}_4 \rightleftharpoons \text{ThCl}_4(\text{g})$			
		234.900 ±5.000		
ThClO <sub>3</sub> <sup>3+</sup>	$\text{ClO}_3^- + \text{Th}^{4+} \rightleftharpoons \text{ThClO}_3^{3+}$			
	1.550 ±0.130	-8.847 ±0.742		
ThBr <sup>3+</sup>	$\text{Br}^- + \text{Th}^{4+} \rightleftharpoons \text{ThBr}^{3+}$			
	1.380 ±0.130	-7.877 ±0.742		
ThBr <sub>4</sub> (g)	$\beta\text{-ThBr}_4 \rightleftharpoons \text{ThBr}_4(\text{g})$			
		221.500 ±5.000		
ThBrO <sub>3</sub> <sup>3+</sup>	$\text{BrO}_3^- + \text{Th}^{4+} \rightleftharpoons \text{ThBrO}_3^{3+}$			
	1.900 ±0.100	-10.845 ±0.571		
ThI <sub>4</sub> (g)	$\text{ThI}_4(\text{cr}) \rightleftharpoons \text{ThI}_4(\text{g})$			
		209.000 ±5.000		
ThIO <sub>3</sub> <sup>3+</sup>	$\text{IO}_3^- + \text{Th}^{4+} \rightleftharpoons \text{ThIO}_3^{3+}$			
	4.140 ±0.100	-23.631 ±0.571		
Th(IO <sub>3</sub> ) <sub>2</sub> <sup>2+</sup>	$2\text{IO}_3^- + \text{Th}^{4+} \rightleftharpoons \text{Th}(\text{IO}_3)_2^{2+}$			
	6.970 ±0.120	-39.785 ±0.685		
Th(IO <sub>3</sub> ) <sub>3</sub> <sup>+</sup>	$3\text{IO}_3^- + \text{Th}^{4+} \rightleftharpoons \text{Th}(\text{IO}_3)_3^+$			
	9.870 ±0.110	-56.338 ±0.628		
ThSO <sub>4</sub> <sup>2+</sup>	$\text{SO}_4^{2-} + \text{Th}^{4+} \rightleftharpoons \text{ThSO}_4^{2+}$			
	6.170 ±0.320	-35.219 ±1.827	20.920 ±0.740	188.292 <sup>(a)</sup> ±6.610

(Continued on next page)

Table III-2 (Continued)

Species	Reaction			
	$\log_{10} K^\circ$	$\Delta_f G_m^\circ$ (kJ·mol <sup>-1</sup> )	$\Delta_f H_m^\circ$ (kJ·mol <sup>-1</sup> )	$\Delta_f S_m^\circ$ (J·K <sup>-1</sup> ·mol <sup>-1</sup> )
Th(SO <sub>4</sub> ) <sub>2</sub> ·9H <sub>2</sub> O(cr)	$9\text{H}_2\text{O(l)} + 2\text{SO}_4^{2-} + \text{Th}^{4+} \rightleftharpoons \text{Th}(\text{SO}_4)_2\cdot9\text{H}_2\text{O(cr)}$			
	11.250 $\pm 0.096$	-64.215 $\pm 0.548$		
Th(SO <sub>4</sub> ) <sub>2</sub> (aq)	$2\text{SO}_4^{2-} + \text{Th}^{4+} \rightleftharpoons \text{Th}(\text{SO}_4)_2(\text{aq})$			
	9.690 $\pm 0.270$	-55.311 $\pm 1.541$	40.380 $\pm 1.080$	320.949 <sup>(a)</sup> $\pm 6.312$
Th(SO <sub>4</sub> ) <sub>3</sub> <sup>2-</sup>	$3\text{SO}_4^{2-} + \text{Th}^{4+} \rightleftharpoons \text{Th}(\text{SO}_4)_3^{2-}$			
	10.748 $\pm 0.076$	-61.352 $\pm 0.434$		
Th(SeO <sub>3</sub> ) <sub>2</sub> (cr)	$\text{Th}(\text{SeO}_3)_2\cdot\text{H}_2\text{O(cr)} \rightleftharpoons \text{H}_2\text{O(g)} + \text{Th}(\text{SeO}_3)_2(\text{cr})$			
	-6.499 $\pm 0.560$	37.094 $\pm 3.195$	94.100 $\pm 2.900$	191.200 $\pm 4.500$
ThN <sub>3</sub> <sup>3+</sup>	$\text{N}_3^- + \text{Th}^{4+} \rightleftharpoons \text{ThN}_3^{3+}$			
	4.440 $\pm 0.640$	-25.344 $\pm 3.653$		
Th(N <sub>3</sub> ) <sub>2</sub> <sup>2+</sup>	$2\text{N}_3^- + \text{Th}^{4+} \rightleftharpoons \text{Th}(\text{N}_3)_2^{2+}$			
	8.590 $\pm 0.640$	-49.032 $\pm 3.653$		
ThNO <sub>3</sub> <sup>3+</sup>	$\text{NO}_3^- + \text{Th}^{4+} \rightleftharpoons \text{ThNO}_3^{3+}$			
	1.300 $\pm 0.200$	-7.420 $\pm 1.142$		
Th(NO <sub>3</sub> ) <sub>2</sub> <sup>2+</sup>	$2\text{NO}_3^- + \text{Th}^{4+} \rightleftharpoons \text{Th}(\text{NO}_3)_2^{2+}$			
	2.300 $\pm 0.400$	-13.128 $\pm 2.283$		
ThH <sub>2</sub> PO <sub>4</sub> <sup>3+</sup>	$\text{H}_3\text{PO}_4(\text{aq}) + \text{Th}^{4+} \rightleftharpoons \text{H}^+ + \text{ThH}_2\text{PO}_4^{3+}$			
	3.450 $\pm 0.320$	-19.693 $\pm 1.827$		
ThH <sub>3</sub> PO <sub>4</sub> <sup>4+</sup>	$\text{H}_3\text{PO}_4(\text{aq}) + \text{Th}^{4+} \rightleftharpoons \text{ThH}_3\text{PO}_4^{4+}$			
	1.890 $\pm 0.310$	-10.788 $\pm 1.769$		
Th(H <sub>2</sub> PO <sub>4</sub> ) <sub>2</sub> <sup>2+</sup>	$2\text{H}_3\text{PO}_4(\text{aq}) + \text{Th}^{4+} \rightleftharpoons 2\text{H}^+ + \text{Th}(\text{H}_2\text{PO}_4)_2^{2+}$			
	6.200 $\pm 0.320$	-35.390 $\pm 1.827$		

(Continued on next page)

Table III-2 (Continued)

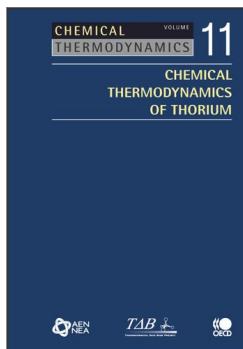
Species	$\log_{10} K^\circ$	Reaction		
		$\Delta_f G_m^\circ$ (kJ·mol <sup>-1</sup> )	$\Delta_f H_m^\circ$ (kJ·mol <sup>-1</sup> )	$\Delta_f S_m^\circ$ (J·K <sup>-1</sup> ·mol <sup>-1</sup> )
$\text{Th}(\text{H}_3\text{PO}_4)(\text{H}_2\text{PO}_4)^{3+}$		$2\text{H}_3\text{PO}_4(\text{aq}) + \text{Th}^{4+} \rightleftharpoons \text{H}^+ + \text{Th}(\text{H}_3\text{PO}_4)(\text{H}_2\text{PO}_4)^{3+}$		
	5.420 $\pm 0.320$		-30.938 $\pm 1.827$	
$\text{Th}(\text{CO}_3)_5^{6-}$		$5\text{CO}_3^{2-} + \text{Th}^{4+} \rightleftharpoons \text{Th}(\text{CO}_3)_5^{6-}$		
	31.000 $\pm 0.700$		-176.949 $\pm 3.996$	
$\text{ThOH}(\text{CO}_3)_4^{5-}$		$4\text{CO}_3^{2-} + \text{OH}^- + \text{Th}^{4+} \rightleftharpoons \text{ThOH}(\text{CO}_3)_4^{5-}$		
	35.600 $\pm 0.500$		-203.206 $\pm 2.854$	
$\text{Th}(\text{OH})_2(\text{CO}_3)_2^{2-}$		$2\text{CO}_3^{2-} + 2\text{OH}^- + \text{Th}^{4+} \rightleftharpoons \text{Th}(\text{OH})_2(\text{CO}_3)_2^{2-}$		
	36.800 $\pm 0.500$		-210.056 $\pm 2.854$	
$\text{Th}(\text{OH})_4(\text{CO}_3)^{2-}$		$\text{CO}_3^{2-} + 4\text{OH}^- + \text{Th}^{4+} \rightleftharpoons \text{Th}(\text{OH})_4(\text{CO}_3)^{2-}$		
	40.400 $\pm 0.600$		-230.605 $\pm 3.425$	
$\text{ThSCN}^{3+}$		$\text{SCN}^- + \text{Th}^{4+} \rightleftharpoons \text{ThSCN}^{3+}$		
	2.000 $\pm 0.500$		-11.416 $\pm 2.854$	
$\text{Th}(\text{SCN})_2^{2+}$		$2\text{SCN}^- + \text{Th}^{4+} \rightleftharpoons \text{Th}(\text{SCN})_2^{2+}$		
	3.400 $\pm 0.800$		-19.407 $\pm 4.566$	
$\text{Na}_6\text{Th}(\text{CO}_3)_5 \cdot 12\text{H}_2\text{O}(\text{cr})$		$5\text{CO}_3^{2-} + 12\text{H}_2\text{O(l)} + 6\text{Na}^+ + \text{Th}^{4+} \rightleftharpoons \text{Na}_6\text{Th}(\text{CO}_3)_5 \cdot 12\text{H}_2\text{O(cr)}$		
	42.200 $\pm 0.800$		-240.879 $\pm 4.566$	

(a) Value calculated internally using  $\Delta_f G_m^\circ = \Delta_f H_m^\circ - T \Delta_f S_m^\circ$ .(b) Value of  $\log_{10} K^\circ$  calculated internally from  $\Delta_f G_m^\circ$

Table III-3: Selected temperature coefficients for heat capacities in the form  $C_{p,m}^o(T) = a + bT + cT^2 + eT^{-2}$ . The functions are valid between the temperatures  $T_{\min}$  and  $T_{\max}$  (in K). Units for  $C_{p,m}^o$  are  $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ .

Compound	<i>a</i>	<i>b</i>	<i>c</i>	<i>e</i>	<i>T</i> (min)	<i>T</i> (max)
Th(cr, $\alpha$ ) (fcc)	$2.34350 \times 10^1$	$8.94500 \times 10^{-3}$	0	$1.14000 \times 10^4$	298.15	1633
Th(g)	$2.41480 \times 10^1$	$-1.45623 \times 10^{-2}$	$1.77473 \times 10^{-5}$	$-5.27700 \times 10^4$	298.15	700
ThO(g)	$2.95010 \times 10^1$	$1.33228 \times 10^{-2}$	$-6.01025 \times 10^{-6}$	$-1.48640 \times 10^5$	298.15	700
ThO <sub>2</sub> (cr)	$7.15780 \times 10^1$	$6.33610 \times 10^{-3}$	$7.44770 \times 10^{-7}$	$-1.04834 \times 10^6$	298.15	2300
ThO <sub>2</sub> (g)	$4.69010 \times 10^1$	$2.01352 \times 10^{-2}$	$-1.02652 \times 10^{-5}$	$-4.57730 \times 10^5$	298.15	800
ThH <sub>2</sub> (cr)	8.29500	$1.25602 \times 10^{-1}$	$-5.05319 \times 10^{-5}$	$-4.04100 \times 10^5$	298.15	1000
ThH <sub>3.75</sub> (cr)	-7.42600	$2.37538 \times 10^{-1}$	$-9.33488 \times 10^{-5}$	$-3.35550 \times 10^5$	298.15	1000
ThF(g) <sup>*</sup>	$3.57170 \times 10^1$	$4.00180 \times 10^{-3}$	$-1.83420 \times 10^{-6}$	$-1.85670 \times 10^5$	298.15	700
ThF <sub>2</sub> (g) <sup>*</sup>	$5.46630 \times 10^1$	$7.46700 \times 10^{-3}$	$-4.51541 \times 10^{-6}$	$-3.62070 \times 10^5$	298.15	600
ThF <sub>3</sub> (g) <sup>*</sup>	$7.71500 \times 10^1$	$1.26203 \times 10^{-2}$	$-7.61875 \times 10^{-6}$	$-6.16320 \times 10^5$	298.15	600
ThF <sub>4</sub> (cr)	$1.21734 \times 10^2$	$9.06400 \times 10^{-3}$	$-2.85740 \times 10^{-7}$	$-1.21821 \times 10^6$	298.15	1383
ThF <sub>4</sub> (g)	$1.02950 \times 10^2$	$7.43050 \times 10^{-3}$	$-2.91682 \times 10^{-6}$	$-1.02068 \times 10^6$	298.15	1300
ThOF(g)	$4.89090 \times 10^1$	$1.90003 \times 10^{-2}$	$-1.12413 \times 10^{-5}$	$-3.59500 \times 10^5$	298.15	600
ThOF <sub>2</sub> (cr)	$9.66560 \times 10^1$	$7.70000 \times 10^{-3}$	$-2.29500 \times 10^{-7}$	$-1.13330 \times 10^6$	298.15	1500
ThCl(g) <sup>*</sup>	$3.73210 \times 10^1$	$1.02980 \times 10^{-3}$	$-3.18700 \times 10^{-8}$	$-1.04870 \times 10^5$	298.15	1900
ThCl <sub>2</sub> (g) <sup>*</sup>	$5.77010 \times 10^1$	$8.49700 \times 10^{-4}$	$-3.99960 \times 10^{-7}$	$-2.34380 \times 10^5$	298.15	1000
ThCl <sub>3</sub> (g) <sup>*</sup>	$8.22270 \times 10^1$	$1.55540 \times 10^{-3}$	$-7.31790 \times 10^{-7}$	$-4.10980 \times 10^5$	298.15	1000
ThCl <sub>4</sub> ( $\beta$ )	$1.20290 \times 10^2$	$2.32672 \times 10^{-2}$	0	$-6.15050 \times 10^5$	298.15	1043
ThCl <sub>4</sub> (g) <sup>*</sup>	$1.07721 \times 10^2$	$2.99300 \times 10^{-4}$	$-6.02300 \times 10^{-8}$	$-5.73880 \times 10^5$	298.15	3000
ThOCl <sub>2</sub> (cr)	$9.59360 \times 10^1$	$1.48040 \times 10^{-2}$	$3.73900 \times 10^{-7}$	$-8.31700 \times 10^5$	298.15	1500
ThBr(g) <sup>*</sup>	$3.74030 \times 10^1$	$1.82430 \times 10^{-3}$	$-2.05000 \times 10^{-9}$	$-5.05800 \times 10^4$	298.15	3000
ThBr <sub>2</sub> (g) <sup>*</sup>	$5.81670 \times 10^1$	$2.85000 \times 10^{-5}$	$-5.82000 \times 10^{-9}$	$-1.28280 \times 10^5$	298.15	3000
ThBr <sub>3</sub> (g) <sup>*</sup>	$8.30940 \times 10^1$	$4.13000 \times 10^{-5}$	$-8.28000 \times 10^{-9}$	$-2.05080 \times 10^5$	298.15	3000
ThBr <sub>4</sub> ( $\beta$ )	$1.27600 \times 10^2$	$1.50624 \times 10^{-2}$	0	$-6.15050 \times 10^5$	298.15	970
ThBr <sub>4</sub> (g) <sup>*</sup>	$1.08009 \times 10^2$	$6.53000 \times 10^{-5}$	$-1.31700 \times 10^{-8}$	$-2.80920 \times 10^5$	298.15	3000
ThI(g) <sup>*</sup>	$3.74110 \times 10^1$	$1.54660 \times 10^{-3}$	$-5.00000 \times 10^{-10}$	$-3.15000 \times 10^4$	298.15	3000
ThI <sub>2</sub> (g) <sup>*</sup>	$5.81910 \times 10^1$	$8.80000 \times 10^{-6}$	$-1.79000 \times 10^{-9}$	$-7.24600 \times 10^4$	298.15	3000
ThI <sub>3</sub> (g) <sup>*</sup>	$8.31280 \times 10^1$	$1.42000 \times 10^{-5}$	$-2.92000 \times 10^{-9}$	$-1.18660 \times 10^5$	298.15	3000
ThI <sub>4</sub> (cr)	$1.40000 \times 10^2$	$1.35000 \times 10^{-2}$	0	$-6.15000 \times 10^5$	298.15	839
ThI <sub>4</sub> (g) <sup>*</sup>	$1.08061 \times 10^2$	$2.27000 \times 10^{-5}$	$-4.55000 \times 10^{-9}$	$-1.69610 \times 10^5$	298.15	3000
ThOI <sub>2</sub> (cr)	$1.05789 \times 10^2$	$9.91800 \times 10^{-3}$	$3.72400 \times 10^{-7}$	$-8.31700 \times 10^5$	298.15	1500
ThS(cr)	$5.01240 \times 10^1$	$5.46000 \times 10^{-3}$	0	$-3.58600 \times 10^5$	298.15	2000
Th(SO <sub>4</sub> ) <sub>2</sub> (cr)	$1.04600 \times 10^2$	$2.3096 \times 10^{-1}$	0		298.15	900
ThN(cr)	$4.78360 \times 10^1$	$1.37750 \times 10^{-2}$	0	$-6.17200 \times 10^5$	298.15	2000
Th <sub>3</sub> N <sub>4</sub> (cr)	$1.81517 \times 10^2$	$2.61810 \times 10^{-2}$	0	$-3.70000 \times 10^6$	298.15	2000
Th <sub>4</sub> (PO <sub>4</sub> ) <sub>4</sub> P <sub>2</sub> O <sub>7</sub> (cr)	$6.96700 \times 10^2$	$1.04550 \times 10^{-1}$	$-1.86250 \times 10^{-7}$	$-1.41590 \times 10^7$	298.15	1273

\* Fitted from heat capacity values calculated from the molecular parameters given in Table E-1.



**From:**  
**Chemical Thermodynamics of Thorium, Volume 11**

**Access the complete publication at:**  
<https://doi.org/10.1787/9789264056688-en>

**Please cite this chapter as:**

OECD/Nuclear Energy Agency (2008), "Selected thorium data", in *Chemical Thermodynamics of Thorium, Volume 11*, OECD Publishing, Paris.

DOI: <https://doi.org/10.1787/9789264056688-4-en>

This work is published under the responsibility of the Secretary-General of the OECD. The opinions expressed and arguments employed herein do not necessarily reflect the official views of OECD member countries.

This document, as well as any data and map included herein, are without prejudice to the status of or sovereignty over any territory, to the delimitation of international frontiers and boundaries and to the name of any territory, city or area. Extracts from publications may be subject to additional disclaimers, which are set out in the complete version of the publication, available at the link provided.

The use of this work, whether digital or print, is governed by the Terms and Conditions to be found at  
<http://www.oecd.org/termsandconditions>.