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FORMATION ENERGETICS OF CERAMIC PHASES RELATED TO SURPLUS PLUTONIUM DISPOSITION

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ABSTRACT

A database of fundamental thermodynamic functions at 298.15 K including entropy, S^o, standard enthalpies and Gibbs free energies of formation, $\Delta_f H^o$ and $\Delta_f G^o$, molar masses, and molar volumes, V^o, for phases related to proposed ceramic waste materials for the disposal of surplus weapons plutonium has been assembled. Previously published as well as newly reported results of measured and predicted quantities for pyrochlore, brannerite, monazite, zircon and other related phases are presented. Where thermodynamic quantities are available for temperatures above 298.15 K, they are included or referenced.

INTRODUCTION

With a landmark record of decision(1), the U.S. Department of Energy has decreed that at least 17 • 10^3 kg of surplus weapons plutonium will be incorporated into a ceramic waste material. Another 33 • 10^3 kg is expected to be used in mixed-oxide (MOX) fuel reactors and the resulting irradiated fuel is to be considered a waste material. Both waste ceramics will be buried in a geological repository such as the proposed Yucca Mountain nuclear waste repository in the state of Nevada in the United States of America. Licensing of each waste material for incorporation into a waste repository will require clear and predictive scientific results on their durability and performance in a geological environment over nearly 10^6 years. Accurate thermodynamic quantities are key to both the development and modeling of these waste materials.

In an effort to facilitate the optimization of a ceramic waste form, enable accurate modeling of its performance in a geological repository, and to provide a thermodynamic basis for production process engineering, we have sought to provide accurate thermodynamic quantities for phases related to these waste materials. Here, we report molar masses, molar volumes, V^o, heat capacities, C_p^o, entropies, S^o, enthalpies, $\Delta_f H^o$, and Gibbs free energies, $\Delta_f G^o$, of formation for phases related to these proposed ceramic waste materials for surplus weapons plutonium. The

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DISCLAIMER

non-MOX plutonium will use a solid solution between Hf-zirconolite, $CaHfTi_2O_7$, and the end member pyrochlores $Gd_2Ti_2O_7$, $CaUTi_2O_7$, and $CaPuTi_2O_7$ as a waste ceramic, while the MOX fuel will be disposed of directly after irradiation.

To date, the energetics of mixing between the end member phases noted above and those that would be used for a MOX fuel are not known. We therefore do not include thermodynamic quantities for mixed phases and solid solutions at this time. We hope to include them in a future revision of this database once they are determined. Such calorimetry work is in progress.

The reader will note that quantities for binary oxides (e.g., MO_x) and elements in their standard states are also reported or referenced along with the thermodynamic quantities for higher order oxide materials. We include these quantities to create an internally consistent database of thermodynamic quantities. Included in this database are all of the fundamental thermodynamic data that have been used in determining the measured or predicted quantities reported here.

NOTATION AND TERMINOLOGY

The symbols and terminology used here for thermochemical quantities and units are consistent with those used in the widely accepted NIST-JANAF thermochemical tables.(2) The standard state pressure is 1 atm (101 325 Pa). The standard state temperature is 298.15 K. Where a quantity is valid at a temperature other than 298.15 K, a superscript T is used to the left of the thermodynamic symbol. (e.g., $\Delta_f H^o$ = the standard enthalpy of formation at 298.15 K and $\Delta_f^T H^o$ = the standard enthalpy of formation at T≠ 298.15 K.) The value of T will be defined in the table where the quantity is listed. Symbols used to designate phases or states of aggregation are as follows: g – gas, cr – crystalline solid, and [allotrope] to designate a specific crystal structure for materials with multiple allotropes (e.g., TiO_2 [cr, anatase] versus TiO_2 [cr, rutile]) Units are standard SI units and are noted in the table column headings. Our reference atomic masses for the elements are taken from reference 3 except for that of Pu. For the atomic mass of Pu we adopt the isotopic mass of ^{239}Pu.(4) ^{239}Pu is the principal isotope found in the surplus weapons material. Molecular masses for compounds listed in Table 1 are calculated in this work from the reference atomic weights as noted above.

THERMODYNAMIC DATA

Table 1 contains a summary of fundamental thermodynamic quantities valid at 298.15 K for several pyrochlore, brannerite, monazite, and zircon compositions as well as other, related, phases. Where noted, some values have been estimated from periodic systematics as described by Putnam[5] previously. Also reported in Table 1, where applicable, are the formation enthalpies of these phases from the binary oxides (equation 1) or from the binary oxides and perovskite, $CaTiO_3$ (equation 2). Examples of these reactions are given below for the formation of zirconolite[6], $CaZrTi_2O_7$.

$$CaO(cr) + ZrO_2(cr, baddeleyite) + 2TiO_2(cr, rutile) = CaZrTi_2O_7(cr, zirconolite) \qquad (1)$$

$$CaTiO_3(cr, perovskite) + ZrO_2(cr, baddeleyite) + TiO_2(cr, rutile) = CaZrTi_2O_7(cr, zirconolite) \qquad (2)$$

A thermodynamically stable phase should have a negative free energy change for reactions of both type (1) and type (2).

Table 2 contains summaries of the fundamental thermodynamic quantities as a function of temperature for some of the higher order oxide materials found in Table 1 and references to similar data on the binary oxides and elements.

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Table 1. Fundamental standard molar thermodynamic functions at 298.15 K. Units are found in the table headings. The standard state pressure is 1 atm (101 325 Pa). Errors are reported in parenthesis () and references and applicable notes are reported in braces { } (e.g., {7,9ac} represents references 7 and 9 and the application of notes a and c). Reported for each compound are: the molar mass (Mw), the molar volume (V^o), the standard molar entropy (S^o), the standard molar enthalpy ($\Delta_f H^o$), the standard molar Gibbs free energy ($\Delta_f G^o$), and the enthalpies of reactions 1 ($\Delta_r H^o(1)$) and 2 ($\Delta_r H^o(2)$) which are the enthalpies of compound formation from the binary oxides and the from the binary oxides plus perovskite, $CaTiO_3$, respectively. Where data is not presently available we leave the table cell blank. Data that has been estimated from systematic trends or in some other way is *italicized* and data derived from our various laboratories are **boldfaced**.

Compound name [phase, allotrope]	**Mw** $g \bullet mol^{-1}$	V^o $cm^3 \bullet mol^{-1}$	S^o $J \bullet K^{-1} \bullet mol^{-1}$	$\Delta_f H^o$ $kJ \bullet mol^{-1}$	$\Delta_f G^o$ $kJ \bullet mol^{-1}$	$\Delta_r H^o(1)$ $kJ \bullet mol^{-1}$	$\Delta_r H^o(2)$ $kJ \bullet mol^{-1}$
Zirconolite / Pyrochlore							
$CaZrTi_2O_7$ [cr]	337.0558 {3a}	76.00 {b}	**193.3 (0.38)** **{7}**	**-3713.7 (4.5)** **{6}**	**-3514.5 (4.5)** **{6}**	**-88.79 (4)** **{6}**	**-8.1 (4.6)** **{6}**
$CaHfTi_2O_7$ [cr]	424.3258 {3a}	76.48 {b}	**194.4 (0.38)** **{8}**	**-3752.27** **(4.9) {9}**	**-552.03 (4.9)** **{9}**	**-111.5 (4.4)** **{9}**	**-29.9 (5.3)** **{b}**
$CaCeTi_2O_7$ [cr]	385.9558 {3a}	79.63 {b}	{c}	**-3666.5 (6.3)** **{10}**	{c}	**-54.7 (5.5)** **{b}**	**+26.9 (6.3)** **{bd}**
$CaPuTi_2O_7$ [cr]	484.888 {3a}	78.11 {b}		***-3636 (6)*** ***{e}***		***-56.9 (5.6)*** ***{e}***	***+25 (6)*** ***{de}***
$CaUTi_2O_7$ [cr]	483.8647 {3a}	79.34 {b}		***-3653 (9)*** ***{e}***		***-44.9 (9.4)*** ***{e}***	***+36.8 (9.8)*** ***{de}***
$CaThTi_2O_7$ [cr]	477.8739 {3a}			***-3782 (9)*** ***{e}***		***-32.1 (9.6)*** ***{e}***	***+49 (10)*** ***{de}***
$Gd_2Ti_2O_7$ [cr]	520.2558 {3a}	80.01 {b}	{c}	**-3820.9 (4.7)** **{b}**	{c}	***-113.3 (2.7)*** ***{10}***	
Brannerite							
$CeTi_2O_6$ [cr]	329.8764 {3a}	67.263 {b}	***174.7 (4.8)*** ***{bf}***	**-2958.4 (5.1)** **{b}**	***-2787.0 (5.5)*** ***{bf}***	**+18.3 (4.7)** **{10d)**	

Compound name [phase, allotrope]	**Mw** **g • mol^{-1}**	V^o **cm^3 • mol^{-1}**	S^o **J • K^{-1} • mol^{-1}**	$\Delta_f H^o$ **kJ • mol^{-1}**	$\Delta_f G^o$ **kJ • mol^{-1}**	$\Delta_r H^o (1)$ **kJ • mol^{-1}**	$\Delta_r H^o (2)$ **kJ • mol^{-1}**
$ThTi_2O_6$ [cr]	421.7945 {3a}	69.348 {b}	***168.5 (4.7)*** ***{bf}***	**-3111 (6)** **{b}**	***-2943.9 (6.1)*** ***{bf}***	**+3.4 (4.6)** **{10d)**	
$PuTi_2O_6$ [cr]	428.8086 {3a}	66.155 {b}	***196.9 (20.1)*** ***{bf}***	***-2896.2 (20.1) {be}***	***-2736.6 (20.)*** ***{bf}***	***+48 (20)*** ***{de}***	
UTi_2O_6 [cr]	427.7853 {3a}	67.249 {b}	***174.4 (4.3)*** ***{bcf}***	**-2979.2 (4.5)** **{b}**	***-2809.4 (4.5)*** ***{bf}***	**-6.1 (4.1)** **{10}**	
Zircon							
$ZrSiO_4$ [cr]	183.3031 {3a}	39.26 {11b}	84.0 (1.3) {11}	-2034.2 (3.1) {11}	-1919.7 (3.1) {11}	-22.9 (3.6) {b}	
$HfSiO_4$ [cr]	270.5731 {3a}	38.79 {b}			*-1973.36* *{12gh}*		
$CeSiO_4$ [cr]	232.2031 {3a}				*-1874.59* *{12ghi}*		
$PuSiO_4$ [cr]	331.1353 {3a}	44.66 {b}			*-1854.37* *{12ghj}*		
$USiO_4$ [cr]	330.112 {3a}	45.84 {b}	118 (12) {13}	-1991.3 (5.4) {13}	-1883.6 (4.0) {13}	+4.4 (5.5) {b}	
$ThSiO_4$ [cr]	324.1212 {3a}	48.41 {b}			-2050.1 (4.3) {14}		
$AmSiO_4$ [cr]	335.0831 {3a}				*-1764.77* *{12gh}*		
Monazite							
$LaPO_4$ [cr]	233.8769 {3a}	45.679 {15k}		**-1955.2 (2.1)** **{b}**		**-306 (2)** **{16}**	
$CePO_4$ [cr]	235.0914 {3a}	44.695 {15k}		**-1959.5 (4.6)** **{b}**		**-309 (2)** **{16}**	

Compound name [phase, allotrope]	**Mw** **$g \bullet mol^{-1}$**	V^o **$cm^3 \bullet mol^{-1}$**	S^o **$J \bullet K^{-1} \bullet mol^{-1}$**	$\Delta_f H^o$ **$kJ \bullet mol^{-1}$**	$\Delta_f G^o$ **$kJ \bullet mol^{-1}$**	$\Delta_r H^o(1)$ **$kJ \bullet mol^{-1}$**	$\Delta_r H^o(2)$ **$kJ \bullet mol^{-1}$**
$NdPO_4$ [cr]	239.2114 {3a}	43.554 {15k}		**-1960.4 (2.0)** **{b}**		**-304 (2)** **{16}**	
$EuPO_4$ [cr]	246.9314 {3a}	42.02 {15k}		**-1850.1 (5.1)** **{b}**		**-272 (3)** **{16}**	
$YbPO_4$ [cr]	268.0114 {3a}	41.73 {15k}		**-1966.1 (2.3)** **{b}**		**-261 (2)** **{16}**	
$LuPO_4$ [cr]	269.9384 {3a}	41.33 {15k}		**-1582.6 (2.5)** **{b}**		**-256 (2.5)** **{16}**	
$PuPO_4$ [cr]	334.0236 {3a}			***-1916 (14)*** ***{b}***		***-264 (14)*** ***{be}***	
UPO_4 [cr]	333.0003 {3a}			***-1752 (17)*** ***{b}***		***-272 (14)*** ***{be}***	
$AmPO_4$ [cr]	337.9714 {3a}			***-1888 (15)*** ***{b}***		***-273 (14)*** ***{be}***	
Other Phases							
$CaTiO_3$ [cr, perovskite]	134.9582 {3a}	33.69 {b}	**93.3 (0.2)** **{17}**	**-1660.8 (3.3)** **{17}**	**-1575.3 (3.3)** **{17}**	**-81.7 (2.9)** **{5}**	
$ZrTiO_4$ [cr]	202.0976 {3a}	39.95 {b}	**111.0 (0.2)** **{18}**	**-2023.8 (4.2)** **{18}**	**-1913.8 (4.3)** **{18}**	**+20.5 (4.1)** **{18d}**	
$HfTiO_4$ [cr]	289.3676 {3a}	40.07 {b}		{c}		{c}	
Binary Oxides							
Am_2O_3 [cr]	533.9982 {3a}	50.51 {19b}	160 (15) {19}	-1690.4 (8.0) {19}	-1613.3 (9.2) {19}		
AmO_2 [cr]	274.9988 {3a}	23.40 {19b}	67 (10) {19}	-932.3 (3.0) {19}	-874.4 (4.3) {19}		

Compound name [phase, allotrope]	**Mw** **$g \bullet mol^{-1}$**	V^o **$cm^3 \bullet mol^{-1}$**	S^o **$J \bullet K^{-1} \bullet mol^{-1}$**	$\Delta_f H^o$ **$kJ \bullet mol^{-1}$**	$\Delta_f G^o$ **$kJ \bullet mol^{-1}$**	$\Delta_r H^o(1)$ **$kJ \bullet mol^{-1}$**	$\Delta_r H^o(2)$ **$kJ \bullet mol^{-1}$**
CaO [cr]	56.0794 {3a}	16.76 {11}	38.1 (0.4) {11}	-625.09(0.88) {11}	-603.1 (0.9) {11}		
Ce_2O_3 [cr, α]	328.2382 {3a}	47.75 {20}	148.8 (0.4) {21}	-1812.4 (1.3) {21}	-1723.1 (1.3) {21}		
CeO_2 [cr]	172.1188 {3a}	23.85 {11}	62.3 (0.1) {11}	-1088.1 (1.5) {11}	-1025.4 (1.9) {11}		
Eu_2O_3 [cr, α]	351.9182 {3a}	44.02 {20}	146.44 (8.5) {20}	-1651.5 (8.4) {20}	-1555.1 (8.4) {20}		
Gd_2O_3 [cr, α]	362.4982 {3a}	43.4 {20}	151.8 (0.85) {20}	-1819.6 (3.6) {20}	-1732.3 (3.6) {20}		
HfO_2 [cr]	210.4888 {3a}	20.82 {11}	59.3 (0.4) {11}	-1117.6 (1.3) {11,22}	-1061.1 (1.3) {11}		
La_2O_3 [cr]	325.8092 {3a}	49.56 {20}	127.32(0.84) {20}	-1793.6(1.59) {20}	-1705.9 (1.6) {20}		
Lu_2O_3 [cr]	397.9322 {3a}	42.22 {20}	109.9 (0.85) {20}	-1878.2 (7.5) {20}	-1788.8 (6.2) {20}		
Nd_2O_3 [cr, α]	336.4782 {3a}	45.92 {20}	158.5 (4.2) {20}	-18079 (1) {20}	-1721.0 (1) {20}		
P_2O_5 [cr]	141.9445 {3a}	59.4 {11}	114.4(0.4) {11}	-1504.9 (0.5) {11}	-1361.6(0.5) {11}		
Pu_2O_3 [cr, α]	526.1026 {3a}	51.57 {23a}	138.9 (1.5) {24,l}	-1715.4 (8.5) {24m}	-1631.6 (8) {24m}		
PuO_2 [cr]	271.051 {3a}	23.65 {23a}	66.13 (0.26) {25}	-1056.2 (0.7) {25}	-997.96(0.7) {25}		
SiO_2 [cr, quartz]	60.0843 {3a}	22.69 {11}	41.5 (0.1) {11}	-910.7 (1) {11}	-856.3(1) {11}		
ThO_2 [cr]	264.0369 {3a}	26.37 {11}	65.2 (0.2) {11}	-1226.4 (3.5) {11}	-1169.2(3.5) {11}		

Compound name [phase, allotrope]	Mw g • mol^{-1}	V^o cm^3 • mol^{-1}	S^o J • K^{-1} • mol^{-1}	$\Delta_f H^o$ kJ • mol^{-1}	$\Delta_f G^o$ kJ • mol^{-1}	$\Delta_r H^o(1)$ kJ • mol^{-1}	$\Delta_r H^o(2)$ kJ • mol^{-1}
TiO_2 [cr, rutile]	78.8788 {3a}	18.82 {11}	50.6 (0.6) {11}	-944.0 (0.9) {11}	-888.8 (1) {11}		
U_2O_3 [cr]	524.056 {3a}		160 (1.6) {25,1}	-1456 (20) {25}	-1382 (13) {25, 1}		
UO_2 [cr]	270.0277 {3a}	24.62 {11}	77.03 (0.2) {26}	-1085 (1) {13}	-1031.8 (1) {13}		
Yb_2O_3 [cr, α]	394.0782 {3a}	44.88 {20}	99.08 (4.2) {20}	-1905.3 (2.2) {20}	-1816.6 (2.4) {20}		
ZrO_2 [cr]	123.2188 {3a}	21.15 {11}	50.4 (0.3) {11}	-1100.6 (1.7) {11}	-1042.9 (1.7) {11}		
Elements							
Am [cr, α]	243 {3}	20.47 {19k}	55.4 (2) {25}				
Ca [cr]	40.08 {3}	26.19 {11}	41.59 (0.4) {11}				
Ce [cr]	140.12 {3}	20.77 {11}	72 (4) {11}				
Eu [cr]	151.96 {3}	28.97 {20}	80.79 (0.16) {20}				
Gd [cr]	157.25 {3}	19.89 {20}	68.45 (1.25) {20}				
Hf [cr]	178.49 {3}	13.47 {20}	43.56 (0.4) {2,1}				
La [cr]	138.9055 {3}	22.47 {20}	56.9 (2.5) {20}				
Lu [cr]	174.967 {3}	17.77 {20}	50.96 (0.84) {20}				

Notes to table 1.

a. Value calculated by the authors from data found in a publication referenced in this work. (e.g., the molar masses found in reference 3.
b. Value calculated by the authors for this work.
c. Measured data forthcoming in a future publication.
d. Metastability predicted or potential for metastability is predicted based on the value and its error margins.
e. Estimated using systematic trends described by Putnam in reference 5.
f. Values of S are estimated based on assumed sample stability at a synthesis temperature of 1623 K (synthesis temp of Ce, U, and Th brannerite samples). Values of G are calculated based on entropy stabilization from binary oxides at 1623 K.
g. Published results corrected for improper conversion from calories to J. as noted by the authors through personal communication.

Compound name [phase, allotrope]	Mw $g \bullet mol^{-1}$	V^o $cm^3 \bullet mol^{-1}$	S^o $J \bullet K^{-1} \bullet mol^{-1}$	$\Delta_f H^o$ $kJ \bullet mol^{-1}$	$\Delta_f G^o$ $kJ \bullet mol^{-1}$	$\Delta_r H^o (1)$ $kJ \bullet mol^{-1}$	$\Delta_r H^o (2)$ $kJ \bullet mol^{-1}$
Nd [cr]	144.24 {3}	20.57 {20}	71.09 (4.18) {20}				
O_2 [g]	31.9988 {3}	24 789.7 {11}	205.14(0.35) {2}				
P [cr, α]	30.97376 {3}	17.3 {11}	41.077(0.08) {2}				
Pu [cr, α]	239.0522 {27}	12.036 {27k}	55.22 (1.67) {28}				
Si [cr]	28.0855 {3}	12.056 {11}	18.81 (0.08) {11}				
Th [cr]	232.0381 {3}	19.79 {11}	51.83 (0.5) {11}				
Ti [cr]	46.88 {3}	10.63 {11}	30.76 (0.1) {11}				
U [cr]	238.0289 {3}	12.5 {11}	50.2 (0.2) {11}				
Yb [cr]	173.4 {3}	24.83 {20}	59.83 (0.17) {20}				
Zr [cr]	91.22 {3}	14.016 {11}	38.87 (0.2) {11}				

Notes to table 1. continued.

h. Uses a linear free energy relationship to predict the Gibbs free energy of formation as noted in reference 12.
i. Predicted definitely to be metastable with respect to decomposition. Delta G for CeO2 + SiO2 = CeSiO4 is calculated to be +7.1 (2.1) at 298.15 K.
j. Predicted to possibly be metastable with respect to decomposition. Delta G for PuO2 + SiO2 = PuSiO4 is calculated to be -0.11 (1.2) at 298.15 K.
k. Calculated for this work from data found in another reference found in this work.
l. Error estimated.
m. Error estimated from multiple published results.

Table 2 Fundamental standard molar thermodynamic functions at temperatures other than 298.15 K. Data that has been derived from our various laboratories are **boldfaced**.

Compound	Thermodynamic Quantities Reported	Valid Temperature range.	Reference
$CaZrTi_2O_7$ [cr]	**C_p, ${}^TS^o$, $\Delta_f^TH^o$, $\Delta_f^TG^o$**	**298.15 to 1500 K**	**6**
$CaHfTi_2O_7$ [cr]	**C_p, ${}^TS^o$, $\Delta_f^TH^o$, $\Delta_f^TG^o$**	**2989.15 to 1500 K**	**9**
$CaCeTi_2O_7$ [cr]	**C_p, ${}^TS^o$, $\Delta_f^TH^o$, $\Delta_f^TG^o$**	**0 to 1500 K**	**Note a**
$Gd_2Ti_2O_7$ [cr]	**C_p, ${}^TS^o$, $\Delta_f^TH^o$, $\Delta_f^TG^o$**	**0 to 1500 K**	**Note a**
$CeTi_2O_6$ [cr]	**C_p, ${}^TS^o$, $\Delta_f^TH^o$, $\Delta_f^TG^o$**	**0 to 1500 K**	**Note a**
$ZrSiO_4$ [cr]	C_p, ${}^TS^o$, $\Delta_f^TH^o$, $\Delta_f^TG^o$	298.15 to 1600K	11
$CaTiO_3$ [cr, perovskite]	**C_p, ${}^TS^o$, $\Delta_f^TH^o$, $\Delta_f^TG^o$**	**0 to 1900 K**	**17**
$ZrTiO_4$ [cr]	**C_p, ${}^TS^o$, $\Delta_f^TH^o$, $\Delta_f^TG^o$**	**0 to 1400 K**	**18**
CaO [cr]	C_p, ${}^TS^o$, $\Delta_f^TH^o$, $\Delta_f^TG^o$	298.15 to 1800 K	11
Ce_2O_3 [cr, α]	C_p, ${}^TS^o$, $\Delta_f^TH^o$, $\Delta_f^TG^o$	298.15 to 1500 K	21
CeO_2 [cr]	C_p, ${}^TS^o$, $\Delta_f^TH^o$, $\Delta_f^TG^o$	298.15 to 1800 K	11
Eu_2O_3 [cr, α]	C_p, ${}^TS^o$, $\Delta_f^TH^o$, $\Delta_f^TG^o$	298.15 to 1800 K	20
Gd_2O_3 [cr, α]	C_p, ${}^TS^o$, $\Delta_f^TH^o$, $\Delta_f^TG^o$	298.15 to 1800 K	20
HfO_2 [cr]	**C_p, ${}^TS^o$, $\Delta_f^TH^o$, $\Delta_f^TG^o$**	**298.15 to 1500 K**	**9**
La_2O_3 [cr]	C_p, ${}^TS^o$, $\Delta_f^TH^o$, $\Delta_f^TG^o$	298.15 to 1800 K	20
Lu_2O_3 [cr]	C_p, ${}^TS^o$, $\Delta_f^TH^o$, $\Delta_f^TG^o$	298.15 to 1800 K	20
Nd_2O_3 [cr, α]	C_p, ${}^TS^o$, $\Delta_f^TH^o$, $\Delta_f^TG^o$	298.15 to 1800 K	20
PuO_2 [cr]	$\Delta_f^TH^o$, $\Delta_f^TG^o$	298.15 to 1500 K	29
SiO_2 [cr, quartz]	C_p, ${}^TS^o$, $\Delta_f^TH^o$, $\Delta_f^TG^o$	298.15 to 1800 K	11
ThO_2 [cr]	C_p, ${}^TS^o$, $\Delta_f^TH^o$, $\Delta_f^TG^o$	298.15 to 1200 K	11
TiO_2 [cr, rutile]	C_p, ${}^TS^o$, $\Delta_f^TH^o$, $\Delta_f^TG^o$	298.15 to 1800 K	11
UO_2 [cr]	C_p, ${}^TS^o$, $\Delta_f^TH^o$, $\Delta_f^TG^o$	298.15 to 1800 K	11
Yb_2O_3 [cr, α]	C_p, ${}^TS^o$, $\Delta_f^TH^o$, $\Delta_f^TG^o$	298.15 to 1800 K	20
ZrO_2 [cr]	C_p, ${}^TS^o$, $\Delta_f^TH^o$, $\Delta_f^TG^o$	298.15 to 1800 K	11
Ca [cr]	C_p, ${}^TS^o$	298.15 to 1800 K	11
Ce [cr]	C_p, ${}^TS^o$	298.15 to 1800 K	11
Eu [cr]	C_p, ${}^TS^o$	298.15 to 1800 K	20
Gd [cr]	C_p, ${}^TS^o$	298.15 to 1800 K	20
Hf [cr]	C_p, ${}^TS^o$	0 to 6000 K	2
La [cr]	C_p, ${}^TS^o$	298.15 to 1800 K	20
Lu [cr]	C_p, ${}^TS^o$	298.15 to 1800 K	20
Nd [cr]	C_p, ${}^TS^o$	298.15 to 1800 K	20
O_2 [g]	C_p, ${}^TS^o$	0 to 6000 K	2
P [cr,]	C_p, ${}^TS^o$	0 to 6000 K	2
Pu [cr, α]	C_p, ${}^TS^o$	260 to 873 K	30
Si [cr]	C_p, ${}^TS^o$	0 to 6000 K	2

Compound	Thermodynamic Quantities Reported	Valid Temperature range.	Reference
Th [cr]	C_p, ${}^{T}S^{o}$	298.15 to 1800 K	11
Ti [cr]	C_p, ${}^{T}S^{o}$	0 to 6000 K	2
U [cr]	C_p, ${}^{T}S^{o}$	298.15 to 1800 K	11
Yb [cr]	C_p, ${}^{T}S^{o}$	298.15 to 1400 K	20
Zr [cr]	C_p, ${}^{T}S^{o}$	0 to 6000 K	2

a. Data forthcoming from our laboratory.

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