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A Computer-Assisted Evaluation of the Thermochemical Data of the Compounds of Thorium

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Abstract

Selected values are given for the thermochemical properties of the compounds of thorium. They are obtained from a computer-assisted least sums-least squares approach to the evaluation of thermodynamic data networks. The properties given, where data are available, are enthalpy of formation, Gibbs energy of formation, and entropy at 298.15 K ($\Delta Hf°(298)$, $\Delta Gf°(298)$, and $S°(298)$). The values are consistent with the CODATA Key Values for Thermodynamics. The reaction catalog from which this self consistent set of values is generated is given with a statistical analysis. Some thermal functions are also given, as well as detailed comments when necessary.

Keywords: Data evaluation; enthalpy; entropy; Gibbs energy; thermochemical data networks; thermochemical tables; thorium compounds.

I. General Description

1. Introduction

This report presents a computer-assisted comprehensive evaluation of the thermochemical properties of compounds of thorium at 298 K that is consistent with the CODATA Key Values for Thermodynamics [75COD][a]. A combined least sums-least squares technique previously described by Garvin et al [76GAR/PAR] has been used. This computer-based evaluation is an extension of the CATCH program developed by J. B. Pedley, University of Sussex who used linear least squares analysis on enthalpy measurements [69GUE/PED].

Thorium represents the first complete analysis of an element and its compounds to be done by this least sums-least squares approach to the evaluation of thermodynamic data networks. A self consistent set of values for $\Delta Hf°$, $\Delta Gf°$, and $S°$ is generated from the given reaction catalog. A detailed analysis of the values leads us to believe that they are as good as and as reliable as those which would be obtained in the traditional sequential method. Comparisons of the performance of the computer-assisted method used here versus the traditional method are given in [76GAR/PAR].

A major advantage of this method is the rapid updating that is possible when new data become available or if the interpretation of the existing data must be revised. Another advantage of this method is that a translation from one scale of auxiliary values (CODATA here) to the NBS Technical Note 270 Scale or some other scale can be made readily.

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[a] References are given in a chronologically ordered bibliography at the end of the report. They are cited in the text in coded form indicating year of publication and the first two authors.

This report provides the following data: the final selceted values for $\Delta Hf°$, $\Delta Gf°$ and $S°$ for the compounds considered and their predicted reliabilities, the values used for auxiliary compounds, a catalog of the measurements upon which the solution is based, some newly developed thermal functions and, where, needed, comments on the interpretation of the data.

The values for properties of auxiliary compounds are either CODATA selections [75COD] or compatible with them [75PAR/WAG].

The reaction catalog (following the selected values), from which the solution is derived, contains the set of experimental enthalpy, Gibbs energy and entropy changes at 298 K as well as entropies at 298 K from low temperature Cp measurements or statistical calculations. It also contains for each reaction the initial assigned uncertainty, the final weighting factor, the residual (i.e., the observed minus the predicted value), the standard deviation of the predicted value (95 per cent confidence level), a coded citation to the Bibliography, and, occasionally, brief comments on corrections made to or interpretation of individual measurements.

Users of the tables and reaction catalog are invited to comment on the selections, correct errors and bring new measurements to our attention.

2. Explanation of the Contents of the Tables

The following material provides definitions and conventions used in the tables.

2.1 Chemical Formulae and Physical States

The tables were reproduced from computer printout in which only capital (upper case) letters are available. Normal one-line chemical formulae are used, with the following modifications:

- Subscripts (counts of atoms) and superscripts (charge) are printed on line: TH'CL'4 = $ThCl_4$; TH'CL'+3 = $ThCl^{3+}$

- The apostrophe ' appears after each letter in a chemical symbol that would normally be written in lower case: TH'N = ThN

- The centered dot, used in hydrates and minerals, is shown as a colon: TH'F4:2.5H2O = $ThF_4 \cdot 2.5H_2O$

- The physical state of the substance is appended to the chemical formula in parentheses: TH'CL'4(C) = $ThCl_4$, crystalline

Conventions with respect to physical state are given in Table A.

2.2 Definition of Symbols for Thermochemical Properties

The headings used in the tabulated Thermochemical Values have the following meanings:

DELTA HF = $\Delta Hf°$, standard enthalpy of formation at 298.15 K;

DELTA GF = $\Delta Gf°$, standard Gibbs energy (formerly free energy), G, of formation at 298.15 K;

+/- SIGMA = Predicted reliability, "one sigma" (see paragraph 4.1)

In the reaction catalog the heading, PROP. MEAS. refers to ΔH, ΔG, and ΔS at 298 K for the process given; the symbols used are H, G, and S; the symbol S means $S°_{298}$ when it refers to a "process" written without reactants:

= TH'CL'4(C) S = 45.5 (standard entropy of cryst. $ThCl_4$)

All H and G relationships are in kcal/mol; all S relationships in cal/(mol·K).

All values refer to one mole of substance for the formula given.

2.3 Conventions Regarding Pure Substances

The values of the thermodynamic properties of the pure substances given in these tables are for the substances in their standard states. These standard states are defined as follows:

For a pure solid or liquid, the standard state at any temperature is the substance in the condensed phase under a pressure of one atmosphere.

For a gas the standard state at any temperature is the hypothetical ideal gas at unit fugacity, in which state the enthalpy is that of the real gas at the same temperature and at zero pressure.

The phase of a substance is indicated in parentheses at the end of the chemical formula. See Table A.

The values of $\Delta Hf°$ and $\Delta Gf°$ given in the tables represent the change in the appropriate thermodynamic quantity when one mole of the substance in its standard state is formed, isothermally at the indicated temperature, from the elements, each in its appropriate standard reference state. The standard reference state at 298 K for each element except phosphorus has been chosen to be the standard state that is thermodynamically stable at 298 K and at one atmosphere pressure. For phosphorus the standard reference state is the crystalline white form; the more stable forms have not been well characterized thermochemically. The same reference states have been maintained for the

elements at 0 K except for the liquid elements bromine and mercury for which the reference states have been chosen as the stable crystalline forms. The standard reference states for the elements are indicated in the tables by the fact that the values of $\Delta Hf°$ and $\Delta Gf°$ are exactly zero.

The values of S° represent the virtual or "thermal" entropy of the substance in the standard state at 298.15 K, omitting contributions from nuclear spins and isotopic mixing. Where data have been available only for a particular isotope, they have been corrected when possible to the normal isotopic composition.

2.4 Convention Regarding Solutions

For all dissolved substances the composition of the solvent is indicated in parentheses following the chemical formula. Except in special cases, discussed below, the number of moles of the solvent associated with one mole of solute is stated explicitly. See Table A for the conventions used.

In some cases the concentration of the solute can not be specified. These are indicated as "AU" (aqueous, unspecified) for water solutions and by "U" for non-aqueous and mixed media. In all these cases the solution may be assumed to be "dilute".

The standard state for a non-dissociated solute in aqueous solution is taken as the hypothetical ideal solution of unit molality, which has been designated as "std. state, m = 1". For strong electrolytes in aqueous solution the conventional standard state is the ideal

solution of unit activity (unit mean molality). The designation "A" is used for strong electrolytes in the standard state and "AO" for undissociated species in water solution. In non-aqueous media two standard states are commonly used. For the mole fraction scale, "std. state, $x_2 = 1$", x is added to the formula of the solvent. For the molal scale, "std. state, m = 1", either s or M is appended to the formula.

The value of $\Delta Hf°$ for a solute in its standard state is equal to the apparent molal enthalpy of formation of the substance in the infinitely dilute real solution, since the enthalpy of dilution of an ideal solution is zero. At this dilution the partial molal enthalpy is equal to the apparent molal quantity. At concentrations other than the standard state, the value of $\Delta Hf°$ represents the apparent enthalpy of the reaction of formation of the solution from the elements comprising the solute, each in its standard reference state, and the appropriate total number of moles of solvent. In this representation the value of $\Delta Hf°$ for the solvent is not required. The experimental value for a heat of dilution is obtained directly as the difference between the two values of $\Delta Hf°$ at the corresponding concentrations. At finite concentrations the partial molal enthalpy of formation differs from the apparent enthalpy.

The values of the thermodynamic properties tabulated for the individual ions in aqueous solution are based on the usual convention

that the values of $\Delta Hf°$, $\Delta Gf°$, $S°$ and $Cp°$ for H^+ (aq, std. state, m = 1) are zero. The properties of a neutral electrolyte in aqueous solution in the standard state are equal to the algebraic sum of these values for the appropriate kinds and numbers of individual ions assumed to constitute the molecule of the given electrolyte. For an ionic aqueous species e.g., HSO_4^-, the properties tabulated refer to that undissociated ion, i.e. they are not equal to the sum of those for its constituent ions. By adopting the above convention with respect to aqueous H^+, it follows that the thermodynamic relation $\Delta Gf° = \Delta Hf° - T(\Delta Sf° + n \cdot 0.5S°(H_2))$ holds for individual ionic species, with n equal to the algebraic value of the charge. For neutral electrolytes the normal consistency relationship applies. See section 4.

3. Unit of Energy and Fundamental Constants

All of the energy values given in these tables are expressed in terms of the thermochemical calorie. This unit, defined as equal to 4.184 joules exactly, is generally accepted for the presentation of chemical thermodynamic data. Values reported in other units have been converted to calories by means of the conversion factors for molecular energy given in Table B.

Values in this report are consistent with the CODATA Fundamental Constants [73COD].

The formula weights in the tables have been calculated from the molecular formula using the 1969 Table of Atomic Weights [70IUP].

Values are given to four decimal places for convenience in the computer processing.

4. Internal Consistency of the Tables

The processes given in the reaction catalog have been obtained from the original articles, using consistent values for all subsidiary and auxiliary quantities. The original data were corrected where possible for differences in energy units, molecular weights, temperature scales, etc. Thus we have sought to maintain a uniform scale of energies for all processes in the tables and catalog. In addition the final tabulated values of the properties of a substance satisfy all the known physical and thermodynamic relationships among these properties. The quantities $\Delta Hf°$, $\Delta Gf°$, and $S°$ at 298.15 K satisfy the relation:

$$\Delta Gf° = \Delta Hf° - T\Delta Sf°$$

to the precision given. The special case of solutions is discussed in section 2.4. Furthermore the calculated value of any thermodynamic quantity for a reaction is independent of the path chosen for the evaluation.

4.1 Uncertainties

The uncertainty reported for a selected value is "one sigma" as developed in the final least squares solution of the reaction data base. The magnitude of the uncertainty reflects the overall fit of the data in the entire network. It is not an estimate made by the data analyst based on how well various small sections of the network fit together.

These uncertainties, when used in the usual "square root of sum of squares" formula overestimate the uncertainty of a process. This is because the selected values (answers) are highly correlated. Better estimates for processes that are in the data network are provided in the listing of the reaction catalog. These estimates allow for the correlations among values.

Since the selected values are computer generated, more places are given than may be warranted by the uncertainty. Although these extra figures in the absolute sense are not significant, the retention and use of these figures ensures that the experimental data from which these values are derived may be recovered with an accuracy equal to that of the original quantities. This is particularly important for enthalpies of solution, dilution and transition.

4.2 Relationship to Other Tables of Thermodynamic Properties

The chemical thermodynamic properties in the present table may be combined with those published by CODATA in order to calculate the change in a property for a process. However, we recommend against these values being combined with those in any other tabulation or with a property reported in an original research paper. In particular, we warn against indiscriminate combination with the NBS Technical Note 270 Series. A conversion to the NBS Technical Note 270 Scale will be made and included in that series.

There are several reasons for avoiding the combination of thermochemical data from more than one table. The most important is that different large-scale tables use different thermochemical properties

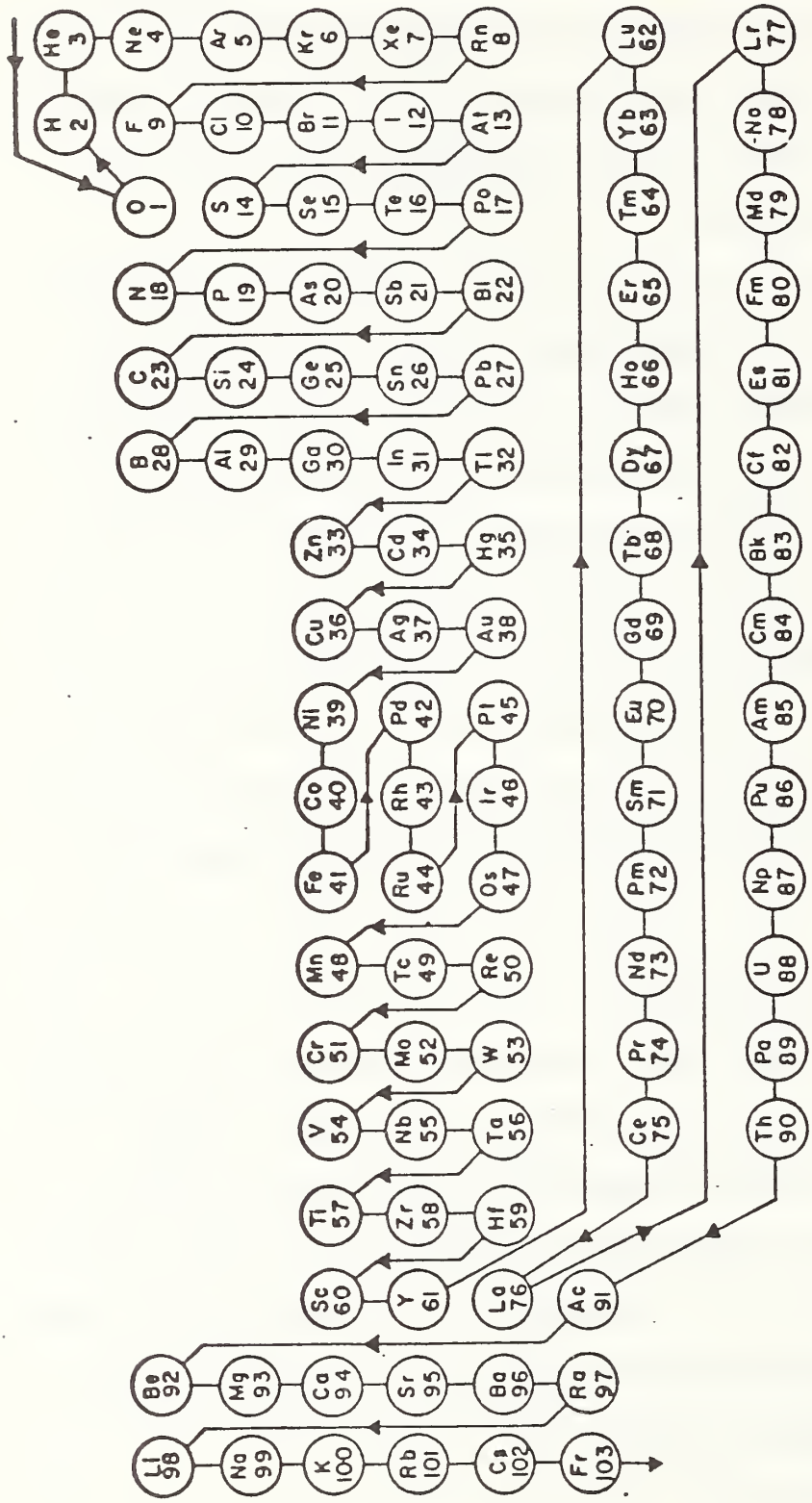
of formation for substances that are ubiquitous in thermochemical measurements. Outstanding examples are in the common inorganic acids and their ions. Another reason is that the groups preparing different tables may have relied on different measurements as the basis for selecting property values.

It is difficult to predict a priori how a change in one selected formation property would affect values assigned to other substances because of the way these are linked by complex networks. In general, it may be expected that the advantage of internal consistency of a table will be lost if values from several sources are combined and the experimental measurements may be reproduced poorly.

No general, simple algorithm can be suggested for overcoming this problem. If it becomes necessary to extend a table of data to substances other than those tabulated, the user is advised to consult the group that prepared the table about the procedure that he plans to use.

5. Arrangement of the Tables

The compounds in the tables are entered according to the Standard Order of Arrangement, (see Figure 1), by the principle of latest position. In this scheme, a compound is listed under the element occurring latest in the list; water of hydration is neglected. Within a given element-table will be found all of the compounds of that element with elements occurring earlier in the order; the arrangement within a table follows the same ordering.



Standard Order of Arrangement of the Elements and Compounds based on the Periodic Classification of the Elements

Figure 1

TABLE A: Physical State Conventions

The following conventions are used to designate the physical state of a substance. These apply to the attached table and to the NBS Thermochemical Data Bank. This information appears in a parenthetical expression appended to the molecular formula. Some of the explanations imply a thermochemical value, particularly those for solutions. These normally are used in describing enthalpy measurements.

Basic Symbols	Explanation
(G)	Gaseous, e.g., HCL'(G) for $HC\ell(g)$
(GS)	Gaseous reference standard state for an element, e.g., O2(GS) for $O_2(g)$
(C)	Crystalline, e.g., NH4CL'(C) for $NH_4C\ell(c)$
(CS)	Crystalline reference standard state for an element, e.g., RB'(CS) for Rb(c)
(L)	Liquid, e.g., H2O(L) for $H_2O(\ell)$
(LS)	Liquid reference standard state for an element, e.g., BR'2(LS) for $Br_2(\ell)$
(AM)	Amorphous
(GL)	Glassy
(A)	Hypothetical standard state of the ideal aqueous solution at unit activity. For a neutral electrolyte the value of a property is equal to the algebraic sum of the values for the ions assumed to constitute the molecule of the electrolyte, e.g. HCL'(A) = H+(A) + CL'-(A). For an ionic species this notation is commonly used to refer to the undissociated ion as written. e.g. HSO4-(A)

Symbol	Explanation
(AO)	Hypothetical standard state of the ideal aqueous solution at unit activity of the undissociated (non-ionized) species, e.g. HF(AO), HF2-(AO). May also be used whenever the designation (A) could be ambiguous. Note that the descriptions HSO4-(A) and HSO4-(AO) are equivalent, but that HF(A) and HF(AO) are not.
(AU)	Aqueous solution of undefined, but usually dilute, concentration, e.g. XE'O3(AU).

The symbols used above occasionally are modified by numbers to distinguish two substances in the same state that have the same molecular weight, as for isomers: (AU2), (C3). They are also used in combination with descriptive material, e.g. (C:HE'), (C:AL') etc. to mean "crystalline, hexagonal", "crystalline, alpha form" etc.

Special notations for substances in solutions

The notations for the "state" of a substance in solution may combine a definition of the system, e.g. HCℓ in 220 moles of water, and a specification of the thermochemical property associated with it. Usually the thermochemical property is the apparent integral enthalpy or free energy of formation or an absolute entropy, i.e. the formation properties of the solvent are not included. If a partial molal property is tabulated the notation D: ("D" for "differential") occurs as the first term in the state bracket. The notations given below illustrate the differences for integral and differential (partial molal) properties, and extrapolated values. Examples are given for aqueous, mixed, and non-aqueous solvents.

Symbol	Explanation
HCL'(200H2O)	An aqueous solution of specified composition, e.g. one mole of $HC\ell$ in 200 moles H_2O. The value of ΔHf represents the apparent integral enthalpy of formation.
HCL'(D:200H2O) and H2O(D:HCL'+200H2O)	These represent the partial molal (enthalpy) of formation of the substance in a solution of specified concentration, e.g. the partial molal enthalpy of formation of $HC\ell$ and H_2O respectively, in a solution consisting of 1 mole $HC\ell$ and 200 moles H_2O.
UCL'4(HCL'O4+50H2O)	This describes a solute dissolved in a mixed solvent, e.g. one mole of $UC\ell_4$ in a mixture of 1 mole of $HC\ell O_4$ and 50 moles H_2O. The value of ΔHf represents the apparent integral enthalpy of formation of the substance, $UC\ell_4$, in the medium.
UCL'4(HCL'O4+ 50H2O:AU)	This represents a solute at an unspecified but usually dilute concentration in a solvent mixture of fixed composition.

TABLE B

CONVERSION FACTORS FOR UNITS OF MOLECULAR ENERGY

	J/mol	cal/mol	cm^3 atm/mol	kWH/mol	Btu/lb-mol	cm^{-1}/molecule	eV/molecule
1 J/mol =	1	2.390057×10^{-1}	9.86923	2.77778×10^{-7}	0.429923	8.35935×10^{-2}	1.036435×10^{-5}
1 cal/mol =	4.184	1	41.2928	1.162222×10^{-6}	1.798796	3.49755×10^{-1}	4.33644×10^{-5}
1 cm^3 atm/mol =	0.1013251	2.42173×10^{-2}	1	2.81458×10^{-8}	4.35619×10^{-2}	8.47011×10^{-3}	1.050166×10^{-6}
1 kWh/mol =	3,600,000	860,421	3.55292×10^{7}	1	1,547,721	300,937	37.3117
1 Btu/lb-mol =	2.32600	5.55927×10^{-1}	22.9558	6.46111×10^{-7}	1	1.944384×10^{-1}	2.41075×10^{-5}
1 cm^{-1}/molecule =	11.96266	2.85914	118.0622	3.32296×10^{-6}	5.14302	1	1.239852×10^{-4}
1 eV/molecule =	96484.56	23060.4	952,230	2.68013×10^{-2}	41480.9	8065.479	1

The underlined numbers represent the fundamental values used in deriving this table. The remaining factors were obtained by applying the relationships:

$$n_{ij} = n_{ik} \cdot n_{kj} \qquad n_{ii} = n_{ik} \cdot n_{ki} = 1$$

II. Tables of Values for $\Delta Hf°$, $\Delta Gf°$ and $S°$ at 298.15 K for the Compounds of Thorium and the Reaction Catalog

NBS CATALOG OF THORIUM THERMOCHEMICAL DATA. 7/27/77 SOLUTION: CODATA COMPATIBLE WEIGHTED SOLN - LST. SQUARES

SEE NOTES AFTER THE LISTING OF AUXILIARY DATA FOR EXPLANATION OF ENTRIES.

HF NO.	COMPOUND	MOL.WT.	DELTA HF +/-SIGMA KCAL.MOL-1	DELTA GF +/-SIGMA KCAL MOL-1	S +/-SIGMA CAL.MOL-1.K-1	REACTIONS
208	TH'(CS')	232.0381	[.000+- .000][.000+- .000][12.761+- .096]			0 [a]
	CODATA TENTATIVE PART V (1975)					
211	TH'(G)	232.0381	[142.900+- 1.400][133.200+- 1.400][45.425+- .010]			0 [a]
	CODATA TENTATIVE PART V (1975)					
214	TH'+(G)	232.0381	283.012+- .863			9 10 11
217	TH'+2(G)	232.0381	550.512+- .992			14
220	TH'+3(G)	232.0381	1012.012+- 1.209			15
223	TH'+4(G)	232.0381	1676.512+- 1.629			16
226	TH'+4(A)	232.0381	[-183.800+- .600][-168.400+- .600][-101.000+- 4.000]			0 [a]
	FUGER,J. AND OETTING, F.L. 'THE CHEMICAL THERMODYNAMICS OF ACTINIDE ELEMENTS AND COMPOUNDS. PART 2. THE ACTINIDE AQUEOUS IONS' IAEA, 1976					
235	TH'O(G)	248.0375	-6.077+- .277	-12.065+- .277	57.350+- .050	19 20 21 22 23 32 33 34 36 343 343 343 18
238	TH'O+(G)	248.0375	135.923+- 1.134			22 23
241	TH'O2(C)	264.0369	[-293.120+- .840][-279.350+- .840][15.590+- .048]			0 [a]
	CODATA TENTATIVE PART V (1975)					
244	TH'O2(G)	264.0369	-118.670+- .672	-120.737+- .688	68.700+- .500	38 39 40 42 344 344 344 37
247	TH'O2+(G)	264.0369	83.330+- .996			40 42
250	TH'H2(C)	234.0541	-32.100+- 1.000	-22.605+- 1.000	12.120+- .030	345 345 345 45 48 46
253	TH'H3.75(C)	235.8181	-48.600+- 1.414	-31.229+- 1.415	13.010+- .030	346 346 346 47 48
256	TH'(OH)+3(A)	249.0455	-246.215+- 1.166	-219.918+- .292	-82.141+- 4.032	49 50 51 53 54 55 56 57 63 347 347 347 52
259	TH'(OH)2+2(A)	266.0529	-306.530+- 1.166	-272.566+- .363	-52.149+- 4.097	58 60 61 62 63 348 348 348 59
268	TH'2(OH)2+6(A)	498.0910		-444.660+- .116		66 67 68 69
274	TH'F(G)	251.0365			61.700+- 1.000	73
277	TH'F+3(A)	251.0365	-265.150+- .797	-246.704+- .173	-71.695+- 2.736	74 75 76 77 78 63 87 352 352 352 352 86 79
280	TH'F2(G)	270.0349	-156.389+- 2.811	-159.161+- 2.827	70.500+- 1.000	353 353 353 80 109
289	TH'F2+2(A)	270.0349	-346.100+- .929	-322.518+- .204	-49.097+- 3.189	82 83 84 85 87 91 92 354 354 354 90 86
292	TH'F3(G)	289.0333	-283.149+- 2.811			110
298	TH'F3+(A)	289.0333	-427.050+- 1.044	-396.241+- .282	-33.512+- 3.627	91 92 93 356 356 356 112 113 90

[a] see note A following the list of Auxiliary Data

NBS CATALOG OF THORIUM THERMOCHEMICAL DATA. 7/27/77 SOLUTION: CODATA COMPATIBLE WEIGHTED SOLN - LST. SQUARES

HF NO.	COMPOUND	MOL.WT.	DELTA HF +/-SIGMA KCAL.MOL-1	DELTA GF +/-SIGMA KCAL MOL-1	S +/-SIGMA CAL.MOL-1.K-1	REACTIONS
301	TH'F4(C)	308.0317	-501.443+- .685	-478.875+- .685	33.953+- .040	95 96 97 98 99 100 105 106 357 357 357 94 115
304	TH'F4(G)	308.0317	-419.509+- 1.426	-411.177+- 1.495	81.700+- 1.500	105 106 358 358 358 103 109 121
307	TH'F4(AO')	308.0317	-508.100+- 1.147	-468.191+- .554	-24.210+- 4.273	360 360 360 112 113
310	TH'F4:2.5H2O(C)	353.0702	-682.230+- 2.272	-624.711+- 2.349	56.000+- 2.000	361 361 361 114 115
313	TH'OF2(C)	286.0343	-398.815+- 2.525	-380.715+- 2.594	25.000+- 2.000	362 362 362 120 121
316	TH'CL'+3(A)	267.4911	-223.733+- 2.088	-201.273+- .135	-82.733+- 7.018	122 123 125 126 128 129 363 363 363 124
319	TH'CL'2+2(A)	302.9441		-232.250+- .226		127 128 129
322	TH'CL'3+(A)	338.3971		-264.790+- .436		130
325	TH'CL'4(C)	373.8501	-283.642+- .484	-261.627+- .768	45.500+- 2.000	132 134 135 136 138 141 146 147 148 149 150 153 154 163 167 170 172 186 188 192 279 281 359 359 359
328	TH'CL'4(G)	373.8501	-230.942+- .484	-223.685+- .768	95.000+- 2.000	133 134 135 136 138 166 168 364 364 364
331	TH'CL'4(A)	373.8501	-343.532+- .606	-293.920+- .606	-47.058+- 2.875	365 365 365 142 143
334	TH'CL'4(AO')	373.8501		-295.640+- 2.090		144
340	TH'CL'4:2H2O(C)	409.8809	-436.072+- .996			157
343	TH'CL'4:4H2O(C)	445.9117	-587.802+- .996			158
346	TH'CL'4:7H2O(C)	499.9579	-804.447+- .996			159
349	TH'CL'4:8H2O(C)	517.9733	-876.162+- .996			160
355	TH'CL'4(HCL'+5.02H2O:AU')	373.8501	-318.553+- .478			146 155
358	TH'CL'4(HCL'+8.16H2O:AU')	373.8501	-328.081+- .478			147 148 149 150 151 156
361	TH'CL'4(HCL'+54.4H2O:AU')	373.8501	-341.043+- .478			153 154 155 156
364	TH'CL'O3+3(A)	315.4893		-170.470+- 1.536		161
367	TH'OCL'2(C)	318.9435	-294.387+- .629	-276.190+- .672	29.520+- .791	163 166 167 168 366 366 366
370	TH'(CL'O4)4(A)	629.8405	-248.130+-10.043			162
373	TH'BR'4(C)	551.6541	-230.783+- .537	-221.684+- .803	55.000+- 2.000	170 172 368 368 368 174 175

NBS CATALOG OF THORIUM THERMOCHEMICAL DATA. 7/27/77 SOLUTION: CODATA COMPATIBLE WEIGHTED SOLN - LST. SQUARES

HF NO.	COMPOUND	MOL.WT.	DELTA HF +/-SIGMA KCAL.MOL-1	DELTA GF +/-SIGMA KCAL MOL-1	S +/-SIGMA CAL.MOL-1.K-1	REACTIONS
376	TH'BR'4(G)	551.6541	-182.383+- .537	-187.595+- .803	103.000+- 2.000	367 367 367 169 174
379	TH'BR'4(AU')	551.6541	-301.483+- 1.343			176
382	TH'BR'4:7H2O(C)	677.7619	-757.288+- 1.023			177
385	TH'BR'4:10H2O(C)	731.8081	-975.133+- 1.023			178
388	TH'BR'4:12H2O(C)	767.8389	-1119.563+- 1.042			179
391	TH'(BR'O3)+3(A)	359.9403		-170.010+- 1.536		181
397	TH'(BR'O3)2+2(A)	487.8425		-170.350+- 2.315		182
400	TH'I4(C)	739.6561	-160.566+- .570	-158.275+- .815	60.595+- 1.955	185 186 188 191 370 370 370 184 195
403	TH'I4(G)	739.6561	-111.766+- 1.831	-124.880+- 1.911	112.262+- 1.835	183 191 369 369 369 184
406	TH'IO3+3(A)	406.9408		-203.840+- 1.536		198
409	TH'OI2(C)	501.8465	-239.792+- .419	-231.763+- .695	38.093+- 1.860	192 193 371 371 371 195
412	TH'(IO3)2+2(A)	581.8435		-237.920+- 2.315		199
415	TH'(IO3)3+(A)	756.7462		-272.530+- 3.219		200
418	TH'(OH)I3:10H2O(C)	809.9130	-949.148+- 1.300			196
421	TH'S(C)	264.0981	-94.540+- 1.500	-93.444+- 1.501	16.685+- .170	372 372 372 202 208 201
424	TH'S2(C)	296.1581	-149.720+- 2.702	-148.241+- 2.703	23.000+- .200	373 373 373 203 211
427	TH'2S3(C)	560.2562	-259.000+- 3.030	-257.471+- 3.093	43.194+- 2.066	375 375 375 204 208 205 206
430	TH'3S7(C)	920.5343	-454.390+- 8.644			210
433	TH'7S12(C)	2008.9867	-988.900+-12.763	-984.663+-13.005	166.315+- 8.326	374 374 374 204 211 205
436	TH'SO4+2(A)	328.0957	-397.240+- .616	-353.785+- .353	-58.585+- 2.383	213 214 215 216 376 376 376 220 212
439	TH'(SO4)2(C)	424.1533	-607.698+- 1.098	-552.158+- 1.295	37.697+- 2.303	217 219 378 378 378 218
442	TH'(SO4)2(AO')	424.1533	-611.030+- .705	-537.582+- .404	-22.363+- 2.725	216 221 222 377 377 377 220
445	TH'(SO4)3-2(A)	520.2109		-716.572+- .831		223
448	TH'(SO4)4-4(A)	616.2685		-891.762+- 1.104		224
451	TH'N(C)	246.0448	-93.031+- 1.178	-86.398+- 1.179	13.400+- .200	227 228 379 379 379 225
454	TH'3N4(C)	752.1411	-314.260+- 2.400			226 227 228
457	TH'NO3+3(A)	294.0430		-196.320+- .825		229 230 231
460	TH'(NO3)2+2(A)	356.0479		-224.370+- 2.579		232
463	TH'(NO3)4(C)	480.0577			80.000+- 3.000	233
466	TH'(NO3)4(A)	480.0577	-382.040+- .721	-274.960+- .721	39.480+- 4.079	235 236 237 263 264 265 266

NBS CATALOG OF THORIUM THERMOCHEMICAL DATA. 7/27/77 SOLUTION: CODATA COMPATIBLE WEIGHTED SOLN - LST. SQUARES

HF NO.	COMPOUND	MOL.WT.	DELTA HF +/-SIGMA KCAL.MOL-1	DELTA GF +/-SIGMA KCAL MOL-1	S +/-SIGMA CAL.MOL-1.K-1	REACTIONS
484	TH'(NO3)4(350H2O)	480.0577	-380.851+- .151			262
493	TH'(NO3)4:4H2O(C)	552.1193	-646.461+- .153			261
496	TH'(NO3)4:5H2O(C)	570.1347	-718.876+- .149	-555.774+- .010	129.830+- .500	260 263 264 265 266 381 381 381
499	TH'(NO3)4(0.9HCL'O4+5000 H2O)	480.0577	-382.570+- .721			250
502	TH'(NO3)4(1.08HCL'O4+600 0H2O)	480.0577	-382.635+- .721			249
505	TH'(NO3)4(1.26HCL'O4+700 0H2O)	480.0577	-382.654+- .721			248
508	TH'(NO3)4(1.8HCL'O4+1000 0H2O)	480.0577	-382.671+- .721			247
511	TH'(NO3)4(5.4HCL'O4+3000 0H2O)	480.0577	-382.609+- .721			246
514	TH'(NO3)4(9HCL'O4+50000H 2O)	480.0577	-382.570+- .721			245
517	TH'(NO3)4(12.6HCL'O4+700 00H2O)	480.0577	-382.548+- .721			244
520	TH'(NO3)4(18HCL'O4+10000 0H2O)	480.0577	-382.528+- .721			243
556	TH'CL'4:NH4CL'(C)	427.3418	-371.924+- .996			284
559	TH'CL'4:2NH4CL':10H2O(C)	660.9875	-1170.156+- 1.016			277
562	TH'CL'4:4NH3(C)	441.9729	-406.762+- 1.061			272
565	TH'(NH3)4CL'4(C2)	441.9729	-431.162+- 1.061			273
568	TH'CL'4:6NH3(C)	476.0343	-459.522+- 1.147			274
571	TH'(NH3)4CL'4:2NH3(C2)	476.0343	-497.122+- 1.147			275
574	TH'CL'4:7NH3(C)	493.0650	-481.802+- 1.183			276
577	TH'(NH3)4CL'4:3NH3(C2)	493.0650	-528.602+- 1.183			278
580	TH'CL'4:12NH3(C)	578.2185	-584.428+- .751			279 283
583	TH'(NH3)6CL'4:6NH3(C2)	578.2185	-631.102+- 1.385			280
586	TH'CL'4:18NH3(C)	680.4027	-698.656+- .751			281 283
589	TH'(NH3)6CL'4:12NH3(C2)	680.4027	-745.482+- 1.661			282
592	TH'P(C)	263.0119	-83.315+- .000			287 288
598	TH'3P4(C)	820.0095	-273.260+- .000			287 288
601	TH'(H2PO4)+3(A)	329.0255		-444.940+- 1.619		289
604	TH'(H2PO4)2+2(A)	426.0129		-720.860+- 1.628		290
607	TH'C(C)	244.0491	-29.818+- .282			291 292
610	TH'C1.94(C)	255.3394	-29.799+- 1.549	-30.084+- 1.550	16.380+- .200	382 382 382 293 294
616	TH'C2(G)	256.0601	167.181+- 5.234			295
619	TH'C2O4+2(A)	320.0577		-342.182+- .391		297 298 299
622	TH'(C2O4)2(AO')	408.0773		-515.893+- .517		300 301 302
625	TH'(C2O4)2:6H2O(C)	516.1697		-864.740+- 2.316		303
628	TH'(C2O4)3-2(A)	496.0969		-686.800+- 3.219		304

NBS CATALOG OF THORIUM THERMOCHEMICAL DATA. 7/27/77 SOLUTION: CODATA COMPATIBLE WEIGHTED SOLN - LST. SQUARES

HF NO.	COMPOUND	MOL.WT.	DELTA HF +/-SIGMA KCAL.MOL-1	DELTA GF +/-SIGMA KCAL MOL-1	S +/-SIGMA CAL.MOL-1.K-1	REACTIONS
631	TH°C2H3O2+3(A)	291.0829		-259.190+- 1.170		305
634	TH°SCN+3(A)	290.1158		-148.534+- .020		307 308
637	TH°(SCN)2+2(A)	348.1935		-128.380+- 1.628		309
640	TH°(SCN)3+(A)	406.2712		-106.780+- 1.643		310
643	TH°(SCN)4(AQ°)	464.3489		-85.980+- 1.664		311
646	TH°SI°(C)	260.1241	-29.000+- 3.000			312
649	TH°SI°2(C)	288.2101	-39.500+- 3.000			313
652	TH°3SI°2(C)	752.2863	-64.700+- 3.000			314
655	TH°3SI°5(C)	836.5443	-110.700+- 3.000			315
658	TH°GE°(C)	304.6281	-19.000+- 3.000			316
661	TH°GE°2(C)	377.2181	-28.000+- 3.000			317
664	TH°GE°3(C)	449.8081	-33.600+- 3.000			318
667	TH°3GE°(C)	768.7043	-26.000+- 3.000			319
670	TH°3GE°2(C)	841.2943	-47.500+- 3.000			320
673	TH°3GE°5(C)	1059.0643	-76.000+- 3.000			321
682	TH°NI°2(C)	349.4581	-30.724+- 1.660	-30.026+- 1.668	24.702+- .499	383 383 383 325 326
685	TH°NI°5(C)	525.5881	-62.059+- 1.778	-59.033+- 1.792	38.314+- .551	385 385 385 325 326 329 330
688	TH°2NI°17(C)	1462.1462	-112.600+- 5.000	-110.066+- 5.048	138.402+- 1.576	386 386 386 329 330 327 328
694	TH°CO°(C)	290.9713	-22.393+- 1.762	-20.368+- 1.770	13.149+- .527	389 389 389 341 342 333 334
697	TH°CO°5(C)	526.7041	-42.824+- 1.778	-39.044+- 1.792	35.985+- .551	390 390 390 335 336 339 340
700	TH°2CO°7(C)	876.6086	-89.753+- 2.856	-80.645+- 2.876	45.235+- .877	388 388 388 333 334 335 336
703	TH°2CO°17(C)	1465.9406	-74.800+- 5.000	-70.298+- 5.048	132.482+- 1.576	391 391 391 339 340 337 338
706	TH°7CO°3(C)	1801.0663	-72.180+-11.311	-69.831+-11.358	102.990+- 3.376	392 392 392 341 342

AUXILIARY DATA USED IN SOLUTION

HF NO.	COMPOUND	MOL.WT.	DELTA HF +/-SIGMA KCAL.MOL-1	DELTA GF +/-SIGMA KCAL MOL-1	S +/-SIGMA CAL.MOL-1.K-1	REACTIONS
1	O2(GS°)	31.9988	.000+- .000	.000+- .000	49.005+- .008	
	CODATA RECOMMENDATIONS (FINAL). 1975					
4	H+(A)	1.0080	.000+- .000	.000+- .000	.000+- .000	
	CONVENTION					
7	H2(GS°)	2.0160	.000+- .000	.000+- .000	31.207+- .008	
	CODATA RECOMMENDATIONS (FINAL). 1975					
10	OH-(A)	17.0074		-37.604+- .011		
	CODATA RECOMMENDATIONS (FINAL). 1975					
13	H2O(L)	18.0154	-68.315+- .010	-56.690+- .010	16.718+- .019	
	CODATA RECOMMENDATIONS (FINAL). 1975					
16	F(G)	18.9984	18.970+- .050			
	BASED ON CODATA TENTATIVE VALUES (1975)					
19	F-(A)	18.9984	-80.150+- .160	-67.340+- .160		
	CODATA RECOMMENDATIONS (FINAL). 1975					
22	F2(GS°)	37.9968	.000+- .000	.000+- .000	48.443+- .010	
	CODATA RECOMMENDATIONS (FINAL). 1975					

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 25 HF(AO°)                        20.0064                          -71.680+-  .100
      SEE FOOTNOTE F(7) OF CODATA RECOMMENDATIONS (FINAL), 1975
 28 CL°-(A)                        35.4530      -39.933+-  .021     -31.380+-  .021
      CODATA RECOMMENDATIONS (FINAL), 1975
 31 CL°2(GS°)                      70.9060          .000+-  .000        .000+-  .000      53.290+-  .010
      CODATA RECOMMENDATIONS (FINAL), 1975
 34 CL°O3-(A)                      83.4512                           -.800+- 1.000
 37 HCL°(1000H2O)                  36.4610      -39.850+-  .010
 40 HCL°(D:55H2O)                  36.4610      -39.286+-  .021
      -39.933(HCL(A),CODATA)+0.407(PHI-L,NSRDS-NBS2)+0.240(DIFF°LDH SEPN. 55H2O)
 43 HCL°(D:54.4H2O)                36.4610      -39.284+-  .010
      CODATA CL- AND L2 (HCL) BASED ON NSRDS/NBS-2
 46 HCL°(D:15H2O)                  36.4610      -38.145+-  .025
      CODATA + L2 BASED ON NSRDS/NBS-2
 49 HCL°(D:8.16H2O)                36.4610      -36.686+-  .010
      CODATA CL- AND L2 (HCL) BASED ON NSRDS/NBS-2
 52 HCL°O4(A)                     100.4586      -30.910+-  .100
 55 BR°2(LS°)                     159.8080          .000+-  .000        .000+-  .000      36.379+-  .010
      CODATA RECOMMENDATIONS (FINAL), 1975. OK VALUE IS FOR BR2(C)
 58 BR°O3-(A)                     127.9022                           .400+- 1.000
 61 HBR°(1000H2O)                  80.9120      -28.958+-  .010
 64 HBR°(D:HCL°+54.4H2O)           80.9120      -28.530+-  .010
      CODATA BR- AND L2 (HBR) BASED ON NSRDS/NBS-2
 67 HBR°(D:HCL°+8.16H2O)           80.9120      -26.201+-  .010
      CODATA BR- AND L2 FOR HBR BASED ON NSRDS/NBS-2
 70 I-(D:HCL°+54.4H2O)            126.9045      -13.268+-  .010
      CODATA + L2 BASED ON NSRDS/NBS-2
 73 I2(CS°)                       253.8090          .000+-  .000        .000+-  .000      27.758+-  .019
      CODATA RECOMMENDATIONS (FINAL), 1975
 76 IO3-(A)                       174.9027                          -30.600+- 1.000
 79 HI(5.4H2O)                    127.9125      -11.710+-  .200
      -13.60(HI(A),CODATA) + 1.89(PHI-L, NSRDS-NBS2)
 82 HI(1000H2O)                   127.9125      -13.106+-  .010
 85 HI(D:HCL°+54.4H2O)            127.9125      -13.265+-  .010
      CODATA I- AND L2 FOR HI BASED ON NSRDS/NBS-2
 88 HI(D:HCL°+8.16H2O)            127.9125      -11.220+-  .010
      CODATA I- AND L2 (HI) BASED ON NSRDS/NBS-2
 91 S(CS°)                         32.0600          .000+-  .000        .000+-  .000       7.600+-  .050
      RHOMBIC
      CODATA TENTATIVE PART V (1975)
 94 S2(G)                          64.1200       30.710+-  .072
      CODATA RECOMMENDATIONS (FINAL), 1975
 97 SO2(G)                         64.0588      -70.939+-  .048                           59.300+-  .014
      CODATA RECOMMENDATIONS (FINAL), 1975
100 SO4-2(A)                       96.0576                         -177.950+-  .096
      CODATA TENTATIVE PART V (1975)
103 HSO4-(A)                       97.0656     -212.900+-  .100    -180.660+-  .100
      BASED ON CODATA TENTATIVE VALUES(1975)
106 N2(GS°)                        28.0134          .000+-  .000        .000+-  .000      45.770+-  .006
      CODATA RECOMMENDATIONS (FINAL), 1975
109 NO2(G)                         46.0055        7.930+-  .100
112 NO3-(A)                        62.0049      -49.560+-  .100     -26.640+-  .100      35.120+-  .200
       CODATA BULL. 10 FOR ION ENTROPY. DHF FROM TN-270-3
115 NH3(G)                         17.0307      -10.980+-  .084
      CODATA RECOMMENDATIONS (FINAL), 1975
118 NH4NO3(30H2O)                  80.0436      -81.945+-  .100
      COMBINES NH4+(CODATA),NO3-(NBS TN 270-3) AND PHI(L) (NSRDS/NBS-2)
121 NH4CL°(C)                      53.4917      -75.332+-  .069
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      TAKEN FROM CODATA IONIC ENTROPY EVALUATION:  SEE CODATA BULL. 10
124 P(G)                        30.9738      75.620+-  .360
      CODATA TENTATIVE PART V (1975)
127 P2(G)                       61.9476      34.370+-  .720
      CODATA TENTATIVE PART V (1975)
130 H3PO4(AQ')                  97.9954                        -273.100+-  .100
133 C(CS')                      12.0110        .000+-  .000       .000+-  .000       1.372+-  .029
      CODATA RECOMMENDATIONS (FINAL), 1975
136 CO(G)                       28.0104     -26.417+-  .041
      CODATA RECOMMENDATIONS (FINAL), 1975
139 CO2(G)                      44.0098     -94.051+-  .031
      CODATA RECOMMENDATIONS (FINAL), 1975
142 C2O4-2(A)                   88.0196                        -161.100+- 1.000
145 C2H3O2-(A)                  59.0448                         -88.290+-  .100
148 HC2H3O2(AQ')                60.0528                         -94.780+-  .100
151 SCN-(A)                     58.0777                          22.150+-  .100
      THIOCYANATE ION
154 SI'(CS')                    28.0860        .000+-  .000
      CODATA RECOMMENDATIONS (FINAL), 1975
157 SI'(G)                      28.0860     107.600+- 1.900
      CODATA RECOMMENDATIONS (FINAL), 1975
160 SI'O(G)                     44.0854     -23.800+- 1.000
163 SI'O2(C)                    60.0848    -217.720+-  .100                          10.000+-  .100
      ALPHA, QUARTZ
166 SI'F4(G)                   104.0796    -385.980+-  .200                          67.555+-  .096
      CODATA RECOMMENDATIONS (FINAL), 1975
169 GE'(CS')                    72.5900        .000+-  .000
172 B(G)                        10.8100     133.800+- 2.900
      CODATA RECOMMENDATIONS (FINAL), 1975
175 AL'(CS')                    26.9815        .000+-  .000
      CODATA RECOMMENDATIONS (FINAL), 1975
178 AL'F3(C)                    83.9767    -360.990+-  .310
      CODATA TENTATIVE PART V (1975)
181 NI'(CS')                    58.7100        .000+-  .000       .000+-  .000       7.140+-  .100
184 NI'F2(C)                    96.7068    -157.200+-  .400                          17.590+-  .100
      RUDZITIS.E., VANDEVENTER.E.H., HUBBARD.W.N., J.CHEM.ENG.DATA.12.133(1967)
187 CO'(CS')                    58.9332        .000+-  .000       .000+-  .000       7.180+-  .100
   ALPHA, HEXAGONAL
190 TI'O2(C3)                   79.8988    -225.800+- 1.000                          12.030+-  .100
   RUTILE
193 TI'I4(G)                   555.5180     -66.400+- 1.000                         103.000+-  .300
      CALC'D FROM DATA OF CLARK AND WILLIS J.CHEM.SOC., 1971, 838
196 Y(G)                        88.9059     100.700+- 1.000
199 YO(G)                      104.9053      -9.300+- 1.000
202 LA'(G)                     138.9055     103.000+- 1.000
205 LA'O(G)                    154.9049     -29.010+-  .100
709 MG'(CS')                    24.3050        .000+-  .000
      CODATA TENTATIVE PART V (1975)
712 MG'F2(C)                    62.3018    -268.690+-  .290
      CODATA TENTATIVE PART V (1975)
715 CA'(G)                      40.0800      42.500+-  .190
      CODATA TENTATIVE PART V (1975)
718 CA'F(G)                     59.0784     -66.000+- 1.000
      CODATA + VBP(75)
721 NA'OH(550H2O)               39.9972    -112.303+-  .010
      CODATA + PHI(L) NSRDS-2
724 NA'CL'(550H2O)              58.4428     -97.282+-  .010
      CODATA (75) + PHI(L) NSRDS/NBS-2
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NOTES ON DELTA HF(298), DELTA GF(298) AND S(298)

THESE ARE PRODUCED IN A SIMULTANEOUS SOLUTION OF THE REACTIONS LISTED SEPARATELY, EITHER BY LEAST SQUARES OR LEAST SUMS. THE REACTIONS IN WHICH A COMPOUND APPEARS AND WHICH ARE USED IN SETTING ITS PROPERTIES ARE LISTED BY NUMBER.

COMPOUNDS ARE LISTED ACCORDING TO THE STANDARD ORDER OF ARRANGEMENT (APPROXIMATELY).

THE PARENTHETICAL EXPRESSION AT THE RIGHT-HAND END OF A CHEMICAL FORMULA SHOWS THE PHYSICAL STATE OF, OR THE MEDIUM CONTAINING THE COMPOUND. COMMON ABBREVIATIONS ARE:
C = CRYSTALLINE, L = LIQUID, G= GASEOUS, OR, FOR ELEMENTS IN THEIR REFERENCE STATES, CS, LS, AND GS.
AM = AMORPHOUS, GL = GLASSY, A = HYPOTHETICAL STANDARD STATE, M = 1, IN AQUEOUS SOLUTION.
AO = AQUEOUS, UNDISSOCIATED, AU = AQUEOUS, UNSPECIFIED CONCENTRATION, USUALLY DILUTE.
250 H2O, ETC. = SOLUTION OF SPECIFIED CONCENTRATION., D:=DIFFERENTIAL (PARTIAL MOLAL) PROPERTY.

FORMULA WEIGHTS ARE ON THE 1969 ATOMIC WEIGHT SCALE.

SIGMA = 1 STANDARD DEVIATION. (NOT DEFINED FOR LEAST SUMS). THE MAGNITUDE OF SIGMA REFLECTS THE OVER-ALL FIT OF THE NETWORK. WHEN SIGMAS ARE USED IN THE USUAL SQUARE-ROOT-OF-SUM-OF-SQUARES FORMULA TO PREDICT THE STD. DEV. OF A PROCESS, THE RESULT IS TOO LARGE BECAUSE PROPERTIES ARE HIGHLY CORRELATED. SEE LIST OF REACTIONS FOR BETTER ESTIMATES.

A VALUE IN THE MAIN LIST THAT IS ENCLOSED IN SQUARE BRACKETS IS AN AUXILIARY, FIXED, DATUM.

Note A: The numbers for the reaction equations in which Th(C,S), Th(G), Th+4(A), and ThO_2(6) appear are not listed in this table because these substances are assigned fixed values. If they had not been fixed they would appear as variables in the following reactions:

Th(G): 2-6, 8-11, 19-21

Th+4(A): 49-63, 66-69, 74-79, 82, 84, 85, 93, 122-127, 141, 144, 212-215, 221, 222, 229-232, 290, 297-305, 307-311

ThO_2(C): 26, 27, 32-34, 36, 38, 39, 100, 121, 162, 163, 166, 193, 217, 218, 226, 291, 292

Note B: A solution obtained when the values for Th(G), Th+4(A), and ThO_2(C) are not fixed, but are solved as variables, results in values for these substances which differ at most by 0.3 kcal from those listed in this table.

NBS CATALOG OF THORIUM THERMOCHEMICAL DATA. 7/27/77 SOLUTION: CODATA COMPATIBLE WEIGHTED SOLN - LST. SQUARES

SEE NOTES AT END OF THE LISTING OF THE REACTIONS FOR EXPLANATION OF ENTRIES.

NO.	REACTION	PROP. MEAS.	OBSVD.	+- UNC.	WT.	RESID. (OB-CAL)	STD. DEV.	AVE. FIT	STD. RES.	REFERENCE
		KCAL/MOL OR CAL/(MOL.K)								
1	= TH°(CS°)	S=	12.76	0.20	-1.0	-.001				53GRI/SKO
	S AND LOW-T THERM. FUNCTS. AS SELECTED BY HULTGREN(FEB. 1967) . HIGH-T THERM. FUNCTS. SOLID TH FROM NBS FIT TO 66LEV: H(ALPHA)-H(ALPHA.298K) = 6.2674T+0.0003325T2+0.0000002346T3-1904(298-1660-K); H(BETA) - H(ALPHA.298K) = 3.7196T+0.001438T2-1185(1660-2020K-); ^H(MELT.2020K) = 3304 . CP(L.ABOVE 2020K) = 11.0 (EST°D BY RAND).									
					CONSTRAINT					
2	= TH°(G)	S=	45.42	0.01	-1.0	-.005				68ZAL
	S AND THERM. FUNCTS. TO 3000K BY NBS FROM 75 ELECTRONIC LEVELS OF 68ZAL TO 20.000 CM-1 .									
					CONSTRAINT					
3	TH°(CS°) = TH°(G)	H=	143.48	1.00	-1.0	.580				72ACK/RAU
	KNUDSEN EFFUSION. 2463 - 2494K; 3RD LAW. RECALCD. BY NBS. INCL. 0.035 CORRN. FOR W SOLY.									
4	TH°(CS°) = TH°(G)	H=	141.2	3.5	-1.0	-1.700				73ACK/RAU
	MASS SPEC. OVER TH(L). THO2; 2020 - 2420K; 2ND LAW. RECALCD. BY NBS .									
5	TH°(CS°) = TH°(G)	H=	142.71	3.00	-1.0	-.190				72ACK/RAU
	MASS SPEC. 2010 - 2460K; 2ND LAW. RECALCD. BY NBS .									
6	TH°(CS°) = TH°(G)	H=	138.5	1.0	-1.0	-4.400				60DAR/MCC
	LANGMUIR EVAP°N. 1757-1956K; 3RD LAW. RECALC°D BY NBS; 2ND LAW GIVES 134.1									
7	TH°(CS°) = TH°(G)	H=	130.6	5.0	-1.0	-12.300				67WEE/MOR
	2ND LAW; 63.6 KCAL TH EXCTN. ENERGY SUBTRACTED									
					LISTED FOR INFORMATION ONLY.					
8	TH°(G) = TH°(CS°)	H=	-143.0	0.5	-1.0	-.100				.NBS
	SELECTED .									
					CONSTRAINT					
9	TH°(G) = TH°+(G)	H=	140.	2.	1.0	-.112	.86	1.06	-.17	74RAU/ACK
10	TH°(G) = TH°+(G)	H=	137.5	7.0	.2	-2.612	.86	4.81	-1.14	73ACK/RAU
	ELECTRON IMPACT. 5.9$0.3EV + 1.48 TO ADJUST TO 298K .									
11	TH°(G) = TH°+(G)	H=	141.7	2.8	.4	1.587	.86	2.19	1.06	73SUG
	CORRELN. IN SPECRUM ANAL.; 6.08 $ 0.12 EV + 1.48 TO ADJUST TO 298K									

NO.	REACTION	PROP. MEAS.	OBSVD. KCAL/MOL OR CAL/(MOL.K)	← UNC.	WT.	RESID. (OB-CAL)	STD. DEV.	AVE. FIT	STD. RES.	REFERENCE
12	TH°(G) = TH°+(G) HOT WIRE SURFACE IONIZATION; 6.95$0.12 EV + 1.48 TO ADJUST TO 298K	H=	161.8	2.8	-1.0	21.687				61ION/MIT
			LISTED FOR INFORMATION ONLY.							
13	TH°(G) = TH°+(G) SURFACE IONIZATION; 7.5$0.6 EV + 1.48 TO ADJUST TO 298K .	H=	174.4	6.9	-1.0	34.288				69SMI/HER
			LISTED FOR INFORMATION ONLY.							
14	TH°+(G) = TH°+2(G) 93000 WAVE NOS. + 1.5 KCAL TO 298 K	H=	267.5	0.2	-1.0	.000				70MOO
15	TH°+2(G) = TH°+3(G) 161000 WAVE NOS. + 1.5 KCAL TO 298 K	H=	461.5	0.4	-1.0	.000				70MOO
16	TH°+3(G) = TH°+4(G) 231900 WAVE NOS. + 1.5 KCAL TO 298 K	H=	664.5	1.0	-1.0	.000				70MOO
17	TH°(CS°) + 4 H+(A) = TH°+4(A) + 2 H2(GS°)	C=	0.0	0.0	-1.0	.000				.DEFINED
					CONSTRAINT					
18	= TH°O(G) LEVELS OF 65EDV/SEL; 1 SIGMA GRD. STATE; MLTPLCTY. 1ST EXC. LEVEL TAKEN TO BE 2 (72WEN/SPI USES 6). SEE ALSO ROSEN .	S=	57.35	0.05	-1.0	.000				.NBS
					CONSTRAINT					
19	YO(G) + TH°(G) = TH°O(G) + Y(G) 2ND AND 3RD LAW; 0.2 KCAL TO 298 K	H=	-39.0	0.2	10.0	-.023	.28	.11	-.08	73ACK/RAU
20	TH°O(G) + SI°(G) = SI°O(G) + TH°(G) THIRD LAW; USING AUTHORS' FIRST SERIES ONLY; 0.4 KCAL TO 298 K	H=	19.4	2.0	.5	1.823	.28	1.91	1.04	74HIL/MUR
21	TH°O(G) + LA°(G) = TH°(G) + LA°O(G) MEAN OF SECOND AND THIRD LAW VALUES	H=	14.9	3.5	.4	-2.067	.28	2.78	-1.05	74NEU/ZMB
22	TH°O(G) = TH°O+(G) ELECTRON IMPACT; 6.1$0.2 EV + 1.481 TO ADJUST TO 298K	H=	142.	2.	1.0	.000	1.10	1.00	.00	74RAU/ACK
23	TH°O(G) = TH°O+(G) MASS SPCTRMTRC. APP. PTNTL.; 6.1$0.15EV + 1.481 TO ADJUST TO 298K	H=	142.	7.	.3	.000	1.10	3.50	.00	73ACK/RAU
24	TH°O(G) = TH°O+(G) MASS SPCTRMTRC.APP.PTNTL.; 6.0$0.2EV+1.481 TO ADJ. TO 298K; VALUES F(T) .	H=	139.8	5.0	-1.0	-2.200				74HIL/MUR
			LISTED FOR INFORMATION ONLY.							

NBS CATALOG OF THORIUM THERMOCHEMICAL DATA, 7/27/77 SOLUTION: CODATA COMPATIBLE WEIGHTED SOLN - LST. SQUARES

NO.	REACTION	PROP. MEAS.	OBSVD.	+- UNC.	WT.	RESID. (OB-CAL)	STD. DEV.	AVE. FIT	STD. RES.	REFERENCE
		KCAL/MOL OR CAL/(MOL.K)								
25	TH°O(G) = TH°O+(G)	H=	188.3	7.0	-1.0	46.300				67ILI/RUT
	8.1±0.1 EV: FOR 0 DEGR K.									
			LISTED FOR INFORMATION ONLY.							
26	= TH°O2(C)	S=	15.59	0.02	-1.0	.000				53OSB/WES
						CONSTRAINT				
27	TH°O2(C) = TH°(CS°) + O2(GS°)	H=	293.12	0.83	-1.0	.000				52HUB/HOL
	DIRECT COMBINATION . SELECTED .									
						CONSTRAINT				
28	TH°(CS°) + O2(GS°) = TH°O2(C)	H=	-293.0	2.0	-1.0	.120				32ROT/BEC
			LISTED FOR INFORMATION ONLY.							
29	TH°(CS°) + O2(GS°) = TH°O2(C)	H=	-288.4	2.0	-1.0	4.720				09WAR
	'IMPURITY' CORRECTION DOES NOT APPLY									
			LISTED FOR INFORMATION ONLY.							
30	TH°O2(C) + 4 H+(A) = TH°+4(A) + 2 H2O(L)	G=	-9.2	2.0	-1.0	-6.770				65BAE/MEY
	PRIV. COMM. FROM AUTHOR(1976), REVISED CORRN. TO 25C 0 IONSTR OF MEAS'D -7.18 AT 95C, IONSTR 1 .									
			LISTED FOR INFORMATION ONLY.							
31	TH°(CS°) + TH°O2(C) = 2 TH°O(G)	H=	278.9	2.0	-1.0	-2.067				61DAR/MCC
	CORRECTED VAPOR PRESSURE DATA									
			LISTED FOR INFORMATION ONLY.							
32	TH°(CS°) + TH°O2(C) = 2 TH°O(G)	H=	279.6	2.0	.6	-1.367	.55	1.68	-.90	73ACK/RAU
	THIRD LAW; INCLUDES 0.1 KCAL FOR 0 TO 298 K									
33	TH°(CS°) + TH°O2(C) = 2 TH°O(G)	H=	278.6	2.0	.5	-2.367	.55	2.18	-1.40	63ACK/RAU
	THIRD LAW; INCLUDES 0.1 KCAL FOR 0 TO 298 K									
34	TH°(CS°) + TH°O2(C) = 2 TH°O(G)	H=	282.4	1.0	.8	1.433	.55	1.22	1.11	74HIL/MUR
	THIRD LAW; INCLUDES 0.1 FOR 0 TO 298 K									
35	TH°(CS°) + TH°O2(C) = 2 TH°O(G)	H=	292.9	2.0	-1.0	11.933				74HIL/MUR
	2ND LAW, RECALCD BY NBS. INCLUDES 0.1 KCAL TO 298 K									
			LISTED FOR INFORMATION ONLY.							
36	TH°(CS°) + TH°O2(C) = 2 TH°O(G)	H=	283.0	2.0	.5	2.033	.55	2.02	1.21	73ACK/RAU
	MEASUREMENTS MADE OVER LIQUID TH. INCLUDES 0.1 KCAL FOR 0 TO 298 K									

NO.	REACTION	PROP. MEAS.	OBSVD.	+- UNC.	WT.	RESID. (OB-CAL)	STD. DEV.	AVE. FIT	STD. RES.	REFERENCE
		KCAL/MOL OR CAL/(MOL.K)								
37	= TH'O2(G)	S=	68.7	0.5	-1.0	.000				.NBS
	CALC'D BY NBS FROM DATA OF 74GAB/REE					CONSTRAINT				
38	TH'O2(C) = TH'O2(G)	H=	175.4	3.4	.6	.950	.67	2.17	1.41	73ACK/RAU
	2ND LAW ; INCLUDES +14.0 KCAL FOR 2600 TO 298 K									
39	TH'O2(C) = TH'O2(G)	H=	173.5	3.4	.6	-.950	.67	2.18	-1.41	63ACK/RAU
	RECALCD. VALUES: 2ND LAW: INCLUDES +14.0 KCAL FOR 2600 TO 298 K									
40	TH'O2(G) = TH'O2+(G)	H=	202.	3.	.7	.000	.74	1.50	.00	74RAU/ACK
41	TH'O2(G) = TH'O2+(G)	H=	186.5	20.0	-1.0	-15.500				74HIL/MUR
	8$1 EV + 1.481 TO ADJUST TO 298K					LISTED FOR INFORMATION ONLY.				
42	TH'O2(G) = TH'O2+(G)	H=	202.	7.	.3	.000	.74	3.50	.00	73ACK/RAU
	8.7$0.3 EV + 1.481 TO ADJUST TO 298K									
43	TH'O2(G) = TH'O2+(G)	H=	188.	7.	-1.0	-14.000				67ILI/RUT
	8.1 $ 0.1 EV + 1.481 TO ADJUST TO 298K					LISTED FOR INFORMATION ONLY.				
44	TH'O2(G) = TH'O2+(G)	H=	253.	5.	-1.0	51.000				67ILI/RUT
	10.9 EV + 1.481 TO ADJUST TO 298K					LISTED FOR INFORMATION ONLY.				
45	= TH'H2(C)	S=	12.12	0.03	-1.0	.000				77FLO
46	TH'(CS') + H2(GS') = TH'H2(C)	H=	-32.1	1.0	-1.0	.000				51MAL/CAM
	2ND LAW, DELCP AS FOR ZRH2: -9.5+0.012T (YOUNG, TRANS. AIME 245,971(1969)) .									
47	= TH'H3.75(C)	S=	13.01	0.03	-1.0	.000				77FLO
48	TH'H2(C) + 0.875 H2(GS') = TH'H3.75(C)	H=	-16.5	1.0	-1.0	.000				52NOT/WIL
	ADJUSTED FROM 500 K BY ASSUMED DCP = -2 CAL/DEGR									
49	TH'+4(A) + H2O(L) = TH'(OH)+3(A) + H+(A)	G=	5.34	1.00	2.0	.168	.29	.58	.24	55PAN/HSE
	AUTHORS' 5.81 AT IONSTR 0.5 ADJ'D BY -0.47									
50	TH'+4(A) + OH-(A) = TH'(OH)+3(A)	G=	-15.50	0.50	.9	-1.586	.29	1.04	-1.47	72USH/SKO
	AS REPORTED AT ICNSTR 0									
51	TH'+4(A) + H2O(L) = TH'(OH)+3(A) + H+(A)	G=	5.14	1.00	1.7	-.032	.29	.52	-.04	65BAE/MEY
	RECALC. BY AUTHORS FROM 54KRA/HOL AUTHORS 5.62 AT IONSTR 1 ADJD -0.48									

NBS CATALOG OF THORIUM THERMOCHEMICAL DATA. 7/27/77 SOLUTION: CODATA COMPATIBLE WEIGHTED SOLN - LST. SQUARES

NO.	REACTION	PROP. MEAS.	OBSVD. +- UNC. KCAL/MOL OR CAL/(MOL.K)		WT.	RESID. (OB-CAL)	STD. DEV.	AVE. FIT	STD. RES.	REFERENCE
52	TH°+4(A) + H2O(L) = TH°(OH)+3(A) + H+(A)	H=	5.9	1.0	-1.0	.000				65BAE/MEY
	AS DERIVED BY AUTHORS FROM THEIR DATA AT 0 AND 95C AND THEIR RECALCN. OF DATA OF 54KRA/HOL AT 25C; EFFECT OF IONSTR 1 IGNORED									
53	TH°+4(A) + OH-(A) = TH°(OH)+3(A)	G=	-16.79	1.00	.5	-2.876	.29	1.94	-1.95	67BER
	AUTHORS' -15.88 AT IONSTR 0.5 ADJ'D BY -0.91									
54	TH°+4(A) + H2O(L) = TH°(OH)+3(A) + H+(A)	G=	3.91	0.50	1.0	-1.262	.29	.88	-1.24	72USH/SKO
	AUTHORS' 4.30 AT IONSTR 0.05 ADJ'D BY -0.38									
55	TH°+4(A) + OH-(A) = TH°(OH)+3(A)	G=	-13.52	0.50	2.8	.394	.29	.45	.70	64NAB/KUD
	AUTHORS'-12.82 AT IONSTR 0.1 ADJ'D BY -0.70									
56	TH°+4(A) + H2O(L) = TH°(OH)+3(A) + H+(A)	G=	6.30	1.50	.8	1.128	.29	1.31	.98	68HIE/SIL
	AUTHORS' 6.78 AT IONSTR 3 ADJ'D BY -0.48.									
57	TH°+4(A) + H2O(L) = TH°(OH)+3(A) + H+(A)	G=	5.45	1.00	1.8	.278	.29	.64	.38	54KRA/HOL
	AUTHORS' 5.93 AT IONSTR 1. ADJ'D BY -0.48									
58	TH°+4(A) + 2 H2O(L) = TH°(OH)2+2(A) + 2 H+(A)	G=	9.66	1.00	1.8	.446	.36	.72	.63	54KRA/HOL
	AUTHORS' 10.59 AT IONSTR ADJ'D BY -0.93 .									
59	TH°+4(A) + 2 H2O(L) = TH°(OH)2+2(A) + 2 H+(A)	H=	13.9	1.0	-1.0	.000				65BAE/MEY
	AS DERIVED BY AUTHORS FROM THEIR DATA AT 0 AND 95C AND FROM THEIR RECALCN. DATA OF 54KRA/HOL AT 25C. EFFECT OF IONSTR 1 IGNORED.									
60	TH°+4(A) + 2 H2O(L) = TH°(OH)2+2(A) + 2 H+(A)	G=	9.72	1.00	1.7	.506	.36	.75	.69	65BAE/MEY
	RECALC. BY AUTHORS FROM 54KRA/HOL. AUTHORS 10.65 AT IONSTR 1 AJD BY -0.93 .									
61	TH°+4(A) + 2 H2O(L) = TH°(OH)2+2(A) + 2 H+(A)	G=	9.57	1.00	2.0	.356	.36	.68	.54	68HIE/SIL
	AUTHORS' 10.50 AT IONSTR 1 ADJ'D BY -0.93									
62	TH°+4(A) + 2 H2O(L) = TH°(OH)2+2(A) + 2 H+(A)	G=	8.27	0.50	1.1	-.944	.36	.72	-1.00	72USH/SKO
	AUTHORS' 8.95 AT IONSTR 0.05 AJD'D BY -0.68									
63	TH°(OH)+3(A) + OH-(A) = TH°(OH)2+2(A)	G=	-15.60	0.10	2.4	-.557	.41	.33	-1.02	67BER
	AUTHORS' -14.73 AT IONSTR 0.5 ADJ'D BY 0.87									
64	TH°(OH)4(C) + 1.3 H2O(L) = TH°(OH)4:1.3H2O(C)	H=	-3.0	0.5	-1.0					11CHA
	FROM ENTHALPY OF SOLUTION IN HCL:15.5H2O									
	NO SOLUTION FOR VARIABLE IN EQUATION.									
65	2 TH°+4(A) + 2 H2O(L) = TH°2(OH)2+6(A) + 2 H+(A)	H=	14.8	1.0	-1.0					65BAE/MEY
	AS DERIVED BY AUTHORS FROM THEIR DATA AT 0 AND 95C AND THEIR RECALCN. DATA OF 54KRA/HOL AT 25C; EFFECT OF IONSTR 1 IGNORED.									
	FOR INFORMATION ONLY. VARIABLE NOT IN SOLUTION.									
66	2 TH°+4(A) + 2 H2O(L) = TH°2(OH)2+6(A) + 2 H+(A)	G=	5.55	1.50	1.3	.030	.12	.76	.15	54KRA/HOL
	AUTHORS' 6.48 AT IONSTR. 1 ADJ'D BY -0.93									

NBS CATALOG OF THORIUM THERMOCHEMICAL DATA, 7/27/77 SOLUTION: CODATA COMPATIBLE WEIGHTED SOLN - LST. SQUARES

NO.	REACTION	PROP. MEAS.	OBSVD. +- UNC.	WT.	RESID. (OB-CAL)	STD. DEV.	AVE. FIT	STD. RES.	REFERENCE
		KCAL/MOL OR CAL/(MOL.K)							
67	2 TH'+4(A) + 2 H2O(L) = TH'2(OH)2+6(A) + 2 H+(A)	G=	5.86 1.50	1.1	.340	.12	.92	1.58	71MIL
	AUTHOR'S 7.01 AT IONSTR 3. ADJ'D BY -1.15								
68	2 TH'+4(A) + 2 H2O(L) = TH'2(OH)2+6(A) + 2 H+(A)	G=	5.36 1.50	1.3	-.160	.12	.83	-.83	65BAE/MEY
	AUTHORS' 6.29 AT IONSTR 1. ADJ'D BY -0.93								
69	2 TH'+4(A) + 2 H2O(L) = TH'2(OH)2+6(A) + 2 H+(A)	G=	5.35 1.50	1.2	-.170	.12	.84	-.84	68HIE/SIL
	AUTHORS' 6.49 AT IONSTR 3. ADJ'D BY -1.15								
70	4 TH'+4(A) + 8 H2O(L) = TH'4(OH)8+8(A) + 8 H+(A)	H=	57.7 1.5	-1.0					65BAE/MEY
	AS DERIVED BY AUTHORS FROM THEIR DATA AT 0 AND 95C AND THEIR RECALCN OF DATA OF 54KRA/HOL AT 25C; EFFECT OF IONSTR 1 IGNORED.								
	FOR INFORMATION ONLY. VARIABLE NOT IN SOLUTION.								
71	4 TH'+4(A) + 8 H2O(L) = TH'4(OH)8+8(A) + 8 H+(A)	G=	23.75 1.50	-1.0					65BAE/MEY
	RECALCD. BY AUTHORS FROM 54KH . AUTHORS' 25.93 AT IONSTR 1 ADJ'D BY -2.18								
	FOR INFORMATION ONLY. VARIABLE NOT IN SOLUTION.								
72	4 TH'+4(A) + 8 H2O(L) = TH'4(OH)8+8(A) + 8 H+(A)	G=	25.90 2.00	-1.0					68HIE/SIL
	AUTHORS' 28.79 AT IONSTR 3 ADJ'D BY -2.89								
	FOR INFORMATION ONLY. VARIABLE NOT IN SOLUTION.								
73	= TH'F(G)	S=	61.7 1.0	-1.0	.000				.NBS
	S AND THERM. FUNCTS. TO 1500K FROM MOLEC. CONSTS. OF 73KMF FOR RIGID-ROT.-HARM.-OSC.; 4 SIGMA STATE ASSUMED.								
	CONSTRAINT								
74	TH'+4(A) + HF(AO') = TH'F+3(A) + H+(A)	G=	-6.17 0.07	2.8	.454	.17	.26	1.29	71KLO/MUK
	AUTHORS' MEASUREMENTS ARE APPARENTLY ACTIVITIES								
75	TH'+4(A) + F-(A) = TH'F+3(A)	G=	-11.39 0.50	2.7	-.426	.17	.46	-1.18	70BAU
	AUTHOR'S -11.02 AT IONSTR .01 ADJ'D BY -0.37								
76	TH'+4(A) + HF(AO') = TH'F+3(A) + H+(A)	G=	-6.79 1.00	1.9	-.166	.17	.58	-.37	50DAY/STO
	AUTHORS' -6.32 AT IONSTR 0.5 ADJ'D BY -0.47								
77	TH'+4(A) + HF(AO') = TH'F+3(A) + H+(A)	G=	-6.82 1.00	2.0	-.196	.17	.60	-.46	49DOD/ROL
	AUTHORS' -6.0K AT IONSTR 0.5 ADJ'D BY -0.47								
78	TH'+4(A) + HF(AO') = TH'F+3(A) + H+(A)	G=	-6.88 1.00	1.9	-.256	.17	.63	-.58	51ZEB/ALT
	AUTHORS' -6.41 AT IONSTR 0.5 ADJ'D BY -0.47								
79	TH'+4(A) + F-(A) = TH'F+3(A)	H=	-1.2 0.5	-1.0	.000				70BAU
	AUTHOR'S VALUE; NOT ADJ'D FOR IONSTR 0.1 .								

NBS CATALOG OF THORIUM THERMOCHEMICAL DATA, 7/27/77 SOLUTION: CODATA COMPATIBLE WEIGHTED SOLN - LST. SQUARES

NO.	REACTION	PROP. MEAS.	OBSVD. +- UNC.	WT.	RESID. (OB-CAL)	STD. DEV.	AVE. FIT	STD. RES.	REFERENCE
		KCAL/MOL OR CAL/(MOL.K)							
80	= TH°F2(G)	S=	70.5 1.0	-1.0	.000				.NBS
	MOLEC. CONSTS. OF 73KMF FOR RIGID-ROT.-HARM.-OSC.; 1 SIGMA STATE ASSUMED								
				CONSTRAINT					
81	TH°F2(G) = TH°F2+(G)	H=	302. 12.	-1.0					70ZMB
	AT 0 DEGR. K								
		FOR INFORMATION ONLY. VARIABLE NOT IN SOLUTION.							
82	TH°+4(A) + 2 HF(AO°) = TH°F2+2(A) + 2 H+(A)	G=	-11.13 1.00	1.7	-.372	.20	.69	-.81	50DAY/STO
	AUTHORS' -10.22 AT IONSTR 0.5 ADJ'D BY -0.91								
83	TH°F+3(A) + HF(AO°) = TH°F2+2(A) + H+(A)	G=	-4.15 0.50	4.0	-.016	.21	.26	-.06	49DOD/ROL
	AUTHORS' -3.84 AT IONSTR 0.05 ADJ'D BY -0.31								
84	TH°+4(A) + 2 HF(AO°) = TH°F2+2(A) + 2 H+(A)	G=	-9.90 0.19	1.6	.858	.20	.52	1.80	71KLO/MUK
	AUTHORS' MEASUREMENTS ARE APPARENTLY ACTIVITIES								
85	TH°+4(A) + 2 HF(AO°) = TH°F2+2(A) + 2 H+(A)	G=	-11.08 1.00	2.0	-.322	.20	.66	-.77	51ZEB/ALT
	AUTHORS' -10.18 AT IONSTR 0.5 ADJ'D BY -0.90								
86	TH°F+3(A) + F-(A) = TH°F2+2(A)	H=	-0.8 0.5	-1.0	-.000				70BAU
	AUTHOR'S VALUE; NOT ADJ'D FOR IONSTR 0.01								
87	TH°F+3(A) + F-(A) = TH°F2+2(A)	G=	-8.98 0.50	2.0	-.506	.21	.50	-1.22	70BAU
	AUTHOR'S -8.68 AT IONSTR 0.01 ADJ'D BY -0.30								
88	= TH°F3(G)	S=	81.1 1.5	-1.0					.NBS
	MOLEC. CONSTS. OF 73KMF FOR RIGID-ROT.-HARM.-OSC.; DEGENERACY TAKEN TO BE 6 AS IN TH+3								
		FOR INFORMATION ONLY. VARIABLE NOT IN SOLUTION.							
89	TH°F3(G) = TH°F3+(G)	H=	179.9 12.0	-1.0					70ZMB
	FOR 0 DEGRK								
		FOR INFORMATION ONLY. VARIABLE NOT IN SOLUTION.							
90	TH°F2+2(A) + F-(A) = TH°F3+(A)	H=	-0.8 0.5	-1.0	-.000				70BAU
	AUTHOR'S VALUE; NOT ADJ'D FOR IONSTR 0.01 .								
91	TH°F2+2(A) + F-(A) = TH°F3+(A)	G=	-6.46 0.50	4.0	-.077	.23	.29	-.33	70BAU
	AUTHOR'S -6.23 AT IONSTR 0.01 ADJ'D BY -0.23								
92	TH°F2+2(A) + HF(AO°) = TH°F3+(A) + H+(A)	G=	-2.26 0.50	3.1	-.217	.23	.36	-.73	49DOD/ROL
	AUTHORS -2.06 AT IONSTR 0.05 ADJ'D BY -0.20 .								
93	TH°+4(A) + 3 HF(AO°) = TH°F3+(A) + 3 H+(A)	G=	-12.1 0.4	1.4	.701	.28	.55	1.47	71KLO/MUK
	AUTHORS' MEASUREMENTS ARE APPARENTLY ACTIVITIES								

NO.	REACTION	PROP. MEAS.	OBSVD. +- UNC.	WT.	RESID. (OB-CAL)	STD. DEV.	AVE. FIT	STD. RES.	REFERENCE
		KCAL/MOL OR CAL/(MOL.K)							
94	= TH'F4(C)	S=	33.953 0.040	-1.0	.000				54LOH/OSB
	ESTD. CP = 29.2 + 0.0020T - 300.000/T2 (298 - 1380K, M. PT.) WAS USED TO ADJUST HIGH-TEMP. REACTIONS INVOVING THF4(C) .				CONSTRAINT				
95	3 TH'F4(C) + 4 AL'(CS') = 3 TH'(CS') + 4 AL'F3(C)	H=	60.24 6.00	.3	-.128	2.06	3.06	-.07	66HEU/EGA
96	TH'F4(C) + 2 NI'(CS') = TH'(CS') + 2 NI'F2(C)	H=	180.95 2.00	.2	-6.093	.69	4.05	-1.82	66HEU/EGA
97	TH'F4(C) + 2 NI'(CS') = TH'(CS') + 2 NI'F2(C)	H=	186.8 8.0	.2	-.243	.69	4.12	-.07	73SKE/PAT
	SOLID STATE . 3RD-LAW CALCN. ON AUTHORS' -2.002V AT 1000K . 2ND LAW ON TEMP. VAR'N GIVES 158.8 .								
98	TH'F4(C) + 2 MG'(CS') = TH'(CS') + 2 MG'F2(C)	H=	-37.19 1.50	.7	-1.253	.69	1.38	-.74	66HEU/EGA
99	TH'F4(C) = TH'(CS') + 2 F2(GS')	H=	504.51 1.20	.5	3.067	.69	2.13	1.49	70DEV/RUD
	DIRECT COMBINATION.								
100	TH'F4(C) + SI'O2(C) = TH'O2(C) + SI'F4(G)	H=	41.1 1.7	.7	1.037	.69	1.37	.61	60DAR 1
	AUTHOR'S 37.52 AT 974K ADJ'D TO 298K BY ESTD. THERM. FUNCTS. .								
101	TH'F4(C) + 2 NI'(CS') = TH'(CS') + 2 NI'F2(C)	S=	-30.5 6.0	-1.0	-30.208				73SKE/PAT
	AUTHORS' -27.30 AT 1018K ADJ'D BY 2ND LAW (NIF2 ENTHALPY FROM BINFORD, J.CHEM.THERMODYN.,2,410(1970) .				LISTED FOR INFORMATION ONLY.				
102	TH'F4(C) + SI'O2(C) = TH'O2(C) + SI'F4(G)	S=	42.6 2.0	-1.0	3.408				60DAR 1
	AUTHOR'S 35.4 AT 974K ADJ'D TO 298K BY ESTD. THERM. FUNCTS. .				LISTED FOR INFORMATION ONLY.				
103	= TH'F4(G)	S=	81.7 1.5	-1.0	.000				.NBS
	MOLECULAR CONSTANTS OF 75RAN .				CONSTRAINT				
104	TH'(CS') + 2 CL'2(GS') = TH'CL'4(C)	H=	-284.5 1.0	-1.0	-.858				69SMI/THA
	AS REPORTED BY AUTHORS; SUM OF TH AND THCL4 INTO HCL+8.09H2O NOT USED BECAUSE OF AMBIGUITY ABOUT CORRECTIONS .				LISTED FOR INFORMATION ONLY.				
105	TH'F4(C) = TH'F4(G)	H=	82.1 2.0	1.0	.167	1.25	1.08	.19	58DAR/KEN
	3RD LAW CALCN. ON KNUDSEN V. P. DATA (1055 - 1297K) .								
106	TH'F4(G) = TH'F4(C)	H=	-81.6 4.0	.5	.333	1.25	2.17	.19	58DAR/KEN
	2ND LAW (LIN. FIT). KNUDSEN V. P. (1055 - 1297K)								

NO.	REACTION	PROP. MEAS.	OBSVD.	+- UNC.	WT.	RESID. (OB-CAL)	STD. DEV.	AVE. FIT	STD. RES.	REFERENCE
		KCAL/MOL OR CAL/(MOL.K)								
107	TH°F4(G) = TH°F(G) + 3 F(G) FOR 0 DEGR. K .	H=	690.	25.	-1.0					70ZMB
	FOR INFORMATION ONLY. VARIABLE NOT IN SOLUTION.									
108	TH°F4(G) = TH°F2+2(G) + 2 F(G) AT 0 DEGR. K .	H=	535.	12.	-1.0					70ZMB
	FOR INFORMATION ONLY. VARIABLE NOT IN SOLUTION.									
109	2 CA°(G) + TH°F4(G) = 2 CA°F(G) + TH°F2(G)	H=	46.12	2.00	-1.0	.000				70ZMB
110	CA°(G) + TH°F4(G) = CA°F(G) + TH°F3(G)	H=	27.86	2.00	-1.0	.000				70ZMB
111	TH°F4(G) = TH°F3+(G) + F(G) FOR 0 DEGRK	H=	334.	12.	-1.0					70ZMB
	FOR INFORMATION ONLY. VARIABLE NOT IN SOLUTION.									
112	TH°F3+(A) + F-(A) = TH°F4(AO°) AUTHOR'S VALUE; NOT ADJ°D FOR IONSTR 0.01	H=	-0.9	0.5	-1.0	.000				70BAU
113	TH°F3+(A) + F-(A) = TH°F4(AO°) AUTHOR'S -4.49 AT IONSTR 0.01 ADJ°D BY -0.12	G=	-4.61	0.50	-1.0	.000				70BAU
114	= TH°F4:2.5H2O(C) ESTIMATED	S=	56.	2.	-1.0	.000				.NBS
115	TH°F4(C) + 2.5 H2O(L) = TH°F4:2.5H2O(C) ESTIMATED FROM ANALOGOUS URANIUM SALTS .	H=	-10.	2.	-1.0	.000				.NBS
116	TH°F4:2.5H2O(C) = TH°+4(A) + 4 F-(A) + 2.5 H2O(L) AUTHORS' VALUE AT IONSTR= 1 BASED ON ACTIVITIES SEE 57D°E/B00 FOR :2.5H2O .	G=	38.59	0.50	-1.0	-6.636				71KLO/MUK
	LISTED FOR INFORMATION ONLY.									
117	TH°F4:2.5H2O(C) = TH°+4(A) + 4 F-(A) + 2.5 H2O(L) AUTHORS' 34.58 KCAL AT IONSTR = 0.1 SEE 57D°E/B00 FOR :2.5H2O .	G=	36.76	1.00	-1.0	-8.466				62NIK/LUK
	LISTED FOR INFORMATION ONLY.									
118	TH°F4:2.5H2O(C) + 3 H+(A) = TH°F+3(A) + 3 HF(AO°) + 2.5 H2O(L) AUTHORS' 13.70 KCAL AT IONSTR = 1.1 SEE 57D°E/B00 FOR :2.5H2O .	G=	14.72	1.00	-1.0	-6.522				62NIK/LUK
	LISTED FOR INFORMATION ONLY.									

NO.	REACTION	PROP. MEAS.	OBSVD.	+- UNC.	WT.	RESID. (OB-CAL)	STD. DEV.	AVE. FIT	STD. RES.	REFERENCE
		KCAL/MOL OR CAL/(MOL.K)								
119	TH°F4:2.5H2O(C) + 2 H+(A) = TH°F2+2(A) + 2 HF(AQ°) + 2.5 H2O(L)	G=	10.14	0.50	-1.0	-6.968				49DOD/ROL
	SOL°Y 5.9$0.5X10-8; 0.27 ADJ°T FOR IONSTR (ASSUMED BETWEEN 0.01 AND 0.4) . SEE 57D°E/BOO FOR :2H2O .									
				LISTED FOR INFORMATION ONLY.						
120	= TH°OF2(C)	S=	25.	2.	-1.0	.000				60DAR 1
	MEASUREMENTS OF 60DAR1 ON THOF2=THO2 + THF4(G) AT 1109-1286K. AGREE WITH EST. OF S AND THERM. FUNCTS.: 0.5(THO2+THF4)(C) .									
121	2 TH°OF2(C) = TH°O2(C) + TH°F4(G)	H=	85.0	5.0	-1.0	-.000				60DAR 1
	2ND LAW; MEASUREMENTS AT 1109 - 1286K .									
122	TH°+4(A) + CL°-(A) = TH°CL°+3(A)	G=	-2.14	0.75	1.2	-.647	.14	.70	-2.07	68OHA/MOR
	ASSIGN 50 PERCENT ERRROR TO AUTHORS° XTRPLTD. K AT IONSTR 0 .									
123	TH°+4(A) + CL°-(A) = TH°CL°+3(A)	G=	-1.28	2.00	1.0	.213	.14	1.11	.61	51ZEB/ALT
	AUTHORS° -0.15 AT IONSTR 4 ADJ°D BY -1.13									
124	TH°+4(A) + CL°-(A) = TH°CL°+3(A)	H=	0.	2.	-1.0	.000				68OHA/MOR
125	TH°+4(A) + CL°-(A) = TH°CL°+3(A)	G=	-1.24	1.00	1.9	.253	.14	.63	1.08	50DAY/STO
	AUTHORS° -0.33 AT IONSTR 0.5 ADJ°D BY -0.91									
126	TH°+4(A) + CL°-(A) = TH°CL°+3(A)	G=	-1.50	0.50	2.8	-.007	.14	.25	-.04	52WAG/STO
	XTRPLTN. OF RESULTS AT 6. 4. 2. 1. 0.7. 0.5 IONSTR									
127	TH°+4(A) + 2 CL°-(A) = TH°CL°2+2(A)	G=	-0.99	2.00	1.0	.100	.23	1.05	.34	51ZEB/ALT
	AUTHORS° 1.25 AT IONSTR 4 ADJ°D BY -2.24 .									
128	TH°CL°+3(A) + CL°-(A) = TH°CL°2+2(A)	G=	0.42	1.50	1.3	.017	.21	.76	.07	52WAG/STO
	AUTHORS° 1.47 AT IONSTR 2 ADJ°D BY 1.05 .									
129	TH°CL°+3(A) + CL°-(A) = TH°CL°2+2(A)	G=	0.28	2.00	1.0	-.123	.21	1.06	-.40	51ZEB/ALT
	AUTHORS° 1.40 AT IONSTR 4 ADJ°D BY -1.12									
130	TH°CL°2+2(A) + CL°-(A) = TH°CL°3+(A)	G=	-1.16	1.00	-1.0	-.000				52WAG/STO
	AUTHORS° 0.20. -0.41 AT IONSTR 4. 2 ADJ°D BY -2.09. -1.01									
131	TH°(CS°) + 2 CL°2(GS°) = TH°CL°4(C)	H=	-268.1	5.0	-1.0	15.542				09WAR
	DIRECT COMB°N . AUTHOR°S °IMPURITY CORRECTION° DOES NOT APPLY .									
				LISTED FOR INFORMATION ONLY.						
132	= TH°CL°4(C)	S=	45.5	2.0	-1.0	.000				.NBS
	EST°D FROM ZRCL4. HFCL4. UF4. UCL4 .									
					CONSTRAINT					

NO.	REACTION	PROP. MEAS.	OBSVD.	+- UNC.	WT.	RESID. (OB-CAL)	STD. DEV.	AVE. FIT	STD. RES.	REFERENCE
		KCAL/MOL OR CAL/(MOL.K)								
133	= TH°CL°4(G)	S=	95.	2.	-1.0	.000				.NBS
	TETRAHEDRAL. FREQS. 310(1). 70(2). 320(3). 75(3) CM-1 FROM 73KRA/MOR. MODIFIED BY EQN. (II.232) OF 45HER; GROUND STATE MULT.=1 .					CONSTRAINT				
134	TH°CL°4(C) = TH°CL°4(G)	H=	52.7	2.0	-1.0	-.000				72KNA/MUL1
	THIRD LAW. 673-854K. SELECTED .					CONSTRAINT				
135	TH°CL°4(C) = TH°CL°4(G)	H=	64.5	2.0	-1.0	11.800				66SU/NOV
	AUTHHORS' 58.76 AT 923-1043K ADJ'D BY THERMAL FUNCTIONS .									
136	TH°CL°4(C) = TH°CL°4(G)	H=	65.1	5.0	-1.0	12.400				39FIS/GEW
	AUTHORS' 59.3 AT 974-1036K ADJ'D BY THERMAL FUNCTIONS .									
137	TH°CL°4(C) = TH°CL°4(G)	H=	57.8	3.0	-1.0	5.100				63YEN/LI
	AUTHORS' 52.2 AT 953-1025K ADJ'D BY THERMAL FUNCTIONS . LISTED FOR INFORMATION ONLY.									
138	TH°CL°4(C) = TH°CL°4(G)	S=	50.1	2.0	-1.0	.600				72KNA/MUL1
	AUTHORS' 43.3 AT 673-854K ADJ'D BY THERMAL FUNCTIONS .									
139	TH°CL°4(C) = TH°CL°4(G)	S=	62.	2.	-1.0	12.500				66SU/NOV
	AUTHORS' 52. AT 923-1043K ADJ'D BY THERMAL FUNCTIONS . LISTED FOR INFORMATION ONLY.									
140	TH°CL°4(C) = TH°CL°4(G)	S=	55.6	3.0	-1.0	6.100				63YEN/LI
	AUTHORS' 45.1 AT 953-1053K ADJ'D BY THERMAL FUNCTIONS . LISTED FOR INFORMATION ONLY.									
141	TH°CL°4(C) = TH°+4(A) + 4 CL°-(A)	H=	-60.	1.	2.0	-.110	.48	.56	-.15	.NBS
	LINEAR EXTRAPOLATION VS. IONSTR . CURVILINEAR EXTRPLTN. (VS. IONSTR) OF NBS SELECTIONS OF IONSTR- ADJ'D VALUES OF ^H(SOLN)(THCL4.C) IN 1.02. 6.85. AND 11.05 MOLAL HCL GIVES -62.7									
142	TH°CL°4(A) = TH°+4(A) + 4 CL°-(A)	H=	0.	0.	-1.0	.000				.DEFINED
						CONSTRAINT				
143	TH°CL°4(A) = TH°+4(A) + 4 CL°-(A)	G=	0.	0.	-1.0	-.000				.DEFINED
						CONSTRAINT				
144	TH°+4(A) + 4 CL°-(A) = TH°CL°4(AQ°)	G=	-1.72	2.00	-1.0	-.000				51ZEB/ALT
	-4.24 ADJUSTMENT FOR IONSTR .									

NO.	REACTION	PROP. MEAS.	OBSVD. KCAL/MOL OR CAL/(MOL.K)	+- UNC.	WT.	RESID. (OB-CAL)	STD. DEV.	AVE. FIT	STD. RES.	REFERENCE
145	TH'CL'4(C) = TH'CL'4(AU')	H=	-56.4	2.0	-1.0					11CHA
	FOR INFORMATION ONLY. VARIABLE NOT IN SOLUTION.									
146	TH'CL'4(C) = TH'CL'4(HCL'+5.02H2O:AU')	H=	-34.93	0.20	10.0	-.019	.19	.11	-.06	49WES/ROB
	DELH (HENCE, DELHF AQ THCL4) LIN. FUNCT. MOLALITY HCL;INDEPENDENT CONCN. THCL4 TO 0.01 MOLAL .									
147	TH'CL'4(C) = TH'CL'4(HCL'+8.16H2O:AU')	H=	-44.91	0.20	3.1	-.471	.19	.34	-.70	73FUG/BRO
148	TH'CL'4(C) = TH'CL'4(HCL'+8.16H2O:AU')	H=	-44.35	0.30	4.9	.089	.19	.19	.17	69SMI/THA
	CORR'D FOR .005MOLAL NA2SIF6(0.3 KCAL) .									
149	TH'CL'4(C) = TH'CL'4(HCL'+8.16H2O:AU')	H=	-44.10	0.20	3.6	.339	.19	.27	.55	49WES/ROB
	NO NA2SIF6 IN AQ-HCL SOLVENT .									
150	TH'CL'4(C) = TH'CL'4(HCL'+8.16H2O:AU')	H=	-44.28	0.15	6.1	.159	.19	.15	.34	50EYR/WES
151	TH'(CS') + 4 HCL'(D:8.16H2O) = TH'CL'4(HCL'+8.1 6H2O:AU') + 2 H2(GS')	H=	-181.19	0.50	4.0	.147	.48	.32	.38	50EYR/WES
	RECALC'D; CORR'D FOR .005MOLAL NA2SIF6 (0.3KCAL); USING AUTHORS' EVAP'N AND IMPURITY CORR'NS .									
152	TH'(CS') + 4 HCL'(D:15H2O) = TH'CL'4(HCL'+15H2O) + 2 H2(GS')	H=	-238.	2.	-1.0					11CHA
	PROB. AT 18 DEGR. C.									
	FOR INFORMATION ONLY. VARIABLE NOT IN SOLUTION.									
153	TH'CL'4(C) = TH'CL'4(HCL'+54.4H2O:AU')	H=	-57.42	0.20	10.0	-.019	.19	.11	-.06	49WES/ROB
	SEE COMMENT ON DETN. THCL4 INTO (HCL+5.02H2O) BY 49WES/ROB.									
154	TH'CL'4(C) = TH'CL'4(HCL'+54.4H2O:AU')	H=	-57.79	0.20	3.5	-.389	.19	.29	-.62	73FUG/BRO
	SEE COMMENT ON DETN. THCL4 INTO (HCL+5.02H2O) BY 49WES/ROB.									
155	TH'CL'4(HCL'+5.02H2O:AU') = TH'CL'4(HCL'+54.4H2 O:AU')	H=	-22.49	0.01	-1.0	-.000				.NBS
	^HF(THCL4 IN AQ. HCL) LIN. FUNCTION MOLALITY HCL, INDEPENDENT CONCN. THCL4 TO 0.01 MOLAL. (SEE SIMILAR DATA FOR THCL4(HCL, 8.16 VS. 54.4H2O))									
						CONSTRAINT				
156	TH'CL'4(HCL'+8.16H2O:AU') = TH'CL'4(HCL'+54.4H2 O:AU')	H=	-12.962	0.010	-1.0	-.000				.NBS
	SEE COMMENT FOR THCL4(HCL,5.02 VS. 54.4H2O)									
						CONSTRAINT				
157	TH'CL'4(C) + 2 H2O(L) = TH'CL'4:2H2O(C)	H=	-15.8	0.5	-1.0	-.000				11CHA
	FROM ENTHALPIES OF SOLUTION IN H2O(L).									

NBS CATALOG OF THORIUM THERMOCHEMICAL DATA. 7/27/77 SOLUTION: CODATA COMPATIBLE WEIGHTED SOLN - LST. SQUARES

NO.	REACTION	PROP. MEAS.	OBSVD.	+- UNC.	WT.	RESID. (OB-CAL)	STD. DEV.	AVE. FIT	STD. RES.	REFERENCE
		KCAL/MOL OR CAL/(MOL.K)								
158	TH'CL'4(C) + 4 H2O(L) = TH'CL'4:4H2O(C)	H=	-30.9	0.5	-1.0	.000				11CHA
	FROM ENTHALPIES OF SOLUTION IN H2O(L).									
159	TH'CL'4(C) + 7 H2O(L) = TH'CL'4:7H2O(C)	H=	-42.6	0.5	-1.0	-.000				11CHA
	FROM ENTHALPIES OF SOLUTION IN H2O(L).									
160	TH'CL'4(C) + 8 H2O(L) = TH'CL'4:8H2O(C)	H=	-46.0	0.5	-1.0	.000				11CHA
	FROM ENTHALPIES OF SOLUTION IN H2O(L).									
161	TH'+4(A) + CL'O3-(A) = TH'CL'O3+3(A)	G=	-1.27	1.00	-1.0	-.000				50DAY/STO
	AUTHORS' -0.36 AT IONSTR 0.5 ADJ'D BY -0.91									
162	TH'(CL'O4)4(A) + 2 H2O(L) = TH'O2(C) + 4 HCL'O4(A)	H=	-32.	10.	-1.0	.000				69ATH/KAL
	HEATS COMBSTN. TH(8-HYDROXYQUINOLINATE)4 AND 8-HYDROXYQUINOLINE									
163	2 TH'OCL'2(C) = TH'CL'4(C) + TH'O2(C)	S=	0.	2.	3.4	-2.050	.47	2.03	-4.34	.NBS
	S OF THOCL2 TAKEN TO BE SUM OF THOSE OF ITS COMPNENTS .									
164	2 TH'OCL'2(C) = TH'O2(C) + TH'CL'4(G)	S=	63.3	2.0	-1.0	11.750				63YEN/LI
	DATA REFITTED; 56.87 AT 940 - 1200K ADJ'D BY ESTD. ^CP=-5 . LISTED FOR INFORMATION ONLY.									
165	2 TH'OCL'2(C) = TH'O2(C) + TH'CL'4(G)	H=	75.3	2.0	-1.0	10.587				63YEN/LI
	DATA REFITTED; 71.45 AT 940 -1200K ADJ'D BY ESTD. ^CP=-5 . LISTED FOR INFORMATION ONLY.									
166	2 TH'OCL'2(C) = TH'O2(C) + TH'CL'4(G)	H=	64.5	2.0	1.0	-.213	1.13	1.11	-.43	72KNA/MUL2
	AUTHORS' 60.83 AT 819-1006K ADJ'D BY EST'D DELCP= -6									
167	TH'CL'4(C) + 2 NA'OH(550H2O) = TH'OCL'2(C) + 2 NA'CL'(550H2O) + H2O(L)	H=	-49.55	2.00	.8	-.532	.60	1.27	-.43	63YEN/LI
168	2 TH'OCL'2(C) = TH'O2(C) + TH'CL'4(G)	S=	53.6	2.0	3.4	2.050	.47	2.02	4.34	72KNA/MUL2
	AUTHORS' 46.93 AT 819-1006K ADJ'D BY EST'D DELCP = -6									
169	= TH'BR'4(G)	S=	103.	2.	-1.0	.000				.NBS
	TETRAHEDRAL. FREQS. 205(1). 58(2). 220(3). 72(3) CM-1 FROM 75RAND . GROUND STATE MULT. = 1 . CONSTRAINT									
170	TH'BR'4(C) + 4 HCL'(D:54.4H2O) = TH'CL'4(C) + 4 HBR'(D:HCL'+54.4H2O)	H=	-9.89	0.25	8.0	-.047	.23	.15	-.13	73FUG/BRO
	OBTAINED FROM COMBINATION OF THEIR HEAT OF SOLN DATA ON SALTS									

NO.	REACTION	PROP. MEAS.	OBSVD. +- UNC. KCAL/MOL OR CAL/(MOL.K)		WT.	RESID. (OB-CAL)	STD. DEV.	AVE. FIT	STD. RES.	REFERENCE
171	TH'BR'4(C) + 4 HCL'(D:8.16H2O) = TH'CL'4(HCL'+8.16H2O:AU') + 4 HBR'(D:HCL'+8.16H2O) COMBINED WITH ANOTHER REACT. TO GIVE DIRECT THBR4-THCL4 ELSEWHERE LISTED FOR INFORMATION ONLY.	H=	-55.90	0.20	-1.0	-.542				73FUG/BRO
172	TH'BR'4(C) + 4 HCL'(D:8.16H2O) = TH'CL'4(C) + 4 HBR'(D:HCL'+8.16H2O) OBTAINED FROM COMBINATION OF THEIR HEAT OF SOLN DATA ON SALTS	H=	-10.90	0.10	20.0	.019	.23	.06	.13	73FUG/BRO
173	TH'BR'4(C) + 4 HCL'(D:54.4H2O) = TH'CL'4(HCL'+54.4H2O:AU') + 4 HBR'(D:HCL'+54.4H2O) COMBINED WITH ANOTHER REACT. TO GIVE DIRECT THBR4-THCL4 ELSEWHERE LISTED FOR INFORMATION ONLY.	H=	-67.69	0.25	-1.0	-.446				73FUG/BRO
174	TH'BR'4(C) = TH'BR'4(G) THIRD LAW, 903(CRYSTAL) - 1126K(LIQUID) . SELECTED .	H=	48.4	2.0	-1.0	.000 CONSTRAINT				39FIS/GEW
175	= TH'BR'4(C)	S=	55.	2.	-1.0	.000 CONSTRAINT				.NBS
176	TH'BR'4(C) = TH'BR'4(AU') NO CONCENTRATION SPECIFIED.	H=	-70.7	1.0	-1.0	.000				11CHA
177	TH'BR'4(C) + 7 H2O(L) = TH'BR'4:7H2O(C) FROM ENTHALPY OF SOLUTION IN H2O, USING C'S DATA FOR THBR4(C).	H=	-48.3	0.5	-1.0	-.000				11CHA
178	TH'BR'4(C) + 10 H2O(L) = TH'BR'4:10H2O(C) FROM ENTHALPY OF SOLUTION IN H2O. USING C'S DATA FOR THBR4(C).	H=	-61.2	0.5	-1.0	-.000				11CHA
179	TH'BR'4(C) + 12 H2O(L) = TH'BR'4:12H2O(C) FROM ENTHALPY OF SOLUTION IN H2O, USING C'S DATA FOR THBR4(C).	H=	-69.0	0.5	-1.0	.000				11CHA
180	TH'BR'4(C) + H2O(L) = TH'OBR'2(C) + 2 HBR'(1000H2O) FROM DIFF.IN AUTHOR'S ENTHALPIES OF SOLN.OF THOBR2, THBR4 ; LEADS TO UNACCEPTABLE DELH(2THOBR2=THO2+THBR4) = +43 FOR INFORMATION ONLY. VARIABLE NOT IN SOLUTION.	H=	-42.2	0.5	-1.0					11CHA
181	TH'+4(A) + BR'O3-(A) = TH'(BR'O3)+3(A) AUTHORS' -1.10 AT IONSTR 0.5 ADJ'D BY -0.91	G=	-2.01	1.00	-1.0	-.000				50DAY/STO
182	TH'+4(A) + 2 BR'O3-(A) = TH'(BR'O3)2+2(A) AUTHORS' -1.25 AT IONSTR 0.5 AJD'D BY -1.50 .	G=	-2.75	1.00	-1.0	.000				50DAY/STO
183	= TH'I4(G) TETRAHEDRAL, FREQS. 137(1), 37(2), 177(3), 43(3) FROM 73KRA/MOR .	S=	112.	2.	3.4	-.262	.55	1.13	-.69	.NBS

N8S CATALOG OF THORIUM THERMOCHEMICAL DATA, 7/27/77 SOLUTION: CODATA COMPATI8LE WEIGHTED SOLN - LST. SQUARES

NO.	REACTION	PROP. MEAS.	O8SVD.	+- UNC.	WT.	RESID. (O8-CAL)	STD. DEV.	AVE. FIT	STD. RES.	REFERENCE
		KCAL/MOL OR CAL/(MOL.K)								
184	TH'I4(G) = TH'I4(C)	H=	-48.8	2.0	-1.0	-.000				60LAN/DAR
	THIRD LAW, 600-800K .									
185	= TH'I4(C)	S=	61.	3.	2.2	.405	.58	1.70	.69	.N8S
186	TH'I4(C) + 4 HCL'(D:54.4H2O) = TH'CL'4(C) + 4 HI(D:HCL'+54.4H2O)	H=	-19.17	0.20	10.0	-.169	.30	.18	-.69	73FUG/BRO
	O8TAINED FROM COM8INATION OF THEIR HEAT OF SOLN DATA ON SALTS									
187	TH'I4(C) + 4 HCL'(D:54.4H2O) = TH'CL'4(HCL'+54.4H2O:AU') + 4 HI(D:HCL'+54.4H2O)	H=	-76.96	0.20	-1.0	-.559				73FUG/BRO
	COM8INED WITH ANOTHER REACT. TO GIVE DIRECT THI4-THCL4 ELSEWHERE LISTED FOR INFORMATION ONLY.									
188	TH'I4(C) + 4 HCL'(D:8.16H2O) = TH'CL'4(C) + 4 HI(D:HCL'+8.16H2O)	H=	-20.96	0.30	6.7	.253	.30	.28	.69	73FUG/BRO
	O8TAINED FROM COM8INATION OF THEIR HEAT OF SOLN DATA ON SALTS									
189	TH'I4(C) + 4 HCL'(D:8.16H2O) = TH'CL'4(HCL'+8.16H2O:AU') + 4 HI(D:HCL'+8.16H2O)	H=	-65.96	0.40	-1.0	-.309				73FUG/8RO
	COMBINED WITH ANOTHER REACT. TO GIVE DIRECT THI4-THCL4 ELSEWHERE LISTED FOR INFORMATION ONLY.									
190	TH'I4(C) = TH'+4(HCL'+54.4H2O:AU') + 4 I-(D:HCL'+54.4H2O)	H=	-75.	3.	-1.0					65SCA/TUR
	FOR INFORMATION ONLY. VARIABLE NOT IN SOLUTION.									
191	TH'I4(G) = TH'I4(C)	S=	-51.8	1.0	6.7	-.133	.43	.57	-.69	60LAN/DAR
	-47.2 AT 640-740K ADJ'D 8Y THERMAL FUNCTIONS .									
192	TH'OI2(C) + 4 HCL'(D:55H2O) = TH'CL'4(C) + 2 HI(5.4H2O) + H2O(L)	H=	20.1	1.2	.7	-1.459	.61	1.33	-1.09	65SCA/TUR
	WITH AUXIL. REACTION FROM 50EYR/WES.									
193	2 TH'OI2(C) + TI'O2(C3) = 2 TH'O2(C) + TI'I4(G)	H=	53.0	1.0	2.0	.255	.84	.63	1.09	60LAN/DAR
	2ND LAW; REINTERPRETATION OF AUTHORS' THI4 + TIO2 = TII4 + THO2.									
194	2 TH'OI2(C) + TI'O2(C3) = 2 TH'O2(C) + TI'I4(G)	S=	62.0	1.0	-1.0	16.035				60LAN/DAR
	2ND LAW; REINTERPRETATION OF AUTHORS' THI4 + TIO2 = TII4 + THO2. LISTED FOR INFORMATION ONLY.									
195	TH'I4(C) + TH'O2(C) = 2 TH'OI2(C)	S=	0.	2.	-1.0	.000				.N8S
	ESTIMATE OF S(THOI2,C) .									

NO.	REACTION	PROP. MEAS.	OBSVD.	+- UNC.	WT.	RESID. (OB-CAL)	STD. DEV.	AVE. FIT	STD. RES.	REFERENCE
		KCAL/MOL OR CAL/(MOL.K)								
196	TH'OI2(C) + HI(1000H2O) + 10 H2O(L) = TH'(OH)I3:10H2O(C) FROM ENTHALPY OF SOLUTION IN H2O(L). USING C'S VALUE FOR THOI2(C)	H=	-13.1	1.0	-1.0	-.000				11CHA
197	TH'CL'4(C) + H2O(L) + 2 HI(1000H2O) = TH'OI2(C) + 4 HCL'(1000H2O) FROM ENTHALPIES OF SOLUTION IN H2O(L).	H=	-35.2	1.0	-1.0	-14.177				11CHA
		LISTED FOR INFORMATION ONLY.								
198	TH'+4(A) + IO3-(A) = TH'IO3+3(A) AUTHORS' -3.93 AT IONSTR 0.5 ADJ'D BY -0.91 .	G=	-4.84	1.00	-1.0	-.000				50DAY/STO
199	TH'+4(A) + 2 IO3-(A) = TH'(IO3)2+2(A) AUTHORS' -6.54 AT IONSTR 0.5 ADJ'D BY -1.31 .	G=	-8.32	1.00	-1.0	-.000				50DAY/STO
200	TH'+4(A) + 3 IO3-(A) = TH'(IO3)3+(A) AUTHORS' - 9.75 AT IONSTR 0.5 ADJ'D BY -2.58 .	G=	-12.33	1.00	-1.0	.000				50DAY/STO
201	= TH'S(C)	S=	16.685	0.170	-1.0	.000				71FLO/OSB
202	TH'(CS') + S(CS') = TH'S(C) ADJSTD BY NBS FROM REACTION FOR THS1.03	H=	-94.54	1.50	-1.0	.000				72ADE/HUB
203	= TH'S2(C)	S=	23.0	0.2	-1.0	.000				59KIN/WEL
204	TH'(CS') + TH'7S12(C) = 4 TH'2S3(C)	S=	-6.3	1.0	-1.0	-.000				67ARO
205	TH'(CS') + TH'7S12(C) = 4 TH'2S3(C) 2ND LAW. ASSUME DELCP = 0.	H=	-47.1	4.0	-1.0	-.000				67ARO
206	2 TH'(CS') + 3 S(CS') = TH'2S3(C) COMBINED WITH TH DISSOL'N REACTION OF 50EYR/WES .	H=	-259.00	3.03	-1.0	.000				53EYR/WES
207	2 TH'(CS') + 3 S(CS') = TH'2S3(C) BY COMBUSTION OF TH2S3 .	H=	-238.	5.	-1.0	21.000				58BEA/MCT
		LISTED FOR INFORMATION ONLY.								
208	TH'(CS') + TH'2S3(C) = 3 TH'S(C) AT 1173K; ^CP TAKEN TO BE 0 .	S=	-5.9	2.0	-1.0	-.000				67ARO
209	TH'(CS') + TH'2S3(C) = 3 TH'S(C)	H=	-26.7	4.0	-1.0	-2.080				67ARO
		LISTED FOR INFORMATION ONLY.								
210	2 TH'3S7(C) = 6 TH'S2(C) + S2(G) 2ND LAW. ASSUME DELCP = 0	H=	41.17	6.00	-1.0	.000				41STR/ZUM

NBS CATALOG OF THORIUM THERMOCHEMICAL DATA. 7/27/77 SOLUTION: CODATA COMPATIBLE WEIGHTED SOLN - LST. SQUARES

NO.	REACTION	PROP. MEAS.	OBSVD.	+- UNC.	WT.	RESID. (OB-CAL)	STD. DEV.	AVE. FIT	STD. RES.	REFERENCE
		KCAL/MOL OR CAL/(MOL.K)								
211	TH'(CS') + 6 TH'S2(C) = TH'7S12(C)	H=	-90.58	10.00	-1.0	.000				67ARO
212	TH'SO4+2(A) + H+(A) = TH'+4(A) + HSO4-(A) CALORIMETRIC .	H=	0.54	0.10	-1.0	.000				59ZIE
213	TH'+4(A) + SO4-2(A) = TH'SO4+2(A) RECALCD. BY AUTHORS FROM DATA OF 59Z .	G=	-8.59	1.00	.8	-1.155	.35	1.08	-1.58	63ALL/MCD
214	TH'+4(A) + HSO4-(A) = TH'SO4+2(A) + H+(A) AUTHOR'S -3.03 AT IONSTR 2 ADJ'D BY -1.31 .	G=	-4.34	1.50	1.3	.385	.35	.94	.73	59ZIE
215	TH'+4(A) + HSO4-(A) = TH'SO4+2(A) + H+(A) AUTHORS' -3.00 AT IONSTR 2 AOJ'D BY -1.31 .	G=	-4.31	1.50	1.3	.415	.35	.96	.78	51ZEB/ALT
216	TH'SO4+2(A) + HSO4-(A) = TH'(SO4)2(AO') + H+(A) AUTHOR'S -1.82 AT IONSTR 2 ADJ'D BY -1.23 .	G=	-3.05	1.50	1.3	.088	.44	.79	.19	59ZIE
217	TH'(SO4)2(C) = TH'O2(C) + 2 SO2(G) + O2(GS') THIRD-LAW ANALYSIS OF DATA, 907.2-1057.2K .	S=	147.8	2.0	3.4	2.302	.69	2.15	3.35	60MAY/OWE
218	TH'(SO4)2(C) = TH'O2(C) + 2 SO2(G) + O2(GS') 3RD LAW(907 -1057K); CALCNS. BY NBS .	H=	172.70	0.70	-1.0	.000				60MAY/OWE
219	= TH'(SO4)2(C) ESIMATE (LATIMER'S METHOD) AND COMPARISON WITH URANIUM COMPOUNDS	S=	40.	2.	3.4	2.303	.69	2.15	3.35	.NBS
220	TH'(SO4)2(AO') + H+(A) = TH'SO4+2(A) + HSO4-(A) CALORIMETRIC .	H=	0.89	0.20	-1.0	.000				59ZIE
221	TH'+4(A) + 2 HSO4-(A) = TH'(SO4)2(AO') + 2 H+(A) AUTHORS' -4.71 AT IONSTR 2 ADJ'D BY -2.75 .	G=	-7.46	1.50	1.3	.402	.40	.95	.82	51ZEB/ALT
222	TH'+4(A) + 2 SO4-2(A) = TH'(SO4)2(AO') RECALCD. BY AUTHORS FROM DATA OF 59ZIE.	G=	-13.92	1.00	1.0	-.638	.40	.82	-1.06	63ALL/MCD
223	TH'(SO4)2(AO') + SO4-2(A) = TH'(SO4)3-2(A) ADJ'D BY AUTHORS TO IONSTR 0 .	G=	-1.04	1.00	-1.0	.000				63ALL/MCD
224	TH'(SO4)3-2(A) + SO4-2(A) = TH'(SO4)4-4(A)	G=	2.76	1.00	-1.0	-.000				63ALL/MCD
225	= TH'N(C) ALSO, USE CP = 11.34+0.002276T-1114400/T2 (298 - 2000K) .	S=	13.4	0.2	-1.0	.000				72OAN/NOV
226	TH'3N4(C) + 3 O2(GS') = 3 TH'O2(C) + 2 N2(GS')	H=	-565.1	3.0	.7	.000	2.40	1.50	.02	34NEU/KRO
227	TH'3N4(C) = 3 TH'N(C) + 0.5 N2(GS') AUTHORS' 2ND-LAW 36.35 AT APPROX. 1923K AOJ'D BY 0.65 USING ESTD. CP(TH3N4) = 39.33+0.00624T-533000/T2 .	H=	37.0	4.5	.4	1.833	2.59	3.17	1.00	66ARO/AUS

NO.	REACTION	PROP. MEAS.	OBSVD.	+- UNC.	WT.	RESID. (OB-CAL)	STD. DEV.	AVE. FIT	STD. RES.	REFERENCE
		KCAL/MOL OR CAL/(MOL.K)								
228	TH'3N4(C) = 3 TH'N(C) + 0.5 N2(GS')	H=	31.5	9.0	.2	-3.667	2.59	6.33	-1.00	71KUS/IMO
	AUTHORS' 2ND-LAW 32.00AT APPROX. 1935K ADJ'D TO 298K BY 0.5 .									
229	TH'+4(A) + NO3-(A) = TH'NO3+3(A)	G=	-1.77	3.00	.7	-.490	.82	1.74	-.32	51ZEB/ALT
	AUTHORS' -0.61 AT IONSTR 2 ADJ'D BY -1.16 .									
230	TH'+4(A) + NO3-(A) = TH'NO3+3(A)	G=	-1.8	1.0	1.9	-.520	.82	.76	-.79	50DAY/STO
	AUTHORS' -0.92 AT IONSTR 0.5 ADJ'D BY -0.91 .									
231	TH'+4(A) + NO3-(A) = TH'NO3+3(A)	G=	1.38	1.00	.5	2.660	.82	1.83	1.41	68OHA/MOR
	AUTHORS' 0.07, -0.65 AT IONSTR 1. 0.1 ADJ'D BY -0.98, -0.69 .									
232	TH'+4(A) + 2 NO3-(A) = TH'(NO3)2+2(A)	G=	-2.69	2.50	-1.0	-.000				51ZEB/ALT
	AUTHORS' 0.38 AT IONSTR 6 ADJ'D BY -2.31 .									
233	= TH'(NO3)4(C)	S=	80.	3.	-1.0	.000				.NBS
	EST'D FROM THE :5H2O LESS 10. UNITS PER :H2O .									
234	TH'(NO3)4(C) = TH'O2(C) + 4 NO2(G) + O2(GS')	H=	71.6	6.0	-1.0					30MIS
	2ND LAW . 70.7$6 (397-434K) ADJ'D BY EST'D CP TH(NO3)4 = 66.									
	FOR INFORMATION ONLY. VARIABLE NOT IN SOLUTION.									
235	TH'(NO3)4(A) = TH'+4(A) + 4 NO3-(A)	H=	0.	0.	-1.0	.000				.DEFINED
						CONSTRAINT				
236	TH'(NO3)4(A) = TH'+4(A) + 4 NO3-(A)	S=	0.0	0.0	-1.0	.000				.DEFINED
						CONSTRAINT				
237	TH'(NO3)4(A) = TH'+4(A) + 4 NO3-(A)	G=	0.	0.	-1.0	-.000				.DEFINED
						CONSTRAINT				
238	TH'(NO3)4(100H2O) = TH'(NO3)4(500H2O)	H=	-0.02	0.05	-1.0					29FRI
			NO SOLUTION FOR VARIABLE IN EQUATION.							
239	TH'(NO3)4(50H2O) = TH'(NO3)4(500H2O)	H=	-0.15	0.05	-1.0					29FRI
			NO SOLUTION FOR VARIABLE IN EQUATION.							
240	TH'(NO3)4(25H2O) = TH'(NO3)4(500H2O)	H=	-0.80	0.05	-1.0					29FRI
			NO SOLUTION FOR VARIABLE IN EQUATION.							
241	TH'(NO3)4(20H2O) = TH'(NO3)4(500H2O)	H=	-1.40	0.05	-1.0					29FRI
			NO SOLUTION FOR VARIABLE IN EQUATION.							
242	TH'(NO3)4(16H2O) = TH'(NO3)4(500H2O)	H=	-2.05	0.05	-1.0					29FRI
			NO SOLUTION FOR VARIABLE IN EQUATION.							
243	TH'(NO3)4(18HCL'O4+100000H2O) = TH'(NO3)4(A)	H=	0.488	0.010	-1.0	.000				76MOR/MCC
	IN 0.01N HCLO4 .									

NBS CATALOG OF THORIUM THERMOCHEMICAL DATA, 7/27/77 SOLUTION: CODATA COMPATIBLE WEIGHTED SOLN - LST. SQUARES

NO.	REACTION	PROP. MEAS.	OBSVD.	+- UNC.	WT.	RESID. (OB-CAL)	STD. DEV.	AVE. FIT	STD. RES.	REFERENCE
		KCAL/MOL OR CAL/(MOL.K)								
244	TH'(NO3)4(12.6HCL'O4+70000H2O) = TH'(NO3)4(A) IN 0.01N HCLO4 .	H=	0.508	0.010	-1.0	.000				76MOR/MCC
245	TH'(NO3)4(9HCL'O4+50000H2O) = TH'(NO3)4(A) IN 0.01N HCLO4 .	H=	0.530	0.010	-1.0	.000				76MOR/MCC
246	TH'(NO3)4(5.4HCL'O4+30000H2O) = TH'(NO3)4(A) IN 0.01N HCLO4 .	H=	0.569	0.010	-1.0	.000				76MOR/MCC
247	TH'(NO3)4(1.8HCL'O4+10000H2O) = TH'(NO3)4(A) IN 0.01N HCLO4 .	H=	0.631	0.010	-1.0	.000				76MOR/MCC
248	TH'(NO3)4(1.26HCL'O4+7000H2O) = TH'(NO3)4(A) IN 0.01N HCLO4 .	H=	0.614	0.010	-1.0	.000				76MOR/MCC
249	TH'(NO3)4(1.08HCL'O4+6000H2O) = TH'(NO3)4(A) IN 0.01N HCLO4 .	H=	0.595	0.010	-1.0	.000				76MOR/MCC
250	TH'(NO3)4(0.9HCL'O4+5000H2O) = TH'(NO3)4(A) IN 0.01N HCLO4 .	H=	0.530	0.010	-1.0	.000				76MOR/MCC
251	TH'(NO3)4(1000000H2O+18HNO3) = TH'(NO3)4(2000000H2O+36HNO3) IN .001 MOLAL HNO3 . DOES NOT CONFORM TO D.-H. EXTRAPOLATION . FOR INFORMATION ONLY. VARIABLE NOT IN SOLUTION.	H=	-0.081	0.050	-1.0					57LAN/MIE
252	TH'(NO3)4(500000H2O+9HNO3) = TH'(NO3)4(2000000H2O+36HNO3) IN .001 MOLAL HNO3 . DOES NOT CONFORM TO D.-H. EXTRAPOLATION . FOR INFORMATION ONLY. VARIABLE NOT IN SOLUTION.	H=	-0.170	0.050	-1.0					57LAN/MIE
253	TH'(NO3)4(500000H2O+9HNO3) = TH'(NO3)4(2000000H2O+36HNO3) IN .001 MOLAL HNO3 . DOES NOT CONFORM TO D.-H. EXTRAPOLATION . FOR INFORMATION ONLY. VARIABLE NOT IN SOLUTION.	H=	-0.311	0.050	-1.0					57LAN/MIE
254	TH'(NO3)4(100000H2O+1.8HNO3) = TH'(NO3)4(2000000H2O+36HNO3) IN .001 MOLAL HNO3 . DOES NOT CONFORM TO D.-H. EXTRAPOLATION . FOR INFORMATION ONLY. VARIABLE NOT IN SOLUTION.	H=	-0.449	0.050	-1.0					57LAN/MIE
255	TH'(NO3)4(50000H2O+0.9HNO3) = TH'(NO3)4(2000000H2O+36HNO3) IN .001 MOLAL HNO3 . DOES NOT CONFORM TO D.-H. EXTRAPOLATION . FOR INFORMATION ONLY. VARIABLE NOT IN SOLUTION.	H=	-0.625	0.050	-1.0					57LAN/MIE

NO.	REACTION	PROP. MEAS.	OBSVD. +- UNC.	WT.	RESID. (OB-CAL)	STD. DEV.	AVE. FIT	STD. RES.	REFERENCE
		KCAL/MOL OR CAL/(MOL.K)							
256	TH'(NO3)4(20000H2O+0.36HNO3) = TH'(NO3)4(200000 0H2O+36HNO3)	H=	-0.925	0.050	-1.0				57LAN/MIE
	IN .001 MOLAL HNO3 . DOES NOT CONFORM TO D.-H. EXTRAPOLATION . FOR INFORMATION ONLY. VARIABLE NOT IN SOLUTION.								
257	TH'(NO3)4(20000H2O+0.36HNO3) = TH'(NO3)4(200000 0H2O+36HNO3)	H=	-1.204	0.050	-1.0				57LAN/MIE
	IN .001 MOLAL HNO3. DOES NOT CONFORM TO D.-H. EXTRAPOLATION . FOR INFORMATION ONLY. VARIABLE NOT IN SOLUTION.								
258	TH'(NO3)4(5000H2O+0.09HNO3) = TH'(NO3)4(2000000 H2O+36HNO3)	H=	-1.531	0.050	-1.0				57LAN/MIE
	IN .001 MOLAL HNO3 . DOES NOT CONFORM TO D.-H. EXTRAPOLATION . FOR INFORMATION ONLY. VARIABLE NOT IN SOLUTION.								
259	TH'(NO3)4(C) = TH'(NO3)4(2500H2O)	H=	-34.7	1.0	-1.0				56FER/KAT
	NO SOLUTION FOR VARIABLE IN EQUATION.								
260	= TH'(NO3)4:5H2O(C)	S=	129.83	0.50	-1.0	.000			75WES
	CONSTRAINT								
261	TH'(NO3)4:4H2O(C) = TH'(NO3)4(350H2O) + 4 H2O(L)	H=	-7.65	0.20	-1.0	-.000			56FER/KAT
262	TH'(NO3)4:5H2O(C) = TH'(NO3)4(350H2O) + 5 H2O(L)	H=	-3.55	0.20	-1.0	.000			56FER/KAT
263	TH'(NO3)4:5H2O(C) = TH'(NO3)4(A) + 5 H2O(L)	S=	-7.07	3.00	-1.0	-.310			76MOR/MCC
	CALC'D BY AUTHORS FROM THEIR ^H SOLN. AND THEIR CALC'N OF ^G .								
264	TH'(NO3)4:5H2O(C) = TH'(NO3)4(A) + 5 H2O(L)	G=	-2.62	1.00	2.0	.016	.01	.51	.47 76MOR/MCC
	CALC'D BY AUTHORS: SOL'Y(3.7MOLAL) OF 73APE/AZO, ACTIVITY AND OSMOTIC COEFF. OF 46ROB/LEV .								
265	TH'(NO3)4:5H2O(C) = TH'(NO3)4(A) + 5 H2O(L)	G=	-2.67	0.50	3.7	-.034	.01	.27	-1.38 .NBS
	FROM SOLY.=3.7 MOLAL(73APE/AZO), MEAN ACT. COEFF. AND OSMOTIC COEF. 46ROB/LEV (USING ACTIVITY AND OSMOTIC COEFF. OF 73APE/AZO GIVES -2.14)								
266	TH'(NO3)4:5H2O(C) = TH'(NO3)4(A) + 5 H2O(L)	H=	-4.734	0.100	20.0	.005	.01	.05	.87 76MOR/MCC
267	TH'(NO3)4:5H2O(C) = TH'(NO3)4(A) + 5 H2O(L)	H=	-3.58	0.50	-1.0	1.159			55FER/KAT
	LISTED FOR INFORMATION ONLY.								

NO.	REACTION	PROP. MEAS.	OBSVD. +- UNC.	WT.	RESID. (OB-CAL)	STD. DEV.	AVE. FIT	STD. RES.	REFERENCE
		KCAL/MOL OR CAL/(MOL.K)							
268	TH°(NO3)4:NH4NO3:H2O(C) = TH°(NO3)4(25H2O) + NH4NO3(30H2O) + H2O(L)	H=	-2.16 0.50	-1.0					40BRA
	ASSUME DIFFL HEAT SOLN 1H2O IN 2M TH(NO3)4-2M NH4NO3 IS 0 .								
	NO SOLUTION FOR VARIABLE IN EQUATION.								
269	TH°(NO3)4:NH4NO3:8H2O(C) = TH°(NO3)4(25H2O) + NH4NO3(30H2O) + 8 H2O(L)	H=	12.3 1.0	-1.0					40BRA
	ASSUME DIFFL HEAT SOLN 8 H2O IN 2M TH(NO3)4-2M NH4NO3 IS 0								
	NO SOLUTION FOR VARIABLE IN EQUATION.								
270	(5TH°(NO3)4):4NH4NO3:11H2O(C) = 5 TH°(NO3)4(25H2O) + 4 NH4NO3(30H2O) + 11 H2O(L)	H=	-7.3 1.5	-1.0					40BRA
	ASSUME DIFFL HEAT SOLN 11H2O IN 2M TH(NO3)4-2M NH4NO3 =0.								
	NO SOLUTION FOR VARIABLE IN EQUATION.								
271	(5TH°(NO3)4):4NH4NO3:25H2O(C) = 5 TH°(NO3)4(25H2O) + 4 NH4NO3(30H2O) + 25 H2O(L)	H=	24.9 2.0	-1.0					40BRA
	ASSUME DIFFL HEAT SOLN 25H2O IN 2M TH(NO3)4-2MNH4NO3 IS ZERO								
	NO SOLUTION FOR VARIABLE IN EQUATION.								
272	TH°CL°4(C) + 4 NH3(G) = TH°CL°4:4NH3(C)	H=	-79.2 0.5	-1.0	.000				11CHA
	FROM ENTHALPY OF SOLUTION IN HCL:55H2O, USING TN 270-3								
	FOR NH3(G) + HCL(AQ) AND C°S VALUE FOR THCL4(C).								
273	TH°CL°4(C) + 4 NH3(G) = TH°(NH3)4CL°4(C2)	H=	-103.6 0.5	-1.0	-.000				11CHA
	FROM ENTHALPY OF SOLUTION IN HCL:55H2O, USING TN 270-3								
	FOR NH3(G) + HCL(AQ) AND C°S VALUE FOR THCL4(C).								
	C2 =TH(NH3)4CL4.								
274	TH°CL°4(C) + 6 NH3(G) = TH°CL°4:6NH3(C)	H=	-110.0 0.5	-1.0	.000				11CHA
	FROM ENTHALPY OF SOLUTION IN HCL:55H2O, USING TN 270-3								
	FOR NH3(G) + HCL(AQ) AND C°S VALUE FOR THCL4(C).								
275	TH°CL°4(C) + 6 NH3(G) = TH°(NH3)4CL°4:2NH3(C2)	H=	-147.6 0.5	-1.0	.000				11CHA
	FROM ENTHALPY OF SOLUTION IN HCL:55H2O, USING TN 270-3								
	FOR NH3(G) + HCL(AQ) AND C°S VALUE FOR THCL4(C).								
	C2 = TH(NH3)4CL4:2NH3(C).								
276	TH°CL°4(C) + 7 NH3(G) = TH°CL°4:7NH3(C)	H=	-121.3 0.5	-1.0	.000				11CHA
	FROM ENTHALPY OF SOLUTION IN HCL:55H2O, USING TN 270-3								
	FOR NH3(G) + HCL(AQ) AND C°S VALUE FOR THCL4(C).								
277	TH°CL°4(C) + 2 NH4CL°(C) + 10 H2O(L) = TH°CL°4:2NH4CL°:10H2O(C)	H=	-52.7 0.5	-1.0	-.000				11CHA
	FROM ENTHALPY OF SOLUTION IN H2O, USING TN 270-3 VALUE								
	FOR NH4CL(C) AND C°S VALUE FOR THCL4(C).								
278	TH°CL°4(C) + 7 NH3(G) = TH°(NH3)4CL°4:3NH3(C2)	H=	-168.1 0.5	-1.0	.000				11CHA
	FROM ENTHALPY OF SOLUTION IN HCL:55H2O, USING TN 270-3								
	FOR NH3(G) + HCL(AQ) AND C°S VALUE FOR THCL4(C).								
	C2 = TH(NH3)4CL4:3NH3(C).								

NO.	REACTION	PROP. MEAS.	OBSVD. +- UNC.	WT.	RESID. (OB-CAL)	STD. DEV.	AVE. FIT	STD. RES.	REFERENCE
		KCAL/MOL OR CAL/(MOL.K)							
279	TH'CL'4(C) + 12 NH3(G) = TH'CL'4:12NH3(C) FROM ENTHALPY OF SOLUTION IN HCL:55H2O, USING TN 270-3 FOR NH3(G) + HCL(AQ) AND C'S VALUE FOR THCL4(C).	H= -169.7	0.5	4.0	-.674	.57	.59	-3.04	11CHA
280	TH'CL'4(C) + 12 NH3(G) = TH'(NH3)6CL'4:6NH3(C2) FROM ENTHALPY OF SOLUTION IN HCL:55H2O, USING TN 270-3 FOR NH3(G) + HCL(AQ) AND C'S VALUE FOR THCL4(C). C2 = AMMINO COMPLEX TH(NH3)6:6NH3(C)	H= -215.7	0.5	-1.0	-.000				11CHA
281	TH'CL'4(C) + 18 NH3(G) = TH'CL'4:18NH3(C) FROM ENTHALPY OF SOLUTION IN HCL:55H2O, USING TN 270-3 FOR NH3(G) + HCL(AQ) AND C'S VALUE FOR THCL4(C).	H= -216.7	0.5	4.0	.674	.57	.59	3.04	11CHA
282	TH'CL'4(C) + 18 NH3(G) = TH'(NH3)6CL'4:12NH3(C2) FROM ENTHALPY OF SOLUTION IN HCL:55H2O, USING TN 270-3 FOR NH3(G) + HCL(AQ) AND C'S VALUE FOR THCL4(C). C2 = AMMINO COMPLEX TH(NH3)6CL4:12NH3(C)	H= -264.2	0.5	-1.0	.000				11CHA
283	TH'CL'4:18NH3(C) = TH'CL'4:12NH3(C) + 6 NH3(G) FROM VAPOR PRESSURES FROM 250-281 K	H= 52.2	3.0	.7	3.852	.75	3.43	3.04	11CHA
284	TH'CL'4(C) + NH4CL'(C) = TH'CL'4:NH4CL'(C) FROM ENTHALPY OF SOLUTION IN H2O(L), USING TN 270-3 VALUE FOR NH4CL(C) AND C'S VALUE FOR THCL4(C).	H= -12.95	0.50	-1.0	.000				11CHA
285	TH'P(G) = TH'(G) + P(G) AT 0 DEGR. K; 3RD-LAW CALCN. BY AUTHOR ON DATA AT 2705. 2804K. USING ESTD. THERM. FUNCTS. FOR INFORMATION ONLY. VARIABLE NOT IN SOLUTION.	H= 90.2	5.0	-1.0					69GIN
286	TH'2(G) + P(G) = TH'P(G) + TH'(G) AT 0 DEGR. K . 3RD-LAW CALCN. BY AUTHOR ON SINGLE MASS-SPEC. MEAS'T AT 2804K WITH ESTD. THERM. FUNCTS.:TH2 99.2CM-1 3.30 ANGSTROMS, THP 360 CM-1 2.67 ANGSTROMS, BOTH ELECTR. MLTPLCTY. 4 . FOR INFORMATION ONLY. VARIABLE NOT IN SOLUTION.	H= -22.2	5.0	-1.0					69GIN
287	3 TH'P(C) + 0.5 P2(G) = TH'3P4(C) ADJSTD FROM 1300 K BY ASSUMED DELCP = -1	H= -40.5	5.0	.4	.000	.00	2.50	.00	64GIN
288	TH'(CS') + TH'3P4(C) = 4 TH'P(C) FROM EMF AT 1173 WITH ASSUMED DELCP=-1 AND ASSUMED DELS=-4.7 AT 298K	H= -60.0	4.0	.5	.000	.00	2.00	.00	66GIN/ARO
289	TH'+4(A) + H3PO4(AO') = TH'(H2PO4)+3(A) + H+(A) AUTHORS' -2.96 AT IONSTR 2 ADJ'D BY -0.48 .	G= -3.44	1.50	-1.0	-.000				51ZEB/ALT

NBS CATALOG OF THORIUM THERMOCHEMICAL DATA. 7/27/77 SOLUTION: CODATA COMPATIBLE WEIGHTED SOLN - LST. SQUARES

NO.	REACTION	PROP. MEAS.	OBSVD. +- UNC.	WT.	RESID. (OB-CAL)	STD. DEV.	AVE. FIT	STD. RES.	REFERENCE
		KCAL/MOL OR CAL/(MOL.K)							
290	TH'+4(A) + 2 H3PO4(AO') = TH'(H2PO4)2+2(A) + 2 H+(A)	G=	-6.26	1.50	-1.0	.000			51ZEB/ALT
	AUTHORS' -5.32 AT IONSTR 2 ADJ'D BY-0.94 .								
291	TH'C(C) + 2 O2(GS') = TH'O2(C) + CO2(G)	H=	-357.65	1.10	1.8	-.297	.28	.70 -1.00	68HUB/HOL
292	TH'O2(C) + 3 C(CS') = TH'C(C) + 2 CO(G)	H=	210.2	1.0	2.0	-.268	.28	.63 -1.00	69LOR/SCH
	AUTHORS' 216.4 AT 1750 - 1940K ADJ'D BY ESTD. ^CP=4.								
293	= TH'C1.94(C)	S=	16.38	0.20	-1.0	.000			65WES/TAK
					CONSTRAINT				
294	TH'C1.94(C) + 2.94 O2(GS') = TH'O2(C) + 1.94 CO2(G)	H=	-445.78	1.30	-1.0	.000			68HUB/HOL
295	TH'C1.94(C) + 0.06 C(CS') = TH'C2(G)	H=	196.98	5.00	-1.0	.000			64JAC/BAR
296	TH'(CS') + TH'C2(C) = 2 TH'C(C)	H=	-22.2	3.0	-1.0				69GIN
	USE ASSUMED DELCP = 0 TO ADJUST FROM 1173K								
	FOR INFORMATION ONLY. VARIABLE NOT IN SOLUTION.								
297	TH'+4(A) + C204-2(A) = TH'C204+2(A)	G=	-12.6	1.5	1.3	.082	.39	.79 .17	70GRE/BRY
	AUTHORS' XTRPLTN. TO 0 IONSTR; NBS ADJUSTMENT OF AUTHORS' -11.7 AT IONSTR 0.5 YIELDS -13.7 .								
298	TH'+4(A) + C204-2(A) = TH'C204+2(A)	G=	-12.0	1.5	1.0	.682	.39	1.09 1.13	70BRY/ROG
	NEGLECT EFFECT OF ION STR.								
299	TH'+4(A) + C204-2(A) = TH'C204+2(A)	G=	-13.4	1.0	1.1	-.718	.39	.86 -1.27	67MOS/ESS
	AUTHORS' -22.2 AT IONSTR 1 ADJ'D BY -2.2; AUTHORS DERIVE -14.4 .								
300	TH'+4(A) + 2 C204-2(A) = TH'(C204)2(AO')	G=	-26.9	1.0	.7	-1.607	.52	1.30 -1.39	67MOS/ESS
	AUTHORS' -22.9 AT IONSTR1 ADJ'D BY -4.0 .								
301	TH'+4(A) + 2 C204-2(A) = TH'(C204)2(AO')	G=	-24.8	1.0	1.5	.493	.52	.75 .71	70GRE/BRY
	AUTHORS' -21.2 AT IONSTR 0.5 ADJ'D BY -3.6 . AUTHORS' XTRPLTN. TO 0 IONSTR YIELDS -22.7 9								
302	TH'+4(A) + 2 C204-2(A) = TH'(C204)2(AO')	G=	-25.1	1.0	2.0	.193	.52	.60 .36	70BRY/ROG
	AUTHORS' -21.0 AT IONSTR 1 ADJ'D BY -4.0 . AUTHORS DERIVE -27.6 .								
303	TH'(C204)2:6H2O(C) = TH'+4(A) + 2 C204-2(A) + 6 H2O(L)	G=	34.0	1.0	-1.0	.000			67MOS/ESS
304	TH'+4(A) + 3 C204-2(A) = TH'(C204)3-2(A)	G=	-35.1	1.0	-1.0	-.000			67MOS/ESS
	AUTHORS' -31.1 AT IONSTR 1 ADJ'D BY -4.0								
305	TH'+4(A) + C2H3O2-(A) = TH'C2H3O2+3(A)	G=	-2.5	1.0	-1.0	.000			72TED/ANO
	AUTHORS' -1.5 AT IONSTR 1 ADJ'D BY -1.0								

NO.	REACTION	PROP. MEAS.	OBSVD.	+- UNC.	WT.	RESID. (OB-CAL)	STD. DEV.	AVE. FIT	STD. RES.	REFERENCE
		KCAL/MOL OR CAL/(MOL.K)								
306	TH'+4(A) + HC2H3O2(AO') = TH'C2H3O2+3(A) + H+(A)	G=	-4.7	1.0	-1.0	-8.690				70SEI/AST
	AUTHORS' -4.2 AT IONSTR 0.5 ADJ'D BY -0.5									
			LISTED FOR INFORMATION ONLY.							
307	TH'+4(A) + SCN-(A) = TH'SCN+3(A)	G=	-2.3	1.0	2.0	-.016	.02	.51	-1.00	50WAG/STO
	AUTHORS' -1.5 AT IONSTR 1 ADJ'D BY -0.8									
308	TH'+4(A) + SCN-(A) = TH'SCN+3(A)	G=	-2.26	1.50	1.3	.024	.02	.76	1.00	71LAU/FOU
	AUTHORS' -1.16 AT IONSTR 3 ADJ'D BY -1.10									
309	TH'+4(A) + 2 SCN-(A) = TH'(SCN)2+2(A)	G=	-4.28	1.50	-1.0	-.000				71LAU/FOU
	AUTHORS' -2.09 AT IONSTR 3 ADJ'D BY -2.19									
310	TH'+4(A) + 3 SCN-(A) = TH'(SCN)3+(A)	G=	-4.83	1.50	-1.0	-.000				71LAU/FOU
	AUTHORS' -1.58 AT IONSTR 3 ADJ'D BY -3.25									
311	TH'+4(A) + 4 SCN-(A) = TH'(SCN)4(AO')	G=	-6.18	1.50	-1.0	-.000				71LAU/FOU
	AUTHORS' -2.06 AT IONSTR 3 ADJ'D BY -4.12									
312	TH'(CS') + SI'(CS') = TH'SI'(C)	H=	-29.0	3.0	-1.0	.000				66ALC/COR
	AT 1800K, ASSUME DELCP=0, AUTHORS DO NOT GIVE REACTION ACTUALLY MEASD.									
313	TH'(CS') + 2 SI'(CS') = TH'SI'2(C)	H=	-39.5	3.0	-1.0	.000				66ALC/COR
	AT 1800K, ASSUME DELCP=0, AUTHORS DO NOT GIVE REACTION ACTUALLY MEASD.									
314	3 TH'(CS') + 2 SI'(CS') = TH'3SI'2(C)	H=	-64.7	3.0	-1.0	.000				66ALC/COR
	AT 1800K, ASSUME DELCP=0									
315	3 TH'(CS') + 5 SI'(CS') = TH'3SI'5(C)	H=	-110.7	3.0	-1.0	.000				66ALC/COR
	AT 1800K. ASSUME DELCP=0, AUTHORS DO NOT GIVE REACTION ACTUALLY MEASD.									
316	TH'(CS') + GE'(CS') = TH'GE'(C)	H=	-19.	3.	-1.0	.000				66ALC/COR
	AT 1100K, ASSUME DELCP=0, AUTHORS DO NOT GIVE REACTION ACTUALLY MEASD.									
317	TH'(CS') + 2 GE'(CS') = TH'GE'2(C)	H=	-28.	3.	-1.0	.000				66ALC/COR
	AT 1100K, ASSUME DELCP=0, AUTHORS DO NOT GIVE REACTION ACTUALLY MEASD.									
318	TH'(CS') + 3 GE'(CS') = TH'GE'3(C)	H=	-33.6	3.0	-1.0	.000				66ALC/COR
	AT 1100K, ASSUME DELCP=0, AUTHORS DO NOT GIVE REACTION ACTUALLY MEASD.									
319	3 TH'(CS') + GE'(CS') = TH'3GE'(C)	H=	-26.	3.	-1.0	.000				66ALC/COR
	AS DERIVED (2ND LAW, 1470 - 1490K) BY AUTHORS FROM GE(G) OVER TH + TH3GE; NBS DERIVES 31. FROM THEIR DATA PLOT. ^CP TAKEN TO BE 0									

NO.	REACTION	PROP. MEAS.	OBSVD. +- UNC.	WT.	RESID. (OB-CAL)	STD. DEV.	AVE. FIT	STD. RES.	REFERENCE
		KCAL/MOL OR CAL/(MOL.K)							
320	3 TH°(CS°) + 2 GE°(CS°) = TH°3GE°2(C)	H=	-47.5	3.0	-1.0	.000			66ALC/COR
	AT 1450K. ASSUME DELCP=0. AUTHORS DO NOT GIVE REACTION ACTUALLY MEASD.								
321	3 TH°(CS°) + 5 GE°(CS°) = TH°3GE°5(C)	H=	-76.	3.	-1.0	.000			66ALC/COR
	AT 1100K. ASSUME DELCP=0, AUTHORS DO NOT GIVE REACTION ACTUALLY MEASD.								
322	TH°P(G) + B(G) = TH°B(G) + P(G)	H=	18.9	5.0	-1.0				69GIN
	AT 0 DEGR. K; 3RD-LAW CALCN. BY AUTHOR ON SINGLE MASS-SPEC. MEAS°T AT2804K WITH ESTD. THERM. FUNCTS.: THB 430 CM-1. 2.38 ANGSTR.. ELECTR. MLTPLCTY. 4								
	FOR INFORMATION ONLY. VARIABLE NOT IN SOLUTION.								
323	TH°(CS°) + TH°NI°2(C) = 2 TH°NI°(C)	H=	20.5	2.5	-1.0				70SKE/MAG
	SOLID STATE EMF: 961-1128K: ASSUME DELCP = 0								
	FOR INFORMATION ONLY. VARIABLE NOT IN SOLUTION.								
324	TH°(CS°) + TH°NI°2(C) = 2 TH°NI°(C)	S=	32.8	7.5	-1.0				70SKE/MAG
	SOLID STATE EMF: 901-1128K: ASSUME DEL CP = 0								
	FOR INFORMATION ONLY. VARIABLE NOT IN SOLUTION.								
325	3 TH°(CS°) + 2 TH°NI°5(C) = 5 TH°NI°2(C)	H=	-29.5	7.5	-1.0	-.000			70SKE/MAG
	SOLID STATE EMF: 963-1121K: ASSUME DELCP = 0								
326	3 TH°(CS°) + 2 TH°NI°5(C) = 5 TH°NI°2(C)	S=	8.6	7.5	-1.0	.000			70SKE/MAG
	SOLID STATE EMF: 963-1121K: ASSUME DELCEP = 0								
327	2 TH°(CS°) + 17 NI°(CS°) = TH°2NI°17(C)	H=	-112.6	5.0	-1.0	.000			70SKE/MAG
	SOLID STATE EMF: 954-1091K: ASSUME DELCP = 0.								
328	2 TH°(CS°) + 17 NI°(CS°) = TH°2NI°17(C)	S=	-8.5	5.0	-1.0	.000			70SKE/MAG
	SOLID STATE EMF: 954-1091K: ASSUME DELCP = 0								
329	7 TH°(CS°) + 5 TH°2NI°17(C) = 17 TH°NI°5(C)	H=	-492.	17.	-1.0	.000			70SKE/MAG
	SOLID STATE EMF: 930-1119K: ASSUME DELCP = 0								
330	7 TH°(CS°) + 5 TH°2NI°17(C) = 17 TH°NI°5(C)	S=	-130.	17.	-1.0	.000			70SKE/MAG
	SOLID STATE EMF: 930-1119K: ASSUME DELCP = 0								
331	4 TH°(CS°) + 3 TH°NI°(C) = TH°7NI°3(C)	H=	-4.5	30.0	-1.0				70SKE/MAG
	SOLID STATE EMF: 956-1141K: ASSUME DELCP = 0								
	NO SOLUTION FOR VARIABLE IN EQUATION.								
332	4 TH°(CS°) + 3 TH°NI°(C) = TH°7NI°3(C)	S=	0.7	30.0	-1.0				70SKE/MAG
	SOLID STATE EMF: 956-1141K: ASSUME DELCP = 0								
	NO SOLUTION FOR VARIABLE IN EQUATION.								

NO.	REACTION	PROP. MEAS.	OBSVD.	+- UNC.	WT.	RESID. (OB-CAL)	STD. DEV.	AVE. FIT	STD. RES.	REFERENCE
		KCAL/MOL OR CAL/(MOL.K)								
333	5 TH°(CS°) + TH°2CO°7(C) = 7 TH°CO°(C) SOLID STATE EMF: 949-1233K: ASSUME DELCP = 0	S=	-17.	12.	-1.0	.000				71SKE/MAG
334	5 TH°(CS°) + TH°2CO°7(C) = 7 TH°CO°(C) SOLID STATE EMF: 949-1233K: ASSUME DELCP = 0	H=	-67.	12.	-1.0	-.000				71SKE/MAG
335	3 TH°(CS°) + 7 TH°CO°5(C) = 5 TH°2CO°7(C) SOLID STATE EMF: 980-1045K: ASSUME DELCP = 0	H=	-149.	7.	-1.0	-.000				71SKE/MAG
336	3 TH°(CS°) + 7 TH°CO°5(C) = 5 TH°2CO°7(C) SOLID STATE EMF: 980-1045K: ASSUME DELCP = 0	S=	-64.	7.	-1.0	.000				71SKE/MAG
337	2 TH°(CS°) + 17 CO°(CS°) = TH°2CO°17(C) SOLID STATE EMF: 951-1100K: ASSUME DELCP = 0	H=	-74.8	5.0	-1.0	.000				71SKE/MAG
338	2 TH°(CS°) + 17 CO°(CS°) = TH°2CO°17(C) SOLID STATE EMF: 951-1100K: ASSUME DELCP = 0	S=	-15.1	5.0	-1.0	.000				71SKE/MAG
339	7 TH°(CS°) + 5 TH°2CO°17(C) = 17 TH°CO°5(C) SOLID STATE EMF: 940-1087K: ASSUME DELCP = 0	H=	-354.	17.	-1.0	-.000				71SKE/MAG
340	7 TH°(CS°) + 5 TH°2CO°17(C) = 17 TH°CO°5(C) SOLID STATE EMF: 940-1087K: ASSUME DELCP = 0	S=	-140.	17.	-1.0	.000				71SKE/MAG
341	4 TH°(CS°) + 3 TH°CO°(C) = TH°7CO°3(C) SOLID STATE EMF: 999-1184K: ASSUME DELCP = 0	H=	-5.	10.	-1.0	.000				71SKE/MAG
342	4 TH°(CS°) + 3 TH°CO°(C) = TH°7CO°3(C) SOLID STATE EMF: 999-1184K: ASSUME DELCP = 0	S=	12.5	10.0	-1.0	.000				71SKE/MAG
343	TH°(CS°) + 0.5 O2(GS°) = TH°O(G)	C=	0.000	0.000	-1.0	.000 CONSTRAINT				HGS
344	TH°(CS°) + O2(GS°) = TH°O2(G)	C=	0.000	0.000	-1.0	.000 CONSTRAINT				HGS
345	TH°(CS°) + H2(GS°) = TH°H2(C)	C=	0.000	0.000	-1.0	.000 CONSTRAINT				HGS
346	TH°(CS°) + 1.875 H2(GS°) = TH°H3.75(C)	C=	0.000	0.000	-1.0	.000 CONSTRAINT				HGS
347	TH°(CS°) + 0.5 H2(GS°) + 0.5 O2(GS°) = TH°(OH)+3(A)	C=	13.956	0.000	-1.0	13.956 CONSTRAINT				HGS
348	TH°(CS°) + H2(GS°) + O2(GS°) = TH°(OH)2+2(A)	C=	9.304	0.000	-1.0	9.304 CONSTRAINT				HGS

NBS CATALOG OF THORIUM THERMOCHEMICAL DATA. 7/27/77 SOLUTION: CODATA COMPATIBLE WEIGHTED SOLN - LST. SQUARES

NO.	REACTION	PROP. MEAS.	OBSVD. +- UNC. KCAL/MOL OR CAL/(MOL.K)	WT.	RESID. (OB-CAL)	STD. DEV.	AVE. FIT	STD. RES.	REFERENCE
349	2 TH°(CS°) + H2(GS°) + O2(GS°) = TH°2(OH)2+6(A)	C=	27.912 0.000	-1.0					HGS
			NO SOLUTION FOR VARIABLE IN EQUATION.						
350	4 TH°(CS°) + 4 H2(GS°) + 4 O2(GS°) = TH°4(OH)8+8(A)	C=	37.216 0.000	-1.0					HGS
			NO SOLUTION FOR VARIABLE IN EQUATION.						
351	TH°(CS°) + 0.5 F2(GS°) = TH°F(G)	C=	0.000 0.000	-1.0	.000				HGS
					CONSTRAINT				
352	TH°(CS°) + 0.5 F2(GS°) = TH°F+3(A)	C=	13.956 0.000	-1.0	13.956				HGS
					CONSTRAINT				
353	TH°(CS°) + F2(GS°) = TH°F2(G)	C=	0.000 0.000	-1.0	.000				HGS
					CONSTRAINT				
354	TH°(CS°) + F2(GS°) = TH°F2+2(A)	C=	9.304 0.000	-1.0	9.304				HGS
					CONSTRAINT				
355	TH°(CS°) + 1.5 F2(GS°) = TH°F3(G)	C=	0.000 0.000	-1.0					HGS
			NO SOLUTION FOR VARIABLE IN EQUATION.						
356	TH°(CS°) + 1.5 F2(GS°) = TH°F3+(A)	C=	4.652 0.000	-1.0	4.652				HGS
					CONSTRAINT				
357	TH°(CS°) + 2 F2(GS°) = TH°F4(C)	C=	0.000 0.000	-1.0	.000				HGS
					CONSTRAINT				
358	TH°(CS°) + 2 F2(GS°) = TH°F4(G)	C=	0.000 0.000	-1.0	.000				HGS
					CONSTRAINT				
359	TH°(CS°) + 2 CL°2(GS°) = TH°CL°4(C)	C=	0.000 0.000	-1.0	.000				HGS
					CONSTRAINT				
360	TH°(CS°) + 2 F2(GS°) = TH°F4(AO°)	C=	0.000 0.000	-1.0	.000				HGS
					CONSTRAINT				
361	TH°(CS°) + 2 F2(GS°) + 2.5 H2(GS°) + 1.25 O2(GS°) = TH°F4:2.5H2O(C)	C=	0.000 0.000	-1.0	.000				HGS
					CONSTRAINT				
362	TH°(CS°) + F2(GS°) + 0.5 O2(GS°) = TH°OF2(C)	C=	0.000 0.000	-1.0	.000				HGS
					CONSTRAINT				
363	TH°(CS°) + 0.5 CL°2(GS°) = TH°CL°+3(A)	C=	13.956 0.000	-1.0	13.956				HGS
					CONSTRAINT				
364	TH°(CS°) + 2 CL°2(GS°) = TH°CL°4(G)	C=	0.000 0.000	-1.0	.000				HGS
					CONSTRAINT				

NO.	REACTION	PROP. MEAS.	OBSVD.	+- UNC.	WT.	RESID. (OB-CAL)	STD. DEV.	AVE. FIT	STD. RES.	REFERENCE
		KCAL/MOL OR CAL/(MOL.K)								
365	TH°(CS°) + 2 CL°2(GS°) = TH°CL°4(A)	C=	0.000	0.000	-1.0	.000 CONSTRAINT				HGS
366	TH°(CS°) + CL°2(GS°) + 0.5 O2(GS°) = TH°OCL°2(C)	C=	0.000	0.000	-1.0	.000 CONSTRAINT				HGS
367	TH°(CS°) + 2 BR°2(LS°) = TH°BR°4(G)	C=	0.000	0.000	-1.0	.000 CONSTRAINT				HGS
368	TH°(CS°) + 2 BR°2(LS°) = TH°BR°4(C)	C=	0.000	0.000	-1.0	.000 CONSTRAINT				HGS
369	TH°(CS°) + 2 I2(CS°) = TH°I4(G)	C=	0.000	0.000	-1.0	.000 CONSTRAINT				HGS
370	TH°(CS°) + 2 I2(CS°) = TH°I4(C)	C=	0.000	0.000	-1.0	.000 CONSTRAINT				HGS
371	TH°(CS°) + I2(CS°) + 0.5 O2(GS°) = TH°OI2(C)	C=	0.000	0.000	-1.0	.000 CONSTRAINT				HGS
372	TH°(CS°) + S(CS°) = TH°S(C)	C=	0.000	0.000	-1.0	.000 CONSTRAINT				HGS
373	TH°(CS°) + 2 S(CS°) = TH°S2(C)	C=	0.000	0.000	-1.0	.000 CONSTRAINT				HGS
374	7 TH°(CS°) + 12 S(CS°) = TH°7S12(C)	C=	0.000	0.000	-1.0	.000 CONSTRAINT				HGS
375	2 TH°(CS°) + 3 S(CS°) = TH°2S3(C)	C=	0.000	0.000	-1.0	.000 CONSTRAINT				HGS
376	TH°(CS°) + S(CS°) + 2 O2(GS°) = TH°SO4+2(A)	C=	9.304	0.000	-1.0	9.304 CONSTRAINT				HGS
377	TH°(CS°) + 2 S(CS°) + 4 O2(GS°) = TH°(SO4)2(AQ°)	C=	0.000	0.000	-1.0	.000 CONSTRAINT				HGS
378	TH°(CS°) + 2 S(CS°) + 4 O2(GS°) = TH°(SO4)2(C)	C=	0.000	0.000	-1.0	.000 CONSTRAINT				HGS
379	TH°(CS°) + 0.5 N2(GS°) = TH°N(C)	C=	0.000	0.000	-1.0	.000 CONSTRAINT				HGS
380	TH°(CS°) + 2 N2(GS°) + 6 O2(GS°) = TH°(NO3)4(C)	C=	0.000	0.000	-1.0	.000 CONSTRAINT				HGS

NBS CATALOG OF THORIUM THERMOCHEMICAL DATA. 7/27/77 SOLUTION: CODATA COMPATIBLE WEIGHTED SOLN - LST. SQUARES

NO.	REACTION	PROP. MEAS.	OBSVD.	+- UNC.	WT.	RESID. (OB-CAL)	STD. DEV.	AVE. FIT	STD. RES.	REFERENCE
		KCAL/MOL OR CAL/(MOL.K)								
381	TH°(CS°) + 2 N2(GS°) + 6 O2(GS°) + 5 H2(GS°) + 2.5 O2(GS°) = TH°(NO3)4:5H2O(C)	C=	0.000	0.000	-1.0	.000				HGS
						CONSTRAINT				
382	TH°(CS°) + 1.94 C(CS°) = TH°C1.94(C)	C=	0.000	0.000	-1.0	.000				HGS
						CONSTRAINT				
383	TH°(CS°) + 2 NI°(CS°) = TH°NI°2(C)	C=	0.000	0.000	-1.0	.000				HGS
						CONSTRAINT				
384	TH°(CS°) + NI°(CS°) = TH°NI°(C)	C=	0.000	0.000	-1.0					HGS
			NO SOLUTION FOR VARIABLE IN EQUATION.							
385	TH°(CS°) + 5 NI°(CS°) = TH°NI°5(C)	C=	0.000	0.000	-1.0	.000				HGS
						CONSTRAINT				
386	2 TH°(CS°) + 17 NI°(CS°) = TH°2NI°17(C)	C=	0.000	0.000	-1.0	.000				HGS
						CONSTRAINT				
387	7 TH°(CS°) + 3 NI°(CS°) = TH°7NI°3(C)	C=	0.000	0.000	-1.0					HGS
			NO SOLUTION FOR VARIABLE IN EQUATION.							
388	2 TH°(CS°) + 7 CO°(CS°) = TH°2CO°7(C)	C=	0.000	0.000	-1.0	.000				HGS
						CONSTRAINT				
389	TH°(CS°) + CO°(CS°) = TH°CO°(C)	C=	0.000	0.000	-1.0	.000				HGS
						CONSTRAINT				
390	TH°(CS°) + 5 CO°(CS°) = TH°CO°5(C)	C=	0.000	0.000	-1.0	.000				HGS
						CONSTRAINT				
391	2 TH°(CS°) + 17 CO°(CS°) = TH°2CO°17(C)	C=	0.000	0.000	-1.0	.000				HGS
						CONSTRAINT				
392	7 TH°(CS°) + 3 CO°(CS°) = TH°7CO°3(C)	C=	0.000	0.000	-1.0	.000				HGS
						CONSTRAINT				

NOTES ON THE LISTING OF THE REACTIONS

REACTION NOS. MATCH THOSE GIVEN WITH THE SOLUTION FOR FORMATION PROPERTIES. STATISTICS FOR REACTIONS ARE BASED ON THAT SOLUTION.

THE REACTIONS LISTED HERE MAY FORM SEVERAL INDEPENDENT NETWORKS. IF SO, THEY WERE SOLVED SEPARATELY.

PRIOR TO SOLVING THE NETWORK, ALL ENTROPY REACTIONS ARE MULTIPLIED BY T/1000 TO PUT THEM ON THE SAME SCALE AS ENTHALPY AND FREE ENERGY REACTIONS. THIS FACTOR HAS BEEN REMOVED BEFORE PRINTING THE CATALOG OF REACTIONS. SEE ALSO DISCUSSION OF WEIGHTS, BELOW.

DEFINITIONS: NETWORKS CONTAIN ALL PROPERTIES THAT ARE OVERDETERMINED. SIDE CHAINS ARE SINGLE MEASUREMENTS THAT SPECIFY INDIVIDUAL PROPERTIES. CONSTRAINTS ARE EXACT RELATIONS BETWEEN TWO OR MORE PROPERTIES.

AN UNCERTAINTY SHOWN IN BRACKETS IS MACHINE-ASSIGNED. IT IS EQUAL TO 10 IN THE LEAST SIGNIFICANT DIGIT OF THE

OBSERVATION, AND IS SUPPLIED WHEN NO ESTIMATE IS PROVIDED BY THE DATA ANALYST.

WT.= WEIGHT FOR THE REACTION. WT. IS POSITIVE FOR REACTIONS THAT ARE IN A NETWORK, AND IS -1 FOR CONSTRAINTS, SIDE-CHAINS AND UNUSED REACTIONS. WEIGHTS PRINTED ABOVE ARE APPLICABLE DIRECTLY TO ENTHALPY AND FREE ENERGY REACTIONS AND TO ENTROPY REACTIONS MULTIPLIED BY T/1000. FOR WEIGHTED SOLUTIONS, WT. IS LIMITED (USUALLY) TO THE RANGE 0.1 TO 20. IT IS EQUAL TO THE RECIPROCAL OF THE UNCERTAINTY OF THE REACTION AFTER ALLOWING FOR THE UNCERTAINTIES IN THE AUXILIARY DATA. CONSTRAINT REACTIONS ARE TREATED AS HAVING ZERO UNCERTAINTIES. IN THE SPECIAL CASE OF A SEQUENTIAL PAIR OF SOLUTIONS, WT. FOR THE SECOND IS EQUAL TO THE RECIPROCAL OF THE AVERAGE FIT OF THE FIRST.

RESID. = OBSERVED- PREDICTED VALUE.

STD.DEV.= 1 STANDARD DEVIATION FOR THE PREDICTED VALUE. NEITHER THE UNCERTAINTY OF THE REACTION NOR THOSE OF THE AUXILIARY DATA ARE INCLUDED EXCEPT TO THE EXTENT THAT THEY INFLUENCE THE WEIGHT USED IN THE SOLUTION.

AVE. FIT = (RESID. + UNCERTAINTY)/2, OR, IN SPECIAL CASES, = UNCERTAINTY/2. IT IS A COMBINED MEASURE OF CONSISTENCY AND EXPECTED ACCURACY.

STD. RES. IS THE RESIDUAL NORMALIZED TO UNITY AT ONE STD. DEVIATION (APPROXIMATELY) OF THE NETWORK. A VALUE LESS THAN 0.5 IS VERY GOOD. A VALUE GREATER THAN 2 MEANS A VERY POOR FIT. DEFINITIONS ARE:

STD.RES.(LEAST SUM) = RESID(I)/((SUM(WT(J)*RESID(J))/DF)/WT(I))

STD.RES.(LEAST SQUARES) = RESID(I)/ SQRT((SPR/WT(I)) - SIGMA(I)**2) , WHERE SPR = SUM(WT(J)*RESID(J)**2)/DF.
FOR BOTH CASES J RUNS OVER ALL REACTIONS, AND DF (DEGREES OF FREEDOM) = (NO. OF REACTIONS) - (NO. OF VARIABLES).

REACTIONS LABELED 'CONSTRAINT' ARE SOLVED EXACTLY, PER INSTRUCTIONS FROM THE DATA ANALYST.

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IV. APPENDIX

Thermal Functions for Thorium Compounds

In reducing high-temperature equilibrium measurements to values at 298 K we have made use of the thermal functions S°, (H°-H°(298)), and G°-H°(298)/T for a number of thorium compounds. This section of the Report contains tables of values of the functions that have been used and gives sources of data from which the tables are derived.

Th(c) The high-temperature enthalpy measurements of Levinson [66 LEV] from 1260-2100 K were fitted empirically to the following equations, which also reproduce the value of Cp at 298 K:

Th(c,α): $Cp = 6.267 \pm 0.000664\ T + 7.02 \times 10^{-7} T^2$ cal/mol·K (298-1660)

Transition (c,α) = (c,β): ΔH = 870 cal/mol at 1653 K

Th(c,β): $Cp = 3.72 + 0.00288T$ cal/mol·K

Fusion (c,β) = (l): ΔH = 3300 cal/mol at 2023 K

Th(l): $Cp = 11.0$ cal/mol·K

The above equations for Th(c,α) yield Cp values significantly lower than those reported by Wallace [60WAL] and Mitkina [59MIT] and reproduce the values of Levinson on Th(c,α) more closely than the equation given by Rand [75RAN].

Th(g) Calculated from the 75 energy levels to 20,000 cm^{-1} given by Zalubas [68ZAL]. Up to 2500 K these values are essentially the same as those given by Rand [75RAN].

ThO(g) Calculated from the molecular constants given by Rosen [70ROS], using a non-rigid rotator, anharmonic oscillator approximation and including contributions from the higher electronic levels. This analysis of the higher levels is different from that used by Rand [75RAN], and consequently our values of S° are lower than Rand's by 0.01, 0.03, and 0.54 $cal \cdot K^{-1} \cdot mol^{-1}$ at 298, 1000, and 2000 K, respectively.

$ThO_2(c)$ The entropy and enthalpy content at 298 K are based on the measurements of Osborne and Westrum [53 OSB/WES]. The high temperature enthalpy data of Victor and Douglas [61 VIC/DOU] (273-1173 K) and Hoch and Johnston [61 HOC/JOH] (1450-2750 K) are well represented by the equation given by Victor and Douglas. The data of Hoch and Johnston show considerable scatter with respect to any simple analytical function in T. The equation used to calculate the thermal functions is:

$$Cp(cal \cdot K^{-1} \cdot mol^{-1}) = 17.060 + 0.001806\ T - \frac{251660}{T^2}$$

$ThO_2(g)$ The molecular constants are taken from Gabelnick et al. [74 GAB/REE] who demonstrated by isotopic substitution that the gaseous molecule is bent with an apex angle of 122°. The low lying frequency is taken as 120 cm^{-1}, based on an estimate by Linevsky [65 LIN].

The available vapor pressure data on ThO_2 are not easily reconciled with the available thermal functions but do satisfy functions for $ThO_2(g)$ as a linear molecule.

$ThX_n(g)$ (X = F, Cl, Br, I, n = 1, 2, 3) The values of ω_e for ThX(g) were estimated using the Guggenheimer equation [46 GUG]; we have estimated the anharmonicity constant $\omega_e x_e$. The degeneracy of the ground state is taken = 4. Values of r_e are taken from Krasnov et al [73 KRA/MOR], who also give values for ω_e.

For $ThX_2(g)$ and $ThX_3(g)$ we have used the molecular constants and frequencies estimated by Krasnov et al. [73 KRA/MOR] for a rigid-rotator-harmonic oscillator. As the ground state of ThO(g) was shown to be $^1\Sigma$, we have taken the degeneracy of the ground state of the dihalides to be unity, whereas we have estimated the degeneracy as 6 for the trihalides $ThX_3(g)$.

$ThF_4(c)$ Values of S° and H-H(0) at 298 K are based on the measurements of Lohr et al. [54 LOH/OSB]. Preliminary unpublished high temperature enthalpy measurements by Dworkin [74 DWO] from 1200 K - 1420 K were used to obtain approximate values of the enthalpy of fusion and heat capacities. The equations used are:

$$Cp(c) = 29.2 + 0.002\ T - 300000/T^2\ cal/mol \cdot K$$

$$\Delta H(fusion) = 10000\ cal/mol\ at\ 1383\ K$$

$$Cp(l) = 32.\ cal/mol \cdot K$$

$ThF_4(g)$ Molecular constants have been estimated by Krasnov et al. [73 KRA/MOR] and by Rand [75 RAN]. Calculations using both sets of frequencies have been made with the vaporization data of Darnell and Keneshea [58 DAR/KEN]. A better fit (Second Law and Third Law] is obtained with Rand's function so these are adopted here.

$ThCl_4(c)$ There are no good low temperature heat capacity data for $ThCl_4(c)$. The measurements by Chauvenet [11 CHA] near room temperature are unreasonable. We have estimated $S°(298\ K) = 45.5\ cal \cdot K^{-1} \cdot mol^{-1}$ based on comparisons with $HfCl_4(c)$, $ZrCl_4(c)$, $UCl_4(c)$, and the $UF_4(c)$-$ThF_4(c)$ difference. We have accepted Rand's heat capacity equation [75 RAN].

The enthalpy and temperature of transition and fusion were determined by Chiotti et al. [66 CHI/GAR].

The equations used are:

$Cp(c) = 28.75 + 0.005561\ T - 147000/T^2$ cal/mol·K [298-1042 K]

$\Delta H(transition) = 1200$ cal/mol at 679 K

$\Delta H(fusion) = 14690$ cal/mol at 1042 K

$Cp(l) = 40$ cal/mol·K

$ThCl_4(g)$ The thermal functions for $ThCl_4(g)$ are calculated assuming a tetrahedral molecule (symmetry = 12), ground state degeneracy = 1, and the Th-Cl bond distance = 2.58 Å. The frequencies and degeneracies are taken to be 300(1), 70(2), 335(3), 75(3). The frequency at 335 cm^{-1} has been observed by Buchler et al. [61 BUC/BER]. The enthalpy and entropy of vaporization data computed from the measurements of Knacke et al. [72 KNA/MUL1] are consistent with the functions given here. The data of Fischer et al. [39 FIS/GEW] on the vapor pressure of $ThCl_4(l)$ and (c) are not very consistent with the selected functions.

$ThBr_4(c)$ The heat capacity of the solid and liquid is based on estimated constants given by Rand [75 RAN]. The enthalpy of fusion is calculated from the vapor pressure data of Fischer et al. [39 FIS/GEW]. The entropy is estimated. The equations used are:

$Cp(c) = 30.5 + 0.0036 + - 147000/T^2$ cal/mol·K [298-952 K]

ΔH(transition) = 1000 cal/mol at 693 K

ΔH(fusion) = 7000 cal/mol at 952 K

$Cp(l) = 41$ cal/mol·K

$ThBr_4(g)$ The functions are calculated for a tetrahedral molecule with Th-Br distance = 2.72Å and frequencies 205(1), 58(2), 220(3), 72(3), as estimated by Rand [75 RAN]. The vapor pressure data of Fischer et al.[39 FIS/GEW] are consistent with these functions for both solid and liquid.

$ThI_4(c)$ The thermal functions for the solid and liquid were calculated from the estimated heat capacity and enthalpy of fusion data given by Rand. The vapor pressure of the solid has been reported by Landis and Darnell [60 LAN/DAR; equation only]; data for the liquid are given by Fischer et al. [39 FIS/GEW]. The two sets of data do not agree at the triple point, and do not yield similar values for the heat of sublimation at 298 K. If it is assumed that the Landis and Darnell equation, log P(atm) = 10.32 - 10700/T should be log P(atm) = 10.32-10300/T (misprint in the report?), both sets of data yield consistent values and indicate that $S°(298) = 61$ cal·K·mol^{-1}.

The equations used are:

$Cp(c) = 31.0 + 0.0031\ T - 147000/T^2$ cal/mol·K [298-839 K]

ΔH(fusion) = 11500 cal/mol at 839 K

$Cp(l) = 42$ cal/mol·K

$ThI_4(g)$ The functions are calculated from the molecular constants and frequencies given by Krasnov et al. [73 KRA/MOR]. These frequencies satisfied the relations given by Herzberg [45 HER] better than did those given by Rand [75 RAN].

Th (c,l)

T	CP CAL/MOL.K	H-H298 CAL/MOL	S CAL/MOL.K	(G-H298)/T CAL/MOL.K
298	6.53	0.	12.76	-12.76
300	6.53	12.	12.80	-12.76
400	6.64	671.	14.69	-13.02
500	6.77	1342.	16.19	-13.51
600	6.92	2026.	17.44	-14.06
700	7.08	2726.	18.52	-14.62
800	7.25	3442.	19.47	-15.17
900	7.43	4176.	20.34	-15.70
1000	7.63	4929.	21.13	-16.20
1100	7.85	5703.	21.87	-16.68
1200	8.07	6499.	22.56	-17.14
1300	8.32	7318.	23.22	-17.59
1400	8.57	8162.	23.84	-18.01
1500	8.84	9033.	24.44	-18.42
1600	9.13	9931.	25.02	-18.81
1653	9.28	10419.	25.32	-19.02

HT= 870 CAL/MOL ST= .52632 CAL/MOL.K AT 1653 K

1653	8.48	11289.	25.85	-19.02
1700	8.62	11691.	26.09	-19.21
1800	8.90	12567.	26.59	-19.61
1900	9.19	13472.	27.08	-19.99
2000	9.48	14405.	27.56	-20.35
2023	9.55	14624.	27.66	-20.44

HT= 3300 CAL/MOL ST= 1.6312 CAL/MOL.K AT 2023 K

2023	11.00	17924.	29.30	-20.44
2100	11.00	18771.	29.71	-20.77
2200	11.00	19871.	30.22	-21.19
2300	11.00	20971.	30.71	-21.59
2400	11.00	22071.	31.18	-21.98
2500	11.00	23171.	31.62	-22.36
2600	11.00	24271.	32.06	-22.72
2700	11.00	25371.	32.47	-23.07
2800	11.00	26471.	32.87	-23.42

Th (g)

T	CP CAL/MOL.K	H-H(0) CAL/MOL	S CAL/MOL.K	(G-H298)/T CAL/MOL.K
298	4.969	1481.2	45.424	-45.424
300	4.969	1490.4	45.454	-45.425
400	4.982	1987.7	46.885	-45.620
500	5.039	2488.2	48.002	-45.988
600	5.171	2998.0	48.931	-46.404
700	5.388	3525.3	49.743	-46.824
800	5.679	4078.1	50.481	-47.236
900	6.024	4662.9	51.169	-47.635
1000	6.398	5283.9	51.823	-48.021
1100	6.780	5942.8	52.451	-48.396
1200	7.154	6639.7	53.057	-48.759
1300	7.509	7373.0	53.644	-49.112
1400	7.837	8140.5	54.212	-49.457
1500	8.138	8939.5	54.763	-49.792
1600	8.409	9767.1	55.297	-50.120
1700	8.653	10620.5	55.815	-50.440
1800	8.870	11496.8	56.316	-50.752
1900	9.063	12393.7	56.800	-51.058
2000	9.235	13308.8	57.270	-51.357
2100	9.388	14240.1	57.724	-51.649
2200	9.523	15185.7	58.164	-51.936
2300	9.642	16144.0	58.590	-52.216
2400	9.746	17113.5	59.003	-52.490
2500	9.837	18092.8	59.402	-52.759
2600	9.915	19080.5	59.790	-53.022
2700	9.980	20075.3	60.165	-53.279
2800	10.034	21076.1	60.529	-53.532
2900	10.077	22081.8	60.882	-53.779
3000	10.109	23091.2	61.224	-54.022

ThO (g)

T	CP CAL/MOL.K	H-H(0) CAL/MOL	S CAL/MOL.K	(G-H298)/T CAL/MOL.K
298	7.473	2109.0	57.351	-57.351
300	7.481	2122.8	57.397	-57.351
400	7.864	2890.8	59.604	-57.649
500	8.150	3692.3	61.391	-58.225
600	8.353	4518.0	62.896	-58.881
700	8.501	5361.1	64.195	-59.550
800	8.621	6217.3	65.339	-60.203
900	8.732	7085.0	66.361	-60.832
1000	8.845	7963.8	67.286	-61.431
1100	8.966	8854.2	68.135	-62.003
1200	9.099	9757.4	68.921	-62.547
1300	9.243	10674.4	69.655	-63.066
1400	9.395	11606.2	70.345	-63.561
1500	9.552	12553.5	70.999	-64.035
1600	9.712	13516.7	71.620	-64.490
1700	9.873	14496.0	72.214	-64.927
1800	10.031	15491.2	72.782	-65.348
1900	10.187	16502.2	73.329	-65.754
2000	10.339	17528.5	73.855	-66.146
2100	10.487	18569.9	74.363	-66.525
2200	10.630	19625.7	74.855	-66.892
2300	10.767	20695.6	75.330	-67.249
2400	10.901	21779.1	75.791	-67.595
2500	11.029	22875.6	76.239	-67.932

MOLECULAR WEIGHT= 248.04

MOLECULAR CONSTANTS ARE LISTED AS:
LEVEL, WE, XEWE, YEWE, BE, ALPHAE, DE, MULTIPLICITY, V00

1	895.77	2.39	0	.33264	1.3020E-3	1.8330E-7	1	0
2	864.1	2.31	0	.32641	.00123	1.8630E-7	2	5305
3	846.4	2.4	0	.32304	1.2940E-3	1.8660E-7	1	10601.
4	842.8	2.18	0	.32497	1.2990E-3	1.9400E-7	2	11129.
5	835.1	2.39	0	.32246	.00128	1.9310E-7	2	14490
6	839.2	2.5	0	.32155	.0013	1.8500E-7	2	15946.
7	829.26	2.3	0	.32309	1.3030E-3	1.9900E-7	1	16320.
8	816.2	2.26	0	.31817	.00124	1.9300E-7	2	17998
9	816.2	2.4	0	.3214	.00124	2.0420E-7	1	18338.

ThO_2 (c)

T	CP CAL/MOL.K	H-H298 CAL/MOL	S CAL/MOL.K	(G-H298)/T CAL/MOL.K
298	14.77	0.	15.59	-15.59
300	14.81	27.	15.68	-15.59
400	16.21	1587.	20.16	-16.19
500	16.96	3248.	23.86	-17.37
600	17.44	4970.	27.00	-18.72
700	17.81	6733.	29.72	-20.10
800	18.11	8530.	32.12	-21.45
900	18.37	10354.	34.26	-22.76
1000	18.61	12204.	36.21	-24.01
1100	18.84	14077.	38.00	-25.20
1200	19.05	15971.	39.65	-26.34
1300	19.26	17887.	41.18	-27.42
1400	19.46	19823.	42.61	-28.45
1500	19.66	21779.	43.96	-29.44
1600	19.85	23754.	45.24	-30.39
1700	20.04	25749.	46.45	-31.30
1800	20.23	27763.	47.60	-32.17
1900	20.42	29796.	48.70	-33.02
2000	20.61	31847.	49.75	-33.83
2100	20.80	33917.	50.76	-34.61
2200	20.98	36006.	51.73	-35.37
2300	21.17	38114.	52.67	-36.10
2400	21.35	40239.	53.57	-36.81
2500	21.53	42384.	54.45	-37.49
2600	21.72	44546.	55.30	-38.16
2700	21.90	46727.	56.12	-38.81
2800	22.08	48927.	56.92	-39.45

ThO_2 (g)

T	CP CAL/MOL.K	H-H(0) CAL/MOL	S CAL/MOL.K	(G-H298)/T CAL/MOL.K
298	11.317	2921.2	68.701	-68.701
300	11.334	2942.2	68.771	-68.701
400	12.110	4116.9	72.145	-69.156
500	12.621	5355.3	74.906	-70.038
600	12.955	6635.3	77.239	-71.049
700	13.180	7942.7	79.254	-72.080
800	13.336	9268.9	81.025	-73.090
900	13.448	10608.4	82.602	-74.061
1000	13.531	11957.5	84.024	-74.987
1100	13.593	13313.9	85.316	-75.868
1200	13.642	14675.7	86.501	-76.706
1300	13.680	16041.9	87.595	-77.502
1400	13.711	17411.5	88.610	-78.260
1500	13.736	18783.9	89.557	-78.981
1600	13.757	20158.6	90.444	-79.670
1700	13.774	21535.1	91.278	-80.329
1800	13.788	22913.2	92.066	-80.959
1900	13.801	24292.7	92.812	-81.564
2000	13.811	25673.3	93.520	-82.144
2100	13.820	27054.8	94.194	-82.702
2200	13.828	28437.3	94.837	-83.239
2300	13.835	29820.4	95.452	-83.757
2400	13.841	31204.2	96.041	-84.256
2500	13.846	32588.6	96.606	-84.739
2600	13.851	33973.5	97.149	-85.206
2700	13.855	35358.8	97.672	-85.658
2800	13.859	36744.6	98.176	-86.096
2900	13.863	38130.6	98.662	-86.521
3000	13.866	39517.1	99.132	-86.934

FREQ 787 CM-1 MULT 1
FREQ 120 CM-1 MULT 1
FREQ 735 CM-1 MULT 1
MOLECULAR WEIGHT 264.037
SYMMETRY 2
MOMENTS 23.486 88.795 112.281 IN AMU A2
GROUND STATE DEGENERACY 1

ThF (g)

T	CP CAL/MOL.K	H-H(0) CAL/MOL	S CAL/MOL.K	(G-H298)/T CAL/MOL.K
298	8.285	2226.8	61.471	-61.471
300	8.292	2242.1	61.523	-61.472
400	8.573	3086.7	63.951	-61.801
500	8.735	3952.8	65.882	-62.430
600	8.839	4831.8	67.485	-63.143
700	8.912	5719.5	68.853	-63.863
800	8.968	6613.7	70.047	-64.563
900	9.014	7512.9	71.105	-65.232
1000	9.054	8416.3	72.057	-65.868
1100	9.090	9323.6	72.922	-66.470
1200	9.123	10234.2	73.714	-67.041
1300	9.155	11148.1	74.445	-67.582
1400	9.185	12065.1	75.124	-68.097
1500	9.215	12985.1	75.758	-68.586
1600	9.244	13908.0	76.353	-69.053
1700	9.273	14833.8	76.914	-69.498
1800	9.302	15762.6	77.445	-69.925
1900	9.331	16694.2	77.948	-70.333
2000	9.361	17628.8	78.426	-70.725
2100	9.390	18566.4	78.883	-71.102
2200	9.420	19506.9	79.320	-71.465
2300	9.450	20450.4	79.738	-71.815
2400	9.481	21397.0	80.140	-72.153
2500	9.512	22346.6	80.527	-72.479

MOLECULAR WEIGHT= 251.04
ALPHAE APPROXIMATED AS 2.0386E-3 STATE 1
DE APPROXIMATED AS 4(BE)↑3/(WE)↑2 1.9931E-7 STATE 1

MOLECULAR CONSTANTS ARE LISTED AS
LEVEL,WE,XEWE,YEWE,BE,ALPHAE,DE,MULTIPLICITY,V00

1 489 4 0 .2284 2.0386E-3 1.9931E-7 4 0

ThF_2 (g)

T	CP CAL/MOL.K	H-H(0) CAL/MOL	S CAL/MOL.K	(G-H298)/T CAL/MOL.K
298	12.527	3111.7	70.533	-70.533
300	12.541	3134.9	70.611	-70.534
400	13.064	4418.0	74.299	-71.033
500	13.343	5739.7	77.247	-71.991
600	13.506	7082.9	79.695	-73.077
700	13.609	8439.0	81.785	-74.175
800	13.677	9803.5	83.607	-75.243
900	13.725	11173.7	85.221	-76.263
1000	13.759	12548.0	86.669	-77.233
1100	13.785	13925.3	87.982	-78.151
1200	13.805	15304.8	89.182	-79.021
1300	13.820	16686.1	90.288	-79.846
1400	13.832	18068.7	91.312	-80.629
1500	13.842	19452.5	92.267	-81.373
1600	13.850	20837.1	93.161	-82.082
1700	13.857	22222.5	94.001	-82.759
1800	13.863	23608.5	94.793	-83.406
1900	13.868	24995.1	95.542	-84.025
2000	13.872	26382.0	96.254	-84.619
2100	13.875	27769.4	96.931	-85.189
2200	13.878	29157.1	97.576	-85.737
2300	13.881	30545.1	98.193	-86.266
2400	13.884	31933.3	98.784	-86.775
2500	13.886	33321.8	99.351	-87.267

FREQ 447 CM-1 MULT 1
FREQ 130 CM-1 MULT 1
FREQ 483 CM-1 MULT 1
MOLECULAR WEIGHT 270.04
SYMMETRY 2
MOMENTS 137.64 25.717 163.36 IN AMU A2
GROUND STATE DEGENERACY 1

ThF_3 (g)

T	CP CAL/MOL.K	H-H(0) CAL/MOL	S CAL/MOL.K	(G-H298)/T CAL/MOL.K
298	17.519	4025.6	81.072	-81.072
300	17.542	4058.0	81.181	-81.072
400	18.431	5861.6	86.363	-81.773
500	18.906	7730.8	90.532	-83.122
600	19.184	9636.5	94.006	-84.654
700	19.358	11564.2	96.977	-86.208
800	19.475	13506.2	99.570	-87.719
900	19.556	15458.0	101.869	-89.166
1000	19.614	17416.6	103.932	-90.541
1100	19.658	19380.3	105.804	-91.845
1200	19.692	21347.9	107.516	-93.081
1300	19.718	23318.5	109.093	-94.253
1400	19.739	25291.4	110.555	-95.365
1500	19.756	27266.1	111.918	-96.424
1600	19.770	29242.5	113.193	-97.433
1700	19.781	31220.0	114.392	-98.395
1800	19.791	33198.7	115.523	-99.316
1900	19.799	35178.2	116.593	-100.197
2000	19.806	37158.5	117.609	-101.043
2100	19.812	39139.4	118.576	-101.855
2200	19.818	41120.9	119.497	-102.636
2300	19.822	43102.9	120.378	-103.388
2400	19.826	45085.4	121.222	-104.114
2500	19.830	47068.2	122.032	-104.815

FREQ 480 CM-1 MULT 1
FREQ 140 CM-1 MULT 1
FREQ 484 CM-1 MULT 2
FREQ 156 CM-1 MULT 2
MOLECULAR WEIGHT 289.033
SYMMETRY 3
MOMENTS 133.691 133.691 224.87 IN AMU A2
GROUND STATE DEGENERACY 6

ThF_4 (c,l)

T	CP CAL/MOL.K	H-H298 CAL/MOL	S CAL/MOL.K	(G-H298)/T CAL/MOL.K
298	26.42	0.	33.95	-33.95
300	26.47	49.	34.11	-33.95
400	28.13	2789.	41.98	-35.01
500	29.00	5649.	48.36	-37.07
600	29.57	8579.	53.70	-39.41
700	29.99	11557.	58.29	-41.78
800	30.33	14574.	62.32	-44.10
900	30.63	17622.	65.91	-46.33
1000	30.90	20699.	69.15	-48.45
1100	31.15	23802.	72.11	-50.47
1200	31.39	26929.	74.83	-52.39
1300	31.62	30080.	77.35	-54.21
1383	31.81	32712.	79.32	-55.66

HT= 10000 CAL/MOL ST= 7.2307 CAL/MOL.K AT 1383 K

1383	32.00	42712.	86.55	-55.66
1400	32.00	43256.	86.94	-56.04
1500	32.00	46456.	89.14	-58.17

ThF_4 (g)

T	CP CAL/MOL.K	H-H(0) CAL/MOL	S CAL/MOL.K	(G-H298)/T CAL/MOL.K
298	22.235	4901.5	81.667	-81.667
300	22.269	4942.6	81.805	-81.668
400	23.598	7243.0	88.413	-82.560
500	24.324	9642.5	93.765	-84.283
600	24.753	12098.0	98.240	-86.246
700	25.025	14587.9	102.078	-88.240
800	25.207	17100.0	105.432	-90.184
900	25.334	19627.4	108.409	-92.047
1000	25.426	22165.7	111.083	-93.819
1100	25.496	24712.0	113.510	-95.500
1200	25.548	27264.3	115.731	-97.095
1300	25.590	29821.3	117.777	-98.608
1400	25.623	32382.0	119.675	-100.046
1500	25.650	34945.7	121.444	-101.414
1600	25.672	37511.8	123.100	-102.719
1700	25.690	40079.9	124.657	-103.964
1800	25.705	42649.7	126.126	-105.155
1900	25.718	45220.9	127.516	-106.295
2000	25.730	47793.3	128.835	-107.390
2100	25.739	50366.8	130.091	-108.441
2200	25.747	52941.1	131.289	-109.452
2300	25.755	55516.2	132.433	-110.427
2400	25.761	58092.0	133.530	-111.367
2500	25.767	60668.4	134.581	-112.274

FREQ 555 CM-1 MULT 1
FREQ 145 CM-1 MULT 2
FREQ 515 CM-1 MULT 3
FREQ 155 CM-1 MULT 3
MOLECULAR WEIGHT 308.03
SYMMETRY 12
MOMENTS 232.01 232.01 232.01 IN AMU A2
GROUND STATE DEGENERACY 1

ThCl (g)

T	CP CAL/MOL.K	H-H(0) CAL/MOL	S CAL/MOL.K	(G-H298)/T CAL/MOL.K
298	8.714	2354.0	64.325	-64.325
300	8.718	2370.1	64.379	-64.325
400	8.865	3250.0	66.910	-64.669
500	8.951	4141.2	68.898	-65.323
600	9.012	5039.5	70.535	-66.059
700	9.061	5943.2	71.928	-66.800
800	9.104	6851.6	73.140	-67.518
900	9.144	7764.0	74.215	-68.203
1000	9.183	8680.4	75.180	-68.853
1100	9.220	9600.5	76.056	-69.468
1200	9.258	10524.4	76.859	-70.051
1300	9.295	11452.0	77.601	-70.602
1400	9.333	12383.4	78.290	-71.126
1500	9.372	13318.7	78.935	-71.625
1600	9.411	14257.8	79.540	-72.100
1700	9.451	15200.9	80.110	-72.553
1800	9.492	16148.1	80.651	-72.987
1900	9.534	17099.4	81.164	-73.403
2000	9.577	18054.9	81.653	-73.802
2100	9.620	19014.7	82.119	-74.186
2200	9.665	19979.0	82.566	-74.555
2300	9.710	20947.7	82.995	-74.911
2400	9.757	21921.1	83.408	-75.255
2500	9.804	22899.1	83.805	-75.587

MOLECULAR WEIGHT= 267.49
ALPHAE APPROXIMATED AS 6.0992E-4 STATE 1
DE APPROXIMATED AS 4(BE)↑3/(WE)↑2 3.3206E-8 STATE 1

MOLECULAR CONSTANTS ARE LISTED AS
LEVEL,WE,XEWE,YEWE,BE,ALPHAE,DE,MULTIPLICITY,V00

1 292 2 0 .08912 6.0992E-4 3.3206E-8 4 0

$ThCl_2$ (g)

T	CP CAL/MOL.K	H-H(0) CAL/MOL	S CAL/MOL.K	(G-H298)/T CAL/MOL.K
298	13.212	3359.9	75.766	-75.766
300	13.220	3384.3	75.848	-75.766
400	13.504	4722.4	79.695	-76.289
500	13.645	6080.5	82.725	-77.284
600	13.724	7449.3	85.220	-78.405
700	13.772	8824.3	87.340	-79.534
800	13.804	10203.2	89.181	-80.627
900	13.826	11584.8	90.808	-81.669
1000	13.842	12968.2	92.266	-82.658
1100	13.854	14353.0	93.586	-83.592
1200	13.863	15738.9	94.792	-84.476
1300	13.870	17125.5	95.901	-85.312
1400	13.875	18512.7	96.929	-86.106
1500	13.880	19900.5	97.887	-86.860
1600	13.883	21288.6	98.783	-87.577
1700	13.886	22677.1	99.625	-88.262
1800	13.889	24065.9	100.418	-88.915
1900	13.891	25454.9	101.169	-89.540
2000	13.893	26844.1	101.882	-90.140
2100	13.895	28233.5	102.560	-90.715
2200	13.896	29623.0	103.206	-91.268
2300	13.897	31012.7	103.824	-91.801
2400	13.898	32402.5	104.415	-92.314
2500	13.899	33792.3	104.983	-92.810

FREQ 308 CM-1 MULT 1
FREQ 84 CM-1 MULT 1
FREQ 315 CM-1 MULT 1
MOLECULAR WEIGHT 302.944
SYMMETRY 2
MOMENTS 372.8 62.09 434.89 IN AMU A2
GROUND STATE DEGENERACY 1

$ThCl_3$ (g)

T	CP CAL/MOL.K	H-H(0) CAL/MOL	S CAL/MOL.K	(G-H298)/T CAL/MOL.K
298	18.643	4466.7	88.331	-88.331
300	18.656	4501.2	88.447	-88.332
400	19.155	6394.9	93.891	-89.070
500	19.403	8324.1	98.195	-90.480
600	19.542	10271.9	101.746	-92.070
700	19.628	12230.7	104.765	-93.674
800	19.684	14196.5	107.390	-95.228
900	19.723	16166.9	109.711	-96.710
1000	19.751	18140.7	111.790	-98.116
1100	19.772	20116.9	113.674	-99.446
1200	19.787	22094.9	115.395	-100.705
1300	19.800	24074.2	116.979	-101.896
1400	19.810	26054.7	118.447	-103.027
1500	19.818	28036.1	119.814	-104.101
1600	19.824	30018.2	121.093	-105.123
1700	19.830	32000.9	122.295	-106.098
1800	19.834	33984.1	123.429	-107.030
1900	19.838	35967.7	124.501	-107.922
2000	19.841	37951.7	125.519	-108.776
2100	19.844	39936.0	126.487	-109.597
2200	19.847	41920.5	127.410	-110.386
2300	19.849	43905.3	128.292	-111.145
2400	19.851	45890.2	129.137	-111.877
2500	19.852	47875.4	129.948	-112.584

FREQ 320 CM-1 MULT 1
FREQ 100 CM-1 MULT 1
FREQ 333 CM-1 MULT 2
FREQ 105 CM-1 MULT 2
MOLECULAR WEIGHT 338.397
SYMMETRY 3
MOMENTS 353.677 353.677 609.06 IN AMU A2
GROUND STATE DEGENERACY 6

$ThCl_4$ (c,l)

T	CP CAL/MOL.K	H-H298 CAL/MOL	S CAL/MOL.K	(G-H298)/T CAL/MOL.K
298	28.75	0.	45.50	-45.50
300	28.78	53.	45.68	-45.50
400	30.06	3000.	54.15	-46.65
500	30.94	6052.	60.95	-48.85
600	31.68	9184.	66.66	-51.36
679	32.21	11708.	70.61	-53.37

HT= 1200 CAL/MOL ST= 1.7673 CAL/MOL.K AT 679 K

679	32.21	12908.	72.38	-53.37
700	32.34	13585.	73.36	-53.96
800	32.97	16851.	77.72	-56.66
900	33.57	20179.	81.64	-59.22
1000	34.16	23565.	85.21	-61.64
1042	34.41	25006.	86.62	-62.62

HT= 14690 CAL/MOL ST= 14.098 CAL/MOL.K AT 1042 K

1042	40.00	39696.	100.72	-62.62
1100	40.00	42016.	102.88	-64.69
1200	40.00	46016.	106.36	-68.02
1300	40.00	50016.	109.57	-71.09
1400	40.00	54016.	112.53	-73.95
1500	40.00	58016.	115.29	-76.61

$ThCl_4$ (g)

T	CP CAL/MOL.K	H-H(0) CAL/MOL	S CAL/MOL.K	(G-H298)/T CAL/MOL.K
298	24.273	5816.7	95.000	-95.000
300	24.290	5861.6	95.150	-95.001
400	24.922	8326.2	102.236	-95.963
500	25.237	10835.8	107.835	-97.797
600	25.414	13369.1	112.453	-99.866
700	25.523	15916.3	116.380	-101.952
800	25.594	18472.4	119.793	-103.973
900	25.644	21034.5	122.810	-105.902
1000	25.679	23600.7	125.514	-107.730
1100	25.706	26170.0	127.963	-109.460
1200	25.726	28741.7	130.201	-111.096
1300	25.742	31315.1	132.260	-112.646
1400	25.754	33889.9	134.169	-114.116
1500	25.764	36465.9	135.946	-115.513
1600	25.773	39042.8	137.609	-116.843
1700	25.780	41620.4	139.172	-118.111
1800	25.785	44198.7	140.645	-119.322
1900	25.790	46777.4	142.039	-120.481
2000	25.794	49356.7	143.362	-121.592
2100	25.798	51936.3	144.621	-122.659
2200	25.801	54516.3	145.821	-123.685
2300	25.804	57096.5	146.968	-124.673
2400	25.806	59677.1	148.067	-125.625
2500	25.808	62257.8	149.120	-126.544

FREQ 300 CM-1 MULT 1
FREQ 70 CM-1 MULT 2
FREQ 335 CM-1 MULT 3
FREQ 75 CM-1 MULT 3
MOLECULAR WEIGHT 373.85
SYMMETRY 12
MOMENTS 629.31 629.31 629.31 IN AMU A2
GROUND STATE DEGENERACY 1

ThBr (g)

T	CP CAL/MOL.K	H-H(0) CAL/MOL	S CAL/MOL.K	(G-H298)/T CAL/MOL.K
298	8.952	2452.9	67.153	-67.153
300	8.955	2469.5	67.209	-67.153
400	9.072	3371.2	69.801	-67.506
500	9.164	4283.1	71.835	-68.175
600	9.249	5203.8	73.513	-68.928
700	9.332	6132.8	74.943	-69.686
800	9.416	7070.2	76.193	-70.421
900	9.504	8016.2	77.305	-71.124
1000	9.595	8971.1	78.308	-71.790
1100	9.691	9935.4	79.224	-72.422
1200	9.790	10909.4	80.069	-73.021
1300	9.894	11893.6	80.852	-73.590
1400	10.003	12888.4	81.585	-74.131
1500	10.116	13894.4	82.274	-74.647
1600	10.234	14911.9	82.926	-75.139
1700	10.357	15941.4	83.544	-75.609
1800	10.485	16983.5	84.133	-76.060
1900	10.617	18038.5	84.696	-76.493
2000	10.754	19107.0	85.237	-76.910
2100	10.895	20189.4	85.757	-77.311
2200	11.042	21286.3	86.258	-77.697
2300	11.193	22398.0	86.743	-78.071
2400	11.349	23525.1	87.212	-78.432
2500	11.510	24668.0	87.668	-78.782

MOLECULAR WEIGHT= 311.94
ALPHAE APPROXIMATED AS 3.0458E-4 STATE 1
DE APPROXIMATED AS 4(BE)↑3/(WE)↑2 7.0029E-9 STATE 1

MOLECULAR CONSTANTS ARE LISTED AS:
LEVEL,WE,XEWE,YEWE,BE,ALPHAE,DE,MULTIPLICITY,V00

1 194 2 0 .04039 3.0458E-4 7.0029E-9 4 0

$ThBr_2$ (g)

T	CP CAL/MOL.K	H-H(0) CAL/MOL	S CAL/MOL.K	(G-H298)/T CAL/MOL.K
298	13.559	3556.7	81.009	-81.009
300	13.563	3581.8	81.093	-81.009
400	13.711	4946.5	85.018	-81.543
500	13.781	6321.4	88.085	-82.556
600	13.820	7701.6	90.602	-83.693
700	13.844	9084.9	92.734	-84.837
800	13.859	10470.1	94.584	-85.942
900	13.870	11856.6	96.217	-86.995
1000	13.877	13244.0	97.678	-87.991
1100	13.883	14632.0	99.001	-88.933
1200	13.887	16020.6	100.210	-89.823
1300	13.891	17409.5	101.321	-90.665
1400	13.893	18798.7	102.351	-91.464
1500	13.896	20188.1	103.309	-92.222
1600	13.897	21577.8	104.206	-92.943
1700	13.899	22967.6	105.049	-93.631
1800	13.900	24357.6	105.843	-94.287
1900	13.901	25747.6	106.595	-94.915
2000	13.902	27137.8	107.308	-95.517
2100	13.903	28528.0	107.986	-96.095
2200	13.903	29918.3	108.633	-96.650
2300	13.904	31308.7	109.251	-97.185
2400	13.904	32699.1	109.843	-97.700
2500	13.905	34089.6	110.410	-98.197

FREQ 196 CM-1 MULT 1
FREQ 61 CM-1 MULT 1
FREQ 232 CM-1 MULT 1
MOLECULAR WEIGHT 391.856
SYMMETRY 2
MOMENTS 123.221 956.989 1080.21 IN AMU A2
GROUND STATE DEGENERACY 1

$ThBr_3$ (g)

T	CP CAL/MOL.K	H-H(0) CAL/MOL	S CAL/MOL.K	(G-H298)/T CAL/MOL.K
298	19.311	4888.1	96.829	-96.829
300	19.317	4923.9	96.949	-96.830
400	19.553	6869.0	102.543	-97.591
500	19.666	8830.6	106.920	-99.035
600	19.728	10800.6	110.511	-100.657
700	19.766	12775.4	113.555	-102.288
800	19.790	14753.3	116.196	-103.865
900	19.807	16733.2	118.528	-105.367
1000	19.820	18714.6	120.616	-106.789
1100	19.829	20697.0	122.505	-108.134
1200	19.835	22680.2	124.231	-109.404
1300	19.841	24664.1	125.819	-110.607
1400	19.845	26648.4	127.289	-111.746
1500	19.848	28633.0	128.659	-112.829
1600	19.851	30618.0	129.940	-113.859
1700	19.854	32603.3	131.143	-114.840
1800	19.856	34588.7	132.278	-115.778
1900	19.857	36574.4	133.352	-116.675
2000	19.859	38560.2	134.370	-117.534
2100	19.860	40546.1	135.339	-118.359
2200	19.861	42532.1	136.263	-119.152
2300	19.862	44518.3	137.146	-119.915
2400	19.863	46504.5	137.991	-120.651
2500	19.863	48490.8	138.802	-121.361

FREQ 200 CM-1 MULT 1
FREQ 68 CM-1 MULT 1
FREQ 223 CM-1 MULT 2
FREQ 66 CM-1 MULT 2
MOLECULAR WEIGHT 471.765
SYMMETRY 3
MOMENTS 872.26 872.26 1563.51 IN AMU A2
GROUND STATE DEGENERACY 6

$ThBr_4$ (c,l)

T	CP CAL/MOL.K	H-H298 CAL/MOL	S CAL/MOL.K	(G-H298)/T CAL/MOL.K
298	29.92	0.	54.50	-54.50
300	29.95	55.	54.69	-54.50
400	31.02	3109.	63.46	-55.69
500	31.71	6247.	70.46	-57.97
600	32.25	9446.	76.29	-60.55
693	32.69	12466.	80.97	-62.98

HT= 1000 CAL/MOL ST= 1.443 CAL/MOL.K AT 693 K

693	32.69	13466.	82.42	-62.98
700	32.72	13695.	82.74	-63.18
800	33.15	16989.	87.14	-65.91
900	33.56	20325.	91.07	-68.49
952	33.77	22075.	92.96	-69.77

HT= 7000 CAL/MOL ST= 7.3529 CAL/MOL.K AT 952 K

952	41.00	29075.	100.31	-69.77
1000	41.00	31043.	102.33	-71.29
1100	41.00	35143.	106.24	-74.29
1200	41.00	39243.	109.81	-77.10
1300	41.00	43343.	113.09	-79.75
1400	41.00	47443.	116.13	-82.24
1500	41.00	51543.	118.95	-84.59

$ThBr_4$ (g)

T	CP CAL/MOL.K	H-H(0) CAL/MOL	S CAL/MOL.K	(G-H298)/T CAL/MOL.K
298	25.064	6228.0	102.720	-102.720
300	25.073	6274.4	102.875	-102.720
400	25.396	8800.0	110.139	-103.709
500	25.551	11348.2	115.824	-105.584
600	25.636	13908.0	120.491	-107.691
700	25.688	16474.4	124.447	-109.809
800	25.722	19045.0	127.879	-111.858
900	25.745	21618.4	130.910	-113.810
1000	25.762	24193.7	133.624	-115.658
1100	25.774	26770.6	136.080	-117.405
1200	25.783	29348.5	138.323	-119.056
1300	25.791	31927.2	140.387	-120.618
1400	25.797	34506.6	142.298	-122.099
1500	25.801	37086.5	144.078	-123.506
1600	25.805	39666.8	145.744	-124.844
1700	25.808	42247.5	147.308	-126.120
1800	25.811	44828.5	148.783	-127.339
1900	25.813	47409.7	150.179	-128.504
2000	25.815	49991.1	151.503	-129.622
2100	25.817	52572.7	152.763	-130.694
2200	25.818	55154.5	153.964	-131.724
2300	25.820	57736.4	155.111	-132.716
2400	25.821	60318.4	156.210	-133.673
2500	25.822	62900.6	157.264	-134.595

FREQ 205 CM-1 MULT 1
FREQ 58 CM-1 MULT 2
FREQ 220 CM-1 MULT 3
FREQ 72 CM-1 MULT 3
MOLECULAR WEIGHT 551.654
SYMMETRY 12
MOMENTS 1576.4 1576.4 1576.4 IN AMU A2
GROUND STATE DEGENERACY 1

ThI (g)

T	CP CAL/MOL.K	H-H(0) CAL/MOL	S CAL/MOL.K	(G-H298)/T CAL/MOL.K
298	8.980	2494.2	68.950	-68.950
300	8.982	2510.8	69.006	-68.950
400	9.066	3413.4	71.602	-69.303
500	9.135	4323.5	73.632	-69.973
600	9.199	5240.2	75.302	-70.725
700	9.262	6163.2	76.724	-71.482
800	9.327	7092.7	77.963	-72.215
900	9.394	8028.7	79.064	-72.915
1000	9.464	8971.6	80.056	-73.578
1100	9.536	9921.5	80.959	-74.207
1200	9.611	10878.9	81.789	-74.802
1300	9.690	11843.9	82.559	-75.367
1400	9.772	12817.0	83.277	-75.904
1500	9.856	13798.3	83.951	-76.415
1600	9.944	14788.3	84.586	-76.902
1700	10.036	15787.3	85.188	-77.368
1800	10.130	16795.5	85.760	-77.814
1900	10.228	17813.4	86.305	-78.242
2000	10.329	18841.2	86.827	-78.654
2100	10.433	19879.3	87.328	-79.050
2200	10.541	20927.9	87.810	-79.431
2300	10.651	21987.5	88.275	-79.799
2400	10.765	23058.3	88.724	-80.155
2500	10.883	24140.7	89.158	-80.500

MOLECULAR WEIGHT= 358.94
ALPHAE APPROXIMATED AS 1.3447E-4 STATE 1
DE APPROXIMATED AS 4(BE)↑3/(WE)↑2 2.8410E-9 STATE 1

MOLECULAR CONSTANTS ARE LISTED AS:
LEVEL,WE,XEWE,YEWE,BE,ALPHAE,DE,MULTIPLICITY,V00

1 151 1 0 .0253 1.3447E-4 2.8410E-9 4 0

ThI_2 (g)

T	CP CAL/MOL.K	H-H(0) CAL/MOL	S CAL/MOL.K	(G-H298)/T CAL/MOL.K
298	13.713	3691.1	84.960	-84.960
300	13.716	3716.5	85.045	-84.961
400	13.799	5092.8	89.004	-85.500
500	13.839	6475.0	92.088	-86.520
600	13.860	7860.0	94.613	-87.665
700	13.874	9246.8	96.751	-88.814
800	13.882	10634.6	98.604	-89.925
900	13.888	12023.1	100.239	-90.982
1000	13.892	13412.1	101.703	-91.982
1100	13.895	14801.5	103.027	-92.927
1200	13.898	16191.2	104.236	-93.820
1300	13.900	17581.0	105.349	-94.664
1400	13.901	18971.1	106.379	-95.465
1500	13.902	20361.2	107.338	-96.225
1600	13.903	21751.5	108.235	-96.948
1700	13.904	23141.9	109.078	-97.637
1800	13.905	24532.3	109.873	-98.295
1900	13.905	25922.8	110.625	-98.924
2000	13.906	27313.3	111.338	-99.527
2100	13.906	28703.9	112.016	-100.106
2200	13.906	30094.5	112.663	-100.662
2300	13.907	31485.2	113.282	-101.197
2400	13.907	32875.9	113.873	-101.713
2500	13.907	34266.6	114.441	-102.211

FREQ 140 CM-1 MULT 1
FREQ 45 CM-1 MULT 1
FREQ 176 CM-1 MULT 1
MOLECULAR WEIGHT 485.847
SYMMETRY 2
MOMENTS 182.08 1753.3 1935.38 IN AMU A2
GROUND STATE DEGENERACY 1

ThI_3 (g)

T	CP CAL/MOL.K	H-H(0) CAL/MOL	S CAL/MOL.K	(G-H298)/T CAL/MOL.K
298	19.550	5117.7	102.733	-102.733
300	19.553	5153.9	102.854	-102.734
400	19.690	7117.0	108.501	-103.503
500	19.755	9089.7	112.902	-104.959
600	19.790	11067.1	116.508	-106.592
700	19.812	13047.3	119.560	-108.232
800	19.826	15029.2	122.207	-109.817
900	19.835	17012.3	124.542	-111.326
1000	19.842	18996.2	126.633	-112.754
1100	19.847	20980.7	128.524	-114.103
1200	19.851	22965.7	130.251	-115.378
1300	19.854	24951.0	131.840	-116.584
1400	19.857	26936.5	133.312	-117.727
1500	19.859	28922.3	134.682	-118.812
1600	19.860	30908.2	135.963	-119.844
1700	19.862	32894.3	137.167	-120.828
1800	19.863	34880.5	138.303	-121.768
1900	19.864	36866.8	139.377	-122.667
2000	19.864	38853.2	140.396	-123.528
2100	19.865	40839.7	141.365	-124.354
2200	19.866	42826.2	142.289	-125.149
2300	19.866	44812.8	143.172	-125.913
2400	19.867	46799.4	144.017	-126.650
2500	19.867	48786.1	144.828	-127.361

FREQ 144 CM-1 MULT 1
FREQ 53 CM-1 MULT 1
FREQ 170 CM-1 MULT 2
FREQ 48 CM-1 MULT 2
MOLECULAR WEIGHT 612.751
SYMMETRY 3
MOMENTS 1559.54 1559.94 2864.51 IN AMU A2
GROUND STATE DEGENERACY 6

ThI_4 (c,l)

T	CP CAL/MOL.K	H-H298 CAL/MOL	S CAL/MOL.K	(G-H298)/T CAL/MOL.K
298	30.27	0.	61.00	-61.00
300	30.30	56.	61.19	-61.00
400	31.32	3142.	70.06	-62.20
500	31.96	6308.	77.12	-64.50
600	32.45	9530.	82.99	-67.11
700	32.87	12796.	88.03	-69.75
800	33.25	16102.	92.44	-72.31
839	33.39	17402.	94.03	-73.29

HT= 11500 CAL/MOL ST= 13.707 CAL/MOL.K AT 839 K

839	42.00	28902.	107.73	-73.29
900	42.00	31464.	110.68	-75.72
1000	42.00	35664.	115.11	-79.44
1100	42.00	39864.	119.11	-82.87
1200	42.00	44064.	122.76	-86.04
1300	42.00	48264.	126.13	-89.00
1400	42.00	52464.	129.24	-91.76
1500	42.00	56664.	132.14	-94.36

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16. ABSTRACT *(A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here.)*

Selected values are given for the thermochemical properties of the compounds of thorium. They are obtained from a computer-assisted least sums-least squares approach to the evaluation of thermodynamic data networks. The properties given, where data are available, are enthalpy of formation, Gibbs energy of formation, and entropy at 298.15 K ($\Delta Hf°(298)$, $\Delta Gf°(298)$, and $S°(298)$). The values are consistent with the CODATA Key Values for Thermodynamics. The reaction catalog from which this self consistent set of values is generated is given with a statistical analysis. Some thermal functions are also given, as well as detailed comments when necessary.

17. KEY WORDS *(six to twelve entries; alphabetical order; capitalize only the first letter of the first key word unless a proper name; separated by semicolons)* Data evaluation; enthalpy; entropy; Gibbs energy; thermochemical data networks; thermochemical tables; thorium compounds

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