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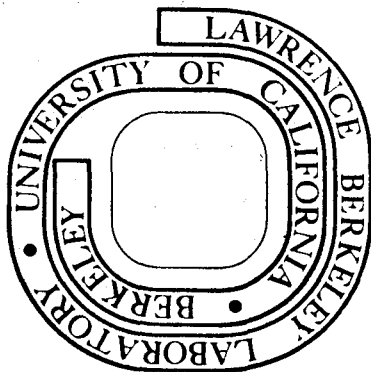
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The Cohesive Energies of the Elements

Leo Brewer*

Hultgren et al. (1) have critically reviewed the thermodynamic data available for the elements and have tabulated values of ΔH_{298}° and ΔH_0° for the atomization of the solid elemental phases. For polymorphic elements, values of ΔH_{298}° were given only for one of the phases, either the one stable at 298.15 K or at 0 K.

This previous compilation has been extended in several respects. Where thermodynamic data were available to relate polymorphic phases of an element, low-temperature heat capacities of the high temperature forms were estimated to evaluate ΔH_{298}° and ΔH_0° for the atomization of each of the polymorphic phases. The uncertainty introduced through use of estimated heat capacities is reflected in the uncertainties assigned to the values in Table I. For some high temperature polymorphs for which entropies of transition were not known but for which equilibrium transition temperatures have been determined, estimates of the entropy of transition and of heat capacities were used to obtain values of ΔH_0° for the atomization. These values are indicated in parentheses. Although the compilation by Hultgren et al. was published in 1973, the evaluations extended over a period of years from 1964 to 1972. Where additional data appeared after the completion of the evaluation of a given element, the references to these data were listed by Hultgren in an appendix. The data in these references and in any other recent publications were examined and a reevaluation of all data made. The compilation by Hultgren was based on the 1948 International Temperature Scale. In the process of reevaluation, all data were converted to the 1968 International Temperature Scale. (2)

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For those elements for which no references are cited, all data were obtained from Hultgren et al. or from the references listed in their appendix. If any additional publications were used to supplement those in Hultgren, they are cited following Table I. For a number of elements, a polymorphic structure occurs at high pressure. Where sufficient thermodynamic data were available and where compressibilities and heat capacities could be estimated, values of ΔH_0° for the atomization of the phase at 1 atm pressure were evaluated.(3) For a number of elements or for some of their polymorphic forms, no experimental data are available. Where it was possible to apply theoretical methods of predicting the thermodynamic properties of polymorphic forms, these values have been given in parentheses with appropriate uncertainties indicated. The models described by Brewer (4,5,6,7,8) were used to predict thermodynamic data for phases for which no experimental data exist.

The first column of Table I lists the elements in alphabetical order with the crystal structure indicated if data are given for polymorphs. Where there are polymorphs, those stable at 1 atm are listed first in order of descending temperature stability. Following the form stable at 0 K are listed the metastable polymorphs.

All values in Table I are given for 0 K at which the difference between ΔH° and ΔE° is negligible. The second column lists the energies of atomization to the ground electronic state of the gaseous atom given in kcal per gram-atom. In those few instances where the ground electronic state is also the valence state, the electronic configuration is indicated. The third column lists energies of atomization to the gaseous valence state which is the gaseous atom with the same electronic configuration

as in the condensed phase of indicated structure. The values in column two are converted to those in column three by addition of the promotion energy to convert the gaseous atom from the ground electronic state to the lowest level of the electronic configuration corresponding to that of the condensed phase. The lowest level is used, rather than the center of gravity of the configuration, because the lowest level is often the least-perturbed and most easily characterized level and because the difference between bonding energies based on the lowest level and those based on the center of gravity vary in a smooth way across the periodic table. Experimental data are often lacking for the levels of a configuration needed to obtain the center of gravity; whereas values for the lowest level for virtually all of the most important configurations involving any number of f or d electrons either with one s electron or with one s plus one p electron are available. (8,9) Values in the third column which are calculated from a theoretical model or which are derived from column two through use of promotion energies of considerable uncertainty are given in parentheses.

The fourth column of Table I lists average bonding energies per electron obtained by dividing the cohesive energies of column three by the number of bonding electrons. In a few instances, where significant bonding is attributed to 5f electrons, their contribution has been subtracted from the cohesive energies of column three and the resulting value divided by the number of non-f bonding electrons. In those instances, the bonding contribution per f electron is also indicated.

Acknowledgments:

I wish to thank Robert H. Lamoreaux and John Ling-Fai Wang for their help in checking some of the recent literature. This work is supported by the Energy Research and Development Administration.

Table I

Cohesive Energies of the Elements

	Atomization Energy to Gaseous Ground State at 0 K. <u>kcal/gram-atom</u>	Atomization Energy to Gaseous Valence State at 0 K. <u>kcal/gram-atom</u>	Valence State Bonding Energy per Bonding Electron. <u>kcal</u>
Ac	98.±3	(143.) (d ^{0.5} sp ^{1.5})	(48.)
Ag (ccp)	68.0±0.2	(201.) (d ^{8.5} sp ^{1.5})	(50.)
Ag (bcc)	(56.)±6. (d ¹⁰ s)		(56.)
Al	78.1±1.	161.1 (sp ²)	53.5
Am (ccp)	(62.9)±2.		
Am (dhcp)	63.±2.	(149.) (f ⁶ dsp)	(47.)+(1.5) per f
Ar	1.848±0.002		
As	68.2±0.6 (s ² p ³)		22.7
At	(22.2)±5. (s ² p ⁵)		(22.)
Au (ccp)	87.96±0.3	(228.) (d ^{8.5} sp ^{1.5})	(57.)
Au (bcc)	(59.)±6. (d ¹⁰ s)		(59.)
B (β)	134±1	>216. (sp ²)	>72
Ba (bcc)	43.7±2.	74.2 (d ^{0.5} sp ^{0.5})	37.
Ba (hcp)	42.6±2.	77.7 (sp)	39.
Be (bcc)	76.0±1.5		
Be (hcp)	76.5±1.5	>139 (sp)	>70.
Bi	50.2±0.5 (s ² p ³)		17.
Bk (ccp)	(68.9)±4.		
Bk (dhcp)	(69)±4.	(135) (f ⁸ dsp)	(45.)
Br	28.183±0.018 (s ² p ⁵)		28.2
C (gr)	169.98±0.15 -0.92	266.5 (sp ³)	66.6
C (dia)	169.40±0.15 -0.92	265.9 (sp ³)	66.5
Ca (bcc)	42.4±0.4	93.1 (d ^{0.5} sp ^{0.5})	46.5
Ca (ccp)	42.5±0.4		
Ca (hcp)	(42.)±2.	(85.) (sp)	(42.5)
Cd	26.73±0.15	112.8 (sp)	56.4
Ce (bcc)	98.8±0.5	121.4 (fd ^{1.5} sp ^{0.5})	40.4
Ce (γccp)	99.3±0.5	(144.) (fd ^{0.5} sp ^{1.5})	(48.)
Ce (dhcp)	99.3±0.5	137.6 (fdsp)	45.9
Ce (αccp)	99.7±0.5	(145.) (fd ^{0.5} sp ^{1.5})	(48.)

Table I contd.

	Atomization Energy to Gaseous Ground State at 0 K. <u>kcal/gram-atom</u>	Atomization Energy to Gaseous Valence State at 0 K. <u>kcal/gram-atom</u>	Valence State Bonding Energy per Bonding Electron. <u>kcal</u>
Cf (ccp)	(41.9)±5.		
Cf (dhcp)	(42.)±5.	(136.) (f ⁹ dsp)	(45.)
Cl	32.195±0.033 (s ² p ⁵)		32.2
Cm (ccp)	(92)±1		
Cm (dhcp)	92.1±1	136. (f ⁷ dsp)	45.
Co (ccp)	101.2±0.5	(194.) (d ^{6.5} sp ^{1.5})	(32.)
Co (hcp)	101.3±0.6	157.3 (d ^{7.2} sp ^{0.8})	34.2
Co (bcc)	(99.5)±3.	(139.5) (d ^{7.5} sp ^{0.5})	(35.)
Cr (bcc)	94.5±1.	130.2 (d ^{4.5} sp ^{0.5})	21.7
Cr (hcp)	(83.)±5.	(154.) (d ⁴ sp)	(26.)
Cs (bcc)	18.54±0.05 (s)		18.5
Cs (ccp)	18.16±0.06		18.2
Cu (ccp)	80.4±0.3	(196.) (d ^{8.5} sp ^{1.5})	(49.)
Cu (bcc)	(60.5)±6. (d ¹⁰ s)		(61.)
Dy (bcc)	69.5±0.5	(127.) (f ⁹ d ^{1.5} sp ^{0.5})	(42.)
Dy (hcp)	70.2±0.1	136. (f ⁹ dsp)	45.3
Er (bcc)	(75.0)±0.5	(136.) (f ¹¹ d ^{1.5} sp ^{0.5})	(45.)
Er (hcp)	75.8±0.1	141.5 (f ¹¹ dsp)	47.2
Es (hcp)	(36.)±5.	(139.) (f ¹⁰ dsp)	(46.)
Eu	42.8±0.2	81.4 (f ⁷ d ^{0.5} sp ^{0.5})	40.6
F	19.37±0.1 (s ² p ⁵)		19.4
Fe (bcc)	98.7±0.3	136.3 (d ^{6.5} sp ^{0.5})	27.3
Fe (ccp)	97.2±0.5	(171.) (d ^{5.5} sp ^{1.5})	(24.)
Fe (hcp)	97.8±0.7	153.1 (d ⁶ sp)	25.5
Fm (hcp)	(34.)±5.	(141.) (f ¹¹ dsp)	(47.)
Fr	(18.)±2. (s)		(18.)
Ga	64.8±0.5	173.4 (sp ²)	57.8
Gd (bcc)	94.8±0.6	124.0 (f ⁷ d ^{1.5} sp ^{0.5})	41.3
Gd (hcp)	95.5±0.5	135.6 (f ⁷ dsp)	45.2
Ge	88.8±0.5	(210.) (sp ³)	(53.)

Table I contd.

	Atomization Energy to Gaseous Ground State at 0 K. <u>kcal/gram-atom</u>	Atomization Energy to Gaseous Valence State at 0 K. <u>kcal/gram-atom</u>	Valence State Bonding Energy per Bonding Electron. <u>kcal</u>
H(para)	51.724±0.002 (s)		(51.7)
He (liq.)	0.014		
Hf (bcc)	(147.)±1.	187. (d ^{2.5} sp ^{0.5})	46.8
Hf (hcp)	148.4±1.	188.5 (d ^{2.3} sp ^{0.7})	47.1
Hg (rhomb)	15.428±0.015	123.0 (sp)	61.5
Hg (tetrag)	15.46±0.02		
Ho (bcc)	71.7±0.5	(132.) (f ¹⁰ d ^{1.5} sp ^{0.5})	(44.)
Ho (hcp)	72.3±0.25	(139.8) (f ¹⁰ dsp)	(46.6)
I	25.612±0.010 (s ² p ⁵)		25.6
In	58.1±0.25	158.1 (sp ²)	52.7
Ir (ccp)	160.1±1.5	(279.) (d ^{6.5} sp ^{1.5})	(46.)
Ir (hcp)	(159.)±4.	(235.) (d ⁷ sp)	(47.)
Ir (bcc)	(156.)±4.	(198.) (d ^{7.5} sp ^{0.5})	(49.5)
K	21.54±0.05 (s)		21.5
Kr	2.676±0.003		
La (bcc)	102.4±1.	125.2 (d ^{1.5} sp ^{0.5})	41.7
La (ccp)	103.0±1.	(144) (d ^{0.5} sp ^{1.5})	(48.)
La (dhcp)	103.1±1.	141.0 (dsp)	47.0
Li (bcc)	37.71±0.2 (s)		37.7
Li (hcp)	37.72±0.2		
Lu (hcp)	102.2±0.2	152.0 (f ¹⁴ dsp)	50.7
Lu (bcc)	(98.)±2.	(151.) (f ¹⁴ d ^{1.5} sp ^{0.5})	(51.)
Lr (hcp)	(73.)±10.	(152.) (f ¹⁴ dsp)	(51.)
Md (hcp)	(27.)±5.	(84.) (f ¹³ sp)—	(42.)
Mg	34.7±0.3	97.2 (sp)	48.6
Mn (bcc)	66.4±1.	117.1 (d ^{5.5} sp ^{0.5})	19.5
Mn (ccp)	67.2±1.	(176.) (d ^{4.5} sp ^{1.5})	(25.)
Mn (β)	66.9±1.	118.7 (d ^{5.2} sp ^{0.8})	18.0
Mn (α)	67.4±1.	118.5 (d ^{5.4} sp ^{0.6})	19.1
Mn (hcp)	(66.)±2	(119.) (d ⁵ sp)	(17.)
Mo (bcc)	157.2±0.5 (d ⁵ s)		26.2
Mo (hcp)	(145.)±5.	(201.) (d ^{4.3} sp ^{0.7})	(34.)

Table I contd.

	Atomization Energy to Gaseous Ground State at 0 K. <u>kcal/gram-atom.</u>	Atomization Energy to Gaseous Valence State at 0 K. <u>kcal/gram-atom</u>	Valence State Bonding Energy per Bonding Electron. <u>kcal</u>
N	113.355±0.01 (s ² p ³)		37.8
Na (bcc)	25.66±0.1 (s)		25.7
Na (hcp)	25.67±0.1		
Nb (bcc)	174.5±4. (d ⁴ s)		34.9
Nb (hcp)	(164.)±5.	(198.) (d ^{3.3} sp ^{0.7})	(40.)
Nd (bcc)	78.0±0.6	119.6 (f ³ d ^{1.5} sp ^{0.5})	39.9
Nd (dhcp)	78.5±0.5	136.5 (f ³ dsp)	45.5
Ne	0.462±0.002		
Ni (ccp)	102.4±0.5	(199.) (d ^{7.5} sp ^{1.5})	(40.)
Ni (bcc)	(96.)±4.	(133.5) (d ^{8.5} sp ^{0.5})	(44.)
Ni (hcp)	(96.)±4.	(148.) (d ^{8.3} sp ^{0.7})	(43.5)
No (hcp)	(26.)±5.	(86.) (f ¹⁴ sp)	(43.)
Np (bcc)	108.±2.	176. (f ³ d ³ s)	(40.)+(5.5) per f
Np (α)	109.±2.		
O	60.03±0.02 (s ² p ⁴)		30.0
Os (hcp)	188.4±0.9	255.5 (d ⁶ sp)	42.6
Os (bcc)	(183.)±5.	(213.) (d ^{6.5} sp ^{0.5})	(45.)
P (red)	79.16±0.25 (s ² p ³)		26.4
P (white)	75.42±0.25 (s ² p ³)		25.1
Pa (bcc)	(145.)±8	(165.) (fd ³ s)	(39.5)+(7) per f
Pa (α)	(146.)±8		
Pb	46.78±0.3 (s ² p ²)		23.4
Pd (ccp)	89.8±0.5	(230.) (d ^{7.5} sp ^{1.5})	(46.)
Pd (bcc)	(82.)±5	(101.) (d ⁹ s)	(51.)
Pm (bcc)	(73.6)±3	(118.8) (f ⁴ d ^{1.5} sp ^{0.5})	(40.)
Pm (dhcp)	(74.2)±3	(136.) (f ⁴ dsp)	(45.)
Po	34.5±2 (s ² p ⁴)		17.3
Pr (bcc)	84.7±0.6	(121.) (f ² d ^{1.5} sp ^{0.5})	(40.)
Pr (dhcp)	85.3±0.5	(137.) (f ² dsp)	(46.)
Pt (ccp)	134.7±0.3	(256.) (d ^{7.5} sp ^{1.5})	(51.)
Pt (hcp)	(127.)±5	(213.) (d ⁸ sp)	(53.)
Pt (bcc)	(124.)±5	(167.) (d ^{8.5} sp ^{0.5})	(56.)

Table I contd.

	Atomization Energy to Gaseous Ground State at 0 K. <u>kcal/gram-atom</u>	Atomization Energy to Gaseous Valence State at 0 K. <u>kcal/gram-atom</u>	Valence State Bonding Energy per Bonding Electron. <u>kcal</u>
Pu (bcc)	81.5±0.5	132.6 (f ⁵ d ^{1.5} sp ^{0.5})	41.+(2.) per f
Pu (ccp)	81.9±0.5	(147) (f ⁵ d ^{0.5} sp ^{1.5})	(46.)+(2.) per f
Pu (γ)	82.1±0.5		
Pu (β)	82.2±0.5		
Pu (α)	83.0±0.5		
Ra	38.2±2	76.5 (d ^{0.5} sp ^{0.5})	38.3
Rb	19.64±0.05 (s)		19.6
Re (hcp)	185.2±1.5	239.4 (d ⁵ sp)	34.2
Re (bcc)	(183.)±4	(227) (d ^{5.5} sp ^{0.5})	(38.)
Rh (ccp)	132.5±1.	(244) (d ^{6.5} sp ^{1.5})	(41.)
Rh (bcc)	(128.)±3. (d ⁸ s)		(43.)
Rn	4.66±0.02		
Ru (hcp)	155.4±1	205. (d ^{6.3} sp ^{0.7})	38.
Ru (bcc)	(153)±2. (d ⁷ s)		(38)
S (monocl.)	65.72±0.03 (s ² p ⁴)		32.9
S (orthorh.)	65.75±0.02 (s ² p ⁴)		32.9
Sb	63.4±1.0 (s ² p ³)		21.1
Sc (bcc)	89.2±1	128.1 (d ^{1.5} sp ^{0.5})	42.7
Sc (hcp)	89.9±1	134.7 (dsp)	44.9
Se	51.8±2 (s ² p ⁴)		25.9
Si	106.7±2	202.0 (sp ³)	50.5
Sm (bcc)	48.7±0.6	(118) (f ⁵ d ^{1.5} sp ^{0.5})	(39.)
Sm (α)	49.3±0.5		
Sm (hcp)	(49.)±1	(133.) (f ⁵ dsp)	(44.)
Sn (β)	72.0±0.5 (s ² p ²)		36.0
Sn (α)	72.4±0.5	185.7 (sp ³)	46.4
Sr (bcc)	39.5±1	85.9 (d ^{0.5} sp ^{0.5})	43.0
Sr (ccp)	39.7±1		
Sr (hcp)	(39.)±2	(80.) (sp)	(40.)
Ta (bcc)	186.8±0.5	225.6 (d ^{3.5} sp ^{0.5})	45.1
Ta (hcp)	(169.)±10	(218) (d ³ sp)	(44.)

Table I contd.

	Atomization Energy to Gaseous Ground State at 0 K. kcal/gram-atom	Atomization Energy to Gaseous Valence State at 0 K. kcal/gram-atom	Valence State Bonding Energy per Bonding Electron. kcal
Tb (bcc)	92.5±0.6	(126.) (f ⁸ d ^{1.5} sp ^{0.5})	(42.)
Tb (hcp)	93.4±0.5	(136.) (f ⁸ dsp)	(45.)
Tc (hcp)	158.±4.	193. (d ^{5.3} sp ^{0.7})	(30.)
Tc (bcc)	(152.)±6.	(179.) (d ^{5.5} sp ^{0.5})	(30.)
Te	51.4±0.2 (s ² p ⁴)		25.7
Th (bcc)	142.6±1.	158.5 (d ³ s)	39.6
Th (ccp)	142.9±1.		
Ti (bcc)	110.5±0.7	142.6 (d ^{2.5} sp ^{0.5})	35.7
Ti (hcp)	111.8±0.5	157.2 (d ² sp)	39.3
Tl	43.4±0.3 (s ² p)		43.4
Tm (bcc)	(55.0)±1.	(136.) (f ¹² d ^{1.5} sp ^{0.5})	(45.)
Tm (hcp)	55.8±1.	139.6 (f ¹² dsp)	46.4
U (bcc)	126.±2	{(170.) (f ² d ³ s) (189.) (fd ⁴ s)}	{(39.5)+6 per f (37.)+6 per f
U (β)	127.±2	188. (f ² d ^{2.4} sp ^{0.6})	(44)+6 per f
U (α)	128.±2		
V (bcc)	122.4±2	148.8 (d ^{3.5} sp ^{0.5})	29.8
V (hcp)	(117.)±3	(164) (d ³ sp)	(33.)
W (bcc)	205.2±1	237.1 (d ^{4.5} sp ^{0.5})	39.5
W (hcp)	(183.)±10	(238.) (d ⁴ sp)	(40.)
Xe	3.798±0.003		
Y (bcc)	99.7±0.8	136.7 (d ^{1.5} sp ^{0.5})	45.6
Y (hcp)	100.8±0.7	143.5 (dsp)	47.8
Yb (bcc)	36.7±0.4	96.4 (f ¹⁴ d ^{0.5} sp ^{0.5})	48.2
Yb (ccp)	37.0±0.3		
Yb (hcp)	37.1±0.8	86.5 (f ¹⁴ sp)	43.2
Zn	31.04±0.05	123.4 (sp)	61.7
Zr (bcc)	143.3±1	165.7 (d ^{2.7} sp ^{0.3})	41.4
Zr (hcp)	144.2±1	178.0 (d ^{2.3} sp ^{0.7})	44.5

APPENDIX

This appendix indicates the source of information used to supplement the tabulations of Hultgren et al.(1). The fifteen elements Ag, Al, B, Br, C, Cl, Cu, F, H, I, N, O, S, Si, and Zn have recently been reviewed by the CODATA committee (10). Except for B, S and Si where the CODATA values were rejected, the Hultgren values were modified where necessary to be consistent with the CODATA values. A small correction was made to the CODATA value for I.

- Ac - Tabulated vapor pressures(1) were combined with estimated entropy and heat capacity values.
- Ag - The recent additional references listed by Hultgren(1) plus the IUPAC summary(11) of interlaboratory measurements were reviewed. Temperature scale corrections were made and a value consistent with the CODATA value (10) was accepted. The bcc value was calculated(5).
- Am - Data given at 1000 K(1) were taken to lower temperatures using estimated entropies and heat capacities.
- As - Values tabulated are based on a revision of Hultgren's tabulation by Professor Gerd Rosenblatt(12) which incorporates recent publications(13-19).
- At - Estimated values from Stull and Sinke(20) were used.
- Au - The additional references listed by Hultgren(1) plus the IUPAC summary(11) of interlaboratory measurements were reviewed. No change was made in Hultgren's value. The value for the bcc phase was calculated(5).
- B - Storms and Mueller (62) and Mar and Bedford (63) have reviewed previous measurements and have presented new data.
- Ba - Recent vapor pressure measurements(21,22) did not change Hultgren's value. High pressure data were used for the hcp phase(3).
- Be - Low temperature heat capacities were estimated for the bcc phase.
- Bi - A review of recent vapor pressure measurements listed by Hultgren(1) and the values cited by Sullivan et al.(23) did not change Hultgren's value.
- Bk - The values were calculated(7,8).

APPENDIX contd.

- Ca - A review of recent references listed by Hultgren and the measurements of DeMaria and Piacente(24) and Petrov and Shmykov(25) did not modify Hultgren's values. Low temperature heat capacities were estimated for the bcc phase. The hcp value was calculated(5).
- Ce - Hultgren's values were corrected on the basis of the recent measurements of Ackermann et al.(26). The bcc data were extrapolated to low temperatures.
- Cf - The values were calculated(7,8).
- Cm - The recent determination of Ward, Ohse, and Paul (61) was considered more accurate than that of Smith, Hale, and Thompson (27).
- Co - The additional vapor pressure measurements listed by Hultgren and more recent papers(28-30) were incorporated. The bcc value was calculated(5).
- Cr - The hcp value was calculated(5).
- Cs - A review of the recent vapor pressure data listed by Hultgren did not change the value. The ccp value was obtained from high pressure data(3).
- Cu - The value was corrected to be consistent with the CODATA value (10). The bcc value was calculated(5).
- Dy - The recent results of McCormack et al.(31) were incorporated. The bcc data were extrapolated to low temperatures.
- Er - The values were obtained in the same manner as for Dy.
- Es - The value was calculated(7,8).
- Eu - Hultgren's values were corrected to be consistent with the entropy and low temperature heat capacity determined by Gerstein et al.(32).
- Fe - The low temperature heat capacities were estimated for ccp Fe. The hcp value came from high pressure data(3). Recent vapor pressure data listed by Hultgren were reviewed.
- Fm - The value was calculated(7,8).
- Fr - The value was estimated.
- Gd - The recent results of Hoenig et al.(33) were incorporated. The heat capacity was estimated for bcc at low temperatures.

APPENDIX contd.

- Hf - The value given by Ackermann and Rauh(34) was accepted. Low temperature heat capacities for bcc were estimated.
- Hg - The value for the tetragonal phase was obtained from high pressure data(3).
- Ho - Low temperature heat capacities for the bcc phase were estimated.
- I - Value was corrected to agree with Barrow and Yee (35).
- Ir - After correcting the data reviewed by Hultgren to the 1968 temperature scale, a different weighting of the data was used to obtain a total change of 0.3 kcal. The bcc and hcp values were calculated(5).
- Kr - The value obtained by Lee et al.(36) was accepted.
- La - Low temperature heat capacities were estimated for bcc and ccp La.
- Li - Recent vapor pressure measurements listed by Hultgren did not change value.
- Lu - The value for metastable bcc Lu was calculated(8).
- Lr - The value was calculated(7,8).
- Md - The value was calculated(7,8).
- Mg - Recent vapor pressure publications listed by Hultgren did not change value.
- Mn - Hultgren's value was not changed by review of recent vapor pressure measurements. The low temperature heat capacities were estimated for the bcc phase. The hcp value was calculated(5).
- Mo - The temperature scale correction and reevaluation of the data yielded a change of 0.3 kcal.
- Nb - The JANAF value(37) was accepted. The hcp value was calculated(5).
- Nd - The low temperature heat capacities for the bcc phase were estimated.
- Ne - The value given McConville(38) was accepted.
- Ni - The recent vapor pressure data listed by Hultgren and those of Vrestal and Kucera(39) and Rutner and Haury(40) did not change Hultgren's value by an amount greater than the temperature scale correction. The values for bcc and hcp Ni were calculated(5).
- No - The value was calculated (7,8).

APPENDIX contd.

- Np - A calculated value (7,8) for α -Np of 109 ± 3 kcal/gram-atom indicated results of Eick and Muford (41) were due to NpO vapor. Recent measurements (60) confirm the calculations.
- Os - The bcc value was calculated(5).
- Pa - The values were calculated(7,8).
- Pb - The recent vapor pressure publications listed by Hultgren did not change value.
- Pd - The bcc value was calculated(5).
- Pm - The values were calculated(8).
- Po - The value given by Stull and Sinke(20) was used.
- Pr - The low temperature heat capacities were estimated for bcc Pr.
- Pt - The value given by Plante et al.(42) was accepted. The values for bcc and hcp Pt were calculated(5).
- Pu - The value given by Kent(43) was accepted. Low temperature heat capacities were estimated for the four high temperature phases.
- Ra - The value is given by the National Bureau of Standards(44).
- Rb - Recent measurements(21,45,46) agree with Hultgren within their experimental uncertainty.
- Re - The bcc value was calculated(5).
- Rh - The results of Piacente et al.(47) were incorporated. The bcc value was calculated(5).
- Ru - The bcc value was calculated(5).
- S - The CODATA value(10) was rejected as Hultgren's evaluation was more up-to-date.
- Sb - Values tabulated are based on a revision of Hultgren's tabulation by Professor Gerd Rosenblatt(12) incorporating Hultgren's list of additional references plus later publications(23,48,49).
- Sc - The low temperature heat capacities were estimated for bcc Sc.
- Se - Hultgren's value was retained but the possibility of a value 4 kcal larger has not been resolved(50).

APPENDIX contd.

- Si - The JANAF value(37) was accepted as being more up-to-date than either the Hultgren(1) or CODATA(10) values.
- Sm - The recent data of Desideri et al.(51) are in good agreement with Hultgren(1). Low temperature heat capacities were estimated for the bcc phase. The hcp value was calculated(7).
- Sr - The results of DeMaria and Piacente(24) were incorporated. The low temperature heat capacity of the bcc phase was estimated. The hcp value was calculated(5).
- Ta - The JANAF value(37) was accepted. The hcp value was calculated(5).
- Tb - The low temperature heat capacities of bcc Tb were estimated.
- Tc - The value of Krikorian et al.(52) was accepted. The bcc value was calculated.
- Te - A review of additional references listed by Hultgren plus more recent publications(53-4) yielded $\Delta H_0^\circ = 20,285 \pm 50$ cal/gram-atom for $\frac{1}{2}\text{Te}_2(\text{g})$. Barrow(55) reviewed recent measurements of $D_0^\circ(\text{Te}_2)$ and selected 62.3 ± 0.2 kcal/mol(50).
- Th - The value of Ackermann and Rauh(34) was accepted. The low temperature heat capacities of the bcc phase were estimated.
- Ti - Hultgren's value were converted to the 1968 Temperature with incorporation of the additional references plus the data presented by Wu and Wahlbeck(56). The low temperature heat capacities of the bcc phase were estimated.
- Tl - Recent measurements(21) were within the uncertainty of Hultgren's value.
- U - The data of Oetting and Leitnaker(57) were incorporated. The low temperature heat capacities of the high temperature forms were estimated.
- V - The JANAF value(37) was accepted. The hcp value was calculated(5).
- W - The value of Plante and Sessions(58) was accepted. The hcp value was calculated(5).
- Y - The data of Ackermann et al.(59) were incorporated. The low temperature heat capacities of the bcc phase were estimated.
- Yb - The data in references listed by Hultgren and by Desideri et al.(51) were evaluated to obtain value 0.5 kcal higher than Hultgren.
- Zr - The value of Ackermann and Rauh(34) was accepted. The low temperature heat capacities of the bcc phase were estimated.

-REFERENCES-

- (1) Unless otherwise indicated, all values of Table I came from the references or the tabulated data listed by R. Hultgren, P. D. Desai, D. T. Hawkins, M. Gleiser, K. K. Kelley, and D. D. Wagman, "Selected Values of the Thermodynamic Properties of the Elements", 1973, American Society for Metals, Metals Park, Ohio.
- (2) F. D. Rossini, *J. Chem. Thermodyn.* 2, 447-459 (1970).
- (3) R. H. Lamoreaux, "Enthalpies of Transition at 0 K for Several Metallic Solid Phase Transitions." LBL Report 3711 (1975).
- (4) L. Brewer, *High-Strength Materials*, V. F. Zackay, ed., Chap. 2, pp. 12-103, John Wiley and Sons, N. Y., 1965.
- (5) L. Brewer: *Phase Stability in Metals and Alloys*, P. Rudman, J. Stringer, R. I. Jaffee, eds., pp. 39-61, 241-49, 344-46, and 560-68, McGraw-Hill, N. Y., 1967.
- (6) L. Brewer: *Plutonium 1970 and other Actinides*, W. N. Miner, ed., pp. 650-58 TMS Nucl. Met. Ser. Vol. 17, Metallurgical Soc. AIME, N. Y., 1970.
- (7) L. Brewer, *Spectra of the Actinides and their Metallurgical Properties*, Abstract 4A1, Third International Trans-Plutonium Element Symposium, Argonne, Ill., Oct. 21, 1971.
- (8) L. Brewer: *J. Opt. Soc. Amer.*, 61, pp. 1101-11, and 1666-82 (1971).
- (9) C. E. Moore: *Atomic Energy Levels*, Nat. Bur. Stand. U. S. Circ. 467, U. S. Govt. Printing Office, Wash., D.C., Vols. 1-3, 1949, 1952, 1958.
- (10) Set of Key Values for Thermodynamics, Parts I, II, and III, CODATA Bulletins 5 and 6 (Dec. 1971), Bulletin 7 (Aug. 1972), and Bulletin 10 (Dec. 1973) and Part IV (Jan. 1974).
- (11) IUPAC Comm. in High Temperatures and Refractory Materials, *Pure Appl. Chem.* 31, 371, 395 (1972).
- (12) G. Rosenblatt, Penn. State Univ., private communication, 1-14-75.
- (13) J. J. Murray, C. Pupp, and R. F. Pottie, *J. Chem. Phys.* 58, 2569-78 (1973); 59, 4572 (1973).
- (14) S. L. Bennett, J. L. Margrave, J. L. Franklin, and J. E. Hudson, *J. Chem. Phys.* 59, 5814-19 (1973).
- (15) S. L. Bennett, unpublished reevaluation of Hudson's electron impact results (1974).
- (16) A. M. Mamedov, S. M. Gadzhiev, and A. A. Kuliev, *Chem. Absts.* 78, 43964 (1973).

Ref. contd.

- (17) P. Perdigon and J. D. Incan, *Can. J. Phys.* 48, 1140 (1970).
- (18) J. Kordis and K. A. Gingerich, *J. Chem. Eng. Data* 18, 135-6 (1973).
- (19) H. Rau, *J. Chem. Thermodyn.* 7, 27-32 (1975).
- (20) D. R. Stull and G. C. Sinke, *Advances in Chem. Ser.*, No. 18 (1956).
- (21) H. E. J. Schins, R. W. M. van Wijk and B. Dorpema, *Z. Metalk* 62, 330-6 (1971).
- (22) M. P. Parshina and P. V. Kovtunencko, *Zh. Fiz. Khim.* 48(2), 483 (1974).
- (23) C. L. Sullivan, J. E. Prusaczyk, and K. D. Carlson, *High. Temp. Science* 4, 1212-21 (1972).
- (24) G. DeMaria and V. Piacente, *J. Chem. Thermodyn.* 6, 1-7 (1974).
- (25) V. S. Petrov and A. A. Shmykov, *Izv. Vyssh. Ucheb. Zaved., Tevet. Met.* 15(6), 74-8 (1972).
- (26) R. J. Ackermann, M. Kojima, E. G. Rauh, and R. R. Walters, *J. Chem. Thermodyn.* 1, 527-33 (1969).
- (27) P. K. Smith, W. H. Hale, M. C. Thompson, *J. Chem. Phys.* 50, 5066-76 (1969).
- (28) R. K. Saxer, Ph.D Thesis, Ohio State Univ., 1962.
- (29) F. M. Wachi and D. E. Gilmartin, *J. Chem. Phys.*, 57, 4713-6 (1972).
- (30) G. M. Fedichkin and A. A. Shmykov, *Izv. Vyssh. Ucheb. Zaved., Tsvet. Met.* 16, 73-5 (1973).
- (31) J. M. McCormack, P. R. Platt, and R. K. Saxer, *J. Chem. Eng. Data* 16, 167-70 (1971).
- (32) B. C. Gerstein, F. J. Jelinek, J. R. Mullaly, W. D. Shickell, and F. H. Spedding, *J. Chem. Phys.* 47, 5194 (1967).
- (33) C. L. Hoenig, N. D. Stout, and P. C. Nordine, *J. Am. Ceram. Soc.* 50, 385-92 (1967).
- (34) R. J. Ackermann and E. G. Rauh, *J. Chem. Thermodyn.* 4 521-32 (1972).
- (35) R. F. Barrow and K. K. Yee, *J. C. S. Faraday II* 69(5), 684-700 (1973).
- (36) M. W. Lee, D. M. Eshelman, and J. Bigeleisen, *J. Chem. Phys.* 56, 4585-92 (1972).

Ref. contd.

- (37) M. W. Chase, JANAF Thermochemical Tables, Dow Chemical Co., Midland, Michigan: Nb-Dec. 31, 1973; Si-Mar. 31, 1967; Ta-Dec. 31, 1972, V-June 30, 1973.
- (38) G. T. McConville, J. Chem. Phys. 60, 4093 (1974).
- (39) J. Vrestal and J. Kucera, Jad. Energ. 17 (5), 158-60 (1971).
- (40) E. Rutner and G. L. Haury, Chem. Absts. 79, 129287 (1973).
- (41) H. A. Eick and R. N. R. Mulford, J. Chem. Phys. 41, 1475-8 (1964).
- (42) E. R. Plante, A. B. Sessoms, and K. R. Fitch, J. Res. Natl. Bur. Stds. 74A, 647-53 (1970).
- (43) R. A. Kent, High Temp. Sci. 1, 169-75 (1969).
- (44) V. B. Parker, D. D. Wagman, and W. H. Evans, NBS Tech. Note 270-6 (1971).
- (45) L. I. Cherneeva, and V. N. Proskurin, Teplofiz. Vys. Temp. 10(4), 765-70 (1972).
- (46) V. Piacente, G. Bardi, and L. Malaspina, J. Chem. Thermodyn. 5, 219-226 (1973).
- (47) V. Piacente, G. Balducci, and G. Bardi, J. Less Common Metals 37, 123-7 (1974).
- (48) H. Gutbier, Z. Naturforschung 169, 268 (1961).
- (49) J. Kordis and K. A. Gingerich, J. Chem. Phys. 58, 5141-9 (1973).
- (50) J. Berkowitz and W. A. Chupka, J. Chem. Phys. 50, 4245-50 (1969).
- (51) A. Desideri, V. Piacente, and S. Nobili, J. Chem. Eng. Data 18, 140-1 (1973).
- (52) O. H. Krikorian, J. H. Carpenter, and R. S. Newbury, High Temp. Sci. 1, 313-30 (1969).
- (53) L. Malaspina, R. Gigli, and G. Bardi, Rev. Inst. Hautes Temp. Refract. 9(1), 131-8 (1972).
- (54) Yu. S. Chernogubov, B. P. Kuznetsov, A. A. Klimenko, and E. V. Podmogil'nyi, Zhur. Fiz. Khim. 46, 275 (1972).
- (55) R. F. Barrow, Spectroscopic Data Relative to Diatomic Molecules, International Tables of Selected Constants 17, Ed. B. Rosen, Pergamon Press, Oxford, 1970.

Ref. contd.

- (56) H. Y. Wu and P. G. Wahlbeck, High Temp. Sci. 3, 469-77 (1971).
- (57) F. L. Oetting and J. M. Leitnaker, J. Chem. Thermodyn. 4, 199-211 (1972).
- (58) E. R. Plante and A. B. Sessions, J. Res. Nat. Bur. Stand., Sect. A 77(2), 237-42 (1973).
- (59) R. J. Ackermann, E. G. Rauh, and R. R. Walters, J. Chem. Thermodyn. 2, 139-149 (1970).
- (60) R. J. Ackermann and E. G. Rauh, J. Chem. Thermodyn. 7, 211-8 (1975).
- (61) J. W. Ward, R. W. Ohse and R. Reul, J. Chem. Phys. 62, 2366-72 (1975).
- (62) E. Storms and B. Mueller, J. Phys. Chem. 81, 318-24 (1977).
- (63) R. W. Mar and R. G. Bedford, High Temp. Sci. 8, 365-76 (1976).

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