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SGTE DATA FOR PURE ELEMENTS

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ABSTRACT

Thermodynamic data for the condensed phases of 78 elements as currently used by SGTE (Scientific Group Thermodata Europe) are tabulated. SGTE is a consortium of seven organisations in Western Europe engaged in the compilation of a comprehensive, self consistent and authoritative thermochemical database for inorganic and metallurgical systems. The data are being published here in the hope that they will become widely adopted within the international community as a sound basis for the critical assessment of thermodynamic data, thereby, perhaps, limiting unnecessary duplication of effort.

The data for each phase of each element considered are presented as expressions showing, as a function of temperature, the variation of (a) $G-H_{SER}$, the Gibbs energy relative to the enthalpy of the "Standard Element Reference" ie the reference phase for the element at 298.15 K and (b) the difference in Gibbs energy between each phase and this reference phase (ie lattice stability). The variation of the heat capacity of the various phases and the Gibbs energy difference between phases are also shown graphically. For certain elements the thermodynamic data have been assessed as a function of pressure as well as temperature. Where appropriate a temperature - pressure phase diagram is also shown.

Throughout this paper the thermodynamic data are expressed in terms of J mol^{-1}. The temperatures of transition between phases have been assessed to be consistent with the 1990 International Temperature Scale (ITS90).

INTRODUCTION

In this paper the thermodynamic data for the pure elements used by SGTE (Scientific Group Thermodata Europe) are tabulated. SGTE is a consortium of seven organisations in Western Europe (LTPCM Grenoble, Association THERMODATA, IRSID, RWTH Aachen, KTH Stockholm, NPL and Harwell) engaged in the compilation of a comprehensive, self consistent and authoritative thermochemical database for inorganic and metallurgical systems (86DIN, 87ANS/SUN). The main purpose of the database lies in its use in the calculation of phase equilibria in multicomponent systems which puts a premium on the interconsistency of the data and thereby on their traceability to the data for the elements. The SGTE element data were first published in September 1989 (89DIN) but since then have undergone a series of revisions and enhancements, the most recent being the conversion of the database as presented here to conform to the 1990 International Temperature Scale (90PRE, 91RUS/HUD). Over the last few years these element data have formed the basis of a number of assessments of binary, ternary and higher order systems which have appeared in the open literature. The purpose behind publishing the data is to encourage other groups outside SGTE but sharing its aims of generating interconsistent data to use the same basic data for the elements as used by SGTE. The benefits of this will be very great. In the past it has been necessary to reassess the thermodynamic data for binary systems to be used in the calculation of multicomponent phase diagrams even where good assessments already existed if different data had been used for the pure components. The

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worldwide use of a single set of element or "unary" data removes this necessity.

Stable and Metastable Phase Data

For a given element data are required for each phase in which it can form or dissolve in either in a stable or a metastable state. The data for the stable phases are, on the whole, well defined although serious anomalies still exist requiring further experimental study. Much more of a problem is encountered when one extrapolates the thermodynamic data from a region of temperature in which a given phase is stable to one in which it is metastable. The traditional CALPHAD approach (70KAU/BER) is to use the enthalpy and entropy of transition to extrapolate the Gibbs energy difference but to neglect any effects due to a difference in heat capacity between the phases. These differences can often be substantial.

The extrapolation of the experimental heat capacity data across a solid state transformation is generally fairly straightforward. The extrapolation of data above and below the fusion temperature is more complicated. If the liquid heat capacity data are extrapolated from above the fusion temperature to lower temperatures there is the possibility that for certain temperatures the liquid phase would have a lower entropy than the solid phases. This is unreasonable and would be prevented in practice by the occurrence of the so called glass transition, which is thought to take place at between 0.5 and 0.75 of the fusion temperature. A similar problem could occur with the extrapolation of the solid phase data to temperatures well above the melting point where under certain circumstances the solid could be predicted to become stable again.

These problems need to be avoided and SGTE has adopted an interim solution for many elements in which the heat capacity of the liquid phase approaches that of the most stable solid phase for temperatures below the melting point (87AND/FERa). In a similar way above the melting temperature the heat capacity of the solid phases approaches that of the liquid phase. This has led to the introduction of terms in T^7 and T^{-9} into expressions for the Gibbs energy and removes the possibility of phases becoming incorrectly stable at high or low temperatures. More recently an alternative method has been used for a number of elements which obtains a smoother extrapolation of the heat capacities of the solid and liquid phases.

Data for phases which, for a given element, are metastable present more of a problem and it has been common to assess these "lattice stabilities", ie expressions for the difference in Gibbs energy between one phase and another, from the critical assessment of data for many binary systems. Many of the lattice stabilities used hitherto have been derived by Kaufman (see for example 70KAU/BER, 77KAU, 78KAU) but are now out of date and need revision. More recently attempts have been made to define new values for the Gibbs energies of transformation (86SAU/MIO, 88SAU/MIO) by considering recent experimental data for stable phase transformations, taking account of the observed correlation between the entropy of fusion and temperature of fusion and better theoretical prediction of the enthalpy difference between two structures for a given element at 0 K. The findings have also been questioned recently for some elements (87AND/FERb, 87FER/HIL). The data given in this document provide, according to the consensus of SGTE members the most reliable data for the elements. The recommended data may change in the course of time as new information becomes available from experimental studies and improved theoretical methods.

Standard Element Reference

The data for each phase are stored in the form of Gibbs energies relative to the "Standard Element Reference" ie the enthalpies of the pure elements in their defined reference phase at 298.15 K (denoted as $G\text{-}H_{SER}$). This reference phase is normally the phase stable at 10^5 Pa and 298.15 K. The exception to this rule is phosphorus for which, by convention, the white form is chosen as the reference phase because the more stable red form is difficult to characterise. This form of data is very convenient to use since all data in a database stored relative to this reference state are interconsistent and can be combined for the calculation of chemical and metallurgical equilibria. Furthermore each dataset contains all the thermodynamic information of interest for a particular phase and does not include any anomalous behaviour in a reference phase. All other thermodynamic functions can be calculated directly from one or more derivatives of the Gibbs energy expression. The concept of $G\text{-}H_{SER}$ can be best understood by noting that a Gibbs energy can be subdivided into its enthalpy and entropy contributions. The entropy of an element in a phase has an absolute value. The enthalpy, on the other hand, and therefore the Gibbs energy, has no absolute value, and a reference state needs to be defined. The most obvious reference state for the enthalpy is that of the element in its reference phase at 298.15 K. This is the reference state used for tabulation of the enthalpy of formation at 298.15 K. Combination of the enthalpy defined in this way with the absolute entropy gives $G\text{-}H_{SER}$. This method of expressing Gibbs energy is also used in the Barin and Knacke tables (73BAR/KNA, 77BAR/KNA).

Representation of data for the elements

The Gibbs energy is represented as a power series in terms of temperature T in the form:

$$G = a + b\,T + c\,T\ln(T) + \sum d\,T^{n}$$

where a, b, c and d are coefficients and n represents a set of integers, typically taking the values of 2, 3 and -1. A number of such expressions are usually required for a given phase to cover the whole temperature range of interest. From this expression for the Gibbs energy other thermodynamic functions can be evaluated:

$$S = -b - c - c\ln(T) - \sum n\,d\,T^{n-1}$$

$$H = a - c\,T - \sum (n-1)\,d\,T^{n}$$

$$Cp = -c - \sum n\,(n-1)\,d\,T^{n-1}$$

In some cases additional terms have been added to the expression for the Gibbs energy in the form of a pressure dependent contribution (Gpres) or a magnetic contribution (Gmag). The pressure dependence for condensed phases is expressed in the form of the Murnaghan equation (44MUR, 85FER/GUS)

$$Gpres = \frac{A\exp(a_0T + a_1T^2/2 + a_2T^3/3 + a_3T^{-1})}{(K_0 + K_1T + K_2T^2)\,(n-1)}\left[1 + nP(K_0 + K_1T + K_2T^2))^{1-1/n} - 1\right]$$

where A, a_0, a_1, a_2, a_3, K_0, K_1, K_2 and n are constants for the particular element and phase and P is the pressure. From the well known relationships:

$$V = \left(\frac{\partial G}{\partial P}\right)_T \qquad \alpha = \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_P \qquad \kappa = -\frac{1}{V}\left(\frac{\partial V}{\partial P}\right)_T$$

where V is the molar volume, α is the expansivity and κ is the compressibility. It can be seen from the above equation that the parameter A is equivalent to the molar volume of the material at a temperature of 0 K and a pressure of 0 Pa. Furthermore the parameters a_0, a_1, a_2 and a_3 represent the thermal expansivity of the material as a function of temperature for a pressure of 0 Pa. In an equivalent way the parameters K_0, K_1 and K_2 represent the variation of the compressibility with temperature at zero pressure.

For typical values of K_0, K_1 and K_2 and a value of P of the order of 10^5 Pa or smaller, the expression can be simplified to give:

$$Gpres = AP\ (1 + a_0 T + a_1\ T^2/2 + a_2\ T^3/3 + a_3\ T^{-1})$$

The contributions to the enthalpy, entropy and heat capacity can also be defined:

$$Spres = -\ AP\ (a_0 + a_1\ T + a_2\ T^2 - a_3\ T^{-2})$$

$$Hpres = AP\ (1 - a_1\ T^2/2 - 2\ a_2\ T^3/3 + 2\ a_3\ T^{-1})$$

$$Cppres = -\ AP\ (a_1 T + 2\ a_2\ T^2 + 2\ a_3\ T^{-2})$$

For applications relating to low or moderate pressures the contribution from the pressure dependence can be ignored.

The magnetic contribution to the thermodynamic properties has been defined by Hillert and Jarl (78HIL/JAR) following the work of Inden (76IND, 81IND). According to Hillert and Jarl the contribution to the Gibbs energy is given by:

$$Gmag = R\ T\ \ln(B_0 + 1)\ g(\tau)$$

where τ is T/T^*, T^* the critical temperature (the Curie temperature T_C for ferromagnetic materials or the Neel temperature T_N for antiferromagnetic materials) and B_0 the average magnetic moment per atom. $g(\tau)$ is given by:

$$g(\tau) = 1 - \left[\frac{79\ \tau^{-1}}{140\ p} + \frac{474}{497}\left(\frac{1}{p} - 1\right)\left(\frac{\tau^3}{6} + \frac{\tau^9}{135} + \frac{\tau^{15}}{600}\right)\right] / D \qquad \ldots\ldots\ldots\ldots \tau \leq 1$$

$$g(\tau) = -\left[\frac{\tau^{-5}}{10} + \frac{\tau^{-15}}{315} + \frac{\tau^{-25}}{1500} \right] / D \qquad \ldots\ldots\ldots\ldots \tau > 1$$

where $$D = \frac{518}{1125} + \frac{11692}{15975}\left(\frac{1}{p} - 1\right)$$

The value of p, which can be thought of as the fraction of the magnetic enthalpy absorbed above the critical temperature, depends on the structure. For the simple BCC_A2 phase p = 0.40 (ie D = 1.55828482) while for other common phases encountered p = 0.28 (ie D = 2.342456517).

In a similar way the magnetic contribution to the other thermodynamic properties can be defined.

$$Smag = -\ R\ \ln(B_0 + 1)\ f(\tau)$$

where $$f(\tau) = 1 - \left[\frac{474}{497}\left(\frac{1}{p} - 1\right)\left(\frac{2\tau^3}{3} + \frac{2\tau^9}{27} + \frac{2\tau^{15}}{75}\right)\right] / D \qquad \ldots\ldots\ldots\ldots \tau \leq 1$$

$$f(\tau) = \left[\frac{2\tau^{-5}}{5} + \frac{2\tau^{-15}}{45} + \frac{2\tau^{-25}}{125} \right] / D \qquad \ldots\ldots\ldots\ldots\ \tau > 1$$

$$Hmag = R\ T \ln(B_0 + 1)\ h(\tau)$$

where $$h(\tau) = \left[-\frac{79\tau^{-1}}{140\,p} + \frac{474}{497}\left(\frac{1}{p} - 1\right)\left(\frac{\tau^3}{2} + \frac{\tau^9}{15} + \frac{\tau^{15}}{40}\right) \right] / D \qquad \ldots\ldots\ldots\ldots\ \tau \le 1$$

$$h(\tau) = -\left[\frac{\tau^{-5}}{2} + \frac{\tau^{-15}}{21} + \frac{\tau^{-25}}{60} \right] / D \qquad \ldots\ldots\ldots\ldots\ \tau > 1$$

$$Cpmag = R \ln(B_0 + 1)\ c(\tau)$$

where $$c(\tau) = \left[\frac{474}{497}\left(\frac{1}{p} - 1\right)\left(2\tau^3 + \frac{2\tau^9}{3} + \frac{2\tau^{15}}{5}\right) \right] / D \qquad \ldots\ldots\ldots\ldots\ \tau \le 1$$

$$c(\tau) = \left[2\tau^{-5} + \frac{2\tau^{-15}}{3} + \frac{2\tau^{-25}}{5} \right] / D \qquad \ldots\ldots\ldots\ldots\ \tau > 1$$

The remainder of this document falls into two parts. The first part is a summary of the transition data between the stable phases for all elements for which SGTE has solid and liquid data. All thermodynamic data refer to units of J mol^{-1}. This is similar to the information presented in the Massalski compilation of binary alloy phase diagrams (91DIN). In this present paper the standard entropies at 298.15 K for certain key elements have been modified to be compatible with the CODATA key values (89COX/WAG). Furthermore all temperatures quoted refer to the ITS-90 temperature scale (90PRE, 91RUS/HUD). These include eight of the fixed points on the temperature scale. The temperatures of transition or fusion for a number of other elements have also been modified from the earlier compilation (89DIN) where the appropriate quantity is known sufficiently accurately. This covers a further 16 elements, some of which were secondary reference points of the IPTS-68 temperature scale. It is felt that transition temperatures for the other elements are not known sufficiently accurately to justify modification (ie the requisite change was significantly smaller than the uncertainty in the measured value).

The second part is a list, for each element, of the data firstly in the form of $G\text{-}H_{SER}$ and secondly relative to the element reference phase. For every element the reference phase is the first phase for which data are given. References are provided to the source of the data used. The references most widely quoted ie Hultgren (73HUL/DES), Saunders et al. (88SAU/MIO), Kaufman (70KAU), TPIS (78GUR/VEI), CODATA (87GAR/PAR) and JANAF (85CHA/DAV) are simply referenced by name. Graphs generated by MTDATA (The NPL Databank for Metallurgical Thermochemistry) (90DAV/DIN) are provided to show the variation of heat capacity of the various phases as a function of temperature and also the difference in Gibbs energy between a given phase and the element reference phase. For certain elements the thermodynamic data have been assessed both as a function of temperature and pressure. Where appropriate a temperature - pressure phase diagram is also shown.

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SGTE PURE ELEMENT TRANSITION DATA

		Atomic wt	H_{298}-H_0	S_{298}	T_{trans}	$\Delta_{trans}H$	$\Delta_{trans}S$	$\Delta_{trans}Cp$
Ag	FCC_A1	107.8682	5745.	42.55	1234.93	11296.8	9.1477	1.5402
Al	FCC_A1	26.98154	4540.	28.30	933.47	10711.04	11.4744	-2.2046
Am	DHCP	243.	6407.00	55.3960	1042.00	870.0	0.8349	-2.7811
	FCC_A1				1350.00	5862.0	4.3422	1.2898
	BCC_A2				1449.00	14393.0	9.9330	2.092
As	RHO_A7	74.922	5117.032	35.6895	1090.00	24442.9	22.4247	0.0
Au	FCC_A1	196.9665	6016.592	47.4884	1337.33	12552.0	9.3859	0.0
B	BET	10.81	1222.0	5.9	2348.00	50200.00	21.3799	0.8362
Ba	BCC_A2	137.33	6910.0	62.50	1000.00	7120.0	7.120	-4.345
Be	HCP_A3	9.01218	1950.0	9.50	1527.00	6849.0	4.4853	-1.892
	BCC_A2				1560.00	7895.0	5.0608	-1.2123
Bi	RHO_A7	208.9804	6426.624	56.735	544.55	11296.80	20.7479	0.6521
C	HEX_A9	12.011	1054.0	5.7423	4765.3	117369.0	24.6300	0.0
Ca	FCC_A1	40.08	5736.0	41.588	716.00	928.85	1.2973	-1.2332
	BCC_A2				1115.00	8539.54	7.6588	-8.2257
Cd	HCP_A3	112.41	6247.	51.80	594.219	6192.32	10.4209	0.1725
Ce	FCC_A1	140.12	7280.16	69.4544	1000.00	2991.56	2.9916	-0.1165
	BCC_A2				1072.00	5460.12	5.0934	0.0836
Co	HCP_A3	58.9332	4765.567	30.0400	694.99	427.59	0.6153	0.000
	FCC_A1				1768.00	16200.00	9.1629	0.8962
Cr	BCC_A2	51.996	4050.0	23.5429	2180.0	21004.00	9.6349	-10.7118
Cs	BCC_A2	132.9054	7711.000	85.23	301.59	2096.00	6.9498	0.1128
Cu	FCC_A1	63.546	5004.	33.15	1357.77	13263.28	9.7684	1.5391
Dy	HCP_A3	162.50	8865.896	75.5630	1659.00	3882.75	2.3404	-0.0381
	BCC_A2				1684.00	10782.17	6.4027	-0.2929
Er	HCP_A3	167.26	7392.2912	73.17816	1802.00	19903.29	11.0451	-4.6468
Eu	BCC_A2	151.96	8004.0	80.79304	1095.00	9213.17	8.4139	-2.9731
Fe	BCC_A2	55.847	4489.0	27.2797	1184.80	1012.87	0.8549	-7.6820
	FCC_A1				1667.50	825.78	0.4953	2.1830
	BCC_A2				1811.00	13806.00	7.6241	4.6537
Ga	ORT	69.72	5572.0	40.7271	302.91	5589.82	18.4535	2.2766
Gd	HCP_A3	157.25	9087.648	67.9482	1535.00	3677.74	2.3959	-1.0745
	BCC_A2				1587.00	9815.66	6.1850	-0.5021
Ge	DIA_A4	72.59	4636.	31.09	1211.40	36944.72	30.4975	-1.1370
Hf	HCP_A3	178.49	5845.0	43.56	2016.00	5860.29	2.9069	-6.6207
	BCC_A2				2506.00	27196.00	10.8524	5.5565
Hg	LIQUID	200.59	9342.	75.90	234.321	2295.34	9.7957	-0.0066

		Atomic wt	H_{298}-H_0	S_{298}	T_{trans}	$\Delta_{trans}H$	$\Delta_{trans}S$	$\Delta_{trans}Cp$
Ho	HCP_A3	164.9304	7995.624	75.0191	1703.00	4271.86	2.5084	-4.0963
	BCC_A2				1745.00	11757.04	6.7376	-4.184
In	TET_A6	114.82	6610.0	57.65	429.75	3283.0	7.6394	0.0148
Ir	FCC_A1	192.22	5267.656	35.5054	2719.00	41124.00	15.1247	12.0550
K	BCC_A2	39.0983	7088.	64.68	336.53	2320.86	6.8964	0.0576
La	DHCP	138.9055	6665.112	56.9024	550.00	364.01	0.6618	-0.569
	FCC_A1				1134.00	3121.26	2.7524	4.515
	BCC_A2				1193.00	6196.50	5.1941	-5.230
Li	BCC_A2	6.941	4632.00	29.12	453.60	2999.93	6.6136	0.6362
Lu	HCP_A3	174.967	6388.968	50.9611	1936.00	18648.09	9.6323	-0.0102
Mg	HCP_A3	24.305	4998.0	32.671	923.00	8476.78	9.1839	2.0821
Mn	BCC_A12	54.9380	4995.696	32.2206	980.00	2253.54	2.2995	-1.5482
	CUB_A13				1360.00	2165.73	1.5924	0.1264
	FCC_A1				1411.00	1908.32	1.3525	3.2651
	BCC_A2				1519.00	12908.94	8.4984	1.7203
Mo	BCC_A2	95.94	4589.0	28.56	2896.00	37479.78	12.9419	-10.5181
Na	BCC_A2	22.98977	6460.	51.3000	370.87	2597.01	7.0025	0.3018
Nb	BCC_A2	92.9064	5220.0	36.27	2750.00	30000.0	10.9091	0.5560
Nd	DHCP	144.24	7133.72	71.0862	1128.00	3029.22	2.6855	-1.435
	BCC_A2				1289.00	7142.09	5.5408	4.2258
Ni	FCC_A1	58.69	4787.0	29.7955	1728.30	17479.82	10.1139	4.248
Np	ORTHO	237.0482	6606.536	50.4590	555.02	4699.92	8.4680	-5.0491
	TETRAG				855.95	3000.12	3.5050	-2.9291
	BCC_A2				916.84	3198.57	3.4887	8.995
Os	HCP_A3	190.2		32.6352	3306.00	57855.00	17.5000	13.8379
P	WHITE	30.97376	5360.0	41.09	317.30	659.0	2.0769	1.9793
Pa	BCT_Aa	231.0359	6439.176	51.882	1443.10	6639.79	4.6011	-2.0962
	BCC_A2				1844.78	12341.18	6.6898	7.5305
Pb	FCC_A1	207.2	6870.	64.80	600.612	4773.94	7.9485	1.1867
Pd	FCC_A1	106.42	5468.488	37.8234	1828.00	16736.00	9.1554	4.5325
Pr	DHCP	140.9077	7418.232	73.9313	1068.00	3167.29	2.9656	-3.557
	BCC_A2				1204.00	6886.86	5.7200	4.5187
Pt	FCC_A1	195.08	5723.712	41.6308	2041.50	22175.00	10.8621	-0.8317
Pu		244.	6902.0	54.4610	397.61	3705.99	9.3207	-3.337
					487.90	478.00	0.9797	-0.563
				593.06	713.02	1.2023	-0.752	
	FCC_A1				736.40	83.35	0.1132	-0.872
	TET_A6				755.67	1841.06	2.4363	-1.84
	BCC_A2				913.00	2824.03	3.0931	8.447
Rb	BCC_A2	85.4678	7489.	76.78	312.46	2192.42	7.0166	-0.5631
Re	HCP_A3	186.207	5355.52	36.5263	3459.00	60428.00	17.4698	7.4703
Rh	FCC_A1	102.9055	(4920.384)	31.5556	2237.00	26593.50	11.8880	1.3593

		Atomic wt	H_{298}-H_0	S_{298}	T_{trans}	$\Delta_{trans}H$	$\Delta_{trans}S$	$\Delta_{trans}Cp$
Ru	HCP_A3	101.07	4602.4	28.6144	2607.00	38589.03	14.8021	0.8342
S	ORTHO	32.06	4412.0	32.054	368.30	401.00	1.0888	0.5363
	MONOCL				388.36	1721.0	4.4315	6.5021
Sb	RHO_A7	121.75	5870.152	45.5219	903.78	19874.00	21.9899	0.4002
Sc	HCP_A3	44.9559	5217.448	34.6435	1608.00	4008.27	2.4927	4.136
	BCC_A2				1814.00	14095.90	7.7706	0.000
Se	HEX_A8	78.96	5514.512	41.9655	494.00	6694.40	13.5514	3.8536
Si	DIA_A4	28.0855	3217.	18.81	1687.00	50208.00	29.7617	-2.0264
Sm	RHO	150.36	7573.04	69.4962	1190.00	3112.90	2.6159	-1.381
	BCC_A2				1345.00	8619.04	6.4082	3.2635
Sn	BCT_A5	118.69	6323.	51.18	505.078	7029.12	13.9169	-1.0252
Sr	FCC_A1	87.62	6568.	55.694	820.00	836.8	1.0207	-2.361
	BCC_A2				1050.00	7431.	7.0771	8.711
Ta	BCC_A2	180.9479	5681.872	41.4718	3290.00	36568.16	11.1149	-2.6340
Tb	HCP_A3	158.9254	9426.552	73.3037	1562.00	4380.65	2.8045	-0.3401
	BCC_A2				1632.00	10150.38	6.2196	0.000
Tc	HCP_A3	98.		32.9856	2430.01	33291.19	13.7000	8.3218
Te	HEX_A8	127.60	6121.192	49.4967	722.66	17489.12	24.2010	2.5841
Th	FCC_A1	232.0381	6350.	51.8	1633.20	3597.02	2.2034	-5.7949
	BCC_A2				2022.99	13807.13	6.8251	6.0679
Ti	HCP_A3	47.88	4824.	30.72	1155.00	4170.00	3.6104	-5.0272
	BCC_A2				1941.00	14146.00	7.2880	8.4656
Tl	HCP_A3	204.383	6831.97	64.2997	507.00	359.82	0.7097	2.0997
	BCC_A2				577.00	4142.16	7.1788	-2.3901
Tm	HCP_A3	168.9342	7397.312	74.01496	1818.00	16840.60	9.2633	3.8918
U	ORT_A20	238.0289	6364.	50.20	942.00	2790.73	2.9626	-5.110
	TET				1049.00	4757.21	4.5350	-4.644
	BCC_A2				1408.00	9142.04	6.4929	10.3764
V	BCC_A2	50.9415	4507.0	30.89	2183.00	21500.0	9.8488	2.3597
W	BCC_A2	183.85	4970.0	32.6176	3695.00	52313.69	14.1580	0.2900
Y	HCP_A3	88.9059	5966.384	44.4341	1752.00	4991.51	2.8490	-2.453
	BCC_A2				1799.00	11397.22	6.3353	8.0751
Yb	FCC_A1	173.04	6711.136	59.8312	1033.00	1748.91	1.6930	4.059
	BCC_A2				1097.00	7656.72	6.9797	0.6695
Zn	HCP_A3	65.38	5657.	41.63	692.68	7322.00	10.5706	1.6653
Zr	HCP_A3	91.22	5566.27	39.1809	1139.45	4103.30	3.6011	-6.3138
	BCC_A2				2127.85	20997.77	9.8681	6.0320

Ag

Source of data: Hultgren [FCC_A1, LIQUID]
Saunders et al. [HCP_A3, BCC_A2]

Data for Ag in the form of G-HSER

FCC_A1

$-7209.512 + 118.202013\ T - 23.8463314\ T\ \ln(T) - 1.790585E\text{-}3\ T^2 - 0.398587E\text{-}6\ T^3 - 12011\ T^{-1}$ *(298.15 < T < 1234.93)*
$-15095.252 + 190.266404\ T - 33.472\ T\ \ln(T) + 1.412E29\ T^{-9}$ *(1234.93 < T < 3000.00)*

LIQUID

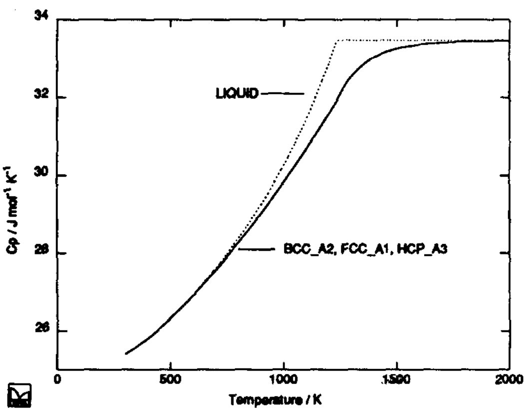
$3815.564 + 109.310993\ T - 23.8463314\ T\ \ln(T) - 1.790585E\text{-}3\ T^2 - 0.398587E\text{-}6\ T^3 - 12011\ T^{-1} - 1.034E\text{-}20\ T^7$
(298.15 < T < 1234.93)
$-3587.111 + 180.964656\ T - 33.472\ T\ \ln(T)$ *(1234.93 < T < 3000.00)*

BCC_A2

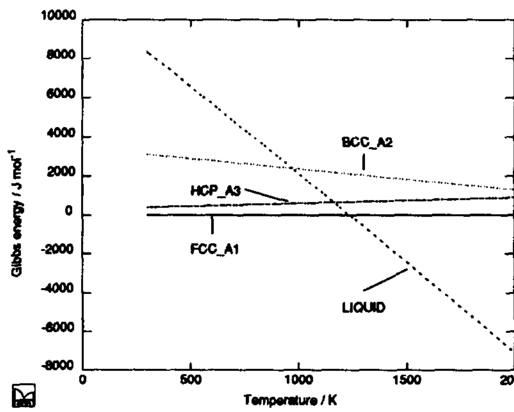
$-3809.512 + 117.152013\ T - 23.8463314\ T\ \ln(T) - 1.790585E\text{-}3\ T^2 - 0.398587E\text{-}6\ T^3 - 12011\ T^{-1}$ *(298.15 < T < 1234.93)*
$-11695.252 + 189.216404\ T - 33.472\ T\ \ln(T) + 1.412E29\ T^{-9}$ *(1234.93 < T < 3000.00)*

HCP_A3

$-6909.512 + 118.502013\ T - 23.8463314\ T\ \ln(T) - 1.790585E\text{-}3\ T^2 - 0.398587E\text{-}6\ T^3 - 12011\ T^{-1}$ *(298.15 < T < 1234.93)*
$-14795.252 + 190.566404\ T - 33.472\ T\ \ln(T) + 1.412E29\ T^{-9}$ *(1234.93 < T < 3000.00)*



Heat capacity of Ag



Gibbs energy of phases of Ag relative to FCC_A1

Data relative to FCC_A1

LIQUID

$11025.076 - 8.891021\ T - 1.034E\text{-}20\ T^7$ *(298.15 < T < 1234.93)*
$11508.141 - 9.301747\ T - 1.412E29\ T^{-9}$ *(1234.93 < T < 3000.00)*

BCC_A2

$3400 - 1.05\ T$ *(298.15 < T < 3000.00)*

HCP_A3

$300 + 0.3\ T$ *(298.15 < T < 3000.00)*

Al

Source of data: JANAF [FCC_A1, LIQUID]
RWTH Aachen, Unpublished work [BCC_A2, BCC_A12]
Kaufman [CUB_A13]
Saunders et al. [HCP_A3]

Data for Al in the form of G-HSER

FCC_A1

-7976.15 + 137.093038 T - 24.3671976 T ln(T) - 1.884662E-3 T^2 - 0.877664E-6 T^3 + 74092 T^{-1} *(298.15 < T < 700)*
-11276.24 + 223.048446 T - 38.5844296 T ln(T) + 18.531982E-3 T^2 - 5.764227E-6 T^3 + 74092 T^{-1} *(700 < T < 933.47)*
-11278.378 + 188.684153 T - 31.748192 T ln(T) - 1.231E28 T^{-9} *(933.47 < T < 2900)*

LIQUID

3028.879 + 125.251171 T - 24.3671976 T ln(T) - 1.884662E-3 T^2 - 0.877664E-6 T^3 + 74092 T^{-1} + 7.934E-20 T^7 *(298.15 < T < 700)*
-271.21 + 211.206579 T - 38.5844296 T ln(T) + 18.531982E-3 T^2 - 5.764227E-6 T^3 + 74092 T^{-1} + 7.934E-20 T^7 *(700 < T < 933.47)*
-795.996 + 177.430178 T - 31.748192 T ln(T) *(933.47 < T < 2900)*

BCC_A12

2107.25 + 132.280038 T - 24.3671976 T ln(T) - 1.884662E-3 T^2 - 0.877664E-6 T^3 + 74092 T^{-1} *(298.15 < T < 700)*
-1192.84 + 218.235446 T - 38.5844296 T ln(T) + 18.531982E-3 T^2 - 5.764227E-6 T^3 + 74092 T^{-1} *(700 < T < 933.47)*
-1194.978 + 183.871153 T - 31.748192 T ln(T) - 1.231E28 T^{-9} *(933.47 < T < 2900)*

BCC_A2

2106.85 + 132.280038 T - 24.3671976 T ln(T) - 1.884662E-3 T^2 - 0.877664E-6 T^3 + 74092 T^{-1} *(298.15 < T < 700)*
-1193.24 + 218.235446 T - 38.5844296 T ln(T) + 18.531982E-3 T^2 - 5.764227E-6 T^3 + 74092 T^{-1} *(700 < T < 933.47)*
-1195.378 + 183.871153 T - 31.748192 T ln(T) - 1.231E28 T^{-9} *(933.47 < T < 2900)*

CUB_A13

2944.29 + 132.281438 T - 24.3671976 T ln(T) - 1.884662E-3 T^2 - 0.877664E-6 T^3 + 74092 T^{-1} *(298.15 < T < 700)*
-355.8 + 218.236846 T - 38.5844296 T ln(T) + 18.531982E-3 T^2 - 5.764227E-6 T^3 + 74092 T^{-1} *(700 < T < 933.47)*
-357.938 + 183.872553 T - 31.748192 T ln(T) - 1.231E28 T^{-9} *(933.47 < T < 2900)*

HCP_A3

-2495.15 + 135.293038 T - 24.3671976 T ln(T) - 1.884662E-3 T^2 - 0.877664E-6 T^3 + 74092 T^{-1} *(298.15 < T < 700)*
-5795.24 + 221.248446 T - 38.5844296 T ln(T) + 18.531982E-3 T^2 - 5.764227E-6 T^3 + 74092 T^{-1} *(700 < T < 933.47)*
-5797.378 + 186.884153 T - 31.748192 T ln(T) - 1.231E28 T^{-9} *(933.47 < T < 2900)*

Data relative to FCC_A1

LIQUID

11005.029 - 11.841867 T + 7.934E-20 T^7 *(298.15 < T < 933.47)*
10482.382 - 11.253974 T + 1.231E28 T^{-9} *(933.47 < T < 2900)*

BCC_A12

10083.4 - 4.813 T *(298.15 < T < 2900)*

BCC_A2

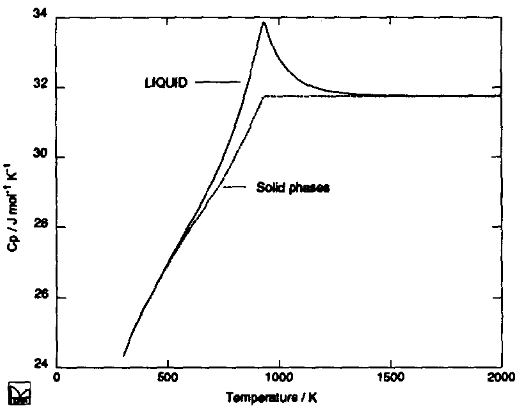
10083 - 4.813 T *(298.15 < T < 2900)*

CUB_A13

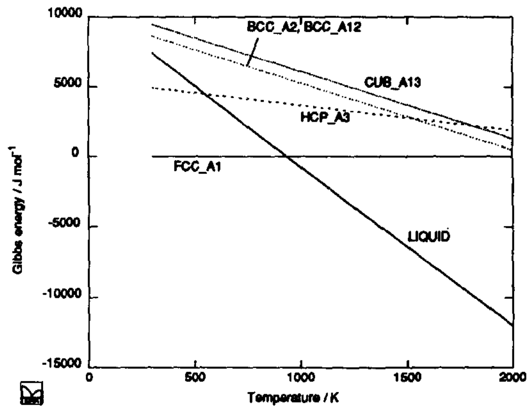
10920.44 - 4.8116 T *(298.15 < T < 2900)*

HCP_A3

5481 - 1.8 T *(298.15 < T < 2900)*



Heat capacity of Al



Gibbs energy of phases of Al relative to FCC_A1

Am

Source of data: M H Rand and A T Dinsdale (unpublished work)

Data for Am in the form of G-HSER

DHCP

$-6639.201 + 89.645685\ T - 21.1868\ T\ \ln(T) - 5.59955E\text{-}3\ T^2 - 0.541038E\text{-}6\ T^3 - 30424\ T^{-1}$	*298.15 < T < 1329.00*
$-21702.938 + 241.107269\ T - 41.84\ T\ \ln(T)$	*1329.00 < T < 3000.00*

FCC_A1

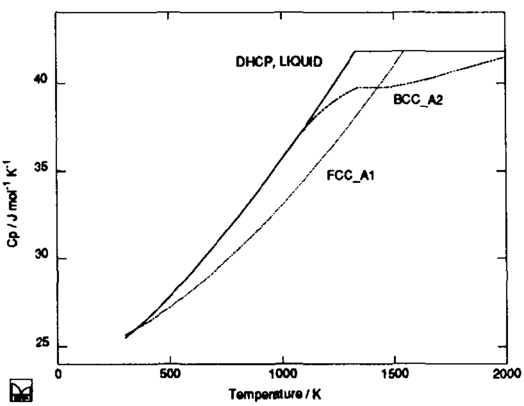
$-5224.899 + 99.204329\ T - 23.1377\ T\ \ln(T) - 2.94694E\text{-}3\ T^2 - 0.664773E\text{-}6\ T^3 - 18507\ T^{-1}$	*298.15 < T < 1018.00*
$-2935.853 + 73.800069\ T - 19.4406\ T\ \ln(T) - 5.418E\text{-}3\ T^2 - 0.375233E\text{-}6\ T^3 - 260435\ T^{-1}$	*1018.00 < T < 1548.70*
$-22179.593 + 241.353807\ T - 41.84\ T\ \ln(T)$	*1548.70 < T < 3000.00*

BCC_A2

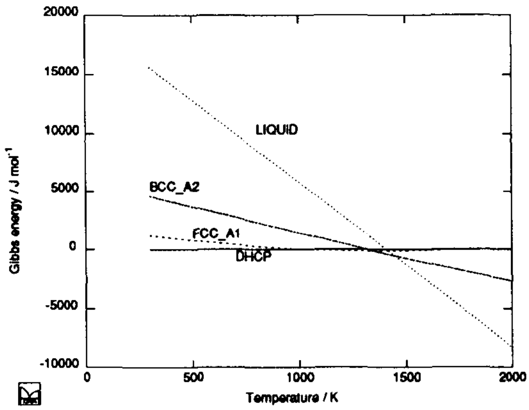
$-665.396 + 85.114354\ T - 21.1868\ T\ \ln(T) - 5.5995E\text{-}3\ T^2 - 0.541033E\text{-}6\ T^3 - 30424\ T^{-1}$	*298.15 < T < 999.00*
$-7800.332 + 63.93115\ T - 15.8832\ T\ \ln(T) - 19.0671E\text{-}3\ T^2 + 2.291117E\text{-}6\ T^3 + 2287195\ T^{-1}$	*999.00 < T < 1339.00*
$-13153.887 + 219.600832\ T - 39.748\ T\ \ln(T)$	*1339.00 < T < 1449.00*
$70352.138 - 326.394464\ T + 33.413\ T\ \ln(T) - 27.36485E\text{-}3\ T^2 + 1.801717E\text{-}6\ T^3 - 17379450\ T^{-1}$	*1449.00 < T < 2183.60*
$-16925.244 + 237.367028\ T - 41.84\ T\ \ln(T)$	*2183.60 < T < 3000.00*

LIQUID

$13271.499 + 75.525185\ T - 21.1868\ T\ \ln(T) - 5.59955E\text{-}3\ T^2 - 0.541038E\text{-}6\ T^3 - 30424\ T^{-1}$	*298.15 < T < 1329.00*
$-1792.238 + 226.986769\ T - 41.84\ T\ \ln(T)$	*1329.00 < T < 3000.00*



Heat capacity of Am



Gibbs energy of phases of Am relative to DHCP

Data for Am relative to DHCP

FCC_A1

$1414.302 + 9.558644\ T - 1.9509\ T \ln(T) + 2.65261E\text{-}3\ T^2 - 0.123735E\text{-}6\ T^3 + 11917\ T^{-1}$ — *298.15 < T < 1018.00*
$3703.348 - 15.845616\ T + 1.7462\ T \ln(T) + 0.18155E\text{-}3\ T^2 + 0.165805E\text{-}6\ T^3 - 230011\ T^{-1}$ — *1018.00 < T < 1329.00*
$18767.085 - 167.307199\ T + 22.3994\ T \ln(T) - 5.418E\text{-}3\ T^2 - 0.375233E\text{-}6\ T^3 - 260435\ T^{-1}$ — *1329.00 < T < 1548.70*
$-476.655 + 0.246538\ T$ — *1548.70 < T < 3000.00*

BCC_A2

$5973.805 - 4.531331\ T + 0.00005E\text{-}3\ T^2 + 0.000005E\text{-}6\ T^3$ — *298.15 < T < 999.00*
$-1161.131 - 25.714535\ T + 5.3036\ T \ln(T) - 13.46755E\text{-}3\ T^2 + 2.832155E\text{-}6\ T^3 + 2317619\ T^{-1}$ — *999.00 < T < 1329.00*
$13902.606 - 177.176119\ T + 25.9568\ T \ln(T) - 19.0671E\text{-}3\ T^2 + 2.291117E\text{-}6\ T^3 + 2287195\ T^{-1}$ — *1329.00 < T < 1339.00*
$8549.052 - 21.506436\ T + 2.092\ T \ln(T)$ — *1339.00 < T < 1449.00*
$92055.076 - 567.501733\ T + 75.253\ T \ln(T) - 27.36485E\text{-}3\ T^2 + 1.801717E\text{-}6\ T^3 - 17379450\ T^{-1}$ — *1449.00 < T < 2183.60*
$4777.694 - 3.740241\ T$ — *2183.60 < T < 3000.00*

LIQUID

$19910.7 - 14.1205\ T$ — *298.15 < T < 3000.00*

As

Source of data: Hultgren modified by I Ansara [RHOMBO_A7, LIQUID]
Saunders et al. [HCP_A3, BCC_A2, FCC_A1]

Data for As in the form of G-HSER

RHOMBO_A7

$-7270.447 + 122.211069\ T - 23.3144\ T \ln(T) - 2.71613E\text{-}3\ T^2 + 11600\ T^{-1}$ — *298.15 < T < 1090.00*
$-10454.913 + 163.457433\ T - 29.216037\ T \ln(T)$ — *1090.00 < T < 1200.00*

LIQUID

$17172.453 + 99.78639\ T - 23.3144\ T \ln(T) - 2.71613E\text{-}3\ T^2 + 11600\ T^{-1}$ — *298.15 < T < 1090.00*
$13987.987 + 141.032754\ T - 29.216037\ T \ln(T)$ — *1090.00 < T < 1200.00*

FCC_A1

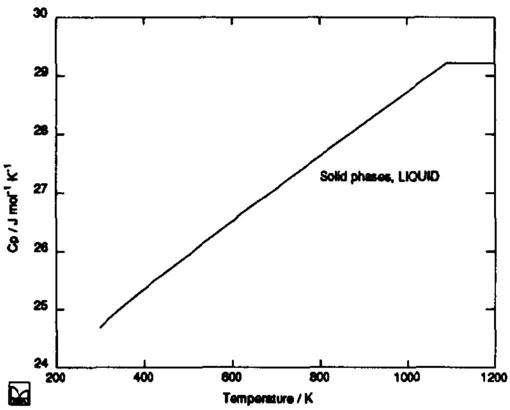
$17603.553 + 107.471069\,T - 23.3144\,T\ln(T) - 2.71613E\text{-}3\,T^2 + 11600\,T^{-1}$	*298.15 < T < 1090.00*
$14419.087 + 148.717433\,T - 29.216037\,T\ln(T)$	*1090.00 < T < 1200.00*

BCC_A2

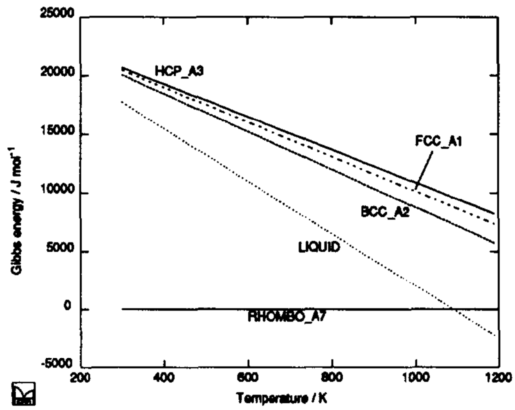
$17603.553 + 106.111069\,T - 23.3144\,T\ln(T) - 2.71613E\text{-}3\,T^2 + 11600\,T^{-1}$	*298.15 < T < 1090.00*
$14419.087 + 147.357433\,T - 29.216037\,T\ln(T)$	*1090.00 < T < 1200.00*

HCP_A3

$17603.553 + 108.211069\,T - 23.3144\,T\ln(T) - 2.71613E\text{-}3\,T^2 + 11600\,T^{-1}$	*298.15 < T < 1090.00*
$14419.087 + 149.457433\,T - 29.216037\,T\ln(T)$	*1090.00 < T < 1200.00*



Heat capacity of As



Gibbs energy of phases of As relative to RHOMBO_A7

Data for As relative to RHOMBO_A7

LIQUID

$24442.9 - 22.424679\,T$	*298.15 < T < 3000.00*

FCC_A1

$24874 - 14.74\,T$	*298.15 < T < 3000.00*

BCC_A2

$24874 - 16.1\,T$	*298.15 < T < 3000.00*

HCP_A3

$24874 - 14.0\,T$	*298.15 < T < 3000.00*

Au

Source of data: Hultgren, revised by M H Rand [FCC_A1, LIQUID]
I Ansara, M H Rand - unpublished work [HCP_A3]
Saunders et al. [BCC_A2]

Data for Au in the form of G-HSER

FCC_A1

$-6938.856 + 106.830098\,T - 22.75455\,T\ln(T) - 3.85924E\text{-}3\,T^2 + 0.379625E\text{-}6\,T^3 - 25097\,T^{-1}$ *(298.15 < T < 929.4)*
$-93586.481 + 1021.69543\,T - 155.7067449\,T\ln(T) + 87.56015E\text{-}3\,T^2 - 11.518713E\text{-}6\,T^3 + 10637210\,T^{-1}$ *(929.4 < T < 1337.33)*
$314067.829 - 2016.378254\,T + 263.2522592\,T\ln(T) - 118.216828E\text{-}3\,T^2 + 8.923844E\text{-}6\,T^3 - 67999832\,T^{-1}$ *(1337.33 < T < 1735.8)*
$-12133.783 + 165.272524\,T - 30.9616\,T\ln(T)$ *(1735.8 < T < 3200)*

BCC_A2

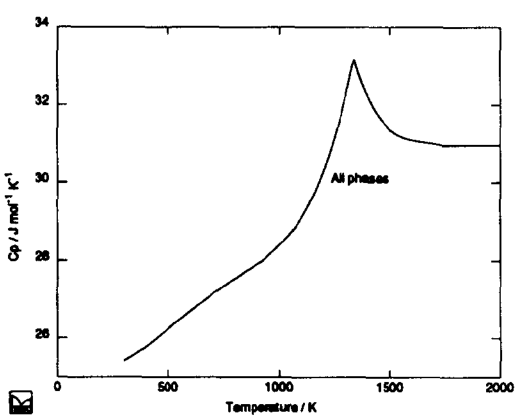
$-2688.856 + 105.730098\,T - 22.75455\,T\ln(T) - 3.85924E\text{-}3\,T^2 + 0.379625E\text{-}6\,T^3 - 25097\,T^{-1}$ *(298.15 < T < 929.4)*
$-89336.481 + 1020.59543\,T - 155.7067449\,T\ln(T) + 87.56015E\text{-}3\,T^2 - 11.518713E\text{-}6\,T^3 + 10637210\,T^{-1}$ *(929.4 < T < 1337.33)*
$318317.829 - 2017.478254\,T + 263.2522592\,T\ln(T) - 118.216828E\text{-}3\,T^2 + 8.923844E\text{-}6\,T^3 - 67999832\,T^{-1}$ *(1337.33 < T < 1735.8)*
$-7883.783 + 164.172524\,T - 30.9616\,T\ln(T)$ *(1735.8 < T < 3200)*

HCP_A3

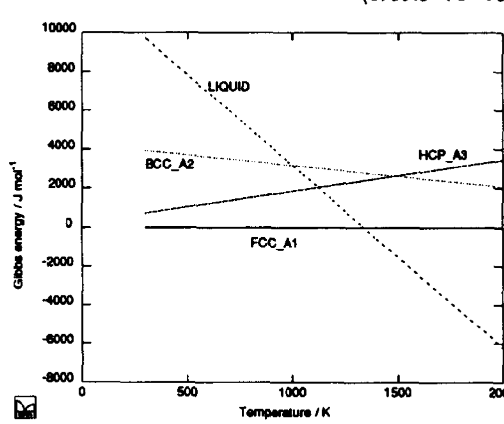
$-6698.106 + 108.430098\,T - 22.75455\,T\ln(T) - 3.85924E\text{-}3\,T^2 + 0.379625E\text{-}6\,T^3 - 25097\,T^{-1}$ *(298.15 < T < 929.4)*
$-93345.731 + 1023.29543\,T - 155.7067449\,T\ln(T) + 87.56015E\text{-}3\,T^2 - 11.518713E\text{-}6\,T^3 + 10637210\,T^{-1}$ *(929.4 < T < 1337.33)*
$314308.579 - 2014.778254\,T + 263.2522592\,T\ln(T) - 118.216828E\text{-}3\,T^2 + 8.923844E\text{-}6\,T^3 - 67999832\,T^{-1}$ *(1337.33 < T < 1735.8)*
$-11893.033 + 166.872524\,T - 30.9616\,T\ln(T)$ *(1735.8 < T < 3200)*

LIQUID

$5613.144 + 97.444232\,T - 22.75455\,T\ln(T) - 3.85924E\text{-}3\,T^2 + 0.379625E\text{-}6\,T^3 - 25097\,T^{-1}$ *(298.15 < T < 929.4)*
$-81034.481 + 1012.309564\,T - 155.7067449\,T\ln(T) + 87.56015E\text{-}3\,T^2 - 11.518713E\text{-}6\,T^3 + 10637210\,T^{-1}$ *(929.4 < T < 1337.33)*
$326619.829 - 2025.76412\,T + 263.2522592\,T\ln(T) - 118.216828E\text{-}3\,T^2 + 8.923844E\text{-}6\,T^3 - 67999832\,T^{-1}$ *(1337.33 < T < 1735.8)*
$418.217 + 155.886658\,T - 30.9616\,T\ln(T)$ *(1735.8 < T < 3200)*



Heat capacity of Au



Gibbs energy of phases of Au relative to FCC_A1

Data relative to FCC_A1

BCC_A2

4250 - 1.1 T (298.15 < T < 3200)

HCP_A3

240.75 + 1.6 T (298.15 < T < 3200)

LIQUID

12552 - 9.385866 T (298.15 < T < 3200)

B

Source of data: TPIS

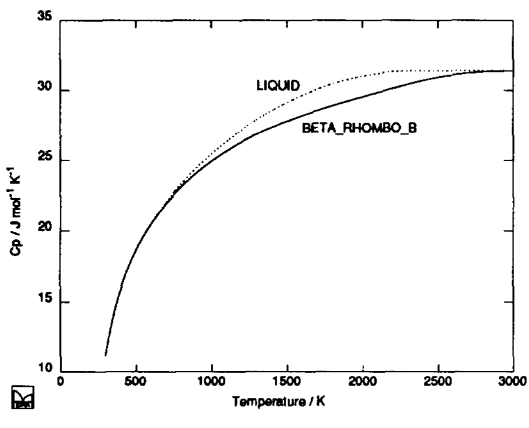
Data for B in the form of G-HSER

BETA_RHOMBO_B

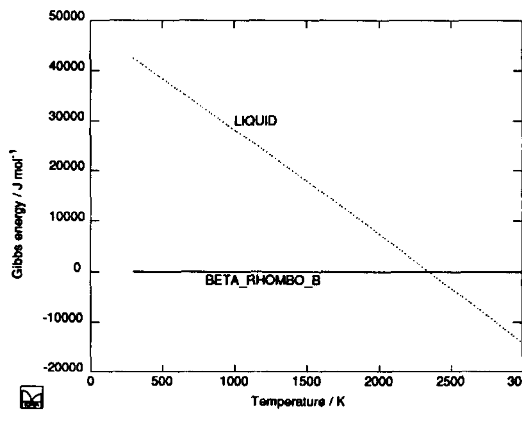
$-7735.284 + 107.111864\,T - 15.6641\,T\ln(T) - 6.864515E{-}3\,T^2 + 0.618878E{-}6\,T^3 + 370843\,T^{-1}$ (298.15 < T < 1100.00)
$-16649.474 + 184.801744\,T - 26.6047\,T\ln(T) - 0.79809E{-}3\,T^2 - 0.02556E{-}6\,T^3 + 1748270\,T^{-1}$ (1100.00 < T < 2348.00)
$-36667.582 + 231.336244\,T - 31.5957527\,T\ln(T) - 1.59488E{-}3\,T^2 + 0.134719E{-}6\,T^3 + 11205883\,T^{-1}$ (2348.00 < T < 3000.00)
$-21530.653 + 222.396264\,T - 31.4\,T\ln(T)$ (3000.00 < T < 6000.00)

LIQUID

$40723.275 + 86.843839\,T - 15.6641\,T\ln(T) - 6.864515E{-}3\,T^2 + 0.618878E{-}6\,T^3 + 370843\,T^{-1}$ (298.15 < T < 500.00)
$41119.703 + 82.101722\,T - 14.9827763\,T\ln(T) - 7.095669E{-}3\,T^2 + 0.507347E{-}6\,T^3 + 335484\,T^{-1}$ (500.00 < T < 2348.00)
$28842.012 + 200.94731\,T - 31.4\,T\ln(T)$ (2348.00 < T < 6000.00)



Heat capacity of B



Gibbs energy of phases of B relative to BETA_RHOMB_B

Data for B relative to BETA_RHOMBO_B

LIQUID

$48458.559 - 20.268024\,T$ (298.15 < T < 500.00)
$48854.986 - 25.010142\,T + 0.6813237\,T\ln(T) - 0.231154E{-}3\,T^2 - 0.111531E{-}6\,T^3 - 35359\,T^{-1}$ (500.00 < T < 1100.00)
$57769.177 - 102.700022\,T + 11.6219237\,T\ln(T) - 6.297579E{-}3\,T^2 + 0.532907E{-}6\,T^3 - 1412786\,T^{-1}$ (1100.00 < T < 2348.00)

$65509.594 - 30.388933\ T + 0.1957527\ T\ \ln(T) + 1.594880E\text{-}3\ T^2 - 0.134719E\text{-}6\ T^3 - 11205883\ T^{-1}$ *(2348.00 < T < 3000.00)*

$50372.664 - 21.448953\ T$ *(3000.00 < T < 6000.00)*

Ba

Source of data: TPIS [BCC_A2, LIQUID]
Saunders et al. [HCP_A3, FCC_A1]

Data for Ba in the form of G-HSER

BCC_A2

$-17685.226 + 233.78606\ T - 42.889\ T\ \ln(T) - 1.8314E\text{-}3\ T^2 - 0.000095E\text{-}6\ T^3 + 705880\ T^{-1}$ *(298.15 < T < 1000.00)*

$-64873.614 + 608.188389\ T - 94.2824199\ T\ \ln(T) + 19.504772E\text{-}3\ T^2 - 1.051353E\text{-}6\ T^3 + 8220192\ T^{-1}$ *(1000.00 < T < 2995.00)*

$8083.889 + 136.780042\ T - 32.2\ T\ \ln(T)$ *(2995.00 < T < 4000.00)*

LIQUID

$-9738.988 + 229.540143\ T - 43.4961089\ T\ \ln(T) - 2.346416E\text{-}3\ T^2 + 0.991223E\text{-}6\ T^3 + 723016\ T^{-1}$ *(298.15 < T < 1000.00)*

$-7381.093 + 235.49642\ T - 45.103\ T\ \ln(T) + 2.154E\text{-}3\ T^2 + 0.000027E\text{-}6\ T^3 - 365\ T^{-1}$ *(1000.00 < T < 2995.00)*

$11940.282 + 132.212\ T - 32.2\ T\ \ln(T)$ *(2995.00 < T < 4000.00)*

HCP_A3

$-15685.226 + 235.08606\ T - 42.889\ T\ \ln(T) - 1.8314E\text{-}3\ T^2 - 0.000095E\text{-}6\ T^3 + 705880\ T^{-1}$ *(298.15 < T < 1000.00)*

$-62873.614 + 609.488389\ T - 94.2824199\ T\ \ln(T) + 19.504772E\text{-}3\ T^2 - 1.051353E\text{-}6\ T^3 + 8220192\ T^{-1}$ *(1000.00 < T < 2995.00)*

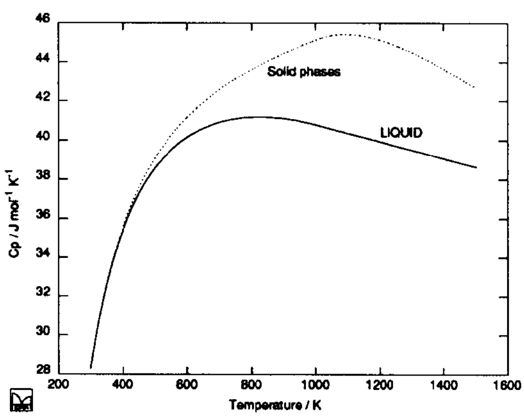
$10083.889 + 138.080042\ T - 32.2\ T\ \ln(T)$ *(2995.00 < T < 4000.00)*

FCC_A1

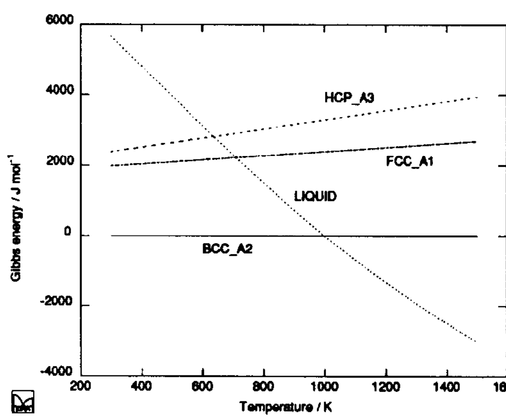
$-15885.226 + 234.38606\ T - 42.889\ T\ \ln(T) - 1.8314E\text{-}3\ T^2 - 0.000095E\text{-}6\ T^3 + 705880\ T^{-1}$ *(298.15 < T < 1000.00)*

$-63073.614 + 608.788389\ T - 94.2824199\ T\ \ln(T) + 19.504772E\text{-}3\ T^2 - 1.051353E\text{-}6\ T^3 + 8220192\ T^{-1}$ *(1000.00 < T < 2995.00)*

$9883.889 + 137.380042\ T - 32.2\ T\ \ln(T)$ *(2995.00 < T < 4000.00)*



Heat capacity of Ba



Gibbs energy of phases of Ba relative to BCC_A2

Data for Ba relative to BCC_A2

LIQUID

$7946.238 - 4.245917\ T - 0.6071089\ T\ \ln(T) - 0.515016E\text{-}3\ T^2 + 0.991318E\text{-}6\ T^3 + 17136\ T^{-1}$ *(298.15 < T < 1000.00)*

$57492.521 - 372.691969\ T + 49.1794199\ T\ln(T) - 17.350772E\text{-}3\ T^2 + 1.051380E\text{-}6\ T^3 - 8220557\ T^{-1}$ *(1000.00 < T < 2995.00)*

$3856.393 - 4.568041\ T$ *(2995.00 < T < 4000.00)*

HCP_A3

$2000 + 1.3\ T$ *(298.15 < T < 4000.00)*

FCC_A1

$1800 + 0.6\ T$ *(298.15 < T < 4000.00)*

Be

Source of data: JANAF, extended by A T Dinsdale [HCP_A3, BCC_A2, LIQUID]
Saunders et al. [FCC_A1]

Data for Be in the form of G-HSER

HCP_A3

$-8553.651 + 137.560219\ T - 21.204\ T\ln(T) - 2.84715E\text{-}3\ T^2 - 0.160413E\text{-}6\ T^3 + 293690\ T^{-1}$ *(298.15 < T < 1527)*
$-121305.858 + 772.405844\ T - 103.9842999\ T\ln(T) + 21.078651E\text{-}3\ T^2 - 1.119065E\text{-}6\ T^3 + 27251743\ T^{-1}$ *(1527 < T < 3000)*

BCC_A2

$-1076.057 + 109.411712\ T - 17.1727841\ T\ln(T) - 8.672487E\text{-}3\ T^2 + 0.961427E\text{-}6\ T^3 + 242309\ T^{-1}$ *(298.15 < T < 1527)*
$-6970.378 + 196.411689\ T - 30\ T\ln(T)$ *(1527 < T < 1560)*
$-2609.973 + 178.131722\ T - 27.7823769\ T\ln(T) - 0.103629E\text{-}3\ T^2 - 0.059331E\text{-}6\ T^3 - 1250847\ T^{-1}$ *(1560 < T < 3000)*

LIQUID

$7511.838 + 120.362788\ T - 20.0497038\ T\ln(T) - 4.821347E\text{-}3\ T^2 + 0.415958E\text{-}6\ T^3 + 281044\ T^{-1}$ *(298.15 < T < 1560)*
$5364.713 + 156.961141\ T - 25.486\ T\ln(T) - 1.0572E\text{-}3\ T^2 - 0.001117E\text{-}6\ T^3 + 15920\ T^{-1}$ *(1560 < T < 3000)*

FCC_A1

$-2204.651 + 136.475219\ T - 21.204\ T\ln(T) - 2.84715E\text{-}3\ T^2 - 0.160413E\text{-}6\ T^3 + 293690\ T^{-1}$ *(298.15 < T < 1527)*
$-114956.858 + 771.320844\ T - 103.9842999\ T\ln(T) + 21.078651E\text{-}3\ T^2 - 1.119065E\text{-}6\ T^3 + 27251743\ T^{-1}$ *(1527 < T < 3000)*

Data for Be relative to HCP_A3

BCC_A2

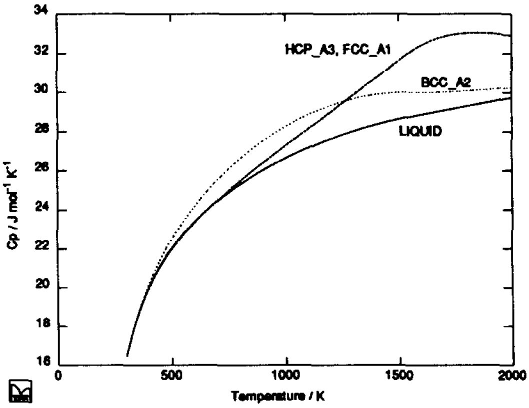
$7477.594 - 28.148507\ T + 4.0312159\ T\ln(T) - 5.825337E\text{-}3\ T^2 + 1.12184E\text{-}6\ T^3 - 51381\ T^{-1}$ *(298.15 < T < 1527.00)*
$114335.48 - 575.994154\ T + 73.9842999\ T\ln(T) - 21.078651E\text{-}3\ T^2 + 1.119065E\text{-}6\ T^3 - 27251743\ T^{-1}$ *(1527.00 < T < 1560.00)*
$118695.885 - 594.274122\ T + 76.201923\ T\ln(T) - 21.182279E\text{-}3\ T^2 + 1.059735E\text{-}6\ T^3 - 28502591\ T^{-1}$ *(1560.00 < T < 3000.00)*

LIQUID

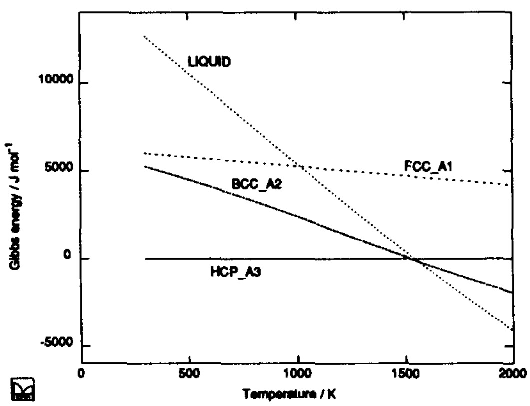
$16065.489 - 17.197431\ T + 1.1542962\ T\ln(T) - 1.974197E\text{-}3\ T^2 + 0.576371E\text{-}6\ T^3 - 12646\ T^{-1}$ *(298.15 < T < 1527.00)*
$128817.697 - 652.043056\ T + 83.9345962\ T\ln(T) - 25.899997E\text{-}3\ T^2 + 1.535023E\text{-}6\ T^3 - 26970699\ T^{-1}$ *(1527.00 < T < 1560.00)*
$126670.571 - 615.444703\ T + 78.4982999\ T\ln(T) - 22.135851E\text{-}3\ T^2 + 1.117948E\text{-}6\ T^3 - 27235823\ T^{-1}$ *(1560.00 < T < 3000.00)*

FCC_A1

$6349 - 1.085\ T$ *(298.15 < T < 3000.00)*



Heat capacity of Be



Gibbs energy of phases of Be relative to HCP_A3

Bi

Source of data: Hultgren [RHOMBO_A7, LIQUID]
P Y Chevalier [TETRAGONAL_A6, BCT_A5, TET_ALPHA1]
Saunders et al. [BCC_A2, FCC_A1, HCP_A3]

Data for Bi in the form of G-HSER

RHOMBO_A7

$-7817.776 + 128.418925\ T - 28.4096529\ T\ln(T) + 12.338888E\text{-}3\ T^2 - 8.381598E\text{-}6\ T^3$ *(298.15 < T < 544.55)*
$30208.022 - 393.650351\ T + 51.8556592\ T\ln(T) - 75.311163E\text{-}3\ T^2 + 13.499885E\text{-}6\ T^3 - 3616168\ T^{-1} + 1.661E25\ T^{-9}$ *(544.55 < T < 800)*
$-11045.664 + 182.548971\ T - 35.9824\ T\ln(T) + 7.4266E\text{-}3\ T^2 - 1.046E\text{-}6\ T^3 + 1.661E25\ T^{-9}$ *(800 < T < 1200)*
$-7581.312 + 124.77144\ T - 27.196\ T\ln(T) + 1.661E25\ T^{-9}$ *(1200 < T < 3000)*

LIQUID

$3428.29 + 107.782415\ T - 28.4096529\ T\ln(T) + 12.338888E\text{-}3\ T^2 - 8.381598E\text{-}6\ T^3 - 5.955E\text{-}19\ T^7$ *(298.15 < T < 544.55)*
$41544.282 - 414.460769\ T + 51.8556592\ T\ln(T) - 75.311163E\text{-}3\ T^2 + 13.499885E\text{-}6\ T^3 - 3616168\ T^{-1}$ *(544.55 < T < 800)*
$290.595 + 161.738553\ T - 35.9824\ T\ln(T) + 7.4266E\text{-}3\ T^2 - 1.046E\text{-}6\ T^3$ *(800 < T < 1200)*
$3754.947 + 103.961022\ T - 27.196\ T\ln(T)$ *(1200 < T < 3000)*

BCC_A2

$3479.224 + 114.518925\ T - 28.4096529\ T\ln(T) + 12.338888E\text{-}3\ T^2 - 8.381598E\text{-}6\ T^3$ *(298.15 < T < 544.55)*
$41505.022 - 407.550351\ T + 51.8556592\ T\ln(T) - 75.311163E\text{-}3\ T^2 + 13.499885E\text{-}6\ T^3 - 3616168\ T^{-1} + 1.661E25\ T^{-9}$ *(544.55 < T < 800)*
$251.336 + 168.648971\ T - 35.9824\ T\ln(T) + 7.4266E\text{-}3\ T^2 - 1.046E\text{-}6\ T^3 + 1.661E25\ T^{-9}$ *(800 < T < 1200)*
$3715.688 + 110.87144\ T - 27.196\ T\ln(T) + 1.661E25\ T^{-9}$ *(1200 < T < 3000)*

BCT_A5

$-3633.706 + 128.418925\ T - 28.4096529\ T\ln(T) + 12.338888E\text{-}3\ T^2 - 8.381598E\text{-}6\ T^3$ *(298.15 < T < 544.55)*
$34392.092 - 393.650351\ T + 51.8556592\ T\ln(T) - 75.311163E\text{-}3\ T^2 + 13.499885E\text{-}6\ T^3 - 3616168\ T^{-1} + 1.661E25\ T^{-9}$ *(544.55 < T < 800)*
$-6861.594 + 182.548971\ T - 35.9824\ T\ln(T) + 7.4266E\text{-}3\ T^2 - 1.046E\text{-}6\ T^3 + 1.661E25\ T^{-9}$ *(800 < T < 1200)*
$-3397.242 + 124.77144\ T - 27.196\ T\ln(T) + 1.661E25\ T^{-9}$ *(1200 < T < 3000)*

FCC_A1

$2082.224 + 115.918925\ T - 28.4096529\ T \ln(T) + 12.338888E\text{-}3\ T^2 - 8.381598E\text{-}6\ T^3$ *(298.15 < T < 544.55)*
$40108.022 - 406.150351\ T + 51.8556592\ T \ln(T) - 75.311163E\text{-}3\ T^2 + 13.499885E\text{-}6\ T^3 - 3616168\ T^{-1} + 1.661E25\ T^{-9}$ *(544.55 < T < 800)*
$-1145.664 + 170.048971\ T - 35.9824\ T \ln(T) + 7.4266E\text{-}3\ T^2 - 1.046E\text{-}6\ T^3 + 1.661E25\ T^{-9}$ *(800 < T < 1200)*
$2318.688 + 112.27144\ T - 27.196\ T \ln(T) + 1.661E25\ T^{-9}$ *(1200 < T < 3000)*

HCP_A3

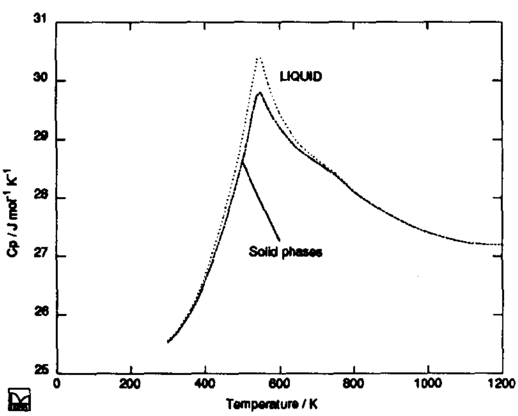
$2082.224 + 116.618925\ T - 28.4096529\ T \ln(T) + 12.338888E\text{-}3\ T^2 - 8.381598E\text{-}6\ T^3$ *(298.15 < T < 544.55)*
$40108.022 - 405.450351\ T + 51.8556592\ T \ln(T) - 75.311163E\text{-}3\ T^2 + 13.499885E\text{-}6\ T^3 - 3616168\ T^{-1} + 1.661E25\ T^{-9}$ *(544.55 < T < 800)*
$-1145.664 + 170.748971\ T - 35.9824\ T \ln(T) + 7.4266E\text{-}3\ T^2 - 1.046E\text{-}6\ T^3 + 1.661E25\ T^{-9}$ *(800 < T < 1200)*
$2318.688 + 112.97144\ T - 27.196\ T \ln(T) + 1.661E25\ T^{-9}$ *(1200 < T < 3000)*

TETRAGONAL_A6

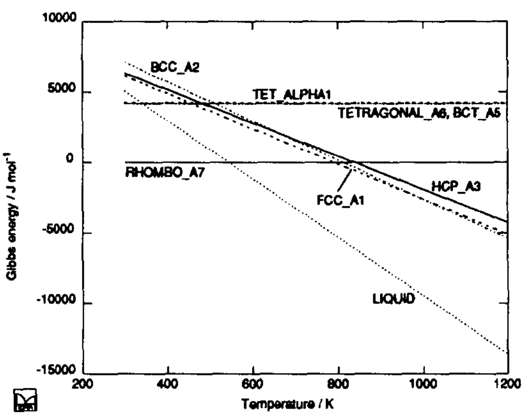
$-3633.706 + 128.418925\ T - 28.4096529\ T \ln(T) + 12.338888E\text{-}3\ T^2 - 8.381598E\text{-}6\ T^3$ *(298.15 < T < 544.55)*
$34392.092 - 393.650351\ T + 51.8556592\ T \ln(T) - 75.311163E\text{-}3\ T^2 + 13.499885E\text{-}6\ T^3 - 3616168\ T^{-1} + 1.661E25\ T^{-9}$ *(544.55 < T < 800)*
$-6861.594 + 182.548971\ T - 35.9824\ T \ln(T) + 7.4266E\text{-}3\ T^2 - 1.046E\text{-}6\ T^3 + 1.661E25\ T^{-9}$ *(800 < T < 1200)*
$-3397.242 + 124.77144\ T - 27.196\ T \ln(T) + 1.661E25\ T^{-9}$ *(1200 < T < 3000)*

TET_ALPHA1

$-3583.776 + 128.418925\ T - 28.4096529\ T \ln(T) + 12.338888E\text{-}3\ T^2 - 8.381598E\text{-}6\ T^3$ *(298.15 < T < 544.55)*
$34442.022 - 393.650351\ T + 51.8556592\ T \ln(T) - 75.311163E\text{-}3\ T^2 + 13.499885E\text{-}6\ T^3 - 3616168\ T^{-1} + 1.661E25\ T^{-9}$ *(544.55 < T < 800)*
$-6811.664 + 182.548971\ T - 35.9824\ T \ln(T) + 7.4266E\text{-}3\ T^2 - 1.046E\text{-}6\ T^3 + 1.661E25\ T^{-9}$ *(800 < T < 1200)*
$-3347.312 + 124.77144\ T - 27.196\ T \ln(T) + 1.661E25\ T^{-9}$ *(1200 < T < 3000)*



Heat capacity of Bi



Gibbs energy of phases of Bi relative to RHOMBO_A7

Data relative to RHOMBO_A7

LIQUID

$11246.067 - 20.63651\ T - 5.955E\text{-}19\ T^7$ *(298.15 < T < 544.55)*
$11336.259 - 20.810418\ T - 1.661E25\ T^{-9}$ *(544.55 < T < 3000)*

BCC_A2

$11297 - 13.9\ T$ *(298.15 < T < 3000)*

BCT_A5

4184.07 *(298.15 < T < 3000)*

FCC_A1

9900 - 12.5 T *(298.15 < T < 3000)*

HCP_A3

9900 - 11.8 T *(298.15 < T < 3000)*

TETRAGONAL_A6

4184.07 *(298.15 < T < 3000)*

TET_ALPHA1

4234 *(298.15 < T < 3000)*

C

Source of data: P Gustafson, Carbon, 1986, 24, 169-76

Data for C in the form of G-HSER

GRAPHITE (HEX_A9)

$A = 5.259E\text{-}6$ $a_0 = 2.32E\text{-}5$ $a_1 = 5.7E\text{-}9$
$K_0 = 3.0E\text{-}11$ $n = 12$

$-17368.441 + 170.73\ T - 24.3\ T\ \ln(T) - 4.723E\text{-}4\ T^2 + 2562600\ T^{-1} - 2.643E8\ T^{-2} + 1.2E10\ T^{-3} + Gpres$
(298.15 < T < 6000.00)

DIAMOND

$A = 3.412E\text{-}6$ $a_0 = 2.43E\text{-}6$ $a_1 = 1.0E\text{-}8$
$K_0 = 1.7E\text{-}12$ $n = 5$

$-16359.441 + 175.61\ T - 24.31\ T\ \ln(T) - 4.723E\text{-}4\ T^2 + 2698000\ T^{-1} - 2.61E8\ T^{-2} + 1.11E10\ T^{-3} + Gpres$
(298.15 < T < 6000.00)

LIQUID

$A = 7.626E\text{-}6$ $a_0 = 2.32E\text{-}5$ $a_1 = 5.7E\text{-}9$
$K_0 = 1.6E\text{-}10$ $n = 2$

$100000.559 + 146.1\ T - 24.3\ T\ \ln(T) - 4.723E\text{-}4\ T^2 + 2562600\ T^{-1} - 2.643E8\ T^{-2} + 1.2E10\ T^{-3} + Gpres$
(298.15 < T < 6000.00)

Data for C relative to GRAPHITE

GRAPHITE

$A = 5.259E\text{-}6$ $a_0 = 2.32E\text{-}5$ $a_1 = 5.7E\text{-}9$
$K_0 = 3.0E\text{-}11$ $n = 12$

Gpres *(298.15 < T < 6000.00)*

DIAMOND

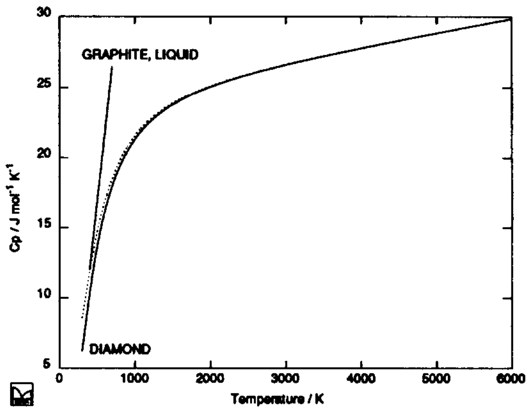
$A = 3.412E\text{-}6$ $a_0 = 2.43E\text{-}6$ $a_1 = 1.0E\text{-}8$
$K_0 = 1.7E\text{-}12$ $n = 5$

$1009 + 4.88\ T - 0.01\ T\ln(T) + 135400\ T^{-1} + 33.0E5\ T^{-2} - 9E8\ T^{-3} + Gpres$ *(298.15 < T < 6000.00)*

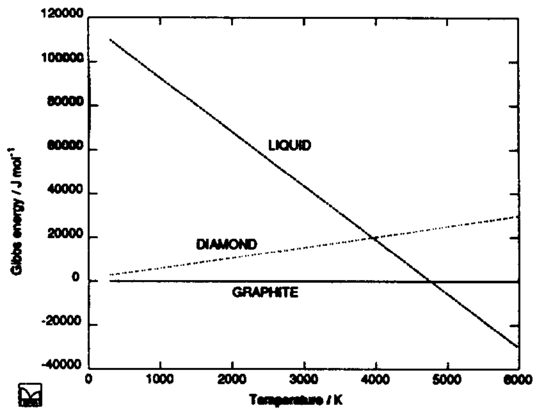
LIQUID

$A = 7.626E\text{-}6$ $a_0 = 2.32E\text{-}5$ $a_1 = 5.7E\text{-}9$
$K_0 = 1.6E\text{-}10$ $n = 2$

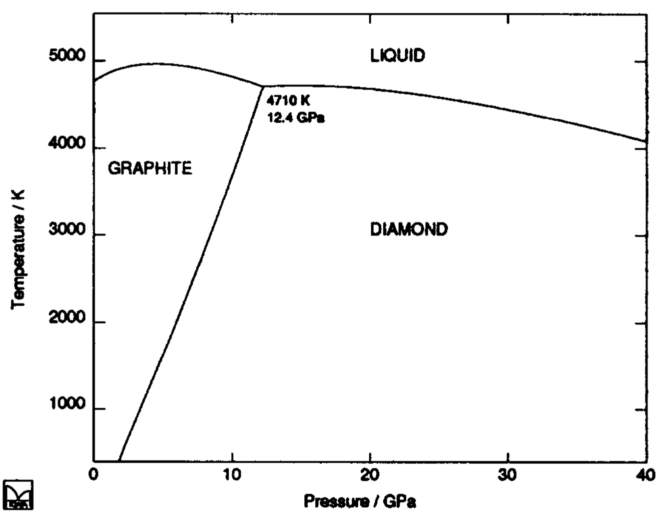
$117369 - 24.63\ T + Gpres$ *(298.15 < T < 6000.00)*



Heat capacity of C



Gibbs energy of phases of C relative to GRAPHITE



P-T phase diagram for C

Ca

Source of data : CODATA extended by A T Dinsdale [FCC_A1, BCC_A2, LIQUID]
Saunders et al. [HCP_A3]

Data for Ca in the form of G-HSER

FCC_A1

$-4955.062 + 72.794266\,T - 16.3138\,T\ln(T) - 11.10455E{-3}\,T^2 - 133574\,T^{-1}$ *(298.15 < T < 1115.00)*
$-107304.428 + 799.982066\,T - 114.2922467\,T\ln(T) + 23.733814E{-3}\,T^2 - 1.2438E{-6}\,T^3 + 18245540\,T^{-1}$
(1115.00 < T < 3000.00)

BCC_A2

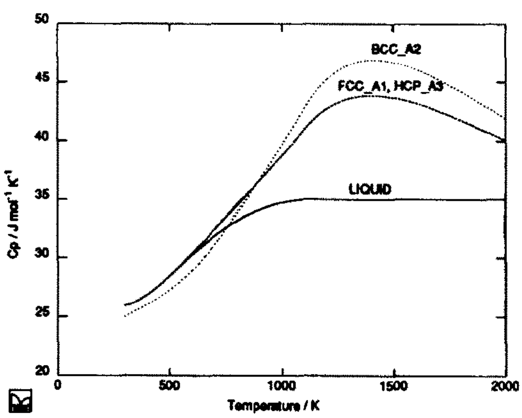
$-7020.852 + 142.970155\,T - 28.2541\,T\ln(T) + 7.2326E{-3}\,T^2 - 4.500217E{-6}\,T^3 + 60578\,T^{-1}$ *(298.15 < T < 716.00)*
$1640.475 + 1.999694\,T - 6.276\,T\ln(T) - 16.1921E{-3}\,T^2 - 523000\,T^{-1}$ *(716.00 < T < 1115.00)*
$-142331.096 + 1023.549046\,T - 143.8726979\,T\ln(T) + 32.543127E{-3}\,T^2 - 1.704079E{-6}\,T^3 + 25353771\,T^{-1}$
(1115.00 < T < 3000.00)

LIQUID

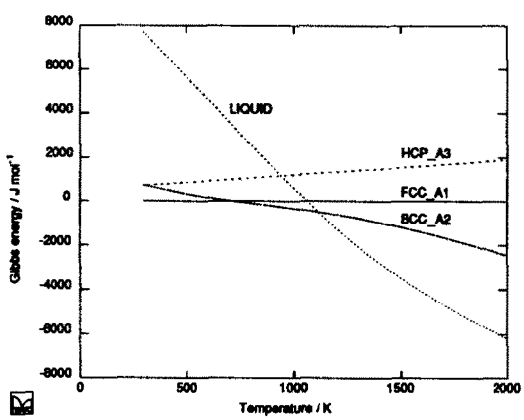
$5844.846 + 62.4838\,T - 16.3138\,T\ln(T) - 11.10455E{-3}\,T^2 - 133574\,T^{-1}$ *(298.15 < T < 500.00)*
$7838.856 + 18.2979\,T - 8.9874787\,T\ln(T) - 22.66537E{-3}\,T^2 + 3.338303E{-6}\,T^3 - 230193\,T^{-1}$ *(500.00 < T < 1115.00)*
$-2654.938 + 188.9223\,T - 35\,T\ln(T)$ *(1115.00 < T < 3000.00)*

HCP_A3

$-4455.062 + 73.494266\,T - 16.3138\,T\ln(T) - 11.10455E{-3}\,T^2 - 133574\,T^{-1}$ *(298.15 < T < 1115.00)*
$-106804.428 + 800.682066\,T - 114.2922467\,T\ln(T) + 23.733814E{-3}\,T^2 - 1.2438E{-6}\,T^3 + 18245540\,T^{-1}$
(1115.00 < T < 3000.00)



Heat capacity of Ca



Gibbs energy of phases of Ca relative to FCC_A1

Data for Ca relative to FCC_A1

BCC_A2

$-2065.79 + 70.175889\,T - 11.9403\,T\ln(T) + 18.33715E{-3}\,T^2 - 4.500217E{-6}\,T^3 + 194152\,T^{-1}$ *(298.15 < T < 716.00)*
$6595.537 - 70.794572\,T + 10.0378\,T\ln(T) - 5.08755E{-3}\,T^2 - 389426\,T^{-1}$ *(716.00 < T < 1115.00)*
$-35026.669 + 223.56698\,T - 29.5804512\,T\ln(T) + 8.809313E{-3}\,T^2 - 0.460278E{-6}\,T^3 + 7108230\,T^{-1}$
(1115.00 < T < 3000.00)

LIQUID

$10799.908 - 10.310466\,T$ *(298.15 < T < 500.00)*

$12793.918 - 54.496366\ T + 7.3263213\ T\ \ln(T) - 11.56082E{-3}\ T^2 + 3.338303E{-6}\ T^3 - 96619\ T^{-1}$ *(500.00 < T < 1115.00)*

$104649.49 - 611.059766\ T + 79.2922467\ T\ \ln(T) - 23.733814E{-3}\ T^2 + 1.2438E{-6}\ T^3 - 18245540\ T^{-1}$ *(1115.00 < T < 3000.00)*

HCP_A3

$500 + 0.700\ T$ *(298.15 < T < 3000.00)*

Cd

Source of data: Hultgren [HCP_A3, LIQUID]

Data for Cd in the form of G-HSER

HCP_A3 (Cd non ideal)

$-7083.469 + 99.506198\ T - 22.0442408\ T\ \ln(T) - 6.273908E{-3}\ T^2 - 6966\ T^{-1}$ *(298.15 < T < 594.219)*

$-20064.971 + 256.812233\ T - 45.1611543\ T\ \ln(T) + 8.832011E{-3}\ T^2 - 0.899604E{-6}\ T^3 + 1241290\ T^{-1}$ *(594.219 < T < 1500)*

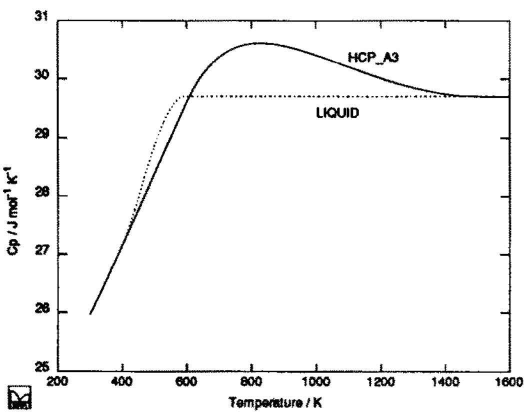
$-9027.489 + 148.20548\ T - 29.7064\ T\ \ln(T)$ *(1500 < T < 1600)*

LIQUID

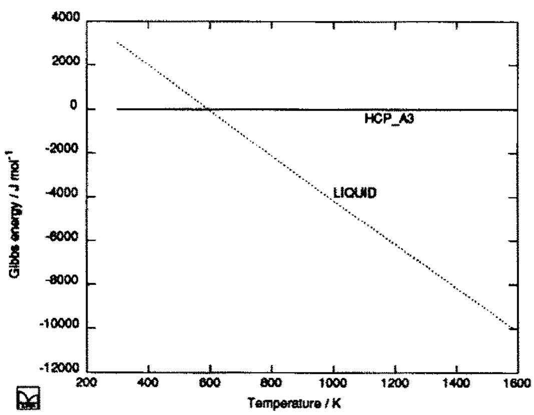
$-955.025 + 89.209282\ T - 22.0442408\ T\ \ln(T) - 6.273908E{-3}\ T^2 - 6966\ T^{-1}$ *(298.15 < T < 400)*

$21716.884 - 371.046869\ T + 53.1313898\ T\ \ln(T) - 115.159917E{-3}\ T^2 + 28.899781E{-6}\ T^3 - 1271815\ T^{-1}$ *(400 < T < 594.219)*

$-3252.303 + 138.251107\ T - 29.7064\ T\ \ln(T)$ *(594.219 < T < 1600)*



Heat capacity of Cd



Gibbs energy of phases of Cd relative to HCP_A3

Data relative to HCP_A3

LIQUID

$6128.444 - 10.296916\ T$ *(298.15 < T < 400)*

$28800.352 - 470.553067\ T + 75.1756306\ T\ \ln(T) - 108.886009E{-3}\ T^2 + 28.899781E{-6}\ T^3 - 1264849\ T^{-1}$ *(400 < T < 594.219)*

$16812.668 - 118.561126\ T + 15.4547543\ T\ \ln(T) - 8.832011E{-3}\ T^2 + 0.899604E{-6}\ T^3 - 1241290\ T^{-1}$ *(594.219 < T < 1500)*

$5775.185 - 9.954373\ T$ *(1500 < T < 1600)*

Ce

Source of data: Hultgren extended by A T Dinsdale [FCC_A1, BCC_A2, LIQUID]

Data for Ce in the form of G-HSER

FCC_A1

-7160.519 + 84.23022 T - 22.3664 T ln(T) - 6.7103E-3 T^2 - 0.320773E-6 T^3 - 18117 T^{-1} *(298.15 < T < 1000)*
-79678.506 + 659.4604 T - 101.3224803 T ln(T) + 26.046487E-3 T^2 - 1.930297E-6 T^3 + 11531707 T^{-1} *(1000 < T < 2000)*
-14198.639 + 190.370192 T - 37.6978 T ln(T) *(2000 < T < 4000)*

BCC_A2

-1354.69 - 5.21501 T - 7.7305867 T ln(T) - 29.098402E-3 T^2 + 4.784299E-6 T^3 - 196303 T^{-1} *(298.15 < T < 1000)*
-12101.106 + 187.449688 T - 37.6142 T ln(T) *(1000 < T < 1072)*
-11950.375 + 186.333811 T - 37.4627992 T ln(T) - 0.057145E-3 T^2 + 0.002348E-6 T^3 - 25897 T^{-1} *(1072 < T < 4000)*

LIQUID

4117.865 - 11.423898 T - 7.5383948 T ln(T) - 29.36407E-3 T^2 + 4.827734E-6 T^3 - 198834 T^{-1} *(298.15 < T < 1000)*
-6730.605 + 183.023193 T - 37.6978 T ln(T) *(1000 < T < 4000)*

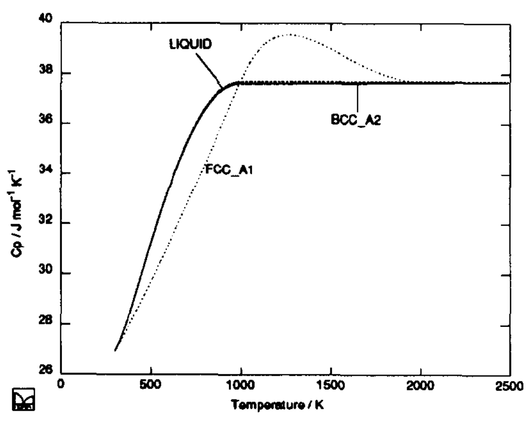
Data relative to FCC_A1

BCC_A2

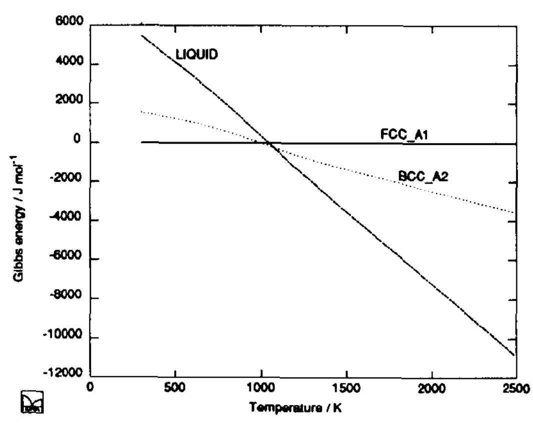
5805.829 - 89.44523 T + 14.6358133 T ln(T) - 22.388102E-3 T^2 + 5.105073E-6 T^3 - 178186 T^{-1} *(298.15 < T < 1000)*
67577.4 - 472.010713 T + 63.7082803 T ln(T) - 26.046487E-3 T^2 + 1.930297E-6 T^3 - 11531707 T^{-1} *(1000 < T < 1072)*
67728.132 - 473.126589 T + 63.8596811 T ln(T) - 26.103632E-3 T^2 + 1.932645E-6 T^3 - 11557604 T^{-1} *(1072 < T < 2000)*
2248.265 - 4.036381 T + 0.2350008 T ln(T) - 0.057145E-3 T^2 + 0.002348E-6 T^3 - 25897 T^{-1} *(2000 < T < 4000)*

LIQUID

11278.385 - 95.654118 T + 14.8280052 T ln(T) - 22.65377E-3 T^2 + 5.148507E-6 T^3 - 180717 T^{-1} *(298.15 < T < 1000)*
72947.901 - 476.437207 T + 63.6246803 T ln(T) - 26.046487E-3 T^2 + 1.930297E-6 T^3 - 11531707 T^{-1} *(1000 < T < 2000)*
7468.034 - 7.346999 T *(2000 < T < 4000)*



Heat capacity of Ce



Gibbs energy of phases of Ce relative to FCC_A1

Co

Source of data: A Fernandez Guillermet, Int. J. Thermophys., 1987, 8(4), 481 [HCP_A3, FCC_A1, LIQUID]
A Fernandez Guillermet, High Temp. - High Press., 1987, 19, 477-9 [BCC_A2]
Weiming Huang, Report, TRITA-MAC-0386 [BCC_A12, CUB_A13]

Data for Co in the form of G-HSER

HCP_A3

$T_C = 1396$ $B_0 = 1.35$
$A = 6.719875E-6$ $a_0 = 3.4581936E-5$ $a_1 = 5.587534E-9$
$K_0 = 4.51216E-12$ $K_1 = 1.60731E-15$ $K_2 = 4.66729E-20$ $n = 4.007$

$310.241 + 133.36601\ T - 25.0861\ T \ln(T) - 2.6547387E-3\ T^2 - 1.7348E-7\ T^3 + 72526.9\ T^{-1}$ + Gmag + Gpres *(298.15 < T < 1768.00)*
$-17197.666 + 253.28374\ T - 40.5\ T \ln(T) + 9.3488E30\ T^{-9}$ + Gmag + Gpres *(1768.00 < T < 6000.00)*

FCC_A1

$T_C = 1396$ $B_0 = 1.35$
$A = 6.752927E-6$ $a_0 = 3.2070159E-5$ $a_1 = 5.868345E-9$
$K_0 = 4.66592E-12$ $K_1 = 1.45933E-15$ $K_2 = 5.17369E-20$ $n = 4.007$

$737.832 + 132.750762\ T - 25.0861\ T \ln(T) - 2.6547387E-3\ T^2 - 1.7348E-7\ T^3 + 72526.9\ T^{-1}$ + Gmag + Gpres *(298.15 < T < 1768.00)*
$-16770.075 + 252.668487\ T - 40.5\ T \ln(T) + 9.3488E30\ T^{-9}$ + Gmag + Gpres *(1768.00 < T < 6000.00)*

LIQUID

$A = 6.465079E-6$ $a_0 = 10.1216993E-5$ $a_1 = -8.3E-9$
$K_0 = 5.06842E-12$ $K_1 = 4.32538E-15$ $n = 4.5925$

$15395.278 + 124.434078\ T - 25.0861\ T \ln(T) - 2.6547387E-3\ T^2 - 1.7348E-7\ T^3 + 72526.9\ T^{-1} - 2.198E-21\ T^7$ + Gpres *(298.15 < T < 1768.00)*
$-846.61 + 243.599944\ T - 40.5\ T \ln(T)$ + Gpres *(1768.00 < T < 6000.00)*

BCC_A2

$T_C = 1450.0$ $B_0 = 1.35$
$A = 6.8147641E-6$ $a_0 = 3.20701588E-5$ $a_1 = 2.93417253E-9$
$K_0 = 4.66591978E-12$ $K_1 = 1.45932922E-15$ $K_2 = 5.173687E-20$ $n = 4.007$

$3248.241 + 132.65221\ T - 25.0861\ T \ln(T) - 2.6547387E-3\ T^2 - 1.7348E-7\ T^3 + 72526.9\ T^{-1}$ + Gmag + Gpres *(298.15 < T < 1768.00)*
$-14259.666 + 252.56994\ T - 40.5\ T \ln(T) + 9.3488E30\ T^{-9}$ + Gmag + Gpres *(1768.00 < T < 6000.00)*

BCC_A12

$4465.241 + 133.36601\ T - 25.0861\ T \ln(T) - 2.6547387E-3\ T^2 - 1.7348E-7\ T^3 + 72526.9\ T^{-1}$ *(298.15 < T < 1768.00)*
$-13042.666 + 253.28374\ T - 40.5\ T \ln(T) + 9.3488E30\ T^{-9}$ *(1768.00 < T < 6000.00)*

CUB_A13

$3465.241 + 133.36601\ T - 25.0861\ T \ln(T) - 2.6547387E-3\ T^2 - 1.7348E-7\ T^3 + 72526.9\ T^{-1}$ *(298.15 < T < 1768.00)*
$-14042.666 + 253.28374\ T - 40.5\ T \ln(T) + 9.3488E30\ T^{-9}$ *(1768.00 < T < 6000.00)*

Data for Co relative to paramagnetic HCP_A3

HCP_A3

$T_C = 1396$ $B_0 = 1.35$
$A = 6.719875E-6$ $a_0 = 3.4581936E-5$ $a_1 = 5.587534E-9$
$K_0 = 4.51216E-12$ $K_1 = 1.60731E-15$ $K_2 = 4.66729E-20$ $n = 4.007$

Gmag + Gpres *(298.15 < T < 6000.00)*

FCC_A1

$T_C = 1396$	$B_0 = 1.35$		
$A = 6.752927E\text{-}6$	$a_0 = 3.2070159E\text{-}5$	$a_1 = 5.868345E\text{-}9$	
$K_0 = 4.66592E\text{-}12$	$K_1 = 1.45933E\text{-}15$	$K_2 = 5.17369E\text{-}20$	$n = 4.007$

427.591 - 0.61525 T + Gmag + Gpres *(298.15 < T < 6000.00)*

LIQUID

$A = 6.465079E\text{-}6$	$a_0 = 10.1216993E\text{-}5$	$a_1 = -8.3E\text{-}9$
$K_0 = 5.06842E\text{-}12$	$K_1 = 4.32538E\text{-}15$	$n = 4.5925$

15085.037 - 8.931932 T - 2.198E-21 T^7 + Gpres *(298.15 < T < 1768.00)*
16351.056 - 9.683796 T - 9.3488E30 T^{-9} + Gpres *(1768.00 < T < 6000.00)*

BCC_A2

$T_C = 1450.0$	$B_0 = 1.35$		
$A = 6.8147641E\text{-}6$	$a_0 = 3.2070159E\text{-}5$	$a_1 = 2.93417253E\text{-}9$	
$K_0 = 4.66592E\text{-}12$	$K_1 = 1.45933E\text{-}15$	$K_2 = 5.17369E\text{-}20$	$n = 4.007$

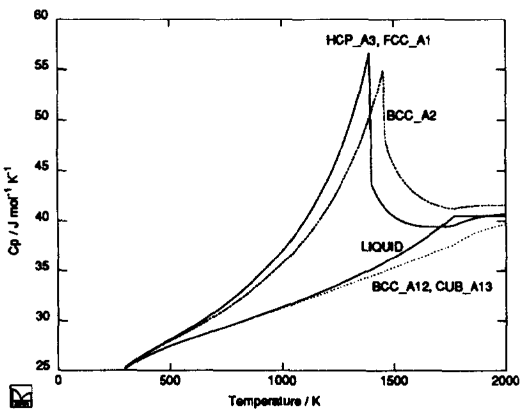
2938 - 0.7138 T + Gmag + Gpres *(298.15 < T < 3000.00)*

BCC_A12

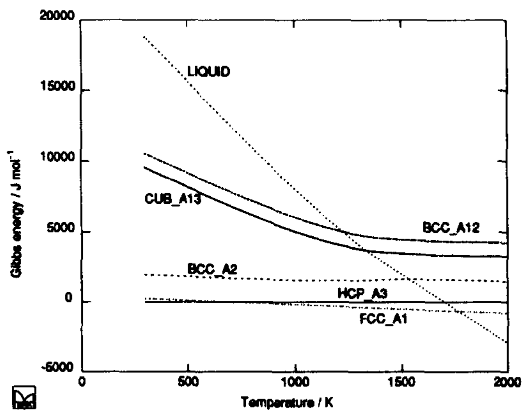
4155 *(298.15 < T < 3000.00)*

CUB_A13

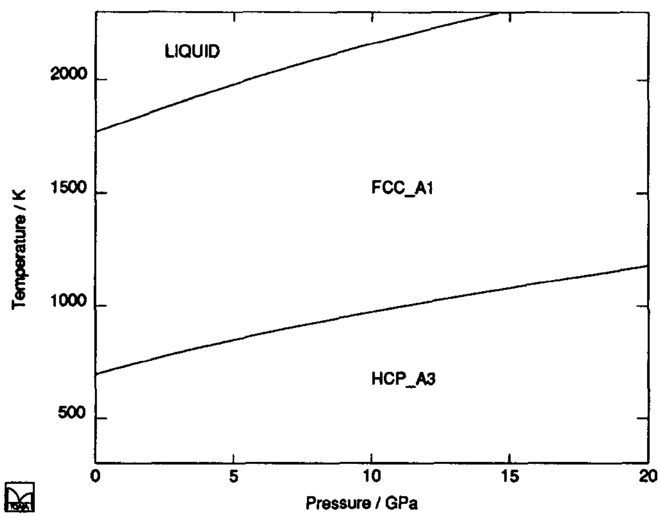
3155 *(298.15 < T < 3000.00)*



Heat capacity of Co



Gibbs energy of phases of Co relative to HCP_A3



P-T phase diagram for Co

Cr

Source of data: J-O Andersson, Int. J. Thermophys., 1985, 6, 411-9 [BCC_A2, LIQUID]
J-O Andersson, A Fernandez Guillermet, P Gustafson, CALPHAD, 1987, 11, 361-4 [HCP_A3, FCC_A1]
Kaufman [CUB_A13, BCC_A12]

Data for Cr in the form of G-HSER

BCC_A2

$T_N = 311.5$ $B_0 = 0.008$
$A = 7.188E\text{-}6$ $a_0 = 1.7E\text{-}5$ $a_1 = 1.84E\text{-}8$
$K_0 = 5.2E\text{-}12$ $n = 5$

$-8856.94 + 157.48\ T - 26.908\ T\ \ln(T) + 0.00189435\ T^2 - 1.47721E\text{-}6\ T^3 + 139250\ T^{-1} + Gmag + Gpres$ *(298.15 < T < 311.5)*
$-8856.94 + 157.48\ T - 26.908\ T\ \ln(T) + 0.00189435\ T^2 - 1.47721E\text{-}6\ T^3 + 139250\ T^{-1} + Gpres$ *(311.5 < T < 2180.00)*
$-34869.344 + 344.18\ T - 50.0\ T\ \ln(T) - 2.88526E32\ T^{-9} + Gpres$ *(2180.00 < T < 6000.00)*

LIQUID

$A = 7.188E\text{-}6$ $a_0 = 1.7E\text{-}5$ $a_1 = 1.84E\text{-}8$
$K_0 = 9.3E\text{-}12$ $n = 5$

$15483.015 + 146.059775\ T - 26.908\ T\ \ln(T) + 0.00189435\ T^2 - 1.47721E\text{-}6\ T^3 + 139250\ T^{-1} + 2.37615E\text{-}21\ T^7 + Gpres$ *(298.15 < T < 2180.00)*
$-16459.984 + 335.616317\ T - 50.0\ T\ \ln(T) + Gpres$ *(2180.00 < T < 6000.00)*

FCC_A1

$T_N = 369.667$ $B_0 = 0.82$

$-1572.94 + 157.643\ T - 26.908\ T\ \ln(T) + 0.00189435\ T^2 - 1.47721E\text{-}6\ T^3 + 139250\ T^{-1}$ *(298.15 < T < 2180.00)*
$-27585.344 + 344.343\ T - 50.0\ T\ \ln(T) - 2.88526E32\ T^{-9}$ *(2180.00 < T < 6000.00)*

HCP_A3

$T_N = 369.667$ $B_0 = 0.82$

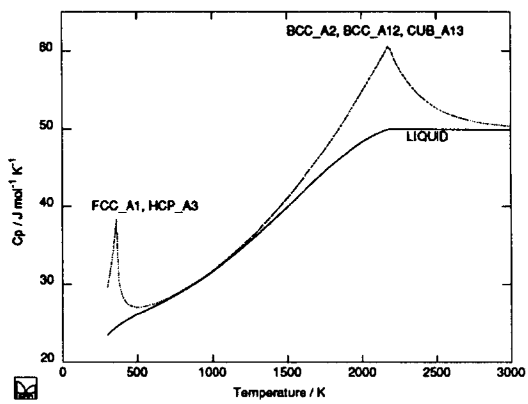
$-4418.94 + 157.48\ T - 26.908\ T\ln(T) + 0.00189435\ T^2 - 1.47721E\text{-}6\ T^3 + 139250\ T^{-1}$ *(298.15 < T < 2180.00)*
$-30431.344 + 344.18\ T - 50.0\ T\ln(T) - 2.88526E32\ T^{-9}$ *(2180.00 < T < 6000.00)*

CUB_A13

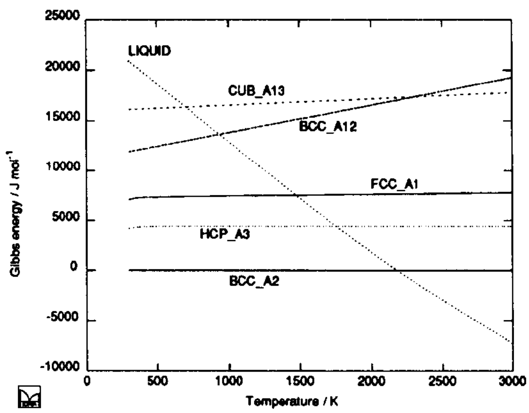
$7042.06 + 158.1076\ T - 26.908\ T\ln(T) + 1.89435E\text{-}3\ T^2 - 1.47721E\text{-}6\ T^3 + 139250\ T^{-1}$ *(298.15 < T < 2180.00)*
$-18970.344 + 344.8076\ T - 50\ T\ln(T) - 2.88526E32\ T^{-9}$ *(2180.00 < T < 6000.00)*

BCC_A12

$2230.06 + 160.1996\ T - 26.908\ T\ln(T) + 1.89435E\text{-}3\ T^2 - 1.47721E\text{-}6\ T^3 + 139250\ T^{-1}$ *(298.15 < T < 2180.00)*
$-23782.344 + 346.8996\ T - 50\ T\ln(T) - 2.88526E32\ T^{-9}$ *(2180.00 < T < 6000.00)*



Heat capacity of Cr



Gibbs energy of phases of Cr relative to BCC_A2

Data for Cr relative to paramagnetic BCC_A2

BCC_A2

$T_N = 311.5$ $B_0 = 0.008$
$A = 7.188E\text{-}6$ $a_0 = 1.7E\text{-}5$ $a_1 = 1.84E\text{-}8$
$K_0 = 5.2E\text{-}12$ $n = 5$

Gmag + Gpres *(298.15 < T < 311.5)*
Gpres *(311.5 < T < 6000.00)*

LIQUID

$A = 7.188E\text{-}6$ $a_0 = 1.7E\text{-}5$ $a_1 = 1.84E\text{-}8$
$K_0 = 9.3E\text{-}12$ $n = 5$

$24339.955 - 11.420225\ T + 2.37615E\text{-}21\ T^7 + \text{Gpres}$ *(298.15 < T < 2180.00)*
$18409.36 - 8.563683\ T + 2.88526E32\ T^{-9} + \text{Gpres}$ *(2180.00 < T < 6000.00)*

FCC_A1

$T_N = 369.667$ $B_0 = 0.82$

$7284 + 0.163\ T$ *(298.15 < T < 6000.00)*

HCP_A3

$T_N = 369.667$ $B_0 = 0.82$

4438 *(298.15 < T < 6000.00)*

CUB_A13

15899 + 0.6276 T *(298.15 < T < 6000.00)*

BCC_A12

11087 + 2.7196 T *(298.15 < T < 6000.00)*

Cs

Source of data: TPIS [BCC_A2, LIQUID]
Saunders et al. [HCP_A3, FCC_A1]

Data for Cs in the form of G-HSER

BCC_A2

$-17373.82 + 436.899787\ T - 90.5212584\ T \ln(T) + 202.9422E{-3}\ T^2 - 127.907669E{-6}\ T^3 + 245245\ T^{-1}$ *(200 < T < 301.59)*
$-13553.817 + 218.689955\ T - 46.7273304\ T \ln(T) + 20.43269E{-3}\ T^2 - 4.074846E{-6}\ T^3 + 181528\ T^{-1} + 7.8E21\ T^{-9}$ *(301.59 < T < 2000)*

LIQUID

$-15282.679 + 429.968752\ T - 90.5212584\ T \ln(T) + 202.9422E{-3}\ T^2 - 127.907669E{-6}\ T^3 + 245245\ T^{-1} - 3.569E{-18}\ T^7$ *(200 < T < 301.59)*
$-11454.038 + 211.728844\ T - 46.7273304\ T \ln(T) + 20.43269E{-3}\ T^2 - 4.074846E{-6}\ T^3 + 181528\ T^{-1}$ *(301.59 < T < 2000)*

HCP_A3

$-16873.82 + 438.899787\ T - 90.5212584\ T \ln(T) + 202.9422E{-3}\ T^2 - 127.907669E{-6}\ T^3 + 245245\ T^{-1}$ *(200 < T < 301.59)*
$-13053.817 + 220.689955\ T - 46.7273304\ T \ln(T) + 20.43269E{-3}\ T^2 - 4.074846E{-6}\ T^3 + 181528\ T^{-1} + 7.8E21\ T^{-9}$ *(301.59 < T < 2000)*

FCC_A1

$-16873.82 + 438.199787\ T - 90.5212584\ T \ln(T) + 202.9422E{-3}\ T^2 - 127.907669E{-6}\ T^3 + 245245\ T^{-1}$ *(200 < T < 301.59)*
$-13053.817 + 219.989955\ T - 46.7273304\ T \ln(T) + 20.43269E{-3}\ T^2 - 4.074846E{-6}\ T^3 + 181528\ T^{-1} + 7.8E21\ T^{-9}$ *(301.59 < T < 2000)*

Data for Cs relative to BCC_A2

LIQUID

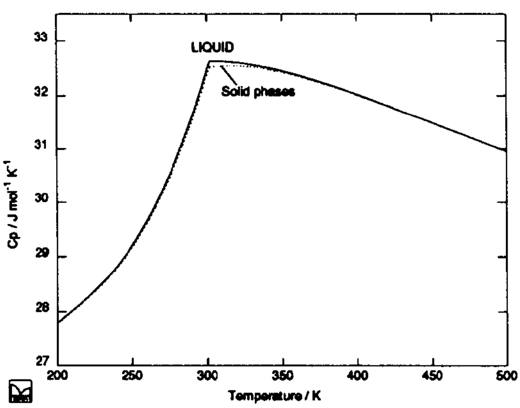
$2091.141 - 6.931035\ T - 3.569E{-18}\ T^7$ *(200.00 < T < 301.59)*
$2099.779 - 6.961111\ T - 7.8E21\ T^{-9}$ *(301.59 < T < 2000.00)*

HCP_A3

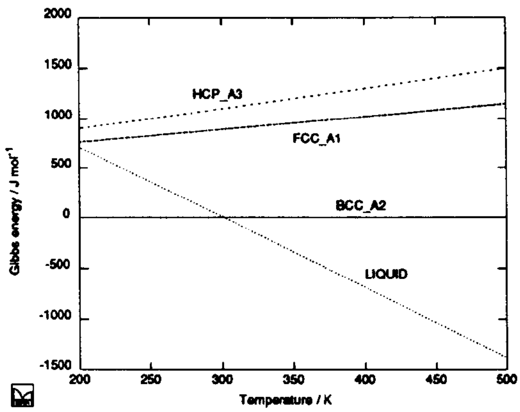
500 + 2.0 T *(298.15 < T < 2000.00)*

FCC_A1

500 + 1.3 T *(298.15 < T < 2000.00)*



Heat capacity of Cs



Gibbs energy of phases of Cs relative to BCC_A2

Cu

Source of data: JANAF [FCC_A1, LIQUID]
Saunders et al. [BCC_A2, HCP_A3]

Data for Cu in the form of G-HSER

FCC_A1

-7770.458 + 130.485235 T - 24.112392 T ln(T) - 2.65684E-3 T^2 + 0.129223E-6 T^3 + 52478 T^{-1} *(298.15 < T < 1357.77)*
-13542.026 + 183.803828 T - 31.38 T ln(T) + 3.642E29 T^{-9} *(1357.77 < T < 3200)*

LIQUID

5194.277 + 120.973331 T - 24.112392 T ln(T) - 2.65684E-3 T^2 + 0.129223E-6 T^3 + 52478 T^{-1} - 5.849E-21 T^7 *(298.15 < T < 1357.77)*
-46.545 + 173.881484 T - 31.38 T ln(T) *(1357.77 < T < 3200)*

BCC_A2

-3753.458 + 129.230235 T - 24.112392 T ln(T) - 2.65684E-3 T^2 + 0.129223E-6 T^3 + 52478 T^{-1} *(298.15 < T < 1357.77)*
-9525.026 + 182.548828 T - 31.38 T ln(T) + 3.642E29 T^{-9} *(1357.77 < T < 3200)*

HCP_A3

-7170.458 + 130.685235 T - 24.112392 T ln(T) - 2.65684E-3 T^2 + 0.129223E-6 T^3 + 52478 T^{-1} *(298.15 < T < 1357.77)*
-12942.026 + 184.003828 T - 31.38 T ln(T) + 3.642E29 T^{-9} *(1357.77 < T < 3200)*

Data relative to FCC_A1

LIQUID

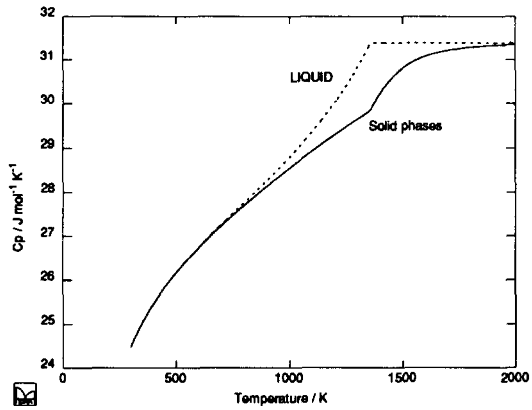
12964.736 - 9.511904 T - 5.849E-21 T^7 *(298.15 < T < 1357.77)*
13495.481 - 9.922344 T - 3.642E29 T^{-9} *(1357.77 < T < 3200)*

BCC_A2

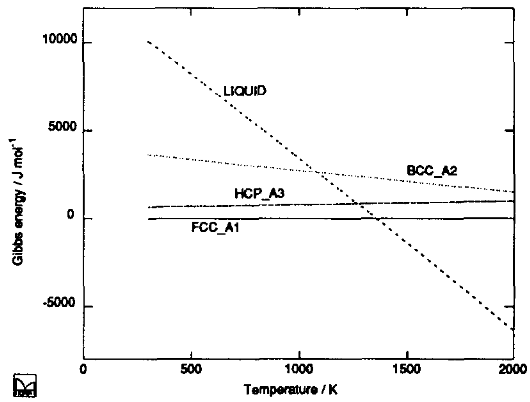
4017 - 1.255 T *(298.15 < T < 3200)*

HCP_A3

600 + 0.2 T *(298.15 < T < 3200)*



Heat capacity of Cu



Gibbs energy of phases of Cu relative to FCC_A1

Dy

Source of data: Hultgren, modified by M H Rand and A T Dinsdale [HCP_A3, BCC_A2, LIQUID]

Data for Dy in the form of G-HSER

HCP_A3

$-9129.216 + 131.734913\ T - 31.3602\ T\ln(T) + 6.14295E\text{-}3\ T^2 - 2.123617E\text{-}6\ T^3 + 31704\ T^{-1}$ *(298.15 < T < 1000.00)*
$46759.596 - 356.59767\ T + 37.102\ T\ln(T) - 29.19595E\text{-}3\ T^2 + 0.999035E\text{-}6\ T^3 - 8228400\ T^{-1}$ *(1000.00 < T < 1400.00)*
$578.987 + 6.964025\ T - 13.3473\ T\ln(T) - 3.82058E\text{-}3\ T^2 - 1.466792E\text{-}6\ T^3$ *(1400.00 < T < 1659.00)*
$-518996.159 + 2659.383552\ T - 353.6421275\ T\ln(T) + 80.893522E\text{-}3\ T^2 - 3.929211E\text{-}6\ T^3 + 137444876\ T^{-1}$ *(1659.00 < T < 3000.00)*

BCC_A2

$-6883.917 + 130.591748\ T - 31.3602\ T\ln(T) + 6.14295E\text{-}3\ T^2 - 2.123617E\text{-}6\ T^3 + 31704\ T^{-1}$ *(298.15 < T < 1000.00)*
$287440.422 - 2533.601262\ T + 344.8751713\ T\ln(T) - 201.179873E\text{-}3\ T^2 + 18.354141E\text{-}6\ T^3 - 42196433\ T^{-1}$ *(1000.00 < T < 1659.00)*
$-32780.012 + 289.980691\ T - 50.208\ T\ln(T)$ *(1659.00 < T < 1684.00)*
$-39830.901 + 328.822231\ T - 55.2727722\ T\ln(T) + 1.523778E\text{-}3\ T^2 - 0.077383E\text{-}6\ T^3 + 1771510\ T^{-1}$ *(1684.00 < T < 3000.00)*

LIQUID

$4010.058 + 124.111866\ T - 31.3602\ T\ln(T) + 6.14295E\text{-}3\ T^2 - 2.123617E\text{-}6\ T^3 + 31704\ T^{-1}$ *(298.15 < T < 1000.00)*
$292367.773 - 2487.678787\ T + 337.5200224\ T\ln(T) - 197.339631E\text{-}3\ T^2 + 18.00701E\text{-}6\ T^3 - 41317706\ T^{-1}$ *(1000.00 < T < 1659.00)*
$-21504.599 + 281.109149\ T - 49.9151\ T\ln(T)$ *(1659.00 < T < 3000.00)*

Data for Dy relative to HCP_A3

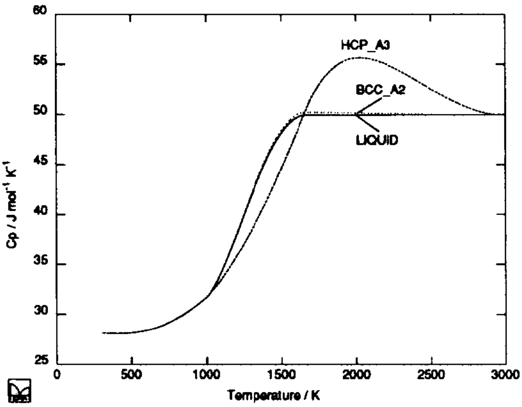
BCC_A2

$2245.298 - 1.143165\ T$ *(298.15 < T < 1000.00)*
$240680.826 - 2177.003592\ T + 307.7731713\ T\ln(T) - 171.983923E\text{-}3\ T^2 + 17.355106E\text{-}6\ T^3 - 33968033\ T^{-1}$ *(1000.00 < T < 1400.00)*
$286861.434 - 2540.565287\ T + 358.2224713\ T\ln(T) - 197.359293E\text{-}3\ T^2 + 19.820933E\text{-}6\ T^3 - 42196433\ T^{-1}$ *(1400.00 < T < 1659.00)*
$486216.147 - 2369.402861\ T + 303.4341275\ T\ln(T) - 80.893522E\text{-}3\ T^2 + 3.929211E\text{-}6\ T^3 - 137444876\ T^{-1}$ *(1659.00 < T < 1684.00)*

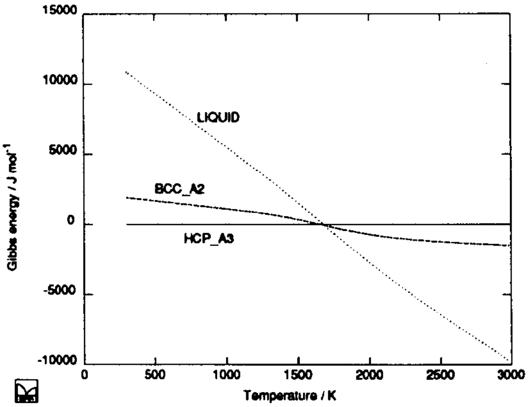
$479165.258 - 2330.561321\ T + 298.3693553\ T\ ln(T) - 79.369744E\text{-}3\ T^2 + 3.851829E\text{-}6\ T^3 - 135673366\ T^{-1}$ *(1684.00 < T < 3000.00)*

LIQUID

$13139.274 - 7.623046\ T$ *(298.15 < T < 1000.00)*
$245608.177 - 2131.081117\ T + 300.4180224\ T\ ln(T) - 168.143681E\text{-}3\ T^2 + 17.007975E\text{-}6\ T^3 - 33089306\ T^{-1}$ *(1000.00 < T < 1400.00)*
$291788.786 - 2494.642812\ T + 350.8673224\ T\ ln(T) - 193.519051E\text{-}3\ T^2 + 19.473802E\text{-}6\ T^3 - 41317706\ T^{-1}$ *(1400.00 < T < 1659.00)*
$497491.560 - 2378.274404\ T + 303.7270275\ T\ ln(T) - 80.893522E\text{-}3\ T^2 + 3.929211E\text{-}6\ T^3 - 137444876\ T^{-1}$ *(1659.00 < T < 3000.00)*



Heat capcacity of Dy



Gibbs energy of phases of Dy relative to HCP_A3

Er

Source of data: Hultgren

Data for Er in the form of G-HSER

HCP_A3

$-8489.136 + 116.698964\ T - 28.3846744\ T\ ln(T) + 0.995792E\text{-}3\ T^2 - 0.952557E\text{-}6\ T^3 + 9581\ T^{-1}$ *(298.15 < T < 1802.00)*
$-445688.206 + 2233.102116\ T - 298.1351305\ T\ ln(T) + 65.950553E\text{-}3\ T^2 - 3.041405E\text{-}6\ T^3 + 123973199\ T^{-1}$ *(1802.00 < T < 3200.00)*

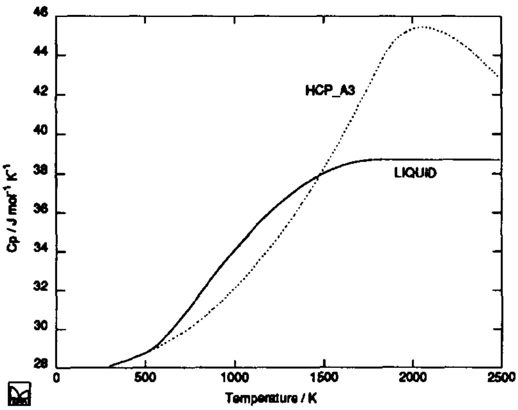
LIQUID

$10892.966 + 106.457118\ T - 28.3846744\ T\ ln(T) + 0.995792E\text{-}3\ T^2 - 0.952557E\text{-}6\ T^3 + 9581\ T^{-1}$ *(298.15 < T < 500.00)*
$17912.678 + 0.355564\ T - 12.0761776\ T\ ln(T) - 14.414687E\text{-}3\ T^2 + 1.316517E\text{-}6\ T^3 - 528122\ T^{-1}$ *(500.00 < T < 1802.00)*
$747.131 + 187.623024\ T - 38.702\ T\ ln(T)$ *(1802.00 < T < 3200.00)*

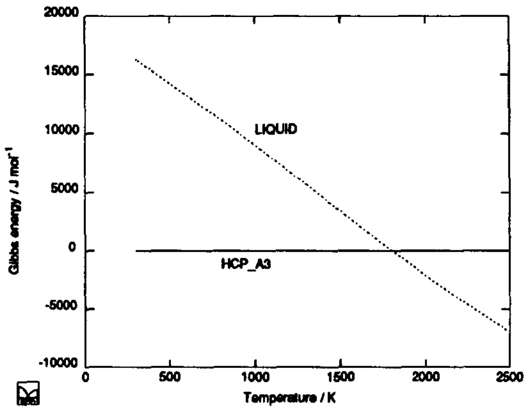
Data for Er relative to HCP_A3

LIQUID

$19382.102 - 10.241846\ T$ *(298.15 < T < 500.00)*
$26401.813 - 116.3434\ T + 16.3084968\ T\ ln(T) - 15.410479E\text{-}3\ T^2 + 2.269074E\text{-}6\ T^3 - 537704\ T^{-1}$ *(500.00 < T < 1802.00)*
$446435.337 - 2045.479093\ T + 259.4331305\ T\ ln(T) - 65.950553E\text{-}3\ T^2 + 3.041405E\text{-}6\ T^3 - 123973199\ T^{-1}$ *(1802.00 < T < 3200.00)*



Heat capacity of Er



Gibbs energy of phases of Er relative to HCP_A3

Eu

Source of data: Hultgren

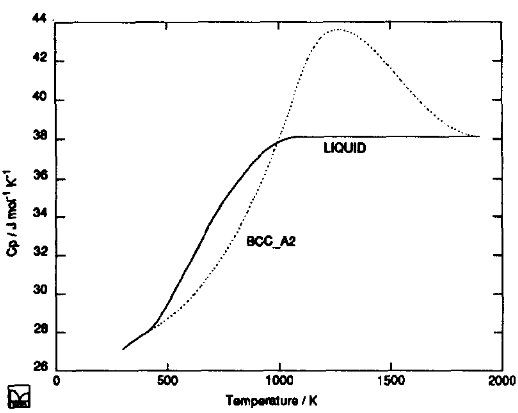
Data for Eu in the form of G-HSER

BCC_A2

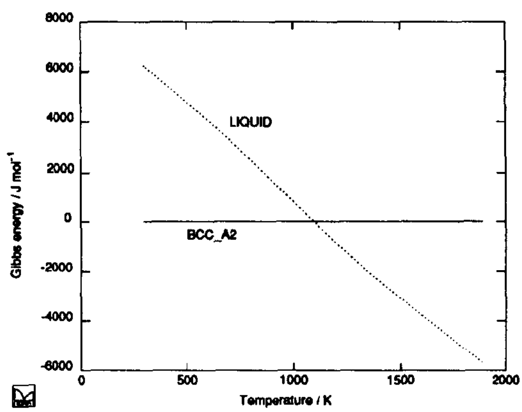
$-9864.965 + 135.836737\ T - 32.8418896\ T\ln(T) + 9.31735E\text{-}3\ T^2 - 4.006564E\text{-}6\ T^3 + 102717\ T^{-1}$ *(298.15 < T < 1095.00)*
$-287423.476 + 2174.733036\ T - 309.3571009\ T\ln(T) + 114.530917E\text{-}3\ T^2 - 8.809866E\text{-}6\ T^3 + 48455305\ T^{-1}$ *(1095.00 < T < 1900.00)*

LIQUID

$-1482.46 + 128.661522\ T - 32.8418896\ T\ln(T) + 9.31735E\text{-}3\ T^2 - 4.006564E\text{-}6\ T^3 + 102717\ T^{-1}$ *(298.15 < T < 400.00)*
$10972.726 - 103.688201\ T + 4.3501554\ T\ln(T) - 36.811218E\text{-}3\ T^2 + 5.452934E\text{-}6\ T^3 - 646908\ T^{-1}$ *(400.00 < T < 1095.00)*
$-6890.641 + 175.517247\ T - 38.11624\ T\ln(T)$ *(1095.00 < T < 1900.00)*



Heat capacity of Eu



Gibbs energy of phases of Eu relative to BCC_A2

Data for Eu relative to BCC_A2

LIQUID

8382.505 - 7.175215 T *(298.15 < T < 400.00)*
20837.691 - 239.524939 T + 37.192045 T ln(T) - 46.128567E-3 T^2 + 9.459498E-6 T^3 - 749625 T^{-1} *(400.00 < T < 1095.00)*
280532.835 - 1999.21579 T + 271.2408609 T ln(T) - 114.530917E-3 T^2 + 8.809866E-6 T^3 - 48455305 T^{-1}
(1095.00 < T < 1900.00)

Fe

Source of data: A Fernandez Guillermet, P Gustafson, High Temp. - High Press., 1985, **16**, 591-610. [BCC_A2, FCC_A1, HCP_A3, LIQUID]
Weiming Huang, TRITA-MAC-0388 [BCC_A12, CUB_A13]

Data for Fe in the form of G-HSER

BCC_A2

T_C = 1043	B_0 = 2.22	
A = 7.042095E-6	a_0 = 2.3987E-5	a_1 = 2.569E-8
K_0 = 5.965E-12	K_1 = 6.5152E-17	n = 4.7041

1225.7 + 124.134 T - 23.5143 T ln(T) - 0.00439752 T^2 - 5.89269E-8 T^3 + 77358.5 T^{-1} + Gmag + Gpres
(298.15 < T < 1811.00)
-25383.581 + 299.31255 T - 46.0 T ln(T) + 2.2960305E31 T^{-9} + Gmag + Gpres *(1811.00 < T < 6000.00)*

FCC_A1

T_N = 67	B_0 = 0.7	
A = 6.688726E-6	a_0 = 7.3097E-5	
K_0 = 6.2951E-12	K_1 = 6.5152E-17	n = 5.1665

-236.7 + 132.416 T - 24.6643 T ln(T) - 0.00375752 T^2 - 5.89269E-8 T^3 + 77358.5 T^{-1} + Gmag + Gpres
(298.15 < T < 1811.00)
-27097.396 + 300.25256 T - 46.0 T ln(T) + 2.78854E31 T^{-9} + Gmag + Gpres *(1811.00 < T < 6000.00)*

HCP_A3

A = 6.59121E-6	a_0 = 7.3646E-5	
K_0 = 6.2951E-12	K_1 = 6.5152E-17	n = 5.1665

-2480.08 + 136.725 T - 24.6643 T ln(T) - 0.00375752 T^2 - 5.89269E-8 T^3 + 77358.5 T^{-1} + Gpres *(298.15 < T < 1811.00)*
-29340.78 + 304.56206 T - 46.0 T ln(T) + 2.78854E31 T^{-9} + Gpres *(1811.00 < T < 6000.00)*

LIQUID

A = 6.62574E-6	a_0 = 10.7895E-5	a_3 = -25.79493
K_0 = 0.75475E-12	K_1 = 485.09E-17	n = 6.59834

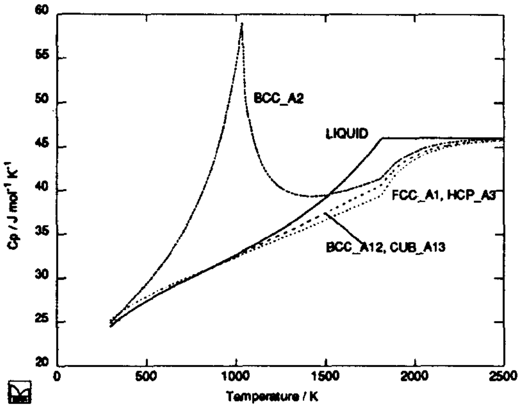
13265.87 + 117.57557 T - 23.5143 T ln(T) - 0.00439752 T^2 - 5.89269E-8 T^3 + 77358.5 T^{-1} - 3.6751551E-21 T^7 + Gpres
(298.15 < T < 1811.00)
-10838.83 + 291.302 T - 46.0 T ln(T) + Gpres *(1811.00 < T < 6000.00)*

BCC_A12

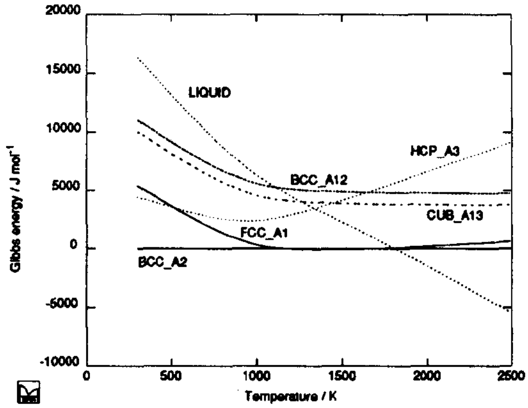
5970.7 + 124.134 T - 23.5143 T ln(T) - 0.00439752 T^2 - 5.89269E-8 T^3 + 77358.5 T^{-1} *(298.15 < T < 1811.00)*
-20638.581 + 299.31255 T - 46.0 T ln(T) + 2.2960305E31 T^{-9} *(1811.00 < T < 6000.00)*

CUB_A13

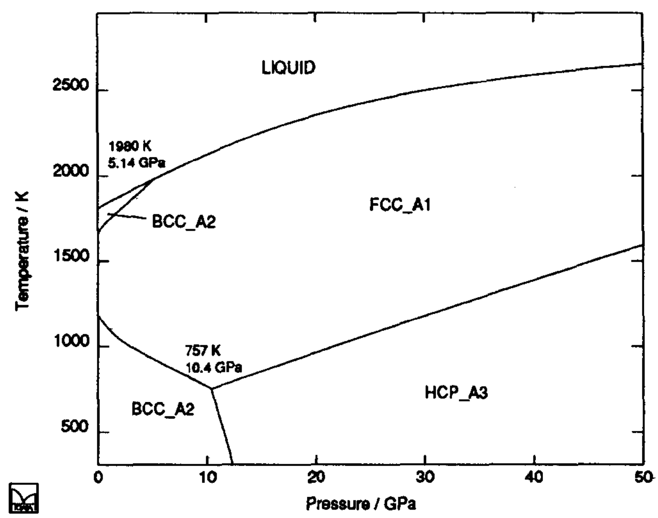
4970.7 + 124.134 T - 23.5143 T ln(T) - 0.00439752 T^2 - 5.89269E-8 T^3 + 77358.5 T^{-1} *(298.15 < T < 1811.00)*
-21638.581 + 299.31255 T - 46.0 T ln(T) + 2.2960305E31 T^{-9} *(1811.00 < T < 6000.00)*



Heat capacity of Fe



Gibbs energy of phases of Fe relative to BCC_A2



P-T phase diagram for Fe

Data for Fe relative to paramagnetic BCC_A2

BCC_A2

$T_C = 1043$	$B_0 = 2.22$	
$A = 7.042095E\text{-}6$	$a_0 = 2.3987E\text{-}5$	$a_1 = 2.569E\text{-}8$
$K_0 = 5.965E\text{-}12$	$K_1 = 6.5152E\text{-}17$	$n = 4.7041$

Gmag + Gpres *(298.15 < T < 6000.00)*

FCC_A1

$T_N = 67$ $B_0 = 0.7$
$A = 6.688726E\text{-}6$ $a_0 = 7.3097E\text{-}5$
$K_0 = 6.2951E\text{-}12$ $K_1 = 6.5152E\text{-}17$ $n = 5.1665$

-1462.4 + 8.282 T - 1.15 T ln(T) + 0.00064 T^2 + Gmag + Gpres *(298.15 < T < 1811.00)*
-1713.815 + 0.94001 T + 0.4925095E31 T^{-9} + Gmag + Gpres *(1811.00 < T < 6000.00)*

HCP_A3

$A = 6.59121E\text{-}6$ $a_0 = 7.3646E\text{-}5$
$K_0 = 6.2951E\text{-}12$ $K_1 = 6.5152E\text{-}17$ $n = 5.1665$

-3705.78 + 12.591 T - 1.15 T ln(T) + 0.00064 T^2 + Gpres *(298.15 < T < 1811.00)*
-3957.199 + 5.24951 T + 0.4925095E31 T^{-9} + Gpres *(1811.00 < T < 6000.00)*

LIQUID

$A = 6.62574E\text{-}6$ $a_0 = 10.7895E\text{-}5$ $a_3 = -25.79493$
$K_0 = 0.75475E\text{-}12$ $K_1 = 485.09E\text{-}17$ $n = 6.59834$

12040.17 - 6.55843 T - 3.6751551E-21 T^7 + Gpres *(298.15 < T < 1811.00)*
14544.751 - 8.01055 T - 2.2960305E31 T^{-9} + Gpres *(1811.00 < T < 6000.00)*

CUB_A13

3745 *(298.15 < T < 6000.00)*

BCC_A12

4745 *(298.15 < T < 6000.00)*

Ga

Source of data : TPIS [ORTHORHOMBIC, LIQUID]
Ansara [BCT_A5]
Saunders et al. [FCC_A1, HCP_A3, BCC_A2, TET_A6]

Data for Ga in the form of G-HSER

ORTHORHOMBIC

-21312.331 + 585.263691 T - 108.2287832 T ln(T) + 227.155636E-3 T^2 - 118.575257E-6 T^3 + 439954 T^{-1} *(298.15 < T < 302.9146)*
-7055.643 + 132.73019 T - 26.0692906 T ln(T) + 0.1506E-3 T^2 - 0.040173E-6 T^3 - 118332 T^{-1} + 1.645E23 T^{-9} *(302.9146 < T < 4000)*

LIQUID

-15821.033 + 567.189696 T - 108.2287832 T ln(T) + 227.155636E-3 T^2 - 118.575257E-6 T^3 + 439954 T^{-1} - 7.017E-17 T^7 *(298.15 < T < 302.9146)*
-1389.188 + 114.049043 T - 26.0692906 T ln(T) + 0.1506E-3 T^2 - 0.040173E-6 T^3 - 118332 T^{-1} *(302.9146 < T < 4000)*

BCC_A2

-16812.331 + 573.563691 T - 108.2287832 T ln(T) + 227.155636E-3 T^2 - 118.575257E-6 T^3 + 439954 T^{-1} *(298.15 < T < 302.9146)*
-2555.643 + 121.03019 T - 26.0692906 T ln(T) + 0.1506E-3 T^2 - 0.040173E-6 T^3 - 118332 T^{-1} + 1.645E23 T^{-9} *(302.9146 < T < 4000)*

BCT_A5

$-17466.331 + 575.463691\ T - 108.2287832\ T\ \ln(T) + 227.155636E\text{-}3\ T^2 - 118.575257E\text{-}6\ T^3 + 439954\ T^{-1}$ *(298.15 < T < 302.9146)*

$-3209.643 + 122.93019\ T - 26.0692906\ T\ \ln(T) + 0.1506E\text{-}3\ T^2 - 0.040173E\text{-}6\ T^3 - 118332\ T^{-1} + 1.645E23\ T^{-9}$ *(302.9146 < T < 4000)*

FCC_A1

$-17512.331 + 575.063691\ T - 108.2287832\ T\ \ln(T) + 227.155636E\text{-}3\ T^2 - 118.575257E\text{-}6\ T^3 + 439954\ T^{-1}$ *(298.15 < T < 302.9146)*

$-3255.643 + 122.53019\ T - 26.0692906\ T\ \ln(T) + 0.1506E\text{-}3\ T^2 - 0.040173E\text{-}6\ T^3 - 118332\ T^{-1} + 1.645E23\ T^{-9}$ *(302.9146 < T < 4000)*

HCP_A3

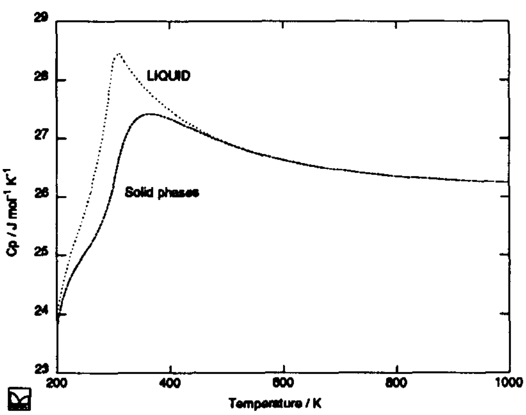
$-16812.331 + 575.763691\ T - 108.2287832\ T\ \ln(T) + 227.155636E\text{-}3\ T^2 - 118.575257E\text{-}6\ T^3 + 439954\ T^{-1}$ *(298.15 < T < 302.9146)*

$-2555.643 + 123.23019\ T - 26.0692906\ T\ \ln(T) + 0.1506E\text{-}3\ T^2 - 0.040173E\text{-}6\ T^3 - 118332\ T^{-1} + 1.645E23\ T^{-9}$ *(302.9146 < T < 4000)*

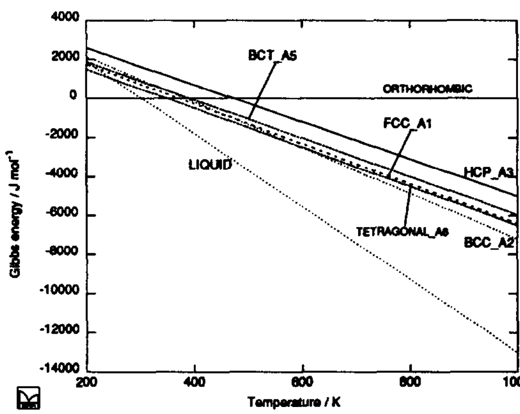
TETRAGONAL_A6

$-17812.331 + 575.263691\ T - 108.2287832\ T\ \ln(T) + 227.155636E\text{-}3\ T^2 - 118.575257E\text{-}6\ T^3 + 439954\ T^{-1}$ *(298.15 < T < 302.9146)*

$-3555.643 + 122.73019\ T - 26.0692906\ T\ \ln(T) + 0.1506E\text{-}3\ T^2 - 0.040173E\text{-}6\ T^3 - 118332\ T^{-1} + 1.645E23\ T^{-9}$ *(302.9146 < T < 4000)*



Heat capacity of Ga



Gibbs energy of phases of Ga relative to ORTHORHOMBIC

Data relative to ORTHORHOMBIC

LIQUID

$5491.298 - 18.073995\ T - 7.017E\text{-}17\ T^7$ *(298.15 < T < 302.9146)*

$5666.455 - 18.681147\ T - 1.645E23\ T^{-9}$ *(302.9146 < T < 4000)*

BCC_A2

$4500 - 11.7\ T$ *(298.15 < T < 4000)*

BCT_A5

$3846 - 9.8\ T$ *(298.15 < T < 4000)*

FCC_A1

3800 - 10.2 T (298.15 < T < 4000)

HCP_A3

4500 - 9.5 T (298.15 < T < 4000)

TETRAGONAL_A6

3500 - 10 T (298.15 < T < 4000)

Gd

Source of data: Hultgren, modified by M H Rand and A T Dinsdale [HCP_A3, BCC_A2 and LIQUID]

Data for Gd in the form of G-HSER

HCP_A3

$T_C = 291.8$ $B_0 = 3.0$

-11600.525 + 151.111948 T - 32.5013 T ln(T) + 2.81265E-3 T^2 - 1.081237E-6 T^3 + 421363 T^{-1} + Gmag (298.15 < T < 1300.00)
-8106.163 + 115.953605 T - 27.459 T ln(T) - 0.276123E-3 T^2 - 0.737325E-6 T^3 + Gmag (1300.00 < T < 1535.00)
-125618.511 + 711.994197 T - 103.4037575 T ln(T) + 15.817949E-3 T^2 - 0.672548E-6 T^3 + 30183452 T^{-1} + Gmag (1535.00 < T < 3600.00)

BCC_A2

-8028.44 + 148.806951 T - 32.5013 T ln(T) + 2.81265E-3 T^2 - 1.081237E-6 T^3 + 421363 T^{-1} (298.15 < T < 1000.00)
86879.486 - 747.960507 T + 95.1961984 T ln(T) - 72.542756E-3 T^2 + 7.116157E-6 T^3 - 12664161 T^{-1} (1000.00 < T < 1535.00)
-14097.626 + 192.503674 T - 37.656 T ln(T) (1535.00 < T < 1587.00)
-18620.027 + 217.622313 T - 40.9284427 T ln(T) + 0.953751E-3 T^2 - 0.041967E-6 T^3 + 1107440 T^{-1} (1587.00 < T < 3600.00)

LIQUID

1957.09 + 142.499221 T - 32.5013 T ln(T) + 2.81265E-3 T^2 - 1.081237E-6 T^3 + 421363 T^{-1} (298.15 < T < 1000.00)
80721.646 - 609.764875 T + 74.8351133 T ln(T) - 61.538012E-3 T^2 + 6.061728E-6 T^3 - 10325075 T^{-1} (1000.00 < T < 1535.00)
-3485.133 + 182.116258 T - 37.1539 T ln(T) (1535.00 < T < 3600.00)

Data for Gd relative to paramagnetic HCP_A3

HCP_A3

$T_C = 291.8$ $B_0 = 3.0$

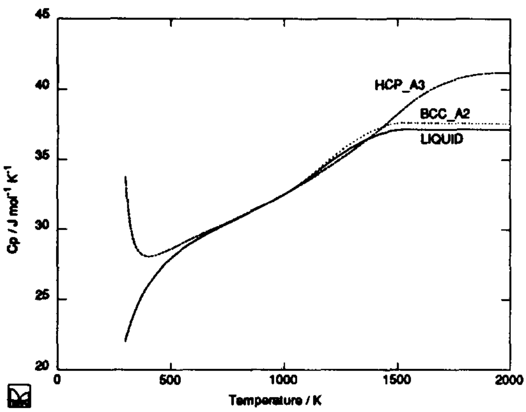
Gmag

BCC_A2

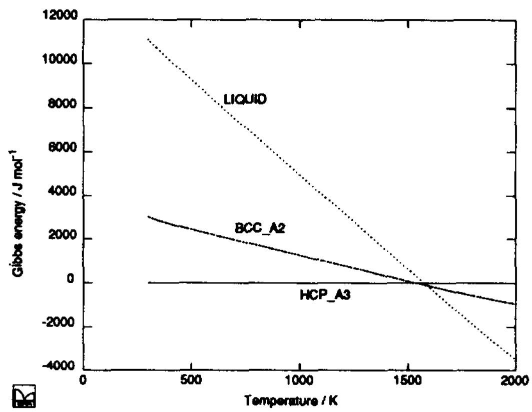
3572.085 - 2.304997 T (298.15 < T < 1000.00)
98480.010 - 899.072455 T + 127.6974984 T ln(T) - 75.355406E-3 T^2 + 8.197393E-6 T^3 - 13085523 T^{-1} (1000.00 < T < 1300.00)
94985.649 - 863.914112 T + 122.6551984 T ln(T) - 72.266633E-3 T^2 + 7.853482E-6 T^3 - 12664161 T^{-1} (1300.00 < T < 1535.00)
111520.885 - 519.490522 T + 65.7477575 T ln(T) - 15.817949E-3 T^2 + 0.672548E-6 T^3 - 30183452 T^{-1} (1535.00 < T < 1587.00)
106998.484 - 494.371883 T + 62.4753149 T ln(T) - 14.864198E-3 T^2 + 0.630581E-6 T^3 - 29076013 T^{-1} (1587.00 < T < 3600.00)

LIQUID

13557.615 - 8.612727 T *(298.15 < T < 1000.00)*
92322.171 - 760.876823 T + 107.3364133 T ln(T) - 64.350662E-3 T^2 + 7.142964E-6 T^3 - 10746438 T^{-1} *(1000.00 < T < 1300.00)*
88827.809 - 725.718480 T + 102.2941133 T ln(T) - 61.261889E-3 T^2 + 6.799053E-6 T^3 - 10325075 T^{-1} *(1300.00 < T < 1535.00)*
122133.378 - 529.877938 T + 66.2498575 T ln(T) - 15.817949E-3 T^2 + 0.672548E-6 T^3 - 30183452 T^{-1} *(1535.00 < T < 3600.00)*



Heat capacity of Gd



Gibbs energy of phases of Gd relative to HCP_A3

Ge

Source of data: Hultgren [DIAMOND_A4, LIQUID]
Saunders et al. [FCC_A1, BCC_A2, HCP_A3]

Data for Ge in the form of G-HSER

DIAMOND_A4

-9486.153 + 165.635573 T - 29.5337682 T ln(T) + 5.568297E-3 T^2 - 1.513694E-6 T^3 + 163298 T^{-1} *(298.15 < T < 900)*
-5689.239 + 102.86087 T - 19.8536239 T ln(T) - 3.672527E-3 T^2 *(900 < T < 1211.4)*
-9548.204 + 156.708024 T - 27.6144 T ln(T) - 8.598E28 T^{-9} *(1211.4 < T < 3200)*

LIQUID

27655.337 + 134.94853 T - 29.5337682 T ln(T) + 5.568297E-3 T^2 - 1.513694E-6 T^3 + 163298 T^{-1} + 8.5663E-21 T^7 *(298.15 < T < 900)*
31452.25 + 72.173826 T - 19.8536239 T ln(T) - 3.672527E-3 T^2 + 8.5663E-21 T^7 *(900 < T < 1211.4)*
27243.473 + 126.324186 T - 27.6144 T ln(T) *(1211.4 < T < 3200)*

BCC_A2

24613.847 + 142.135573 T - 29.5337682 T ln(T) + 5.568297E-3 T^2 - 1.513694E-6 T^3 + 163298 T^{-1} *(298.15 < T < 900)*
28410.761 + 79.36087 T - 19.8536239 T ln(T) - 3.672527E-3 T^2 *(900 < T < 1211.4)*
24551.796 + 133.208024 T - 27.6144 T ln(T) - 8.598E28 T^{-9} *(1211.4 < T < 3200)*

FCC_A1

26513.847 + 143.335573 T - 29.5337682 T ln(T) + 5.568297E-3 T^2 - 1.513694E-6 T^3 + 163298 T^{-1} *(298.15 < T < 900)*
30310.761 + 80.56087 T - 19.8536239 T ln(T) - 3.672527E-3 T^2 *(900 < T < 1211.4)*
26451.796 + 134.408024 T - 27.6144 T ln(T) - 8.598E28 T^{-9} *(1211.4 < T < 3200)*

HCP_A3

$25513.847 + 144.135573\,T - 29.5337682\,T\ln(T) + 5.568297E\text{-}3\,T^2 - 1.513694E\text{-}6\,T^3 + 163298\,T^{-1}$ *(298.15 < T < 900)*
$29310.761 + 81.36087\,T - 19.8536239\,T\ln(T) - 3.672527E\text{-}3\,T^2$ *(900 < T < 1211.4)*
$25451.796 + 135.208024\,T - 27.6144\,T\ln(T) - 8.598E28\,T^{-9}$ *(1211.4 < T < 3200)*

Data relative to DIAMOND_A4

LIQUID

$37141.49 - 30.687044\,T + 8.5663E\text{-}21\,T^7$ *(298.15 < T < 1211.4)*
$36791.677 - 30.383838\,T + 8.598E28\,T^{-9}$ *(1211.4 < T < 3200)*

BCC_A2

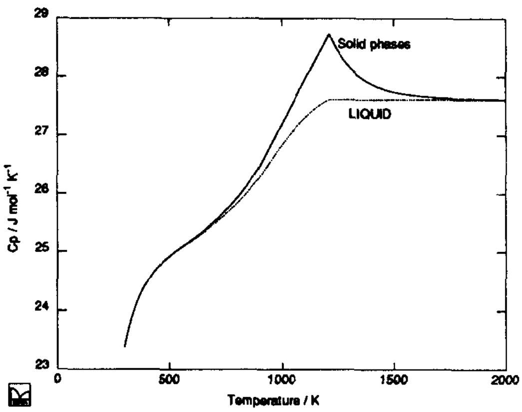
$34100 - 23.5\,T$ *(298.15 < T < 3200)*

FCC_A1

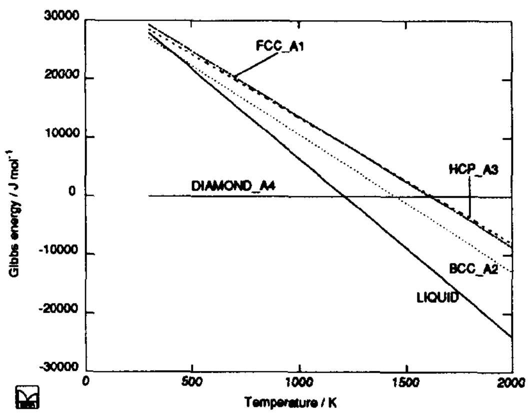
$36000 - 22.3\,T$ *(298.15 < T < 3200)*

HCP_A3

$35000 - 21.5\,T$ *(298.15 < T < 3200)*



Heat capacity of Ge



Gibbs energy of phases of Ge relative to DIAMOND_A4

Hf

Source of data: N Saunders and A T Dinsdale, Unpublished work.

Data for Hf in the form of G-HSER

HCP_A3

$-6987.297 + 110.744026\,T - 22.7075\,T\ln(T) - 4.146145E\text{-}3\,T^2 - 0.000477E\text{-}6\,T^3 - 22590\,T^{-1}$ *(298.15 < T < 2506.00)*
$-1446776.329 + 6193.609991\,T - 787.5363829\,T\ln(T) + 173.5215E\text{-}3\,T^2 - 7.575759E\text{-}6\,T^3 + 501742495\,T^{-1}$ *(2506.00 < T < 3000.00)*

BCC_A2

$5370.703 + 103.836026\,T - 22.8995\,T\ln(T) - 4.206605E\text{-}3\,T^2 + 0.871923E\text{-}6\,T^3 - 22590\,T^{-1} - 0.1446E\text{-}9\,T^4$ *(298.15 < T < 2506.00)*

$1912456.771 - 8624.20573\ T + 1087.6141247\ T\ \ln(T) - 286.857065E{-3}\ T^2 + 13.427829E{-6}\ T^3 - 610085091\ T^{-1}$ *(2506.00 < T < 3000.00)*

LIQUID

$20414.959 + 99.790933\ T - 22.7075\ T\ \ln(T) - 4.146145E{-3}\ T^2 - 0.000477E{-6}\ T^3 - 22590\ T^{-1}$ *(298.15 < T < 1000.00)*
$49731.499 - 149.91739\ T + 12.116812\ T\ \ln(T) - 21.262021E{-3}\ T^2 + 1.376466E{-6}\ T^3 - 4449699\ T^{-1}$ *(1000.00 < T < 2506.00)*
$-4247.217 + 265.470523\ T - 44\ T\ \ln(T)$ *(2506.00 < T < 3000.00)*

FCC_A1

$3012.703 + 108.544026\ T - 22.7075\ T\ \ln(T) - 4.146145E{-3}\ T^2 - 0.000477E{-6}\ T^3 - 22590\ T^{-1}$ *(298.15 < T < 2506.00)*
$-1436776.329 + 6191.409991\ T - 787.5363829\ T\ \ln(T) + 173.5215E{-3}\ T^2 - 7.575759E{-6}\ T^3 + 501742495\ T^{-1}$ *(2506.00 < T < 3000.00)*

Data for Hf relative to HCP_A3

BCC_A2

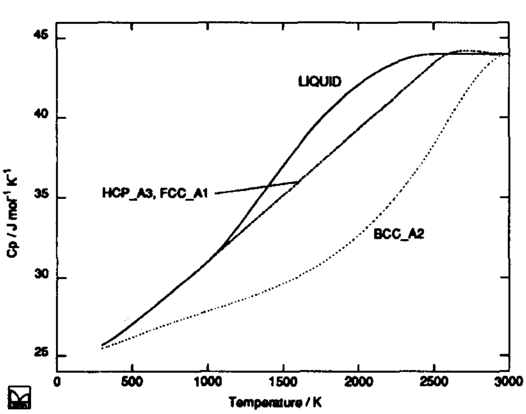
$12358.0 - 6.908\ T - 0.192\ T\ \ln(T) - 0.06046E{-3}\ T^2 + 0.8724E{-6}\ T^3 - 0.1446E{-9}\ T^4$ *(298.15 < T < 2506.00)*
$3359233.1 - 14817.815721\ T + 1875.1505076\ T\ \ln(T) - 460.378566E{-3}\ T^2 + 21.003588E{-6}\ T^3 - 1111827587\ T^{-1}$ *(2506.00 < T < 3000.00)*

LIQUID

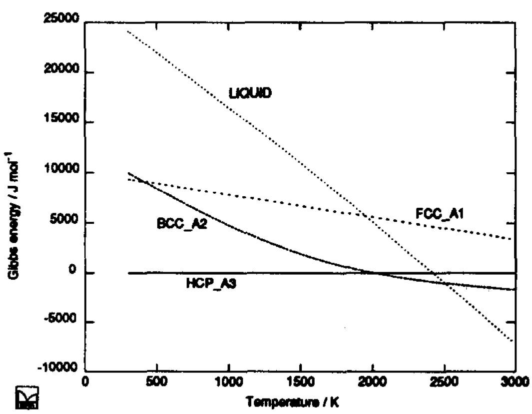
$27402.256 - 10.953094\ T$ *(298.15 < T < 1000.00)*
$56718.796 - 260.661417\ T + 34.824312\ T\ \ln(T) - 17.115876E{-3}\ T^2 + 1.376943E{-6}\ T^3 - 4427109\ T^{-1}$ *(1000.00 < T < 2506.00)*
$1442529.112 - 5928.139468\ T + 743.5363829\ T\ \ln(T) - 173.521500E{-3}\ T^2 + 7.575759E{-6}\ T^3 - 501742495\ T^{-1}$ *(2506.00 < T < 3000.00)*

FCC_A1

$10000.0 - 2.2\ T$ *(298.15 < T < 3000.00)*



Heat capacity of Hf



Gibbs energy of phases of Hf relative to HCP_A3

Hg

Source of data: Hultgren [RHOMBO_A10, LIQUID]

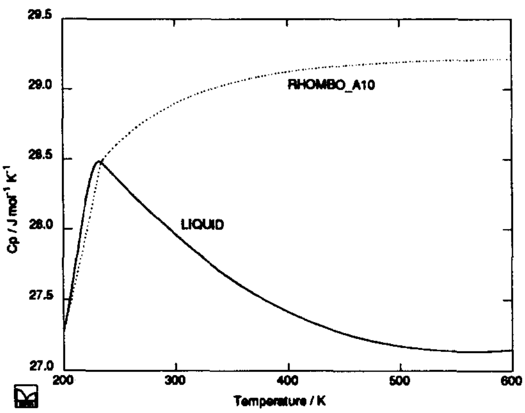
Data for Hg in the form of G-HSER

LIQUID

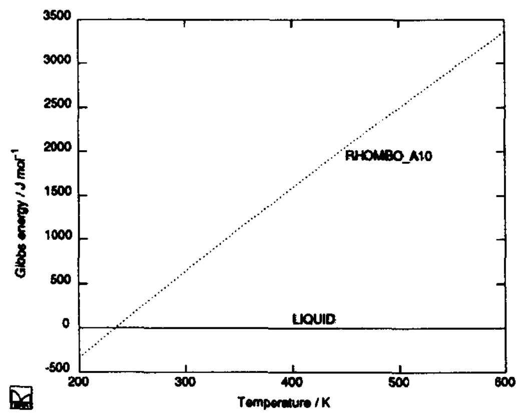
$82356.855 - 3348.194658 T + 618.1933082 T \ln(T) - 2028.2337E-3 T^2 + 1183.982129E-6 T^3 - 2366612 T^{-1}$ $(200 < T < 234.321)$
$-8961.207 + 135.232291 T - 32.257 T \ln(T) + 9.7977E-3 T^2 - 3.20695E-6 T^3 + 6670 T^{-1}$ $(234.321 < T < 400)$
$-7970.627 + 112.33345 T - 28.414 T \ln(T) + 3.18535E-3 T^2 - 1.077802E-6 T^3 - 41095 T^{-1}$ $(400 < T < 700)$
$-7161.338 + 90.797305 T - 24.87 T \ln(T) - 1.66775E-3 T^2 + 0.008737E-6 T^3 - 27495 T^{-1}$ $(700 < T < 2000)$

RHOMBO_A10

$-10668.401 + 123.274598 T - 28.847 T \ln(T) + 16.99705E-3 T^2 - 24.555667E-6 T^3 + 13330 T^{-1}$ $(200 < T < 234.321)$
$-11425.394 + 135.928158 T - 30.2091 T \ln(T) + 1.07555E-3 T^2 - 0.228298E-6 T^3 + 35545 T^{-1}$ $(234.321 < T < 2000)$



Heat capacity of Hg



Gibbs energy of phases of Hg relative to LIQUID

Data relative to LIQUID

RHOMBO_A10

$-93025.255 + 3471.469256 T - 647.0403082 T \ln(T) + 2045.23075E-3 T^2 - 1208.537796E-6 T^3 + 2379942 T^{-1}$ $(200 < T < 234.321)$
$-2464.187 + 0.695868 T + 2.0479 T \ln(T) - 8.72215E-3 T^2 + 2.978652E-6 T^3 + 28875 T^{-1}$ $(234.321 < T < 400)$
$-3454.767 + 23.594708 T - 1.7951 T \ln(T) - 2.1098E-3 T^2 + 0.849503E-6 T^3 + 76640 T^{-1}$ $(400 < T < 700)$
$-4264.056 + 45.130853 T - 5.3391 T \ln(T) + 2.7433E-3 T^2 - 0.237035E-6 T^3 + 63040 T^{-1}$ $(700 < T < 2000)$

Ho

Source of data: Hultgren, modified by M H Rand and A T Dinsdale [HCP_A3, BCC_A2, LIQUID]

Data for Ho in the form of G-HSER

HCP_A3

$-7612.429 + 86.593171 T - 23.4879 T \ln(T) - 8.27315E-3 T^2 + 2.375467E-6 T^3$ $(298.15 < T < 600.00)$
$-10917.688 + 182.475691 T - 39.6932 T \ln(T) + 18.20065E-3 T^2 - 4.829733E-6 T^3$ $(600.00 < T < 900.00)$
$46646.188 - 421.474473 T + 48.0595 T \ln(T) - 42.4634E-3 T^2 + 3.233133E-6 T^3 - 7185900 T^{-1}$ $(900.00 < T < 1200.00)$
$27786.061 - 156.162846 T + 8.28608 T \ln(T) - 10.82725E-3 T^2 - 1.112352E-6 T^3 - 6183850 T^{-1}$ $(1200.00 < T < 1703.00)$
$-825364.662 + 4248.379056 T - 558.9506818 T \ln(T) + 139.111904E-3 T^2 - 6.824652E-6 T^3 + 219952973 T^{-1}$ $(1703.00 < T < 3000.00)$

BCC_A2

-3881.2 + 84.532855 T - 23.4879 T ln(T) - 8.27315E-3 T^2 + 2.375467E-6 T^3 *(298.15 < T < 600.00)*
-7186.458 + 180.415375 T - 39.6932 T ln(T) + 18.20065E-3 T^2 - 4.829733E-6 T^3 *(600.00 < T < 900.00)*
50377.417 - 423.53479 T + 48.0595 T ln(T) - 42.4634E-3 T^2 + 3.233133E-6 T^3 - 7185900 T^{-1} *(900.00 < T < 1000.00)*
185512.056 - 1635.740669 T + 218.9372486 T ln(T) - 135.16576E-3 T^2 + 12.168911E-6 T^3 - 26729747 T^{-1} *(1000.00 < T < 1703.00)*
-28867.901 + 272.946988 T - 48.116 T ln(T) *(1703.00 < T < 1745.00)*
-152754.148 + 939.764197 T - 134.7930638 T ln(T) + 25.544089E-3 T^2 - 1.287517E-6 T^3 + 32050889 T^{-1} *(1745.00 < T < 3000.00)*

LIQUID

9649.743 + 76.600977 T - 23.4879 T ln(T) - 8.27315E-3 T^2 + 2.375467E-6 T^3 *(298.15 < T < 600.00)*
6344.484 + 172.483497 T - 39.6932 T ln(T) + 18.20065E-3 T^2 - 4.829733E-6 T^3 *(600.00 < T < 900.00)*
63908.36 - 431.466667 T + 48.0595 T ln(T) - 42.4634E-3 T^2 + 3.233133E-6 T^3 - 7185900 T^{-1} *(900.00 < T < 1000.00)*
124706.283 - 994.683024 T + 127.9577778 T ln(T) - 88.196514E-3 T^2 + 8.008222E-6 T^3 - 15727191 T^{-1} *(1000.00 < T < 1703.00)*
-9809.781 + 230.793918 T - 43.932 T ln(T) *(1703.00 < T < 3000.00)*

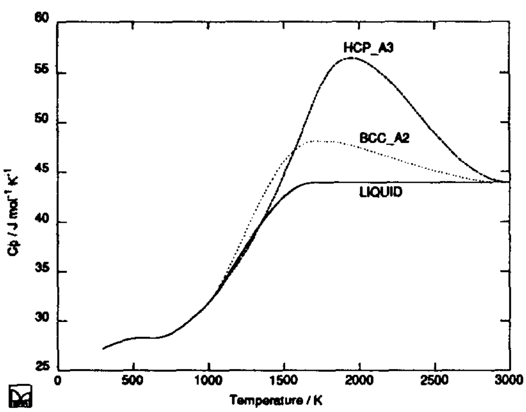
Data for Ho relative to HCP_A3

BCC_A2

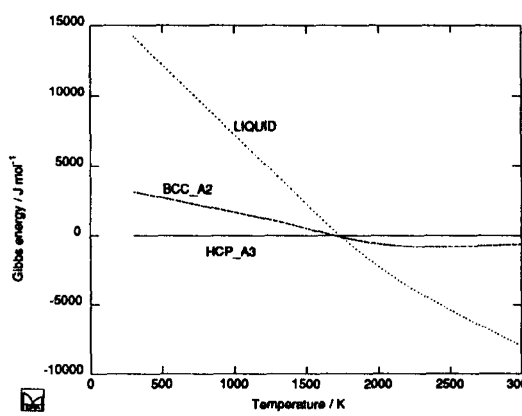
3731.229 - 2.060317 T *(298.15 < T < 1000.00)*
138865.868 - 1214.266196 T + 170.8777486 T ln(T) - 92.702360E-3 T^2 + 8.935778E-6 T^3 - 19543847 T^{-1} *(1000.00 < T < 1200.00)*
157725.995 - 1479.577823 T + 210.6511686 T ln(T) - 124.338510E-3 T^2 + 13.281263E-6 T^3 - 20545897 T^{-1} *(1200.00 < T < 1703.00)*
796496.760 - 3975.432068 T + 510.8346818 T ln(T) - 139.111904E-3 T^2 + 6.824652E-6 T^3 - 219952973 T^{-1} *(1703.00 < T < 1745.00)*
672610.514 - 3308.614860 T + 424.1576180 T ln(T) - 113.567815E-3 T^2 + 5.537135E-6 T^3 - 187902084 T^{-1} *(1745.00 < T < 3000.00)*

LIQUID

17262.172 - 9.992194 T *(298.15 < T < 1000.00)*
78060.095 - 573.208551 T + 79.8982778 T ln(T) - 45.733114E-3 T^2 + 4.775089E-6 T^3 - 8541291 T^{-1} *(1000.00 < T < 1200.00)*
96920.222 - 838.520178 T + 119.6716978 T ln(T) - 77.369264E-3 T^2 + 9.120574E-6 T^3 - 9543341 T^{-1} *(1200.00 < T < 1703.00)*
815554.880 - 4017.585139 T + 515.0186818 T ln(T) - 139.111904E-3 T^2 + 6.824652E-6 T^3 - 219952973 T^{-1} *(1703.00 < T < 3000.00)*



Heat capacity of Ho



Gibbs energy of phases of Ho relative to HCP_A3

In

Source of data: TPIS [TETRAGONAL_A6, LIQUID]
I Ansara, Unpublished work, 1989 [HCP_A3, FCC_A1]
Saunders et al. [BCC_A2]
J P Nabot, I Ansara, Bull. Alloy Phase Diag., 1987, 8, 246 [TET_ALPHA1]

Data for In in the form of G-HSER

TETRAGONAL_A6

$-6978.89 + 92.338115\,T - 21.8386\,T\ln(T) - 5.72566E\text{-}3\,T^2 - 2.120321E\text{-}6\,T^3 - 22906\,T^{-1}$ *(298.15 < T < 429.75)*
$-7033.516 + 124.476588\,T - 27.4562\,T\ln(T) + 0.54607E\text{-}3\,T^2 - 0.08367E\text{-}6\,T^3 - 211708\,T^{-1} + 3.53E22\,T^{-9}$ *(429.75 < T < 3800)*

LIQUID

$-3696.798 + 84.701255\,T - 21.8386\,T\ln(T) - 5.72566E\text{-}3\,T^2 - 2.120321E\text{-}6\,T^3 - 22906\,T^{-1} - 5.59E\text{-}20\,T^7$ *(298.15 < T < 429.75)*
$-3749.81 + 116.835784\,T - 27.4562\,T\ln(T) + 0.54607E\text{-}3\,T^2 - 0.08367E\text{-}6\,T^3 - 211708\,T^{-1}$ *(429.75 < T < 3800)*

BCC_A2

$-6178.89 + 91.538115\,T - 21.8386\,T\ln(T) - 5.72566E\text{-}3\,T^2 - 2.120321E\text{-}6\,T^3 - 22906\,T^{-1}$ *(298.15 < T < 429.75)*
$-6233.516 + 123.676588\,T - 27.4562\,T\ln(T) + 0.54607E\text{-}3\,T^2 - 0.08367E\text{-}6\,T^3 - 211708\,T^{-1} + 3.53E22\,T^{-9}$ *(429.75 < T < 3800)*

FCC_A1

$-6855.89 + 92.139315\,T - 21.8386\,T\ln(T) - 5.72566E\text{-}3\,T^2 - 2.120321E\text{-}6\,T^3 - 22906\,T^{-1}$ *(298.15 < T < 429.75)*
$-6910.516 + 124.277788\,T - 27.4562\,T\ln(T) + 0.54607E\text{-}3\,T^2 - 0.08367E\text{-}6\,T^3 - 211708\,T^{-1} + 3.53E22\,T^{-9}$ *(429.75 < T < 3800)*

HCP_A3

$-6445.89 + 91.651315\,T - 21.8386\,T\ln(T) - 5.72566E\text{-}3\,T^2 - 2.120321E\text{-}6\,T^3 - 22906\,T^{-1}$ *(298.15 < T < 429.75)*
$-6500.516 + 123.789788\,T - 27.4562\,T\ln(T) + 0.54607E\text{-}3\,T^2 - 0.08367E\text{-}6\,T^3 - 211708\,T^{-1} + 3.53E22\,T^{-9}$ *(429.75 < T < 3800)*

TET_ALPHA1

$-6785.89 + 92.173325\,T - 21.8386\,T\ln(T) - 5.72566E\text{-}3\,T^2 - 2.120321E\text{-}6\,T^3 - 22906\,T^{-1}$ *(298.15 < T < 429.75)*
$-6840.516 + 124.311798\,T - 27.4562\,T\ln(T) + 0.54607E\text{-}3\,T^2 - 0.08367E\text{-}6\,T^3 - 211708\,T^{-1} + 3.53E22\,T^{-9}$ *(429.75 < T < 3800)*

Data relative to TETRAGONAL_A6

LIQUID

$3282.092 - 7.63686\,T - 5.59E\text{-}20\,T^7$ *(298.15 < T < 429.75)*
$3283.706 - 7.640804\,T - 3.53E22\,T^{-9}$ *(429.75 < T < 3800)*

BCC_A2

$800 - 0.8\,T$ *(298.15 < T < 3800)*

FCC_A1

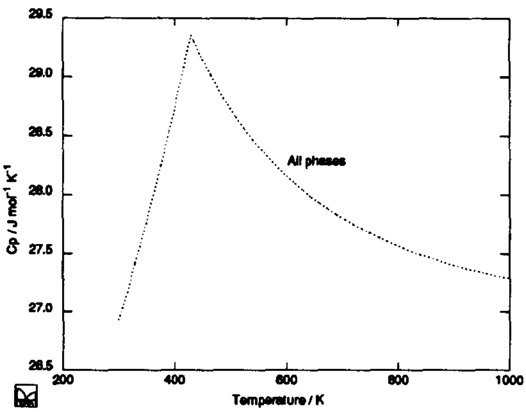
$123 - 0.1988\,T$ *(298.15 < T < 3800)*

HCP_A3

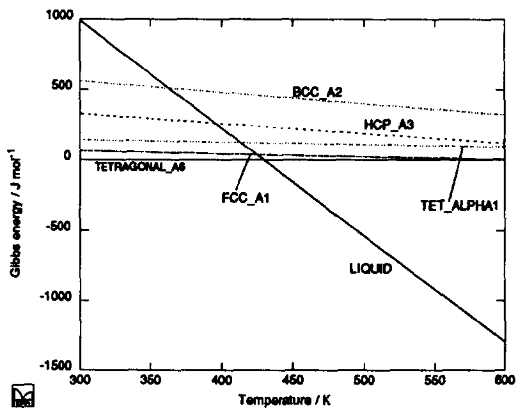
$533 - 0.6868\,T$ *(298.15 < T < 3800)*

TET_ALPHA1

193 - 0.16479 T *(298.15 < T < 3800)*



Heat capacity of In



Gibbs energy of phases of In relative to TETRAGONAL_A6

Ir

Source of data: A T Dinsdale, Unpublished work [FCC_A1, LIQUID]
Saunders et al. [BCC_A2, HCP_A3]

Data for Ir in the form of G-HSER

FCC_A1

-6936.288 + 118.780119 T - 22.7944 T ln(T) - 3.091976E-3 T^2 - 20083 T^{-1} *(298.15 < T < 1215)*
-8123.73 + 140.066697 T - 26.085 T ln(T) - 0.47969E-6 T^3 *(1215 < T < 2719)*
290529.037 - 1258.352965 T + 152.4988737 T ln(T) - 47.176402E-3 T^2 + 1.844977E-6 T^3 - 92987250 T^{-1} *(2719 < T < 4000)*

LIQUID

16518.956 + 112.46806 T - 22.7944 T ln(T) - 3.091976E-3 T^2 - 20083 T^{-1} *(298.15 < T < 1000)*
102217.789 - 587.632815 T + 73.9517579 T ln(T) - 46.38802E-3 T^2 + 2.761831E-6 T^3 - 13382612 T^{-1} *(1000 < T < 2719)*
-38347.217 + 411.234043 T - 59.418 T ln(T) *(2719 < T < 4000)*

BCC_A2

25063.712 + 111.880119 T - 22.7944 T ln(T) - 3.091976E-3 T^2 - 20083 T^{-1} *(298.15 < T < 1215)*
23876.27 + 133.166697 T - 26.085 T ln(T) - 0.47969E-6 T^3 *(1215 < T < 2719)*
322529.037 - 1265.252965 T + 152.4988737 T ln(T) - 47.176402E-3 T^2 + 1.844977E-6 T^3 - 92987250 T^{-1} *(2719 < T < 4000)*

HCP_A3

-2936.288 + 118.180119 T - 22.7944 T ln(T) - 3.091976E-3 T^2 - 20083 T^{-1} *(298.15 < T < 1215)*
-4123.73 + 139.466697 T - 26.085 T ln(T) - 0.47969E-6 T^3 *(1215 < T < 2719)*
294529.037 - 1258.952965 T + 152.4988737 T ln(T) - 47.176402E-3 T^2 + 1.844977E-6 T^3 - 92987250 T^{-1} *(2719 < T < 4000)*

Data relative to FCC_A1

LIQUID

$23455.244 - 6.312059\ T$ *(298.15 < T < 1000)*

$109154.077 - 706.412934\ T + 96.7461579\ T\ln(T) - 43.296044E\text{-}3\ T^2 + 2.761831E\text{-}6\ T^3 - 13362528\ T^{-1}$ *(1000 < T < 1215)*

$110341.519 - 727.699512\ T + 100.0367579\ T\ln(T) - 46.38802E\text{-}3\ T^2 + 3.241521E\text{-}6\ T^3 - 13382612\ T^{-1}$ *(1215 < T < 2719)*

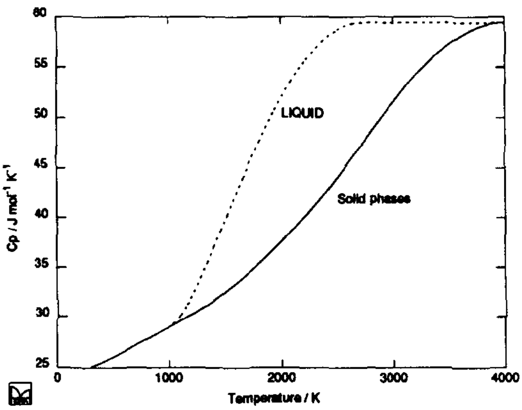
$-328876.254 + 1669.587008\ T - 211.9168737\ T\ln(T) + 47.176402E\text{-}3\ T^2 - 1.844977E\text{-}6\ T^3 + 92987250\ T^{-1}$ *(2719 < T < 4000)*

BCC_A2

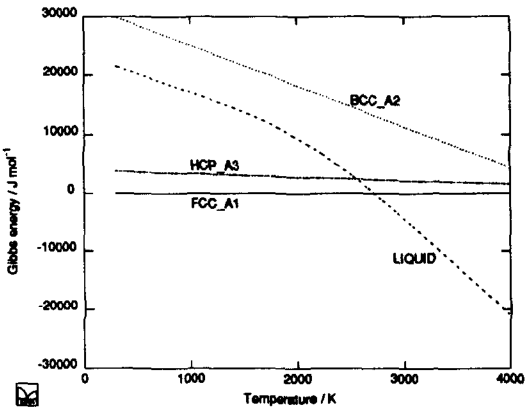
$32000 - 6.9\ T$ *(298.15 < T < 4000)*

HCP_A3

$4000 - 0.6\ T$ *(298.15 < T < 4000)*



Heat capacity of Ir



Gibbs energy of phases of Ir relative to FCC_A1

K

Source of data: TPIS [BCC_A2, LIQUID]
Saunders et al. [FCC_A1, HCP_A3]

Data for K in the form of G-HSER

BCC_A2

$-16112.929 + 389.624197\ T - 77.0571464\ T\ln(T) + 146.211135E\text{-}3\ T^2 - 84.949147E\text{-}6\ T^3 + 243385\ T^{-1}$ *(200 < T < 336.53)*

$-11122.441 + 192.586544\ T - 39.2885968\ T\ln(T) + 12.167386E\text{-}3\ T^2 - 2.64387E\text{-}6\ T^3 + 43251\ T^{-1} + 1.192E22\ T^{-9}$ *(336.53 < T < 2200)*

LIQUID

$-13794.833 + 382.737338\ T - 77.0571464\ T\ln(T) + 146.211135E\text{-}3\ T^2 - 84.949147E\text{-}6\ T^3 + 243385\ T^{-1} - 9.44E\text{-}19\ T^7$ *(200 < T < 336.53)*

$-8799.422 + 185.684327\ T - 39.2885968\ T\ln(T) + 12.167386E\text{-}3\ T^2 - 2.64387E\text{-}6\ T^3 + 43251\ T^{-1}$ *(336.53 < T < 2200)*

FCC_A1

-16062.929 + 390.924197 T - 77.0571464 T ln(T) + 146.211135E-3 T^2 - 84.949147E-6 T^3 + 243385 T^{-1}
(200 < T < 336.53)
-11072.441 + 193.886544 T - 39.2885968 T ln(T) + 12.167386E-3 T^2 - 2.64387E-6 T^3 + 43251 T^{-1} + 1.192E22 T^{-9}
(336.53 < T < 2200)

HCP_A3

-16062.929 + 391.624197 T - 77.0571464 T ln(T) + 146.211135E-3 T^2 - 84.949147E-6 T^3 + 243385 T^{-1}
(200 < T < 336.53)
-11072.441 + 194.586544 T - 39.2885968 T ln(T) + 12.167386E-3 T^2 - 2.64387E-6 T^3 + 43251 T^{-1} + 1.192E22 T^{-9}
(336.53 < T < 2200)

Data relative to BCC_A2

LIQUID

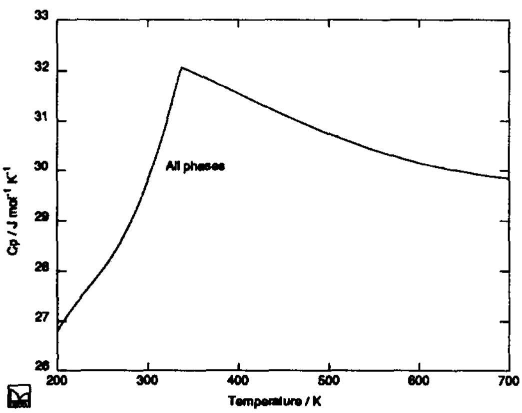
2318.096 - 6.886859 T - 9.44E-19 T^7 *(298.15 < T < 336.53)*
2323.018 - 6.902217 T - 1.192E22 T^{-9} *(336.53 < T < 2200)*

FCC_A1

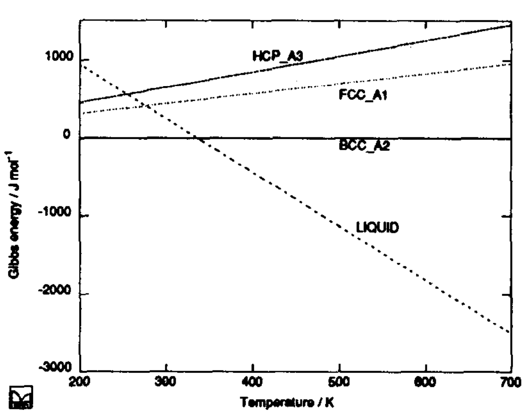
50 + 1.3 T *(298.15 < T < 2200)*

HCP_A3

50 + 2 T *(298.15 < T < 2200)*



Heat capacity of K



Gibbs energy of phases of K relative to BCC_A2

La

Source of data: Hultgren, modified by A T Dinsdale [DHCP, FCC_A1, BCC_A2, LIQUID]

Data for La in the form of G-HSER

DHCP

$-7968.403 + 120.284604\ T - 26.34\ T\ \ln(T) - 1.295165E{-3}\ T^2$ *(298.15 < T < 550.00)*
$-3381.413 + 59.06113\ T - 17.1659411\ T\ \ln(T) - 8.371705E{-3}\ T^2 + 0.68932E{-6}\ T^3 - 399448\ T^{-1}$ *(550.00 < T < 2000.00)*
$-15608.882 + 181.390071\ T - 34.3088\ T\ \ln(T)$ *(2000.00 < T < 4000.00)*

FCC_A1

$-6109.797 + 89.878761\ T - 21.7919\ T\ \ln(T) - 4.045175E{-3}\ T^2 - 0.525865E{-6}\ T^3$ *(298.15 < T < 1134.00)*
$-124598.976 + 955.878375\ T - 139.3467411\ T\ \ln(T) + 42.032405E{-3}\ T^2 - 3.066199E{-6}\ T^3 + 20994153\ T^{-1}$ *(1134.00 < T < 2000.00)*
$-12599.386 + 178.54399\ T - 34.3088\ T\ \ln(T)$ *(2000.00 < T < 4000.00)*

BCC_A2

$-3952.161 + 88.072353\ T - 21.7919\ T\ \ln(T) - 4.045175E{-3}\ T^2 - 0.525865E{-6}\ T^3$ *(298.15 < T < 800.00)*
$321682.673 - 3565.082518\ T + 513.4407077\ T\ \ln(T) - 387.295093E{-3}\ T^2 + 49.547989E{-6}\ T^3 - 36581228\ T^{-1}$ *(800.00 < T < 1134.00)*
$-16377.894 + 218.492988\ T - 39.5388\ T\ \ln(T)$ *(1134.00 < T < 1193.00)*
$-136609.91 + 1123.343974\ T - 163.4130738\ T\ \ln(T) + 53.968535E{-3}\ T^2 - 4.056395E{-6}\ T^3 + 21167204\ T^{-1}$ *(1193.00 < T < 2000.00)*
$-8205.988 + 174.836315\ T - 34.3088\ T\ \ln(T)$ *(2000.00 < T < 4000.00)*

LIQUID

$5332.653 + 18.23012\ T - 11.0188191\ T\ \ln(T) - 20.171603E{-3}\ T^2 + 2.93775E{-6}\ T^3 - 133541\ T^{-1}$ *(298.15 < T < 1134.00)*
$-3942.004 + 171.018431\ T - 34.3088\ T\ \ln(T)$ *(1134.00 < T < 4000.00)*

Data for La relative to DHCP

FCC_A1

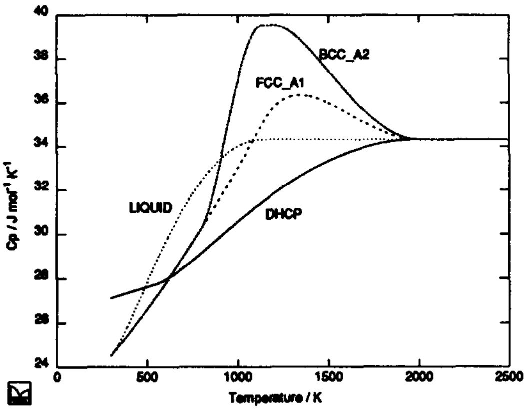
$1858.605 - 30.405844\ T + 4.5481\ T\ \ln(T) - 2.75001E{-3}\ T^2 - 0.525865E{-6}\ T^3$ *(298.15 < T < 550.00)*
$-2728.384 + 30.817631\ T - 4.6259589\ T\ \ln(T) + 4.32653E{-3}\ T^2 - 1.215185E{-6}\ T^3 + 399448\ T^{-1}$ *(550.00 < T < 1134.00)*
$-121217.563 + 896.817245\ T - 122.1808\ T\ \ln(T) + 50.404111E{-3}\ T^2 - 3.755519E{-6}\ T^3 + 21393601\ T^{-1}$ *(1134.00 < T < 2000.00)*
$3009.496 - 2.84608\ T$ *(2000.00 < T < 4000.00)*

BCC_A2

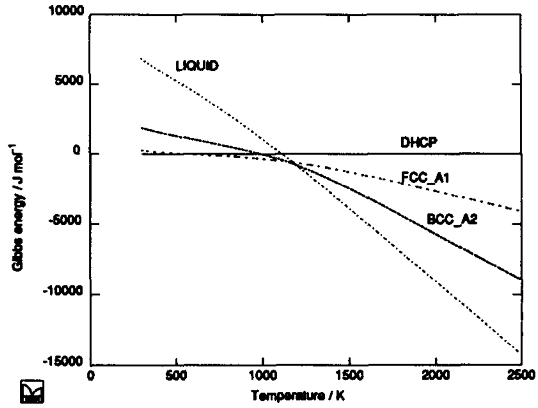
$4016.242 - 32.212251\ T + 4.5481\ T\ \ln(T) - 2.75001E{-3}\ T^2 - 0.525865E{-6}\ T^3$ *(298.15 < T < 550.00)*
$-570.748 + 29.011224\ T - 4.6259589\ T\ \ln(T) + 4.32653E{-3}\ T^2 - 1.215185E{-6}\ T^3 + 399448\ T^{-1}$ *(550.00 < T < 800.00)*
$325064.086 - 3624.143648\ T + 530.6066488\ T\ \ln(T) - 378.923388E{-3}\ T^2 + 48.858668E{-6}\ T^3 - 36181779\ T^{-1}$ *(800.00 < T < 1134.00)*
$-12996.481 + 159.431858\ T - 22.3728589\ T\ \ln(T) + 8.371705E{-3}\ T^2 - 0.68932E{-6}\ T^3 + 399448\ T^{-1}$ *(1134.00 < T < 1193.00)*
$-133228.497 + 1064.282844\ T - 146.2471326\ T\ \ln(T) + 62.34024E{-3}\ T^2 - 4.745715E{-6}\ T^3 + 21566652\ T^{-1}$ *(1193.00 < T < 2000.00)*
$7402.895 - 6.553756\ T$ *(2000.00 < T < 4000.00)*

LIQUID

$13301.055 - 102.054485\ T + 15.3211809\ T\ \ln(T) - 18.876438E{-3}\ T^2 + 2.93775E{-6}\ T^3 - 133541\ T^{-1}$ *(298.15 < T < 550.00)*
$8714.066 - 40.83101\ T + 6.1471221\ T\ \ln(T) - 11.799898E{-3}\ T^2 + 2.24843E{-6}\ T^3 + 265907\ T^{-1}$ *(550.00 < T < 1134.00)*
$-560.591 + 111.957302\ T - 17.1428589\ T\ \ln(T) + 8.371705E{-3}\ T^2 - 0.68932E{-6}\ T^3 + 399448\ T^{-1}$ *(1134.00 < T < 2000.00)*
$11666.878 - 10.371639\ T$ *(2000.00 < T < 4000.00)*



Heat capacity of La



Gibbs energy of phases of La relative to DHCP

Li

Source of data: TPIS [BCC_A2, LIQUID]
Saunders et al. [FCC_A1, HCP_A3]

Data for Li in the form of G-HSER

BCC_A2

-10583.817 + 217.637482 T - 38.940488 T ln(T) + 35.466931E-3 T^2 - 19.869816E-6 T^3 + 159994 T^{-1} *(200 < T < 453.6)*
-559579.123 + 10547.879893 T - 1702.8886493 T ln(T) + 2258.329444E-3 T^2 - 571.066077E-6 T^3 + 33885874 T^{-1} *(453.6 < T < 500)*
-9062.994 + 179.278285 T - 31.2283718 T ln(T) + 2.633221E-3 T^2 - 0.438058E-6 T^3 - 102387 T^{-1} *(500 < T < 3000)*

LIQUID

-7883.612 + 211.841861 T - 38.940488 T ln(T) + 35.466931E-3 T^2 - 19.869816E-6 T^3 + 159994 T^{-1} *(200 < T < 250)*
12015.027 - 362.187078 T + 61.6104424 T ln(T) - 182.426463E-3 T^2 + 63.955671E-6 T^3 - 559968 T^{-1} *(250 < T < 453.6)*
-6057.31 + 172.652183 T - 31.2283718 T ln(T) + 2.633221E-3 T^2 - 0.438058E-6 T^3 - 102387 T^{-1} *(453.6 < T < 3000)*

FCC_A1

-10691.817 + 218.937482 T - 38.940488 T ln(T) + 35.466931E-3 T^2 - 19.869816E-6 T^3 + 159994 T^{-1} *(200 < T < 453.6)*
-559687.123 + 10549.179893 T - 1702.8886493 T ln(T) + 2258.329444E-3 T^2 - 571.066077E-6 T^3 + 33885874 T^{-1} *(453.6 < T < 500)*
-9170.994 + 180.578285 T - 31.2283718 T ln(T) + 2.633221E-3 T^2 - 0.438058E-6 T^3 - 102387 T^{-1} *(500 < T < 3000)*

HCP_A3

-10737.817 + 219.637482 T - 38.940488 T ln(T) + 35.466931E-3 T^2 - 19.869816E-6 T^3 + 159994 T^{-1} *(200 < T < 453.6)*
-559733.123 + 10549.879893 T - 1702.8886493 T ln(T) + 2258.329444E-3 T^2 - 571.066077E-6 T^3 + 33885874 T^{-1} *(453.6 < T < 500)*
-9216.994 + 181.278285 T - 31.2283718 T ln(T) + 2.633221E-3 T^2 - 0.438058E-6 T^3 - 102387 T^{-1} *(500 < T < 3000)*

Data relative to BCC_A2

LIQUID

2700.205 - 5.795621 T *(200 < T < 250)*
22598.844 - 579.824561 T + 100.5509304 T ln(T) - 217.893394E-3 T^2 + 83.825487E-6 T^3 - 719962 T^{-1} *(250 < T < 453.6)*

553521.814 - 10375.227710 T + 1671.6602775 T ln(T) - 2255.696223E-3 T^2 + 570.628019E-6 T^3 - 33988260 T^{-1} *(453.6 < T < 500)*

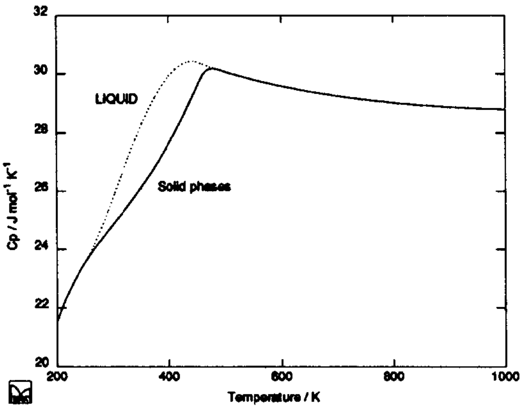
3005.685 - 6.626102 T *(500 < T < 3000)*

FCC_A1

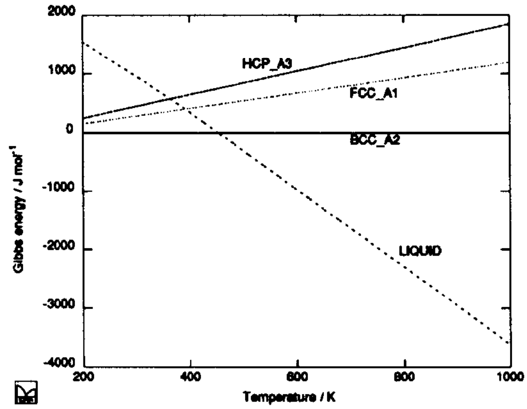
-108 + 1.3 T *(200 < T < 3000)*

HCP_A3

-154 + 2 T *(200 < T < 3000)*



Heat capacity of Li



Gibbs energy of phases of Li relative to BCC_A2

Lu

Source of data: Hultgren [HCP_A3, LIQUID]

Data for Lu in the form of G-HSER

HCP_A3

-8788.329 + 146.536283 T - 29.812 T ln(T) + 5.19165E-3 T^2 - 1.790717E-6 T^3 + 39723 T^{-1} *(298.15 < T < 700.00)*
-9043.057 + 142.327643 T - 29.0095 T ln(T) + 3.71416E-3 T^2 - 1.50147E-6 T^3 + 141549 T^{-1} *(700.00 < T < 1700.00)*
6940.092 - 46.91844 T - 1.83986 T ln(T) - 11.9001E-3 T^2 *(1700.00 < T < 1936.00)*
-404023.691 + 1829.379425 T - 239.019502 T ln(T) + 41.800748E-3 T^2 - 1.661174E-6 T^3 + 124825465 T^{-1} *(1936.00 < T < 3700.00)*

LIQUID

3983.791 + 141.5374 T - 29.812 T ln(T) + 5.19165E-3 T2 - 1.790717E-6 T^3 + 39723 T^{-1} *(298.15 < T < 600.00)*
30389.863 - 198.378793 T + 20.9392663 T ln(T) - 34.238743E-3 T^2 + 2.890636E-6 T^3 - 2398650 T^{-1} *(600.00 < T < 1936.00)*
-18994.687 + 292.091104 T - 47.9068 T ln(T) *(1936.00 < T < 3700.00)*

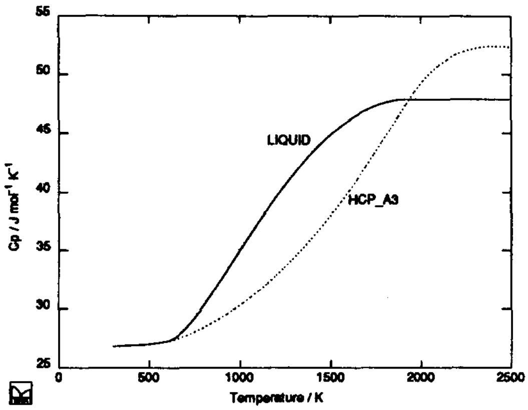
Data for Lu relative to HCP_A3

LIQUID

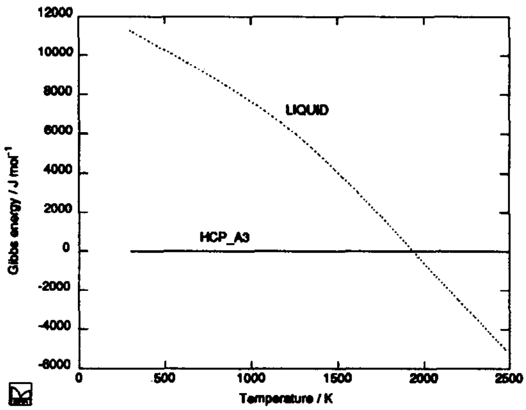
12772.12 - 4.998884 T *(298.15 < T < 600.00)*
39178.192 - 344.915076 T + 50.7512663 T ln(T) - 39.430393E-3 T^2 + 4.681352E-6 T^3 - 2438373 T^{-1} *(600.00 < T < 700.00)*
39432.92 - 340.706436 T + 49.9487663 T ln(T) - 37.952903E-3 T^2 + 4.392106E-6 T^3 - 2540199 T^{-1} *(700.00 < T < 1700.00)*

23449.77 - 151.460353 T + 22.7791263 T ln(T) - 22.338643E-3 T^2 + 2.890636E-6 T^3 - 2398650 T^{-1} *(1700.00 < T < 1936.00)*

385029.004 - 1537.288322 T + 191.112702 T ln(T) - 41.800748E-3 T^2 + 1.661174E-6 T^3 - 124825465 T^{-1} *(1936.00 < T < 3700.00)*



Heat capacity of Lu



Gibbs energy of phases of Lu relative to HCP_A3

Mg

Source of data: CODATA [HCP_A3, LIQUID]
Hack (unpublished work) [BCC_A12]
Tibbals (unpublished work) [CUB_A13]
Saunders et al. [BCC_A2, FCC_A1]

Data for Mg in the form of G-HSER

HCP_A3

-8367.34 + 143.675547 T - 26.1849782 T ln(T) + 0.4858E-3 T^2 - 1.393669E-6 T^3 + 78950 T^{-1} *(298.15 < T < 923)*
-14130.185 + 204.716215 T - 34.3088 T ln(T) + 1.0382E28 T^{-9} *(923 < T < 3000)*

LIQUID

-165.097 + 134.838617 T - 26.1849782 T ln(T) + 0.4858E-3 T^2 - 1.393669E-6 T^3 + 78950 T^{-1} - 8.0176E-20 T^7 *(298.15 < T < 923)*
-5439.869 + 195.324057 T - 34.3088 T ln(T) *(923 < T < 3000)*

BCC_A12

-3764.94 + 140.664547 T - 26.1849782 T ln(T) + 0.4858E-3 T^2 - 1.393669E-6 T^3 + 78950 T^{-1} *(298.15 < T < 923)*
-9527.785 + 201.705215 T - 34.3088 T ln(T) + 1.0382E28 T^{-9} *(923 < T < 3000)*

BCC_A2

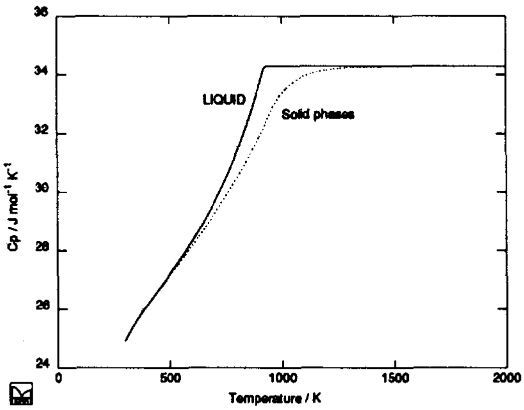
-5267.34 + 141.575547 T - 26.1849782 T ln(T) + 0.4858E-3 T^2 - 1.393669E-6 T^3 + 78950 T^{-1} *(298.15 < T < 923)*
-11030.185 + 202.616215 T - 34.3088 T ln(T) + 1.0382E28 T^{-9} *(923 < T < 3000)*

CUB_A13

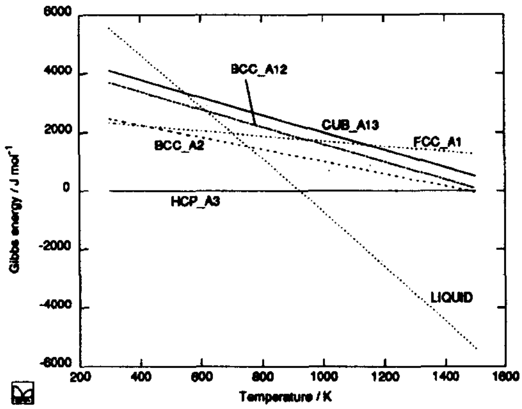
-3367.34 + 140.675547 T - 26.1849782 T ln(T) + 0.4858E-3 T^2 - 1.393669E-6 T^3 + 78950 T^{-1} *(298.15 < T < 923)*
-9130.185 + 201.716215 T - 34.3088 T ln(T) + 1.0382E28 T^{-9} *(923 < T < 3000)*

FCC_A1

$-5767.34 + 142.775547\ T - 26.1849782\ T\ln(T) + 0.4858E{-}3\ T^2 - 1.393669E{-}6\ T^3 + 78950\ T^{-1}$ *(298.15 < T < 923)*
$-11530.185 + 203.816215\ T - 34.3088\ T\ln(T) + 1.0382E28\ T^{-9}$ *(923 < T < 3000)*



Heat capacity of Mg



Gibbs energy of phases of Mg relative to HCP_A3

Data relative to HCP_A3

LIQUID

$8202.243 - 8.83693\ T - 8.0176E{-}20\ T^7$ *(298.15 < T < 923)*
$8690.316 - 9.392159\ T - 1.0382E28\ T^{-9}$ *(923 < T < 3000)*

BCC_A12

$4602.4 - 3.011\ T$ *(298.15 < T < 3000)*

BCC_A2

$3100 - 2.1\ T$ *(298.15 < T < 3000)*

CUB_A13

$5000 - 3\ T$ *(298.15 < T < 3000)*

FCC_A1

$2600 - 0.9\ T$ *(298.15 < T < 3000)*

Mn

Source of data: A Fernandez Guillermet, W Huang, Int. J. Thermophys., 1990, 11, 949-69 [BCC_A12, CUB_A13, FCC_A1, BCC_A2, LIQUID]
Saunders et al. [HCP_A3]

Data for Mn in the form of G-HSER

BCC_A12

$T_N = 95$ $B_0 = 0.22$

$-8115.28 + 130.059\ T - 23.4582\ T\ln(T) - 7.34768E{-}3\ T^2 + 69827.1\ T^{-1} + Gmag$ *(298.15 < T < 1519.00)*
$-28733.41 + 312.2648\ T - 48.0\ T\ln(T) + 1.656847E30\ T^{-9} + Gmag$ *(1519.00 < T < 2000.00)*

CUB_A13

$-5800.4 + 135.995\ T - 24.8785\ T\ln(T) - 5.83359E\text{-}3\ T^2 + 70269.1\ T^{-1}$ *(298.15 < T < 1519.00)*
$-28290.76 + 311.2933\ T - 48.0\ T\ln(T) + 3.9675699E30\ T^{-9}$ *(1519.00 < T < 2000.00)*

FCC_A1

$T_N = 540$ $B_0 = 0.62$

$-3439.3 + 131.884\ T - 24.5177\ T\ln(T) - 6.0E\text{-}3\ T^2 + 69600\ T^{-1} + Gmag$ *(298.15 < T < 1519.00)*
$-26070.1 + 309.6664\ T - 48.0\ T\ln(T) + 3.8619645E30\ T^{-9} + Gmag$ *(1519.00 < T < 2000.00)*

BCC_A2

$T_N = 580$ $B_0 = 0.27$

$-3235.3 + 127.85\ T - 23.7\ T\ln(T) - 7.44271E\text{-}3\ T^2 + 60000\ T^{-1} + Gmag$ *(298.15 < T < 1519.00)*
$-23188.83 + 307.7043\ T - 48.0\ T\ln(T) + 1.265152E30\ T^{-9} + Gmag$ *(1519.00 < T < 2000.00)*

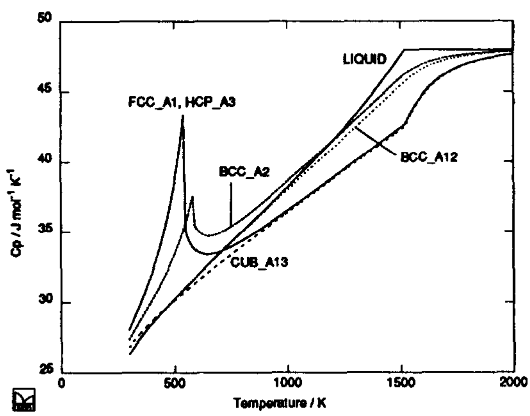
LIQUID

$9744.63 + 117.4382\ T - 23.4582\ T\ln(T) - 7.34768E\text{-}3\ T^2 + 69827.1\ T^{-1} - 4.4192927E\text{-}21\ T^7$ *(298.15 < T < 1519.00)*
$-9993.9 + 299.036\ T - 48.0\ T\ln(T)$ *(1519.00 < T < 2000.00)*

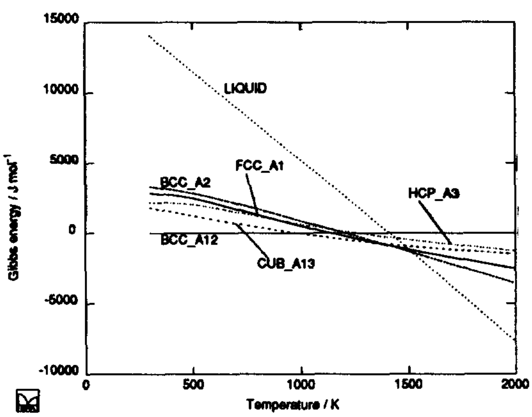
HCP_A3

$T_N = 540$ $B_0 = 0.62$

$-4439.3 + 133.007\ T - 24.5177\ T\ln(T) - 6.0E\text{-}3\ T^2 + 69600\ T^{-1} + Gmag$ *(298.15 < T < 1519.00)*
$-27070.1 + 310.7894\ T - 48.0\ T\ln(T) + 3.8619645E30\ T^{-9} + Gmag$ *(1519.00 < T < 2000.00)*



Heat capacity of Mn



Gibbs energy of phases of Mn relative to BCC_A12

Data for Mn relative to paramagnetic BCC_A12

BCC_A12

$T_N = 95$ $B_0 = 0.22$

Gmag

CUB_A13

$2314.88 + 5.936\ T - 1.4203\ T\ln(T) + 1.51409E\text{-}3\ T^2 + 442\ T^{-1}$ *(298.15 < T < 1519.00)*
$442.65 - 0.9715\ T + 2.3107229E30\ T^{-9}$ *(1519.00 < T < 2000.00)*

FCC_A1

$T_N = 540$ $B_0 = 0.62$

$4675.98 + 1.825\ T - 1.0595\ T\ \ln(T) + 1.34768E\text{-}3\ T^2 - 227\ T^{-1} + Gmag$ *(298.15 < T < 1519.00)*
$2663.31 - 2.5984\ T + 2.2051175E30\ T^{-9} + Gmag$ *(1519.00 < T < 2000.00)*

BCC_A2

$T_N = 580$ $B_0 = 0.27$

$4879.98 - 2.209\ T - 0.2418\ T\ \ln(T) - 0.09503E\text{-}3\ T^2 - 9827\ T^{-1} + Gmag$ *(298.15 < T < 1519.00)*
$5544.58 - 4.5605\ T - 3.916950E29\ T^{-9}$ *(1519.00 < T < 2000.00)*

LIQUID

$17859.91 - 12.6208\ T - 4.4192927E\text{-}21\ T^7$ *(298.15 < T < 1519.00)*
$18739.51 - 13.2288\ T - 1.656847E30\ T^{-9}$ *(1519.00 < T < 2000.00)*

HCP_A3

$T_N = 540$ $B_0 = 0.62$

$3675.98 + 2.948\ T - 1.0595\ T\ \ln(T) + 1.34768E\text{-}3\ T^2 - 227\ T^{-1} + Gmag$ *(298.15 < T < 1519.00)*
$1663.31 - 1.4754\ T + 2.2051175E30\ T^{-9} + Gmag$ *(1519.00 < T < 2000.00)*

Mo

Source of data: A Fernandez Guillermet, Int. J. Thermophys, 1985, **6**, 263-393 [BCC_A2, LIQUID]
J-O Andersson, A Fernandez Guillermet, P Gustafson, CALPHAD, 1987, **11**, 361-4 [HCP_A3, FCC_A1]

Data for Mo in the form of G-HSER

BCC_A2

$A = 9.34372E\text{-}6$	$a_0 = 1.4378E\text{-}5$	$a_1 = 4.66062E\text{-}10$	$a_2 = 3.44061E\text{-}12$
$K_0 = 3.5027E\text{-}12$	$K_1 = 1.5E\text{-}16$	$K_2 = 3.9E\text{-}20$	$n = 3.25$

$-7746.302 + 131.9197\ T - 23.56414\ T\ \ln(T) - 0.003443396\ T^2 + 5.662834E\text{-}7\ T^3 - 1.309265E\text{-}10\ T^4 + 65812.39\ T^{-1} + Gpres$ *(298.15 < T < 2896.00)*
$-30556.41 + 283.559746\ T - 42.63829\ T\ \ln(T) - 4.849315E33\ T^{-9} + Gpres$ *(2896.00 < T < 4000.00)*

LIQUID

$A = 9.75079E\text{-}6$	$a_0 = 1.4378E\text{-}5$	$a_1 = 4.66062E\text{-}10$	$a_2 = 3.44061E\text{-}12$
$K_0 = 3.5027E\text{-}12$	$K_1 = 1.5E\text{-}16$	$K_2 = 3.9E\text{-}20$	$n = 3.25$

$34085.045 + 117.224788\ T - 23.56414\ T\ \ln(T) - 0.003443396\ T^2 + 5.662834E\text{-}7\ T^3 - 1.309265E\text{-}10\ T^4 + 65812.39\ T^{-1} + 4.24519E\text{-}22\ T^7 + Gpres$ *(298.15 < T < 2896.00)*
$3538.963 + 271.6697\ T - 42.63829\ T\ \ln(T) + Gpres$ *(2896.00 < T < 4000.00)*

FCC_A1

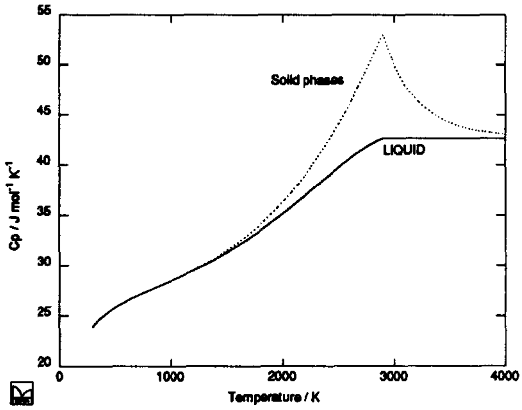
$A = 9.34372E\text{-}6$	$a_0 = 1.4378E\text{-}5$	$a_1 = 4.66062E\text{-}10$	$a_2 = 3.44061E\text{-}12$
$K_0 = 3.5027E\text{-}12$	$K_1 = 1.5E\text{-}16$	$K_2 = 3.9E\text{-}20$	$n = 3.25$

$7453.698 + 132.5497\ T - 23.56414\ T\ \ln(T) - 0.003443396\ T^2 + 5.662834E\text{-}7\ T^3 - 1.309265E\text{-}10\ T^4 + 65812.39\ T^{-1} + Gpres$ *(298.15 < T < 2896.00)*
$-15356.41 + 284.189746\ T - 42.63829\ T\ \ln(T) - 4.849315E33\ T^{-9} + Gpres$ *(2896.00 < T < 4000.00)*

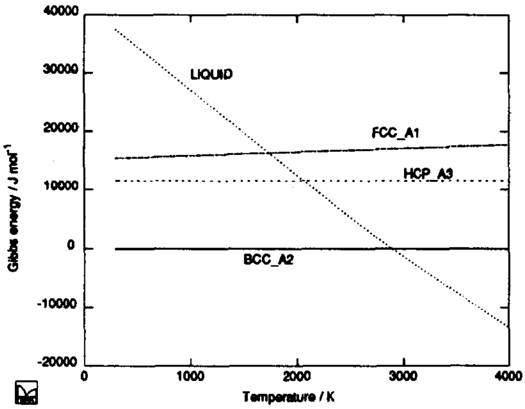
HCP_A3

A = 9.34372E-6	a_0 = 1.4378E-5	a_1 = 4.66062E-10	a_2 = 3.44061E-12
K_0 = 3.5027E-12	K_1 = 1.5E-16	K_2 = 3.9E-20	n = 3.25

3803.698 + 131.9197 T - 23.56414 T ln(T) - 0.003443396 T^2 + 5.662834E-7 T^3 - 1.309265E-10 T^4 + 65812.39 T^{-1} + Gpres *(298.15 < T < 2896.00)*
-19006.41 + 283.559746 T - 42.63829 T ln(T) - 4.849315E33 T^{-9} + Gpres *(2896.00 < T < 4000.00)*



Heat capacity of Mo



Gibbs energy of phases of Mo relative to BCC_A2

Data for Mo relative to BCC_A2

BCC_A2

A = 9.34372E-6	a_0 = 1.4378E-5	a_1 = 4.66062E-10	a_2 = 3.44061E-12
K_0 = 3.5027E-12	K_1 = 1.5E-16	K_2 = 3.9E-20	n = 3.25

Gpres *(298.15 < T < 4000.00)*

LIQUID

A = 9.75079E-6	a_0 = 1.4378E-5	a_1 = 4.66062E-10	a_2 = 3.44061E-12
K_0 = 3.5027E-12	K_1 = 1.5E-16	K_2 = 3.9E-20	n = 3.25

41831.347 - 14.694912 T + 4.24519E-22 T^7 + Gpres *(298.15 < T < 2896.00)*
34095.373 - 11.890046 T + 4.849315E33 T^{-9} + Gpres *(2896.00 < T < 4000.00)*

FCC_A1

A = 9.34372E-6	a_0 = 1.4378E-5	a_1 = 4.66062E-10	a_2 = 3.44061E-12
K_0 = 3.5027E-12	K_1 = 1.5E-16	K_2 = 3.9E-20	n = 3.25

15200 + 0.63 T + Gpres *(298.15 < T < 4000.00)*

HCP_A3

A = 9.34372E-6	a_0 = 1.4378E-5	a_1 = 4.66062E-10	a_2 = 3.44061E-12
K_0 = 3.5027E-12	K_1 = 1.5E-16	K_2 = 3.9E-20	n = 3.25

11550 + Gpres *(298.15 < T < 4000.00)*

N

Soure of data: K Frisk, TRITA-MAC-0393, April 1989 [GAS, LIQUID]

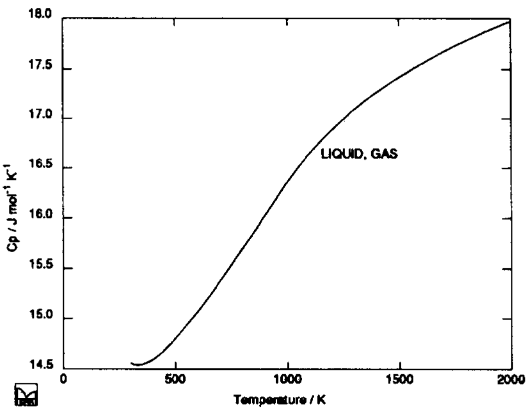
Data for N in the form of G-HSER

GAS (1/2 N2)

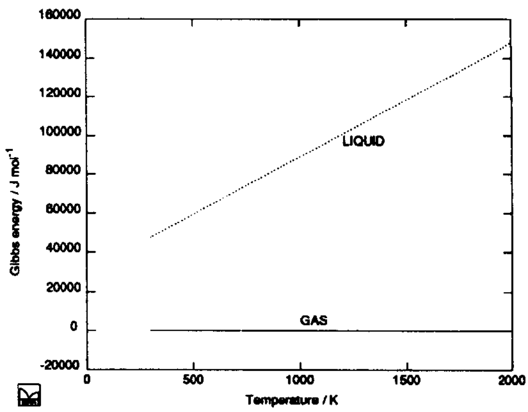
-3750.675 - 9.45425 T - 12.7819 T ln(T) - 0.00176686 T^2 + 2.680735E-9 T^3 - 32374 T^{-1} *(298.15 < T < 950.00)*
-7358.85 + 17.2003 T - 16.3699 T ln(T) - 6.5107E-4 T^2 + 3.0097E-8 T^3 + 563070 T^{-1} *(950.00 < T < 3350.00)*
-16392.8 + 50.26 T - 20.4695 T ln(T) + 2.397545E-4 T^2 - 8.3331E-9 T^3 + 4596375 T^{-1} *(3350.00 < T < 6000.00)*

LIQUID

26199.325 + 49.56575 T - 12.7819 T ln(T) - 0.00176686 T^2 + 2.680735E-9 T^3 - 32374 T^{-1} *(298.15 < T < 950.00)*
22591.15 + 76.2203 T - 16.3699 T ln(T) - 6.5107E-4 T^2 + 3.0097E-8 T^3 + 563070 T^{-1} *(950.00 < T < 3350.00)*
13557.2 + 109.28 T - 20.4695 T ln(T) + 2.397545E-4 T^2 - 8.3331E-9 T^3 + 4596375 T^{-1} *(3350.00 < T < 6000.00)*



Heat capacity of N



Gibbs energy of phases of N relative to GAS

Data for N relative to GAS

LIQUID

29950 + 59.02 T *(298.15 < T < 6000.00)*

Na

Source of data: TPIS [BCC_A2, LIQUID]
Saunders et al. [HCP_A3, FCC_A1]

Data for Na in the form of G-HSER

BCC_A2

-11989.434 + 260.548732 T - 51.0393608 T ln(T) + 72.306633E-3 T^2 - 43.638283E-6 T^3 + 132154 T^{-1} *(200 < T < 370.87)*
-11009.884 + 199.619999 T - 38.1198801 T ln(T) + 9.745854E-3 T^2 - 1.70664E-6 T^3 + 34342 T^{-1} + 1.651E23 T^{-9}
(370.87 < T < 2300)

LIQUID

-9408.414 + 253.596552 T - 51.0393608 T ln(T) + 72.306633E-3 T^2 - 43.638283E-6 T^3 + 132154 T^{-1} - 2.7613E-18 T^7
(200 < T < 370.87)
-8400.44 + 192.587343 T - 38.1198801 T ln(T) + 9.745854E-3 T^2 - 1.70664E-6 T^3 + 34342 T^{-1} *(370.87 < T < 2300)*

FCC_A1

$-12039.434 + 261.848732\ T - 51.0393608\ T \ln(T) + 72.306633E\text{-}3\ T^2 - 43.638283E\text{-}6\ T^3 + 132154\ T^{-1}$ *(200 < T < 370.87)*
$-11059.884 + 200.919999\ T - 38.1198801\ T \ln(T) + 9.745854E\text{-}3\ T^2 - 1.70664E\text{-}6\ T^3 + 34342\ T^{-1} + 1.651E23\ T^{-9}$ *(370.87 < T < 2300)*

HCP_A3

$-12093.434 + 262.548732\ T - 51.0393608\ T \ln(T) + 72.306633E\text{-}3\ T^2 - 43.638283E\text{-}6\ T^3 + 132154\ T^{-1}$ *(200 < T < 370.87)*
$-11113.884 + 201.619999\ T - 38.1198801\ T \ln(T) + 9.745854E\text{-}3\ T^2 - 1.70664E\text{-}6\ T^3 + 34342\ T^{-1} + 1.651E23\ T^{-9}$ *(370.87 < T < 2300)*

Data relative to BCC_A2

LIQUID

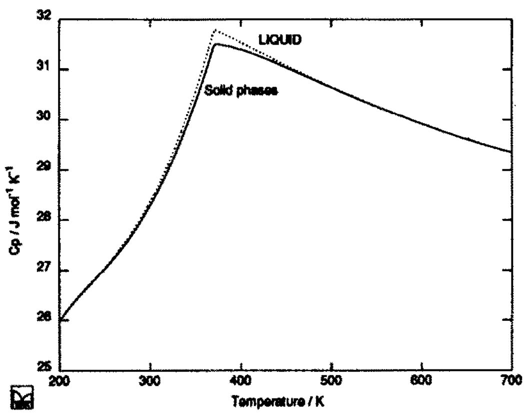
$2581.02 - 6.95218\ T - 2.7613E\text{-}18\ T^7$ *(200 < T < 370.87)*
$2609.445 - 7.032656\ T - 1.651E23\ T^{-9}$ *(370.87 < T < 2300)*

FCC_A1

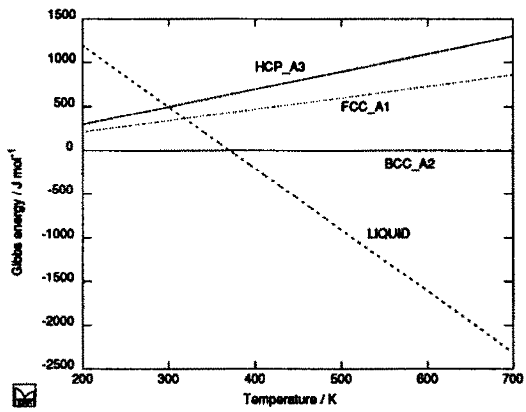
$-50 + 1.3\ T$ *(200 < T < 2300)*

HCP_A3

$-104 + 2\ T$ *(200 < T < 2300)*



Heat capacity of Na



Gibbs energy of phases of Na relative to BCC_A2

Nb

Source of data: TPIS [BCC_A2, LIQUID]
A Fernandez Guillermet, W Huang, Z. Metallkde., 1988, 79, 88-95, [FCC_A1, HCP_A3]

Data for Nb in the form of G-HSER

BCC_A2

$-8519.353 + 142.045475\ T - 26.4711\ T \ln(T) + 0.203475E\text{-}3\ T^2 - 0.350119E\text{-}6\ T^3 + 93399\ T^{-1}$ *(298.15 < T < 2750.00)*
$-37669.3 + 271.720843\ T - 41.77\ T \ln(T) + 1.52824E32\ T^{-9}$ *(2750.00 < T < 6000.00)*

LIQUID

$21262.202 + 131.229057\ T - 26.4711\ T \ln(T) + 0.203475E\text{-}3\ T^2 - 0.350119E\text{-}6\ T^3 + 93399\ T^{-1} - 3.06098E\text{-}23\ T^7$ *(298.15 < T < 2750.00)*

$-7499.398 + 260.756148\ T - 41.77\ T\ \ln(T)$ *(2750.00 < T < 6000.00)*

FCC_A1

$4980.647 + 143.745475\ T - 26.4711\ T\ \ln(T) + 0.203475E\text{-}3\ T^2 - 0.350119E\text{-}6\ T^3 + 93399\ T^{-1}$ *(298.15 < T < 2750.00)*
$-24169.3 + 273.420843\ T - 41.77\ T\ \ln(T) + 1.52824E32\ T^{9}$ *(2750.00 < T < 6000.00)*

HCP_A3

$1480.647 + 144.445475\ T - 26.4711\ T\ \ln(T) + 0.203475E\text{-}3\ T^2 - 0.350119E\text{-}6\ T^3 + 93399\ T^{-1}$ *(298.15 < T < 2750.00)*
$-27669.3 + 274.120843\ T - 41.77\ T\ \ln(T) + 1.52824E32\ T^{9}$ *(2750.00 < T < 6000.00)*

Data from Nb relative to BCC_A2

LIQUID

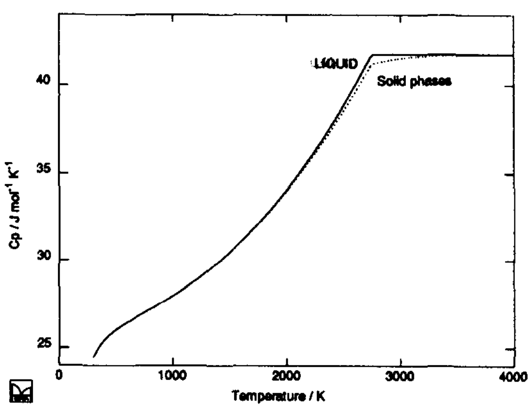
$29781.555 - 10.816417\ T - 3.06098E\text{-}23\ T^7$ *(298.15 < T < 2750.00)*
$30169.901 - 10.964695\ T - 1.52824E32\ T^{-9}$ *(2750.00 < T < 6000.00)*

FCC_A1

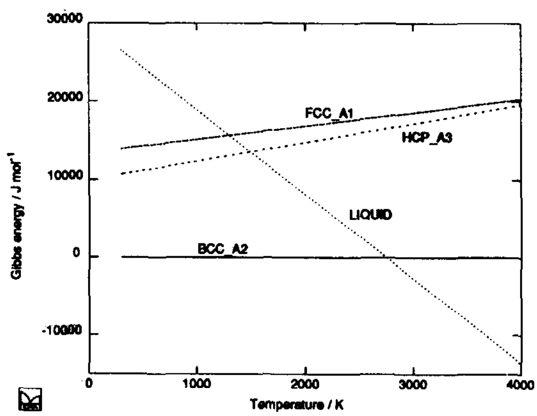
$13500 + 1.7\ T$ *(298.15 < T < 6000.00)*

HCP_A3

$10000 + 2.4\ T$ *(298.15 < T < 6000.00)*



Heat capacity of Nb



Gibbs energy of phases of Nb relative to BCC_A2

Nd

Source of data: Hultgren extended by A T Dinsdale [DHCP, BCC_A2, LIQUID]

Data for Nd in the form of G-HSER

DHCP

$-8402.93 + 111.10239\ T - 27.0858\ T\ \ln(T) + 0.556125E\text{-}3\ T^2 - 2.6923E\text{-}6\ T^3 + 34887\ T^{-1}$ *(298.15 < T < 900.00)*
$-6984.083 + 83.662617\ T - 22.7536\ T\ \ln(T) - 4.20402E\text{-}3\ T^2 - 1.802E\text{-}6\ T^3$ *(900.00 < T < 1128.00)*
$-225610.846 + 1673.040749\ T - 238.1828733\ T\ \ln(T) + 78.615997E\text{-}3\ T^2 - 6.048207E\text{-}6\ T^3 + 38810350\ T^{-1}$
(1128.00 < T < 1800.00)

BCC_A2

-6965.635 + 110.556109 T - 27.0858 T ln(T) + 0.556125E-3 T^2 - 2.6923E-6 T^3 + 34887 T^{-1} *(298.15 < T < 400.00)*
7312.2 - 153.033976 T + 14.9956777 T ln(T) - 50.479E-3 T^2 + 7.287217E-6 T^3 - 831810 T^{-1} *(400.00 < T < 1128.00)*
-18030.266 + 239.677322 T - 44.5596 T ln(T) *(1128.00 < T < 1289.00)*
334513.017 - 2363.919899 T + 311.409193 T ln(T) - 156.030778E-3 T^2 + 12.408421E-6 T^3 - 64319604 T^{-1}
(1289.00 < T < 1800.00)

LIQUID

5350.01 - 86.593963 T + 5.357301 T ln(T) - 46.955463E-3 T^2 + 6.860782E-6 T^3 - 374380 T^{-1} *(298.15 < T < 1128.00)*
-16335.232 + 268.625903 T - 48.7854 T ln(T) *(1128.00 < T < 1800.00)*

Data for Nd relative to DHCP

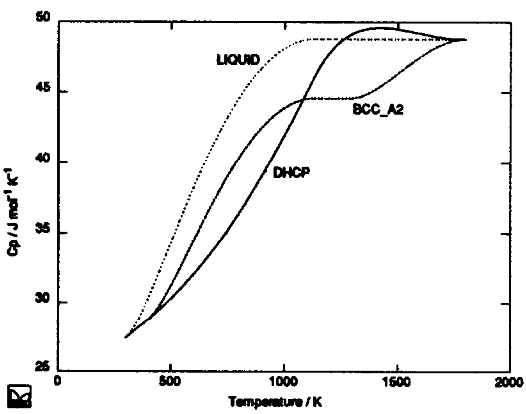
BCC_A2

1437.295 - 0.546281 T *(298.15 < T < 400.00)*
15715.13 - 264.136366 T + 42.0814777 T ln(T) - 51.035125E-3 T^2 + 9.979517E-6 T^3 - 866697 T^{-1} *(400.00 < T < 900.00)*
14296.283 - 236.696593 T + 37.7492777 T ln(T) - 46.27498E-3 T^2 + 9.089217E-6 T^3 - 831810 T^{-1} *(900.00 < T < 1128.00)*
207580.58 - 1433.363427 T + 193.6232733 T ln(T) - 78.615997E-3 T^2 + 6.048207E-6 T^3 - 38810350 T^{-1}
(1128.00 < T < 1289.00)
560123.863 - 4036.960648 T + 549.5920663 T ln(T) - 234.646775E-3 T^2 + 18.456628E-6 T^3 - 103129955 T^{-1}
(1289.00 < T < 1800.00)

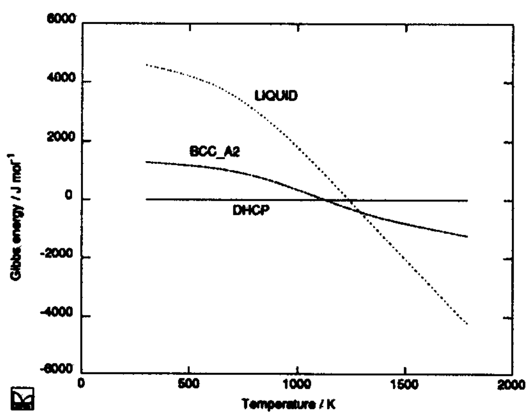
LIQUID

13752.941 - 197.696353 T + 32.443101 T ln(T) - 47.511588E-3 T^2 + 9.553082E-6 T^3 - 409267 T^{-1} *(298.15 < T < 900.00)*
12334.094 - 170.25658 T + 28.110901 T ln(T) - 42.751443E-3 T^2 + 8.662782E-6 T^3 - 374380 T^{-1} *(900.00 < T < 1128.00)*
209275.614 - 1404.414846 T + 189.3974733 T ln(T) - 78.615997E-3 T^2 + 6.048207E-6 T^3 - 38810350 T^{-1}

(1128.00 < T < 1800.00)



Heat capacity of Nd



Gibbs energy of phases of Nd relative to DHCP

Ni

Source of data: A T Dinsdale, unpublished work [FCC_A1, LIQUID, BCC_A2]
A Fernandez Guillermet, Z. Metallkde., 1987, **78**, 639-47 [HCP_A3]
Kaufman [BCC_A12, CUB_A13]

Data for Ni in the form of G-HSER

FCC_A1

$T_C = 633$	$B_0 = 0.52$		
$A = 6.533939E-6$	$a_0 = 3.103614E-5$	$a_1 = 2.418404E-8$	
$K_0 = 5.3297107E-12$	$K_1 = 4.5132279E-16$	$K_2 = 9.7669517E-19$	$n = 4.651$

-5179.159 + 117.854 T - 22.096 T ln(T) - 4.8407E-3 T^2 + Gmag + Gpres *(298.15 < T < 1728.00)*
-27840.655 + 279.135 T - 43.10 T ln(T) + 1.12754E31 T^{-9} + Gmag + Gpres *(1728.00 < T < 3000.00)*

LIQUID

11235.527 + 108.457 T - 22.096 T ln(T) - 4.8407E-3 T^2 - 3.82318E-21 T^7 *(298.15 < T < 1728.00)*
-9549.775 + 268.598 T - 43.10 T ln(T) *(1728.00 < T < 3000.00)*

BCC_A2

$T_C = 575$ $B_0 = 0.85$

3535.925 + 114.298 T - 22.096 T ln(T) - 4.8407E-3 T^2 + Gmag *(298.15 < T < 1728.00)*
-19125.571 + 275.579 T - 43.10 T ln(T) + 1.12754E31 T^{-9} + Gmag *(1728.00 < T < 3000.00)*

HCP_A3

$T_C = 633$ $B_0 = 0.52$

-4133.159 + 119.109 T - 22.096 T ln(T) - 4.8407E-3 T^2 + Gmag *(298.15 < T < 1728.00)*
-26794.655 + 280.39 T - 43.10 T ln(T) + 1.12754E31 T^{-9} + Gmag *(1728.00 < T < 3000.00)*

CUB_A13

-3087.159 + 117.854 T - 22.096 T ln(T) - 4.8407E-3 T^2 + Gmag *(298.15 < T < 1728.00)*
-25748.655 + 279.135 T - 43.10 T ln(T) + 1.12754E31 T^{-9} + Gmag *(1728.00 < T < 3000.00)*

BCC_A12

-1623.159 + 117.854 T - 22.096 T ln(T) - 4.8407E-3 T^2 + Gmag *(298.15 < T < 1728.00)*
-24284.655 + 279.135 T - 43.10 T ln(T) + 1.12754E31 T^{-9} + Gmag *(1728.00 < T < 3000.00)*

Data for Ni relative to paramagnetic FCC_A1

FCC_A1

$T_C = 633$	$B_0 = 0.52$		
$A = 6.533939E-6$	$a_0 = 3.103614E-5$	$a_1 = 2.418404E-8$	
$K_0 = 5.3297107E-12$	$K_1 = 4.5132279E-16$	$K_2 = 9.7669517E-19$	$n = 4.651$

Gmag + Gpres *(298.15 < T < 3000.00)*

LIQUID

16414.686 - 9.397 T - 3.82318E-21 T^7 *(298.15 < T < 1728.00)*
18290.88 - 10.537 T - 1.12754E31 T^{-9} *(1728.00 < T < 3000.00)*

BCC_A2

$T_C = 575$ $B_0 = 0.85$

$8715.084 - 3.556\ T + Gmag$ $(298.15 < T < 3000.00)$

HCP_A3

$T_C = 633$ $B_0 = 0.52$

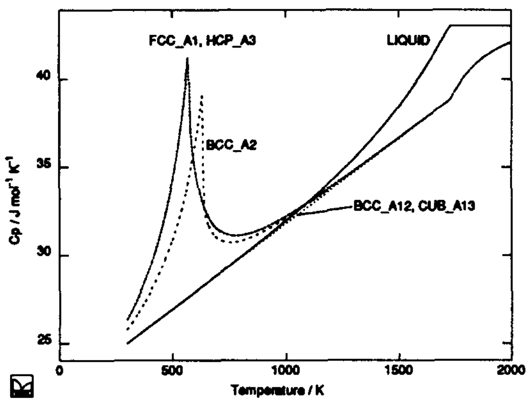
$1046 + 1.2552\ T + Gmag$ $(298.15 < T < 3000.00)$

CUB_A13

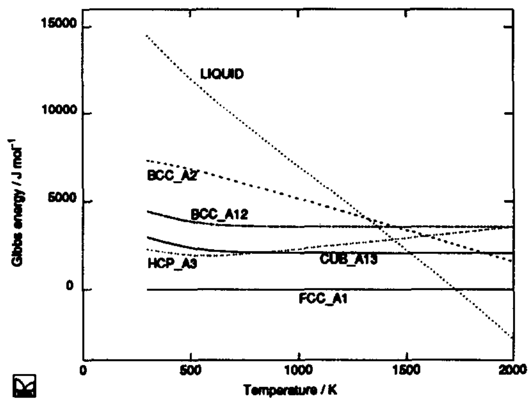
2092 $(298.15 < T < 3000.00)$

BCC_A12

3556 $(298.15 < T < 3000.00)$



Heat capacity of Ni



Gibbs energy of phases of Ni relative to FCC_A1

Np

Source of data: M H Rand (Unpublished work)

ORTHO_Ac

$241.888 - 57.531347\ T + 4.0543\ T\ \ln(T) - 41.27725E\text{-}3\ T^2 - 402857\ T^{-1}$ $(298.15 < T < 553.00)$
$-57015.112 + 664.27337\ T - 102.523\ T\ \ln(T) + 28.4592E\text{-}3\ T^2 - 2.483917E\text{-}6\ T^3 + 4796910\ T^{-1}$ $(553.00 < T < 1799.00)$
$-12092.736 + 255.780866\ T - 45.3964\ T\ \ln(T)$ $(1799.00 < T < 4000.00)$

TETRAG_Ad

$-10157.32 + 183.829213\ T - 34.11\ T\ \ln(T) - 16.1186E\text{-}3\ T^2 + 4.98465E\text{-}6\ T^3 + 532825\ T^{-1}$ $(298.15 < T < 555.00)$
$-7873.688 + 207.01896\ T - 39.33\ T\ \ln(T)$ $(555.00 < T < 856.00)$
$19027.98 - 46.64846\ T - 3.4265\ T\ \ln(T) - 19.21045E\text{-}3\ T^2 + 1.52726E\text{-}6\ T^3 - 3564640\ T^{-1}$ $(856.00 < T < 1999.00)$
$-16070.82 + 256.707037\ T - 45.3964\ T\ \ln(T)$ $(1999.00 < T < 4000.00)$

BCC_A2

$-3224.664 + 174.911817\ T - 35.177\ T\ \ln(T) - 2.51865E\text{-}3\ T^2 + 0.514743E\text{-}6\ T^3 + 302225\ T^{-1}$ $(298.15 < T < 856.00)$
$-2366.486 + 180.807719\ T - 36.401\ T\ \ln(T)$ $(856.00 < T < 917.00)$
$50882.281 - 297.324358\ T + 30.7734\ T\ \ln(T) - 34.3483E\text{-}3\ T^2 + 2.707217E\text{-}6\ T^3 - 7500100\ T^{-1}$ $(917.00 < T < 1999.00)$
$-14879.686 + 254.773087\ T - 45.3964\ T\ \ln(T)$ $(1999.00 < T < 4000.00)$

LIQUID

-4627.18 + 160.024959 T - 31.229 T ln(T) - 16.3885E-3 T^2 + 2.941883E-6 T^3 + 439915 T^{-1}	*(298.15 < T < 917.00)*
-7415.255 + 247.671446 T - 45.3964 T ln(T)	*(917.00 < T < 4000.00)*

Data for Np relative to ORTHO_Ac

TETRAG_Ad

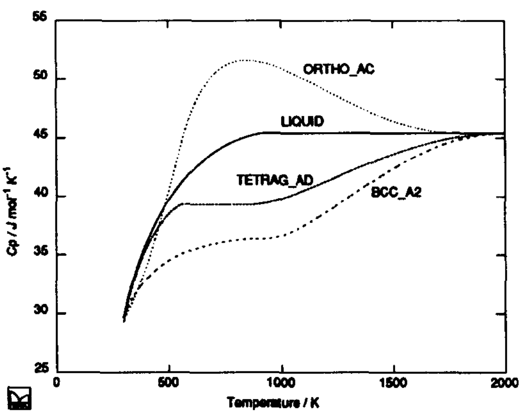
-10399.208 + 241.36056 T - 38.1643 T ln(T) + 25.15865E-3 T^2 + 4.98465E-6 T^3 + 935681 T^{-1}	*(298.15 < T < 553.00)*
46857.793 - 480.444157 T + 68.413 T ln(T) - 44.5778E-3 T^2 + 7.468567E-6 T^3 - 4264085 T^{-1}	*(553.00 < T < 555.00)*
49141.424 - 457.25441 T + 63.193 T ln(T) - 28.4592E-3 T^2 + 2.483917E-6 T^3 - 4796910 T^{-1}	*(555.00 < T < 856.00)*
76043.092 - 710.92183 T + 99.0965 T ln(T) - 47.66965E-3 T^2 + 4.011177E-6 T^3 - 8361550 T^{-1}	*(856.00 < T < 1799.00)*
31120.716 - 302.429326 T + 41.9699 T ln(T) - 19.21045E-3 T^2 + 1.52726E-6 T^3 - 3564640 T^{-1}	*(1799.00 < T < 1999.00)*
-3978.084 + 0.926171 T	*(1999.00 < T < 4000.00)*

BCC_A2

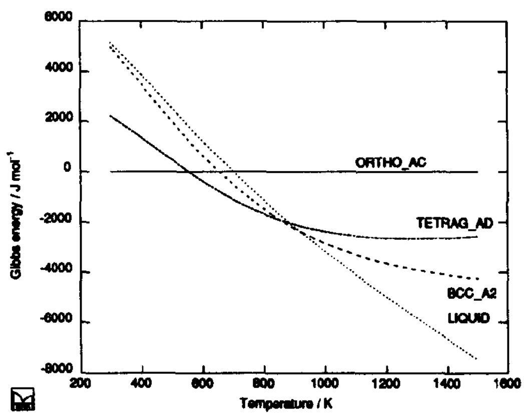
-3466.552 + 232.443163 T - 39.2313 T ln(T) + 38.7586E-3 T^2 + 0.514743E-6 T^3 + 705081 T^{-1}	*(298.15 < T < 553.00)*
53790.448 - 489.361554 T + 67.346 T ln(T) - 30.97785E-3 T^2 + 2.99866E-6 T^3 - 4494685 T^{-1}	*(553.00 < T < 856.00)*
54648.626 - 483.465652 T + 66.122 T ln(T) - 28.4592E-3 T^2 + 2.483917E-6 T^3 - 4796910 T^{-1}	*(856.00 < T < 917.00)*
107897.393 - 961.597728 T + 133.2964 T ln(T) - 62.8075E-3 T^2 + 5.191133E-6 T^3 - 12297010 T^{-1}	*(917.00 < T < 1799.00)*
62975.017 - 553.105224 T + 76.1698 T ln(T) - 34.3483E-3 T^2 + 2.707217E-6 T^3 - 7500100 T^{-1}	*(1799.00 < T < 1999.00)*
-2786.950 - 1.007779 T	*(1999.00 < T < 4000.00)*

LIQUID

-4869.068 + 217.556306 T - 35.2833 T ln(T) + 24.88875E-3 T^2 + 2.941883E-6 T^3 + 842771 T^{-1}	*(298.15 < T < 553.00)*
52387.933 - 504.248411 T + 71.294 T ln(T) - 44.8477E-3 T^2 + 5.4258E-6 T^3 - 4356995 T^{-1}	*(553.00 < T < 917.00)*
49599.858 - 416.601925 T + 57.1266 T ln(T) - 28.4592E-3 T^2 + 2.483917E-6 T^3 - 4796910 T^{-1}	*(917.00 < T < 1799.00)*
4677.481 - 8.10942 T	*(1799.00 < T < 4000.00)*



Heat capacity of Np



Gibbs energy of phases of Np relative to ORTHO_Ac

O

Source of data: JANAF [GAS]
R Schmidt, Metall. Trans., 1983, **14B**, 473-81 [LIQUID]
B Sundman, J. Phase Equil., 1991, **12**(1), 127-40 [BCC_A2, FCC_A1]

Data for O in the form of G-HSER

GAS (1/2O2<g>)

-3480.870 - 25.503038 T - 11.136 T ln(T) - 5.09888E-3 T^2 + 0.661846E-6 T^3 - 38365.0 T^{-1} *(298.15 < T < 1000.00)*
-6568.763 + 12.65988 T - 16.8138 T ln(T) - 0.595798E-3 T^2 + 0.006781E-6 T^3 + 262905 T^{-1} *(1000.00 < T < 3300.00)*
-13986.728 + 31.259625 T - 18.9536 T ln(T) - 0.425243E-3 T^2 + 0.010721E-6 T^3 + 4383200 T^{-1} *(3300.00 < T < 6000.00)*

LIQUID

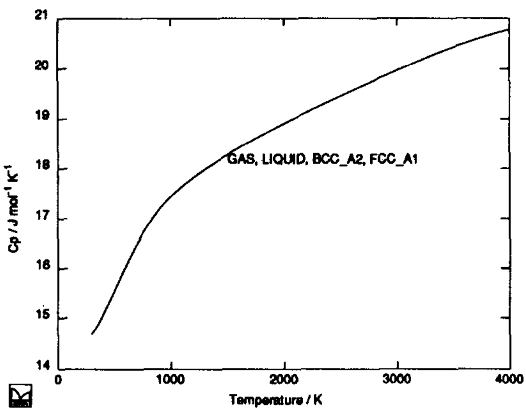
-6129.770 + 5.936962 T - 11.136 T ln(T) - 5.09888E-3 T^2 + 0.661846E-6 T^3 - 38365.0 T^{-1} *(298.15 < T < 1000.00)*
-9217.663 + 44.09988 T - 16.8138 T ln(T) - 0.595798E-3 T^2 + 0.006781E-6 T^3 + 262905 T^{-1} *(1000.00 < T < 3300.00)*
-16635.628 + 62.699625 T - 18.9536 T ln(T) - 0.425243E-3 T^2 + 0.010721E-6 T^3 + 4383200 T^{-1} *(3300.00 < T < 6000.00)*

BCC_A2

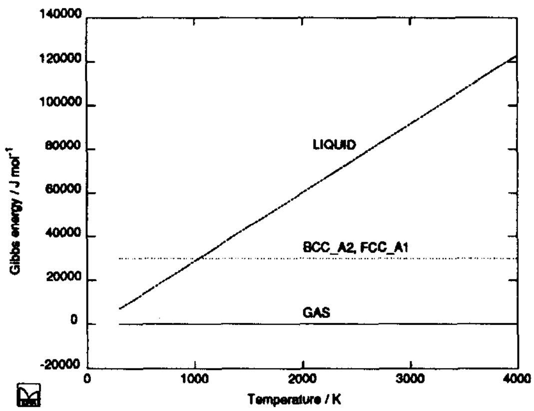
26519.13 - 25.503038 T - 11.136 T ln(T) - 5.09888E-3 T^2 + 0.661846E-6 T^3 - 38365.0 T^{-1} *(298.15 < T < 1000.00)*
23431.237 + 12.65988 T - 16.8138 T ln(T) - 0.595798E-3 T^2 + 0.006781E-6 T^3 + 262905 T^{-1} *(1000.00 < T < 3300.00)*
16013.272 + 31.259625 T - 18.9536 T ln(T) - 0.425243E-3 T^2 + 0.010721E-6 T^3 + 4383200 T^{-1} *(3300.00 < T < 6000.00)*

FCC_A1

26519.13 - 25.503038 T - 11.136 T ln(T) - 5.09888E-3 T^2 + 0.661846E-6 T^3 - 38365.0 T^{-1} *(298.15 < T < 1000.00)*
23431.237 + 12.65988 T - 16.8138 T ln(T) - 0.595798E-3 T^2 + 0.006781E-6 T^3 + 262905 T^{-1} *(1000.00 < T < 3300.00)*
16013.272 + 31.259625 T - 18.9536 T ln(T) - 0.425243E-3 T^2 + 0.010721E-6 T^3 + 4383200 T^{-1} *(3300.00 < T < 6000.00)*



Heat capacity of O



Gibbs energy of phases of O relative to GAS

Data for O relative to 0.5O2<GAS>

LIQUID

-2648.9 + 31.44 T *(298.15 < T < 6000.00)*

BCC_A2

30000 *(298.15 < T < 6000.00)*

FCC_A1

30000 *(298.15 < T < 6000.00)*

Os

Source of data: Hultgren [HCP_A3]
Saunders et al. [LIQUID, FCC_A1, BCC_A2]

Data for Os in the form of G-HSER

HCP_A3

$-7196.978 + 126.369531\ T - 23.5710242\ T\ \ln(T) - 1.90427E\text{-}3\ T^2$ *(298.15 < T < 3306.00)*
$644910.07 - 1935.213696\ T + 224.9980343\ T\ \ln(T) - 42.489827E\text{-}3\ T^2 + 1.173861E\text{-}6\ T^3 - 312569031\ T^{-1}$ *(3306.00 < T < 5500.00)*

LIQUID

$29263.192 + 117.895788\ T - 23.5710242\ T\ \ln(T) - 1.90427E\text{-}3\ T^2$ *(298.15 < T < 1000.00)*
$68715.318 - 198.324341\ T + 19.9382156\ T\ \ln(T) - 20.464464E\text{-}3\ T^2 + 1.014279E\text{-}6\ T^3 - 6237261\ T^{-1}$ *(1000.00 < T < 3306.00)*
$-15903.192 + 336.874526\ T - 50\ T\ \ln(T)$ *(3306.00 < T < 5500.00)*

FCC_A1

$5803.022 + 123.869531\ T - 23.5710242\ T\ \ln(T) - 1.90427E\text{-}3\ T^2$ *(298.15 < T < 3306.00)*
$657910.07 - 1937.713696\ T + 224.9980343\ T\ \ln(T) - 42.489827E\text{-}3\ T^2 + 1.173861E\text{-}6\ T^3 - 312569031\ T^{-1}$ *(3306.00 < T < 5500.00)*

BCC_A2

$36303.022 + 117.369531\ T - 23.5710242\ T\ \ln(T) - 1.90427E\text{-}3\ T^2$ *(298.15 < T < 3306.00)*
$688410.07 - 1944.213696\ T + 224.9980343\ T\ \ln(T) - 42.489827E\text{-}3\ T^2 + 1.173861E\text{-}6\ T^3 - 312569031\ T^{-1}$ *(3306.00 < T < 5500.00)*

Data for Os relative to HCP_A3

LIQUID

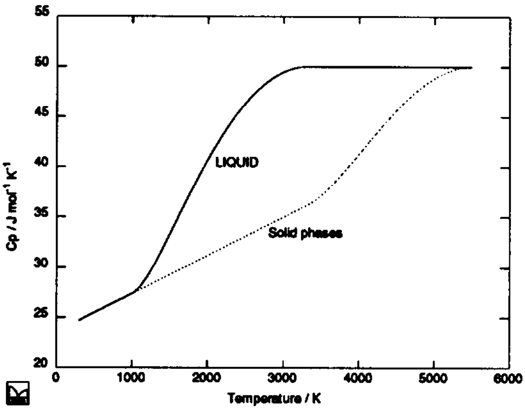
$36460.170 - 8.473742\ T$ *(298.15 < T < 1000.00)*
$75912.296 - 324.693872\ T + 43.5092398\ T\ \ln(T) - 18.560194E\text{-}3\ T^2 + 1.014279E\text{-}6\ T^3 - 6237261\ T^{-1}$ *(1000.00 < T < 3306.00)*
$-660813.262 + 2272.088222\ T - 274.9980343\ T\ \ln(T) + 42.489827E\text{-}3\ T^2 - 1.173861E\text{-}6\ T^3 + 312569031\ T^{-1}$ *(3306.00 < T < 5500.00)*

FCC_A1

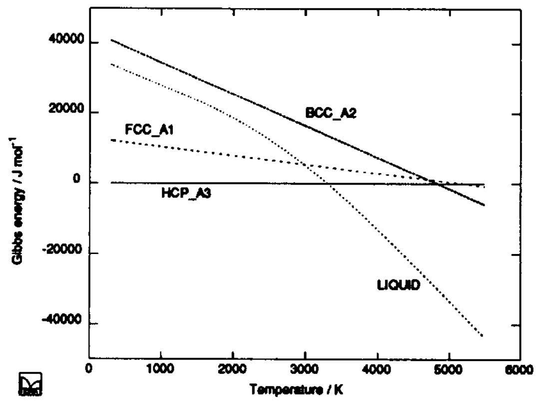
$13000 - 2.5\ T$ *(298.15 < T < 5500.00)*

BCC_A2

$43500 - 9.0\ T$ *(298.15 < T < 5500.00)*



Heat capacity of Os



Gibbs energy of phases of Os relative to HCP_A3

P

Source of data: JANAF [WHITE_P, RED_P, LIQUID]
B Uhrenius (unpublished work) [BCC_A2]
Kaufman [FCC_A1]

Note: By convention the WHITE_P form is taken as reference phase although the RED_P is very much more stable.

Data for P in the form of G-HSER

WHITE_P

$-43821.799 + 1026.693886\ T - 178.426\ T\ \ln(T) + 290.708E\text{-}3\ T^2 - 104.022667E\text{-}6\ T^3 + 1632695\ T^{-1}$ *(250 < T < 317.3)*
$-9587.448 + 152.341487\ T - 28.7335301\ T\ \ln(T) + 1.715669E\text{-}3\ T^2 - 0.22829E\text{-}6\ T^3 + 172966\ T^{-1}$ *(317.3 < T < 1000)*
$-8093.075 + 135.876831\ T - 26.326\ T\ \ln(T)$ *(1000 < T < 3000)*

LIQUID

$-26316.111 + 434.930931\ T - 70.7440584\ T\ \ln(T) - 2.898936E\text{-}3\ T^2 + 39.049371E\text{-}6\ T^3 + 1141147\ T^{-1}$ *(250 < T < 317.3)*
$-7232.449 + 133.291873\ T - 26.326\ T\ \ln(T)$ *(317.3 < T < 3000)*

RED_P

$-25976.559 + 148.672002\ T - 25.55\ T\ \ln(T) + 3.4121E\text{-}3\ T^2 - 2.418867E\text{-}6\ T^3 + 160095\ T^{-1}$ *(250 < T < 500)*
$-21723.721 + 77.671736\ T - 14.368\ T\ \ln(T) - 9.57685E\text{-}3\ T^2 + 0.393917E\text{-}6\ T^3 - 141375\ T^{-1}$ *(500 < T < 852.35)*
$-119408.413 + 1026.02962\ T - 149.4495562\ T\ \ln(T) + 67.272364E\text{-}3\ T^2 - 6.651929E\text{-}6\ T^3 + 12495943\ T^{-1}$
(852.35 < T < 1500)
$-24524.119 + 153.839181\ T - 26.326\ T\ \ln(T)$ *(1500 < T < 3000)*

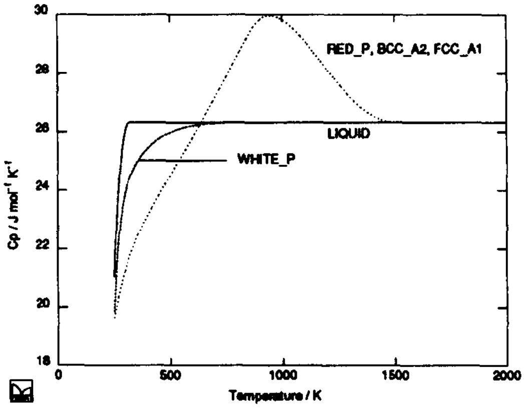
BCC_A2

$18792.241 + 135.412002\ T - 25.55\ T\ \ln(T) + 3.4121E\text{-}3\ T^2 - 2.418867E\text{-}6\ T^3 + 160095\ T^{-1}$ *(250 < T < 500)*
$23045.079 + 64.411737\ T - 14.368\ T\ \ln(T) - 9.57685E\text{-}3\ T^2 + 0.393917E\text{-}6\ T^3 - 141375\ T^{-1}$ *(500 < T < 852.35)*
$-74639.613 + 1012.76962\ T - 149.4495562\ T\ \ln(T) + 67.272364E\text{-}3\ T^2 - 6.651929E\text{-}6\ T^3 + 12495943\ T^{-1}$
(852.35 < T < 1500)
$20244.681 + 140.579181\ T - 26.326\ T\ \ln(T)$ *(1500 < T < 3000)*

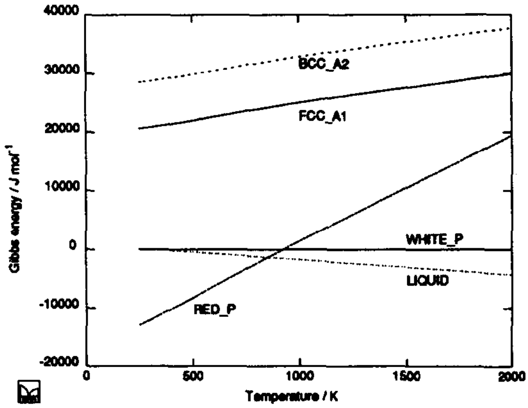
FCC_A1

$10842.441 + 135.534002\ T - 25.55\ T\ \ln(T) + 3.4121E\text{-}3\ T^2 - 2.418867E\text{-}6\ T^3 + 160095\ T^{-1}$ *(250 < T < 500)*
$15095.279 + 64.533737\ T - 14.368\ T\ \ln(T) - 9.57685E\text{-}3\ T^2 + 0.393917E\text{-}6\ T^3 - 141375\ T^{-1}$ *(500 < T < 852.35)*
$-82589.413 + 1012.89162\ T - 149.4495562\ T\ \ln(T) + 67.272364E\text{-}3\ T^2 - 6.651929E\text{-}6\ T^3 + 12495943\ T^{-1}$
(852.35 < T < 1500)

$12294.881 + 140.701181\ T - 26.326\ T \ln(T)$ *(1500 < T < 3000)*



Heat capacity of P



Gibbs energy of phases of P relative to WHITE_P

Data relative to WHITE_P

LIQUID

$17505.688 - 591.762955\ T + 107.6819416\ T \ln(T) - 293.606936E\text{-}3\ T^2 + 143.072038E\text{-}6\ T^3 - 491548\ T^{-1}$ *(250 < T < 317.3)*
$2354.999 - 19.049614\ T + 2.4075301\ T \ln(T) - 1.715669E\text{-}3\ T^2 + 0.22829E\text{-}6\ T^3 - 172966\ T^{-1}$ *(317.3 < T < 1000)*
$860.626 - 2.584958\ T$ *(1000 < T < 3000)*

RED_P

$17845.24 - 878.021884\ T + 152.876\ T \ln(T) - 287.2959E\text{-}3\ T^2 + 101.6038E\text{-}6\ T^3 - 1472600\ T^{-1}$ *(250 < T < 317.3)*
$-16389.111 - 3.669485\ T + 3.1835301\ T \ln(T) + 1.696431E\text{-}3\ T^2 - 2.190577E\text{-}6\ T^3 - 12871\ T^{-1}$ *(317.3 < T < 500)*
$-12136.273 - 74.669751\ T + 14.3655301\ T \ln(T) - 11.292519E\text{-}3\ T^2 + 0.622207E\text{-}6\ T^3 - 314341\ T^{-1}$ *(500 < T < 852.35)*
$-109820.965 + 873.688133\ T - 120.7160261\ T \ln(T) + 65.556695E\text{-}3\ T^2 - 6.423639E\text{-}6\ T^3 + 12322977\ T^{-1}$ *(852.35 < T < 1000)*
$-111315.338 + 890.152789\ T - 123.1235562\ T \ln(T) + 67.272364E\text{-}3\ T^2 - 6.651929E\text{-}6\ T^3 + 12495943\ T^{-1}$ *(1000 < T < 1500)*
$-16431.044 + 17.96235\ T$ *(1500 < T < 3000)*

BCC_A2

$62614.04 - 891.281884\ T + 152.876\ T \ln(T) - 287.2959E\text{-}3\ T^2 + 101.6038E\text{-}6\ T^3 - 1472600\ T^{-1}$ *(250 < T < 317.3)*
$28379.689 - 16.929485\ T + 3.1835301\ T \ln(T) + 1.696431E\text{-}3\ T^2 - 2.190577E\text{-}6\ T^3 - 12871\ T^{-1}$ *(317.3 < T < 500)*
$32632.527 - 87.929751\ T + 14.3655301\ T \ln(T) - 11.292519E\text{-}3\ T^2 + 0.622207E\text{-}6\ T^3 - 314341\ T^{-1}$ *(500 < T < 852.35)*
$-65052.165 + 860.428133\ T - 120.7160261\ T \ln(T) + 65.556695E\text{-}3\ T^2 - 6.423639E\text{-}6\ T^3 + 12322977\ T^{-1}$ *(852.35 < T < 1000)*
$-66546.538 + 876.892789\ T - 123.1235562\ T \ln(T) + 67.272364E\text{-}3\ T^2 - 6.651929E\text{-}6\ T^3 + 12495943\ T^{-1}$ *(1000 < T < 1500)*
$28337.756 + 4.70235\ T$ *(1500 < T < 3000)*

FCC_A1

$54664.24 - 891.159884\ T + 152.876\ T \ln(T) - 287.2959E\text{-}3\ T^2 + 101.6038E\text{-}6\ T^3 - 1472600\ T^{-1}$ *(250 < T < 317.3)*
$20429.889 - 16.807485\ T + 3.1835301\ T \ln(T) + 1.696431E\text{-}3\ T^2 - 2.190577E\text{-}6\ T^3 - 12871\ T^{-1}$ *(317.3 < T < 500)*
$24682.727 - 87.807751\ T + 14.3655301\ T \ln(T) - 11.292519E\text{-}3\ T^2 + 0.622207E\text{-}6\ T^3 - 314341\ T^{-1}$ *(500 < T < 852.35)*
$-73001.965 + 860.550133\ T - 120.7160261\ T \ln(T) + 65.556695E\text{-}3\ T^2 - 6.423639E\text{-}6\ T^3 + 12322977\ T^{-1}$ *(852.35 < T < 1000)*
$-74496.338 + 877.014789\ T - 123.1235562\ T \ln(T) + 67.272364E\text{-}3\ T^2 - 6.651929E\text{-}6\ T^3 + 12495943\ T^{-1}$ *(1000 < T < 1500)*
$20387.956 + 4.82435\ T$ *(1500 < T < 3000)*

Pa

Source of data: M H Rand, Unpublished work

Data for Pa in the form of G-HSER

BCT_Aa

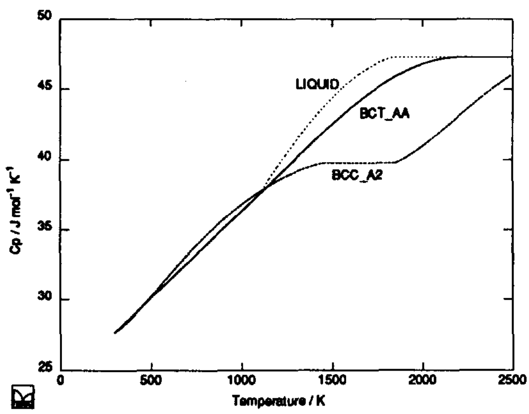
$-7681.561 + 111.973215\ T - 23.9116\ T\ ln(T) - 6.21325E\text{-}3\ T^2$	*(298.15 < T < 1443.00)*
$27955.763 - 177.320253\ T + 16.305\ T\ ln(T) - 26.3416E\text{-}3\ T^2 + 1.884933E\text{-}6\ T^3 - 5908900\ T^{-1}$	*(1443.00 < T < 2176.00)*
$-29949.683 + 288.308639\ T - 47.2792\ T\ ln(T)$	*(2176.00 < T < 4000.00)*

BCC_A2

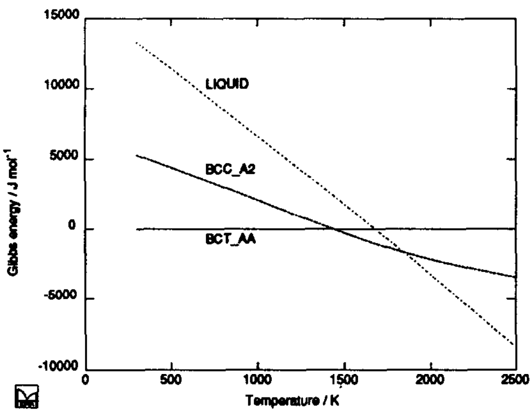
$781.847 + 71.957409\ T - 18.203\ T\ ln(T) - 13.22095E\text{-}3\ T^2 + 1.337387E\text{-}6\ T^3 - 101600\ T^{-1}$	*(298.15 < T < 1443.00)*
$-10955.948 + 220.478519\ T - 39.748\ T\ ln(T)$	*(1443.00 < T < 1845.00)*
$284495.194 - 1397.150521\ T + 171.108\ T\ ln(T) - 63.7105E\text{-}3\ T^2 + 3.343867E\text{-}6\ T^3 - 74992000\ T^{-1}$	*(1845.00 < T < 2710.00)*
$-27885.171 + 286.096187\ T - 47.2792\ T\ ln(T)$	*(2710.00 < T < 4000.00)*

LIQUID

$8499.539 + 102.429215\ T - 23.9116\ T\ ln(T) - 6.21325E\text{-}3\ T^2$	*(298.15 < T < 1088.00)*
$48013.96 - 278.789916\ T + 30.336\ T\ ln(T) - 37.2478E\text{-}3\ T^2 + 3.075017E\text{-}6\ T^3 - 5064250\ T^{-1}$	*(1088.00 < T < 1845.00)*
$-12508.174 + 277.955437\ T - 47.2792\ T\ ln(T)$	*(1845.00 < T < 4000.00)*



Heat capacity of Pa



Gibbs energy of phases of Pa relative to BCT_Aa

Data for Pa relative to BCT_Aa

BCC_A2

$8463.408 - 40.015805\ T + 5.7086\ T\ ln(T) - 7.0077E\text{-}3\ T^2 + 1.337387E\text{-}6\ T^3 - 101600\ T^{-1}$	*(298.15 < T < 1443.00)*
$-38911.711 + 397.798772\ T - 56.053\ T\ ln(T) + 26.3416E\text{-}3\ T^2 - 1.884933E\text{-}6\ T^3 + 5908900\ T^{-1}$	*(1443.00 < T < 1845.00)*
$256539.43 - 1219.830269\ T + 154.803\ T\ ln(T) - 37.3689E\text{-}3\ T^2 + 1.458933E\text{-}6\ T^3 - 69083100\ T^{-1}$	*(1845.00 < T < 2176.00)*
$314444.877 - 1685.45916\ T + 218.3872\ T\ ln(T) - 63.7105E\text{-}3\ T^2 + 3.343867E\text{-}6\ T^3 - 74992000\ T^{-1}$	*(2176.00 < T < 2710.00)*
$2064.512 - 2.212452\ T$	*(2710.00 < T < 4000.00)*

LIQUID

$16181.1 - 9.544\ T$	*(298.15 < T < 1088.00)*
$55695.52 - 390.76313\ T + 54.2476\ T\ ln(T) - 31.03455E\text{-}3\ T^2 + 3.075017E\text{-}6\ T^3 - 5064250\ T^{-1}$	*(1088.00 < T < 1443.00)*
$20058.197 - 101.469663\ T + 14.031\ T\ ln(T) - 10.9062E\text{-}3\ T^2 + 1.190083E\text{-}6\ T^3 + 844650\ T^{-1}$	*(1443.00 < T < 1845.00)*
$-40463.937 + 455.275689\ T - 63.5842\ T\ ln(T) + 26.3416E\text{-}3\ T^2 - 1.884933E\text{-}6\ T^3 + 5908900\ T^{-1}$	*(1845.00 < T < 2176.00)*
$17441.509 - 10.353203\ T$	*(2176.00 < T < 4000.00)*

Pb

Source of data: JANAF [FCC_A1, LIQUID]
T L Ngai, Y A Chang, CALPHAD, 1981, 5, 267 [BCT_A5]
Saunders et al. [HCP_A3, BCC_A2]
J P Nabot, I Ansara, Bull. Alloy Phase Diag., 1987, 8, 246 [TET_ALPHA1]

Data for Pb in the form of G-HSER

FCC_A1

$-7650.085 + 101.700244\,T - 24.5242231\,T\ln(T) - 3.65895E\text{-}3\,T^2 - 0.24395E\text{-}6\,T^3$ *(298.15 < T < 600.612)*
$-10531.095 + 154.243182\,T - 32.4913959\,T\ln(T) + 1.54613E\text{-}3\,T^2 + 8.054E25\,T^{-9}$ *(600.612 < T < 1200)*
$4157.616 + 53.139072\,T - 18.9640637\,T\ln(T) - 2.882943E\text{-}3\,T^2 + 0.098144E\text{-}6\,T^3 - 2696755\,T^{-1} + 8.054E25\,T^{-9}$ *(1200 < T < 2100)*

LIQUID

$-2977.961 + 93.949561\,T - 24.5242231\,T\ln(T) - 3.65895E\text{-}3\,T^2 - 0.24395E\text{-}6\,T^3 - 6.019E\text{-}19\,T^7$ *(298.15 < T < 600.612)*
$-5677.958 + 146.176046\,T - 32.4913959\,T\ln(T) + 1.54613E\text{-}3\,T^2$ *(600.612 < T < 1200)*
$9010.753 + 45.071937\,T - 18.9640637\,T\ln(T) - 2.882943E\text{-}3\,T^2 + 0.098144E\text{-}6\,T^3 - 2696755\,T^{-1}$ *(1200 < T < 2100)*

BCC_A2

$-5250.085 + 100.600244\,T - 24.5242231\,T\ln(T) - 3.65895E\text{-}3\,T^2 - 0.24395E\text{-}6\,T^3$ *(298.15 < T < 600.612)*
$-8131.095 + 153.143182\,T - 32.4913959\,T\ln(T) + 1.54613E\text{-}3\,T^2 + 8.054E25\,T^{-9}$ *(600.612 < T < 1200)*
$6557.616 + 52.039072\,T - 18.9640637\,T\ln(T) - 2.882943E\text{-}3\,T^2 + 0.098144E\text{-}6\,T^3 - 2696755\,T^{-1} + 8.054E25\,T^{-9}$ *(1200 < T < 2100)*

BCT_A5

$-7161.085 + 105.220244\,T - 24.5242231\,T\ln(T) - 3.65895E\text{-}3\,T^2 - 0.24395E\text{-}6\,T^3$ *(298.15 < T < 600.612)*
$-10042.095 + 157.763182\,T - 32.4913959\,T\ln(T) + 1.54613E\text{-}3\,T^2 + 8.054E25\,T^{-9}$ *(600.612 < T < 1200)*
$4646.616 + 56.659072\,T - 18.9640637\,T\ln(T) - 2.882943E\text{-}3\,T^2 + 0.098144E\text{-}6\,T^3 - 2696755\,T^{-1} + 8.054E25\,T^{-9}$ *(1200 < T < 2100)*

HCP_A3

$-7350.085 + 102.700244\,T - 24.5242231\,T\ln(T) - 3.65895E\text{-}3\,T^2 - 0.24395E\text{-}6\,T^3$ *(298.15 < T < 600.612)*
$-10231.095 + 155.243182\,T - 32.4913959\,T\ln(T) + 1.54613E\text{-}3\,T^2 + 8.054E25\,T^{-9}$ *(600.612 < T < 1200)*
$4457.616 + 54.139072\,T - 18.9640637\,T\ln(T) - 2.882943E\text{-}3\,T^2 + 0.098144E\text{-}6\,T^3 - 2696755\,T^{-1} + 8.054E25\,T^{-9}$ *(1200 < T < 2100)*

TET_ALPHA1

$-7466.885 + 102.153384\,T - 24.5639065\,T\ln(T) - 3.656801E\text{-}3\,T^2 - 0.24395E\text{-}6\,T^3$ *(298.15 < T < 600.612)*
$-10347.895 + 154.696322\,T - 32.5310793\,T\ln(T) + 1.548279E\text{-}3\,T^2 + 8.054E25\,T^{-9}$ *(600.612 < T < 1200)*
$4340.816 + 53.592212\,T - 19.0037471\,T\ln(T) - 2.880795E\text{-}3\,T^2 + 0.098144E\text{-}6\,T^3 - 2696755\,T^{-1} + 8.054E25\,T^{-9}$ *(1200 < T < 2100)*

Data relative to FCC_A1

LIQUID

$4672.123 - 7.750683\,T - 6.019E\text{-}19\,T^7$ *(298.15 < T < 600.612)*
$4853.138 - 8.067136\,T - 8.054E25\,T^{-9}$ *(600.612 < T < 2100)*

BCC_A2

$2400 - 1.1\,T$ *(298.15 < T < 2100)*

BCT_A5

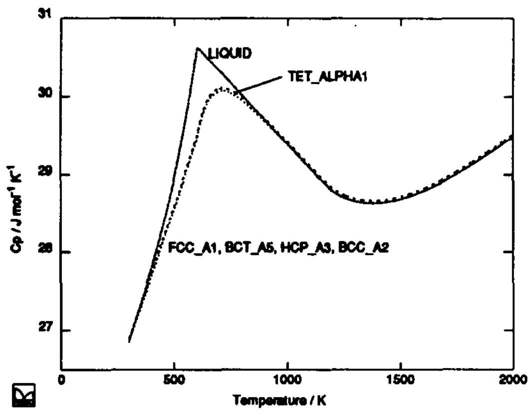
$489 + 3.52\,T$ *(298.15 < T < 2100)*

HCP_A3

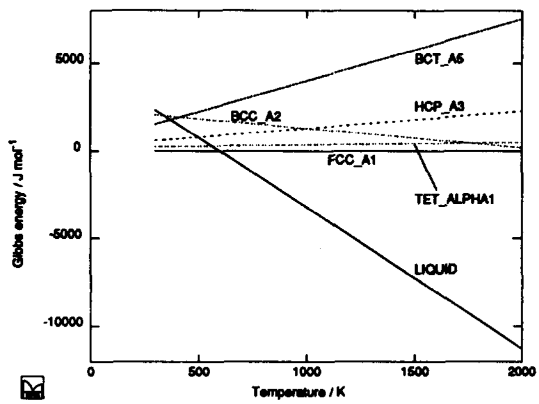
$300 + 1\ T$ *(298.15 < T < 2100)*

TET_ALPHA1

$183.2 + 0.45314\ T - 0.0396834\ T\ln(T) + 0.002149E\text{-}3\ T^2$ *(298.15 < T < 2100)*



Heat capacity of Pb



Gibbs energy of phases of Pb relative to FCC_A1

Pd

Source of data: A T Dinsdale, Unpublished work [FCC_A1, LIQUID]
Saunders et al. [BCC_A2, HCP_A3]

Data for Pd in the form of G-HSER

FCC_A1

$-10204.027 + 176.076315\ T - 32.211\ T\ln(T) + 7.120975E\text{-}3\ T^2 - 1.919875E\text{-}6\ T^3 + 168687\ T^{-1}$ *(298.15 < T < 900)*
$917.062 + 49.659892\ T - 13.5708\ T\ln(T) - 7.17522E\text{-}3\ T^2 + 0.191115E\text{-}6\ T^3 - 1112465\ T^{-1}$ *(900 < T < 1828)*
$-67161.018 + 370.102147\ T - 54.2067086\ T\ln(T) + 2.091396E\text{-}3\ T^2 - 0.062811E\text{-}6\ T^3 + 18683526\ T^{-1}$ *(1828 < T < 4000)*

LIQUID

$1302.731 + 170.964153\ T - 32.211\ T\ln(T) + 7.120975E\text{-}3\ T^2 - 1.919875E\text{-}6\ T^3 + 168687\ T^{-1}$ *(298.15 < T < 600)*
$23405.778 - 116.918419\ T + 10.8922031\ T\ln(T) - 27.266568E\text{-}3\ T^2 + 2.430675E\text{-}6\ T^3 - 1853674\ T^{-1}$ *(600 < T < 1828)*
$-12373.637 + 251.416903\ T - 41.17\ T\ln(T)$ *(1828 < T < 4000)*

BCC_A2

$295.973 + 174.276315\ T - 32.211\ T\ln(T) + 7.120975E\text{-}3\ T^2 - 1.919875E\text{-}6\ T^3 + 168687\ T^{-1}$ *(298.15 < T < 900)*
$11417.062 + 47.859892\ T - 13.5708\ T\ln(T) - 7.17522E\text{-}3\ T^2 + 0.191115E\text{-}6\ T^3 - 1112465\ T^{-1}$ *(900 < T < 1828)*
$-56661.018 + 368.302147\ T - 54.2067086\ T\ln(T) + 2.091396E\text{-}3\ T^2 - 0.062811E\text{-}6\ T^3 + 18683526\ T^{-1}$ *(1828 < T < 4000)*

HCP_A3

$-8204.027 + 176.176315\ T - 32.211\ T\ln(T) + 7.120975E\text{-}3\ T^2 - 1.919875E\text{-}6\ T^3 + 168687\ T^{-1}$ *(298.15 < T < 900)*
$2917.062 + 49.759892\ T - 13.5708\ T\ln(T) - 7.17522E\text{-}3\ T^2 + 0.191115E\text{-}6\ T^3 - 1112465\ T^{-1}$ *(900 < T < 1828)*
$-65161.018 + 370.202147\ T - 54.2067086\ T\ln(T) + 2.091396E\text{-}3\ T^2 - 0.062811E\text{-}6\ T^3 + 18683526\ T^{-1}$ *(1828 < T < 4000)*

Data relative to FCC_A1

LIQUID

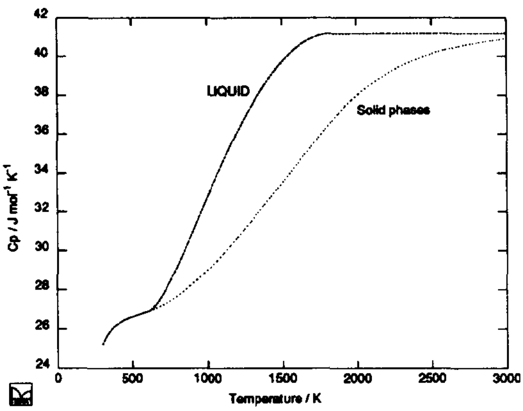
$11506.758 - 5.112161\ T$ *(298.15 < T < 600)*
$33609.804 - 292.994734\ T + 43.1032031\ T\ln(T) - 34.387543E\text{-}3\ T^2 + 4.35055E\text{-}6\ T^3 - 2022361\ T^{-1}$ *(600 < T < 900)*
$22488.716 - 166.578311\ T + 24.4630031\ T\ln(T) - 20.091348E\text{-}3\ T^2 + 2.23956E\text{-}6\ T^3 - 741209\ T^{-1}$ *(900 < T < 1828)*
$54787.381 - 118.685244\ T + 13.0367086\ T\ln(T) - 2.091396E\text{-}3\ T^2 + 0.062811E\text{-}6\ T^3 - 18683526\ T^{-1}$ *(1828 < T < 4000)*

BCC_A2

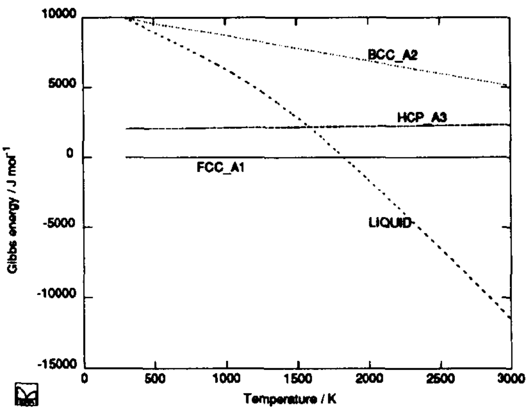
$10500 - 1.8\ T$ *(298.15 < T < 4000)*

HCP_A3

$2000 + 0.1\ T$ *(298.15 < T < 4000)*



Heat capacity of Pd



Gibbs energy of phases of Pd relative to FCC_A1

Pr

Source of data: Hultgren

DHCP

$-18803.379 + 356.587384\ T - 68.9176\ T\ln(T) + 72.929E\text{-}3\ T^2 - 25.184333E\text{-}6\ T^3 + 507385\ T^{-1}$ *(298.15 < T < 500.00)*
$-7246.848 + 82.427384\ T - 22.8909\ T\ln(T) - 4.97126E\text{-}3\ T^2 - 1.22951E\text{-}6\ T^3$ *(500.00 < T < 800.00)*
$95411.023 - 1073.551114\ T + 146.764\ T\ln(T) - 128.8205E\text{-}3\ T^2 + 15.592233E\text{-}6\ T^3 - 11588800\ T^{-1}$
(800.00 < T < 1068.00)
$-481663.131 + 4234.333112\ T - 606.1203107\ T\ln(T) + 305.181506E\text{-}3\ T^2 - 30.994702E\text{-}6\ T^3 + 70926840\ T^{-1}$
(1068.00 < T < 1204.00)
$-20014.678 + 227.685155\ T - 42.9697\ T\ln(T)$ *(1204.00 < T < 3800.00)*

BCC_A2

$-2863.651 + 28.274853\ T - 13.7470527\ T\ln(T) - 22.84377E\text{-}3\ T^2 + 3.542468E\text{-}6\ T^3 - 87486\ T^{-1}$ *(298.15 < T < 1068.00)*
$-11985.919 + 188.657121\ T - 38.451\ T\ln(T)$ *(1068.00 < T < 1204.00)*
$953.224 + 100.826281\ T - 26.6824313\ T\ln(T) - 4.106833E\text{-}3\ T^2 + 0.176214E\text{-}6\ T^3 - 2473024\ T^{-1}$ *(1204.00 < T < 3800.00)*

LIQUID

$3848.961 - 29.099465\ T - 4.7344931\ T\ln(T) - 35.119723E\text{-}3\ T^2 + 5.427467E\text{-}6\ T^3 - 207406\ T^{-1}$ *(298.15 < T < 1068.00)*
$-10539.574 + 219.508806\ T - 42.9697\ T\ln(T)$ *(1068.00 < T < 3800.00)*

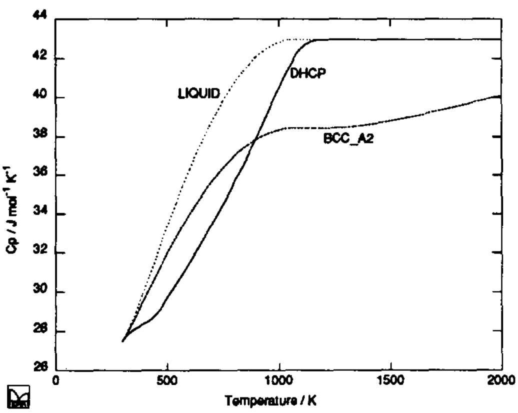
Data for Pr relative to DHCP

BCC_A2

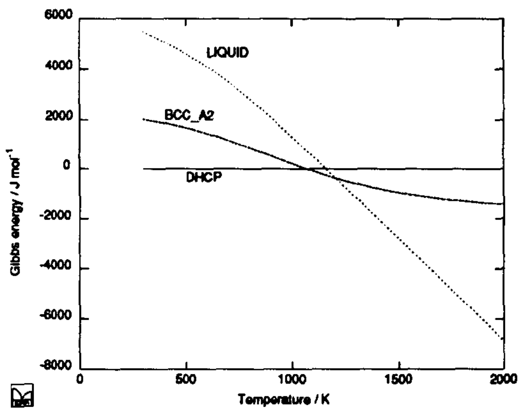
15939.728 - 328.31253 T + 55.1705473 T ln(T) - 95.77277E-3 T^2 + 28.726802E-6 T^3 - 594871 T^{-1} *(298.15 < T < 500.00)*
4383.197 - 54.15253 T + 9.1438473 T ln(T) - 17.87251E-3 T^2 + 4.771978E-6 T^3 - 87486 T^{-1} *(500.00 < T < 800.00)*
-98274.674 + 1101.825967 T - 160.5110527 T ln(T) + 105.97673E-3 T^2 - 12.049765E-6 T^3 + 11501314 T^{-1} *(800.00 < T < 1068.00)*
469677.211 - 4045.675992 T + 567.6693107 T ln(T) - 305.181506E-3 T^2 + 30.994702E-6 T^3 - 70926840 T^{-1} *(1068.00 < T < 1204.00)*
20967.901 - 126.858874 T + 16.2872687 T ln(T) - 4.106833E-3 T^2 + 0.176214E-6 T^3 - 2473024 T^{-1} *(1204.00 < T < 3800.00)*

LIQUID

22652.34 - 385.686848 T + 64.1831069 T ln(T) - 108.048723E-3 T^2 + 30.6118E-6 T^3 - 714791 T^{-1} *(298.15 < T < 500.00)*
11095.809 - 111.526848 T + 18.1564069 T ln(T) - 30.148463E-3 T^2 + 6.656977E-6 T^3 - 207406 T^{-1} *(500.00 < T < 800.00)*
-91562.062 + 1044.451649 T - 151.4984931 T ln(T) + 93.700777E-3 T^2 - 10.164767E-6 T^3 + 11381394 T^{-1} *(800.00 < T < 1068.00)*
471123.557 - 4014.824307 T + 563.1506107 T ln(T) - 305.181506E-3 T^2 + 30.994702E-6 T^3 - 70926840 T^{-1} *(1068.00 < T < 1204.00)*
9475.104 - 8.176349 T *(1204.00 < T < 3800.00)*



Heat capacity of Pr



Gibbs energy of phases of Pr relative to DHCP

Pt

Source of data: A T Dinsdale, Unpublished work, [FCC_A1, LIQUID]
Saunders et al. [BCC_A2, HCP_A3]

Data for Pt in the form of G-HSER

FCC_A1

-7595.631 + 124.388275 T - 24.5526 T ln(T) - 2.48297E-3 T^2 - 0.020138E-6 T^3 + 7974 T^{-1} *(298.15 < T < 1300)*
-9253.174 + 161.529615 T - 30.2527 T ln(T) + 2.321665E-3 T^2 - 0.656946E-6 T^3 - 272106 T^{-1} *(1300 < T < 2041.5)*
-222048.216 + 1019.358919 T - 136.192996 T ln(T) + 20.454938E-3 T^2 - 0.759259E-6 T^3 + 71539020 T^{-1} *(2041.5 < T < 4000)*

LIQUID

12518.385 + 115.113092 T - 24.5526 T ln(T) - 2.48297E-3 T^2 - 0.020138E-6 T^3 + 7974 T^{-1} *(298.15 < T < 600)*
19023.49 + 32.94182 T - 12.3403769 T ln(T) - 11.551507E-3 T^2 + 0.931516E-6 T^3 - 601426 T^{-1} *(600 < T < 2041.5)*
1404.468 + 205.858962 T - 36.5 T ln(T) *(2041.5 < T < 4000)*

BCC_A2

$7404.369 + 121.988275\ T - 24.5526\ T\ \ln(T) - 2.48297E\text{-}3\ T^2 - 0.020138E\text{-}6\ T^3 + 7974\ T^{-1}$ *(298.15 < T < 1300)*
$5746.826 + 159.129615\ T - 30.2527\ T\ \ln(T) + 2.321665E\text{-}3\ T^2 - 0.656946E\text{-}6\ T^3 - 272106\ T^{-1}$ *(1300 < T < 2041.5)*
$-207048.216 + 1016.958919\ T - 136.192996\ T\ \ln(T) + 20.454938E\text{-}3\ T^2 - 0.759259E\text{-}6\ T^3 + 71539020\ T^{-1}$ *(2041.5 < T < 4000)*

HCP_A3

$-5095.631 + 124.488275\ T - 24.5526\ T\ \ln(T) - 2.48297E\text{-}3\ T^2 - 0.020138E\text{-}6\ T^3 + 7974\ T^{-1}$ *(298.15 < T < 1300)*
$-6753.174 + 161.629615\ T - 30.2527\ T\ \ln(T) + 2.321665E\text{-}3\ T^2 - 0.656946E\text{-}6\ T^3 - 272106\ T^{-1}$ *(1300 < T < 2041.5)*
$-219548.216 + 1019.458919\ T - 136.192996\ T\ \ln(T) + 20.454938E\text{-}3\ T^2 - 0.759259E\text{-}6\ T^3 + 71539020\ T^{-1}$ *(2041.5 < T < 4000)*

Data relative to FCC_A1

LIQUID

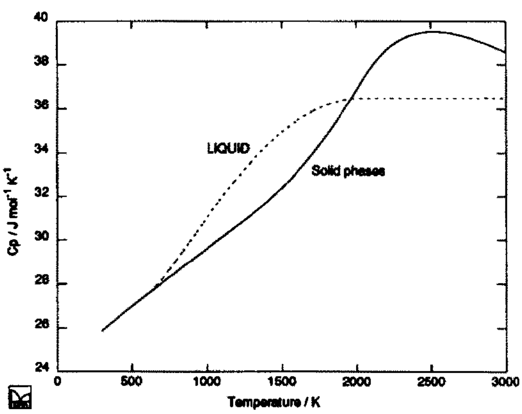
$20114.016 - 9.275183\ T$ *(298.15 < T < 600)*
$26619.122 - 91.446456\ T + 12.2122231\ T\ \ln(T) - 9.068537E\text{-}3\ T^2 + 0.951653E\text{-}6\ T^3 - 609399\ T^{-1}$ *(600 < T < 1300)*
$28276.664 - 128.587796\ T + 17.9123231\ T\ \ln(T) - 13.873172E\text{-}3\ T^2 + 1.588462E\text{-}6\ T^3 - 329320\ T^{-1}$ *(1300 < T < 2041.5)*
$223452.683 - 813.499957\ T + 99.692996\ T\ \ln(T) - 20.454938E\text{-}3\ T^2 + 0.759259E\text{-}6\ T^3 - 71539020\ T^{-1}$ *(2041.5 < T < 4000)*

BCC_A2

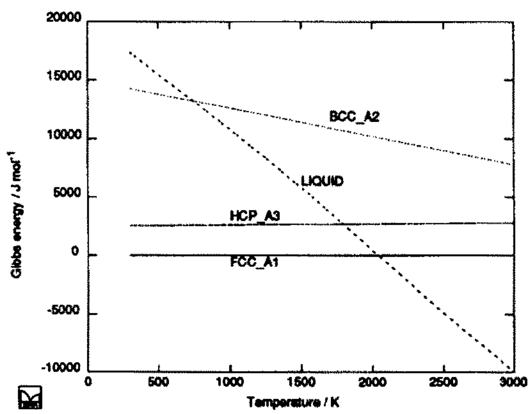
$15000 - 2.4\ T$ *(298.15 < T < 4000)*

HCP_A3

$2500 + 0.1\ T$ *(298.15 < T < 4000)*



Heat capacity of Pt



Gibbs energy of phases of Pt relative to FCC_A1

Pu

Source of data: M H Rand and A T Dinsdale, Unpublished work

Data for Pu in the form of G-HSER

ALPHA

-7396.309 + 80.301382 T - 18.1258 T ln(T) - 22.41E-3 T^2	*(298.15 < T < 400.00)*
-16605.962 + 236.786603 T - 42.4187 T ln(T) - 1.34493E-3 T^2 + 0.263443E-6 T^3 + 579325 T^{-1}	*(400.00 < T < 944.00)*
-14462.156 + 232.961553 T - 42.248 T ln(T)	*(944.00 < T < 3000.00)*

BETA

-4873.654 + 123.249151 T - 27.416 T ln(T) - 6.53E-3 T^2	*(298.15 < T < 679.50)*
2435.094 + 43.566585 T - 15.7351 T ln(T) - 15.4772E-3 T^2 + 1.524942E-6 T^3 - 864940 T^{-1}	*(679.50 < T < 1464.00)*
-13959.062 + 228.221615 T - 42.248 T ln(T)	*(1464.00 < T < 3000.00)*

GAMMA

-16766.303 + 419.402655 T - 77.5802 T ln(T) + 81.6415E-3 T^2 - 28.103833E-6 T^3 + 574825 T^{-1}	*(298.15 < T < 487.90)*
-2942.77 + 88.325069 T - 22.0233 T ln(T) - 11.4795E-3 T^2	*(487.90 < T < 593.90)*
-9336.967 + 160.314641 T - 32.3405 T ln(T) - 7.0383E-3 T^2 + 0.692887E-6 T^3 + 630600 T^{-1}	*(593.90 < T < 1179.00)*
-12435.75 + 226.131617 T - 42.248 T ln(T)	*(1179.00 < T < 3000.00)*

FCC_A1

-3920.781 + 127.586536 T - 28.4781 T ln(T) - 5.4035E-3 T^2	*(298.15 < T < 990.00)*
3528.208 + 41.52572 T - 15.7351 T ln(T) - 15.4772E-3 T^2 + 1.524942E-6 T^3 - 864940 T^{-1}	*(990.00 < T < 1464.00)*
-12865.948 + 226.18075 T - 42.248 T ln(T)	*(1464.00 < T < 3000.00)*

TETRAGONAL_A6

-496.178 + 54.586547 T - 16.43 T ln(T) - 24.006E-3 T^2 + 5.166667E-6 T^3 - 158470 T^{-1}	*(298.15 < T < 736.00)*
-6122.307 + 173.35008 T - 35.56 T ln(T)	*(736.00 < T < 757.00)*
3982.078 + 63.890352 T - 19.756 T ln(T) - 9.37295E-3 T^2 + 0.659882E-6 T^3 - 1112565 T^{-1}	*(757.00 < T < 2157.00)*
-15200.539 + 228.05641 T - 42.248 T ln(T)	*(2157.00 < T < 3000.00)*

BCC_A2

-1358.984 + 116.603882 T - 27.094 T ln(T) - 9.105E-3 T^2 + 2.061667E-6 T^3 + 20863 T^{-1}	*(298.15 < T < 745.00)*
-2890.817 + 156.878957 T - 33.72 T ln(T)	*(745.00 < T < 956.00)*
29313.619 - 132.788248 T + 6.921 T ln(T) - 20.23305E-3 T^2 + 1.426922E-6 T^3 - 4469245 T^{-1}	*(956.00 < T < 2071.00)*
-15400.585 + 227.421855 T - 42.248 T ln(T)	*(2071.00 < T < 3000.00)*

LIQUID

-788.209 + 67.788082 T - 18.1258 T ln(T) - 22.41E-3 T^2	*(298.15 < T < 400.00)*
-9997.862 + 224.273303 T - 42.4187 T ln(T) - 1.34493E-3 T^2 + 0.263443E-6 T^3 + 579325 T^{-1}	*(400.00 < T < 944.00)*
-7854.056 + 220.448253 T - 42.248 T ln(T)	*(944.00 < T < 3000.00)*

Data for Pu relative to ALPHA

BETA

2522.654 + 42.947769 T - 9.2902 T ln(T) + 15.88E-3 T^2	*(298.15 < T < 400.00)*
11732.307 - 113.537453 T + 15.0027 T ln(T) - 5.18507E-3 T^2 - 0.263443E-6 T^3 - 579325 T^{-1}	*(400.00 < T < 679.50)*
19041.056 - 193.220018 T + 26.6836 T ln(T) - 14.13227E-3 T^2 + 1.261498E-6 T^3 - 1444265 T^{-1}	*(679.50 < T < 944.00)*
16897.25 - 189.394968 T + 26.5129 T ln(T) - 15.4772E-3 T^2 + 1.524942E-6 T^3 - 864940 T^{-1}	*(944.00 < T < 1464.00)*
503.094 - 4.739938 T	*(1464.00 < T < 3000.00)*

GAMMA

-9369.994 + 339.101274 T - 59.4544 T ln(T) + 104.0515E-3 T^2 - 28.103833E-6 T^3 + 574825 T^{-1}	*(298.15 < T < 400.00)*
-160.341 + 182.616052 T - 35.1615 T ln(T) + 82.98643E-3 T^2 - 28.367277E-6 T^3 - 4500 T^{-1}	*(400.00 < T < 487.90)*

$13663.192 - 148.461534\ T + 20.3954\ T\ \ln(T) - 10.13457E\text{-}3\ T^2 - 0.263443E\text{-}6\ T^3 - 579325\ T^{-1}$ *(487.90 < T < 593.90)*
$7268.994 - 76.471962\ T + 10.0782\ T\ \ln(T) - 5.69337E\text{-}3\ T^2 + 0.429443E\text{-}6\ T^3 + 51275\ T^{-1}$ *(593.90 < T < 944.00)*
$5125.189 - 72.646912\ T + 9.9075\ T\ \ln(T) - 7.0383E\text{-}3\ T^2 + 0.692887E\text{-}6\ T^3 + 630600\ T^{-1}$ *(944.00 < T < 1179.00)*
$2026.406 - 6.829936\ T$ *(1179.00 < T < 3000.00)*

FCC_A1

$3475.528 + 47.285155\ T - 10.3523\ T\ \ln(T) + 17.0065E\text{-}3\ T^2$ *(298.15 < T < 400.00)*
$12685.181 - 109.200067\ T + 13.9406\ T\ \ln(T) - 4.05857E\text{-}3\ T^2 - 0.263443E\text{-}6\ T^3 - 579325\ T^{-1}$ *(400.00 < T < 944.00)*
$10541.375 - 105.375017\ T + 13.7699\ T\ \ln(T) - 5.4035E\text{-}3\ T^2$ *(944.00 < T < 990.00)*
$17990.364 - 191.435833\ T + 26.5129\ T\ \ln(T) - 15.4772E\text{-}3\ T^2 + 1.524942E\text{-}6\ T^3 - 864940\ T^{-1}$ *(990.00 < T < 1464.00)*
$1596.208 - 6.780803\ T$ *(1464.00 < T < 3000.00)*

TETRAGONAL_A6

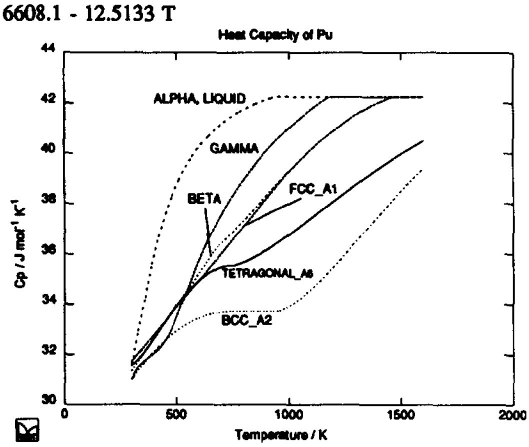
$6900.131 - 25.714834\ T + 1.6958\ T\ \ln(T) - 1.596E\text{-}3\ T^2 + 5.166667E\text{-}6\ T^3 - 158470\ T^{-1}$ *(298.15 < T < 400.00)*
$16109.784 - 182.200056\ T + 25.9887\ T\ \ln(T) - 22.66107E\text{-}3\ T^2 + 4.903223E\text{-}6\ T^3 - 737795\ T^{-1}$ *(400.00 < T < 736.00)*
$10483.655 - 63.436524\ T + 6.8587\ T\ \ln(T) + 1.34493E\text{-}3\ T^2 - 0.263443E\text{-}6\ T^3 - 579325\ T^{-1}$ *(736.00 < T < 757.00)*
$20588.039 - 172.896251\ T + 22.6627\ T\ \ln(T) - 8.02802E\text{-}3\ T^2 + 0.396438E\text{-}6\ T^3 - 1691890\ T^{-1}$ *(757.00 < T < 944.00)*
$18444.234 - 169.071201\ T + 22.492\ T\ \ln(T) - 9.37295E\text{-}3\ T^2 + 0.659882E\text{-}6\ T^3 - 1112565\ T^{-1}$ *(944.00 < T < 2157.00)*
$-738.383 - 4.905143\ T$ *(2157.00 < T < 3000.00)*

BCC_A2

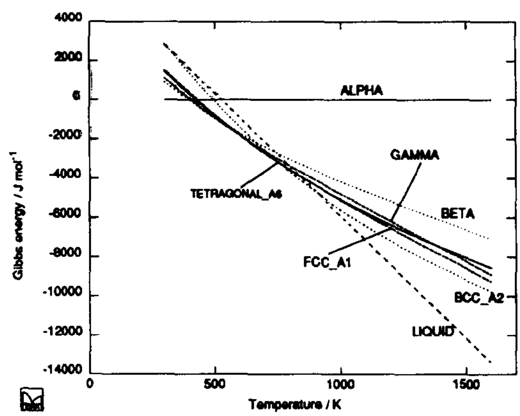
$6037.325 + 36.302501\ T - 8.9682\ T\ \ln(T) + 13.305E\text{-}3\ T^2 + 2.061667E\text{-}6\ T^3 + 20863\ T^{-1}$ *(298.15 < T < 400.00)*
$15246.978 - 120.182721\ T + 15.3247\ T\ \ln(T) - 7.76007E\text{-}3\ T^2 + 1.798223E\text{-}6\ T^3 - 558463\ T^{-1}$ *(400.00 < T < 745.00)*
$13715.145 - 79.907646\ T + 8.6987\ T\ \ln(T) + 1.34493E\text{-}3\ T^2 - 0.263443E\text{-}6\ T^3 - 579325\ T^{-1}$ *(745.00 < T < 944.00)*
$11571.34 - 76.082596\ T + 8.528\ T\ \ln(T)$ *(944.00 < T < 956.00)*
$43775.776 - 365.749801\ T + 49.169\ T\ \ln(T) - 20.23305E\text{-}3\ T^2 + 1.426922E\text{-}6\ T^3 - 4469245\ T^{-1}$ *(956.00 < T < 2071.00)*
$-938.428 - 5.539698\ T$ *(2071.00 < T < 3000.00)*

LIQUID

$6608.1 - 12.5133\ T$ *(298.15 < T < 3000.00)*



Heat capacity of Pu



Gibbs energy of phases of Pu relative to ALPHA

Rb

Source of data: TPIS [BCC_A2, LIQUID]
Saunders et al. [HCP_A3, FCC_A1]

Data for Rb in the form of G-HSER

BCC_A2

$-21669.733 + 583.580988\ T - 115.2825888\ T\ \ln(T) + 262.77612E\text{-}3\ T^2 - 152.236932E\text{-}6\ T^3 + 385754\ T^{-1}$ *(200 < T < 312.46)*

$-7823.397 + 117.050578\ T - 29.1775424\ T\ \ln(T) + 0.412369E\text{-}3\ T^2 - 0.46822E\text{-}6\ T^3 - 126310\ T^{-1} - 5.55E22\ T^{-9}$ *(312.46 < T < 900)*

$-39488.142 + 450.974149\ T - 77.7006456\ T\ \ln(T) + 33.795632E\text{-}3\ T^2 - 4.829082E\text{-}6\ T^3 + 3778006\ T^{-1} - 5.55E22\ T^{-9}$ *(900 < T < 1600)*

$-159742.511 + 1287.789466\ T - 191.2627736\ T\ \ln(T) + 81.61687E\text{-}3\ T^2 - 8.61653E\text{-}6\ T^3 + 27738456\ T^{-1} - 5.55E22\ T^{-9}$ *(1600 < T < 2100)*

LIQUID

$-19452.181 + 576.470502\ T - 115.2825888\ T\ \ln(T) + 262.77612E\text{-}3\ T^2 - 152.236932E\text{-}6\ T^3 + 385754\ T^{-1} + 1.441E\text{-}17\ T^7$ *(200 < T < 312.46)*

$-5650.532 + 110.090262\ T - 29.1775424\ T\ \ln(T) + 0.412369E\text{-}3\ T^2 - 0.46822E\text{-}6\ T^3 - 126310\ T^{-1}$ *(312.46 < T < 900)*

$-37315.276 + 444.013833\ T - 77.7006456\ T\ \ln(T) + 33.795632E\text{-}3\ T^2 - 4.829082E\text{-}6\ T^3 + 3778006\ T^{-1}$ *(900 < T < 1600)*

$-157569.646 + 1280.829151\ T - 191.2627736\ T\ \ln(T) + 81.61687E\text{-}3\ T^2 - 8.61653E\text{-}6\ T^3 + 27738456\ T^{-1}$ *(1600 < T < 2100)*

FCC_A1

$-21469.733 + 584.880988\ T - 115.2825888\ T\ \ln(T) + 262.77612E\text{-}3\ T^2 - 152.236932E\text{-}6\ T^3 + 385754\ T^{-1}$ *(200 < T < 312.46)*

$-7623.397 + 118.350578\ T - 29.1775424\ T\ \ln(T) + 0.412369E\text{-}3\ T^2 - 0.46822E\text{-}6\ T^3 - 126310\ T^{-1} - 5.55E22\ T^{-9}$ *(312.46 < T < 900)*

$-39288.142 + 452.274149\ T - 77.7006456\ T\ \ln(T) + 33.795632E\text{-}3\ T^2 - 4.829082E\text{-}6\ T^3 + 3778006\ T^{-1} - 5.55E22\ T^{-9}$ *(900 < T < 1600)*

$-159542.511 + 1289.089466\ T - 191.2627736\ T\ \ln(T) + 81.61687E\text{-}3\ T^2 - 8.61653E\text{-}6\ T^3 + 27738456\ T^{-1} - 5.55E22\ T^{-9}$ *(1600 < T < 2100)*

HCP_A3

$-21469.733 + 585.580988\ T - 115.2825888\ T\ \ln(T) + 262.77612E\text{-}3\ T^2 - 152.236932E\text{-}6\ T^3 + 385754\ T^{-1}$ *(200 < T < 312.46)*

$-7623.397 + 119.050578\ T - 29.1775424\ T\ \ln(T) + 0.412369E\text{-}3\ T^2 - 0.46822E\text{-}6\ T^3 - 126310\ T^{-1} - 5.55E22\ T^{-9}$ *(312.46 < T < 900)*

$-39288.142 + 452.974149\ T - 77.7006456\ T\ \ln(T) + 33.795632E\text{-}3\ T^2 - 4.829082E\text{-}6\ T^3 + 3778006\ T^{-1} - 5.55E22\ T^{-9}$ *(900 < T < 1600)*

$-159542.511 + 1289.789466\ T - 191.2627736\ T\ \ln(T) + 81.61687E\text{-}3\ T^2 - 8.61653E\text{-}6\ T^3 + 27738456\ T^{-1} - 5.55E22\ T^{-9}$ *(1600 < T < 2100)*

Data relative to BCC_A2

LIQUID

$2217.553 - 7.110485\ T + 1.441E\text{-}17\ T^7$ *(200 < T < 312.46)*

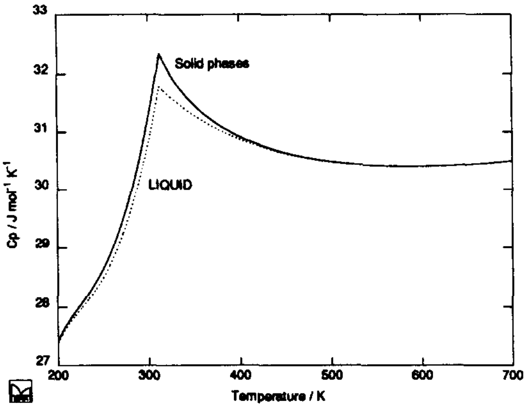
$2172.865 - 6.960316\ T + 5.55E22\ T^{-9}$ *(312.46 < T < 2100)*

FCC_A1

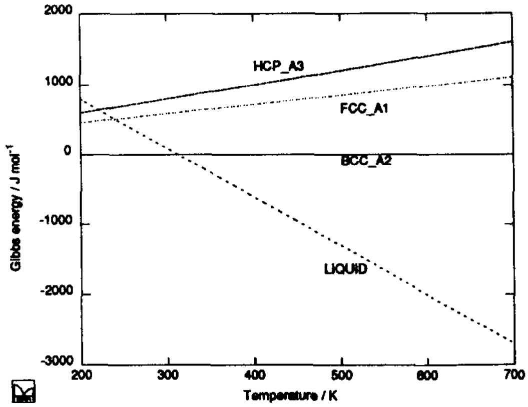
$200 + 1.3\ T$ *(200 < T < 2100)*

HCP_A3

$200 + 2\ T$ *(200 < T < 2100)*



Heat capacity of Rb



Gibbs energy of phases of Rb relative to BCC_A2

Re

Source of data: Hultgren [HCP_A3]
Saunders and Dinsdale, Unpublished work [LIQUID]
Saunders et al. [BCC_A2, FCC_A1]

Data for Re in the form of G-HSER

HCP_A3

-7305.045 + 123.758773 T - 23.6892641 T ln(T) - 2.723387E-3 T^2 *(298.15 < T < 3459.00)*
38514.17 - 65.920606 T + 0.0645635 T ln(T) - 8.050184E-3 T^2 + 0.219551E-6 T^3 - 15938253 T^{-1} *(3459.00 < T < 6000.00)*

LIQUID

37991.663 + 112.574475 T - 23.6892641 T ln(T) - 2.723387E-3 T^2 *(298.15 < T < 1000.00)*
66060.979 - 113.540121 T + 7.4580354 T ln(T) - 16.183804E-3 T^2 + 0.769496E-6 T^3 - 4421721 T^{-1} *(1000.00 < T < 3459.00)*
-5301.43 + 328.158541 T - 50 T ln(T) *(3459.00 < T < 6000.00)*

BCC_A2

21894.955 + 117.758773 T - 23.6892641 T ln(T) - 2.723387E-3 T^2 *(298.15 < T < 3459.00)*
67714.17 - 71.920606 T + 0.0645635 T ln(T) - 8.050184E-3 T^2 + 0.219551E-6 T^3 - 15938253 T^{-1} *(3459.00 < T < 6000.00)*

FCC_A1

3694.955 + 122.258773 T - 23.6892641 T ln(T) - 2.723387E-3 T^2 *(298.15 < T < 3459.00)*
49514.17 - 67.420606 T + 0.0645635 T ln(T) - 8.050184E-3 T^2 + 0.219551E-6 T^3 - 15938253 T^{-1} *(3459.00 < T < 6000.00)*

Data for Re relative to HCP_A3

LIQUID

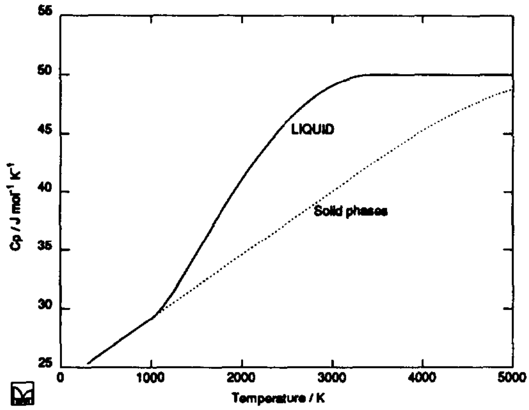
45296.708 - 11.184298 T *(298.15 < T < 1000.00)*
73366.024 - 237.298894 T + 31.1472995 T ln(T) - 13.460417E-3 T^2 + 0.769496E-6 T^3 - 4421721 T^{-1} *(1000.00 < T < 3459.00)*
-43815.600 + 394.079147 T - 50.0645635 T ln(T) + 8.050184E-3 T^2 - 0.219551E-6 T^3 + 15938253 T^{-1} *(3459.00 < T < 6000.00)*

BCC_A2

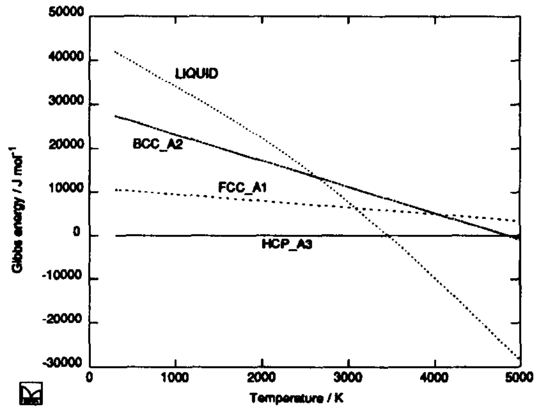
29200 - 6.0 T *(298.15 < T < 6000.00)*

FCC_A1

11000 - 1.50 T *(298.15 < T < 6000.00)*



Heat capacity of Re



Gibbs energy of phases of Re relative to HCP_A3

Rh

Source of data: L.B. Pankratz, Bureau of Mines Bull. 672 [FCC_A1, LIQUID]
Saunders et al. [HCP_A3, BCC_A2]

Data for Rh in the form of G-HSER

FCC_A1

-7848.828 + 132.020923 T - 24.0178336 T ln(T) - 3.424186E-3 T^2 - 0.168032E-6 T^3 + 55846 T^{-1} *(298.15 < T < 1200.00)*
-28367.852 + 305.771019 T - 48.3766632 T ln(T) + 9.66345E-3 T^2 - 1.512774E-6 T^3 + 3348162 T^{-1} *(1200.00 < T < 2237.00)*
-6237470.481 + 30151.634226 T - 3874.2105805 T ln(T) + 1049.213607E-3 T^2 - 53.978814E-6 T^3 + 1880362184 T^{-1} *(2237.00 < T < 2450.00)*
-44863.489 + 344.889895 T - 50.58456 T ln(T) *(2450.00 < T < 2500.00)*

LIQUID

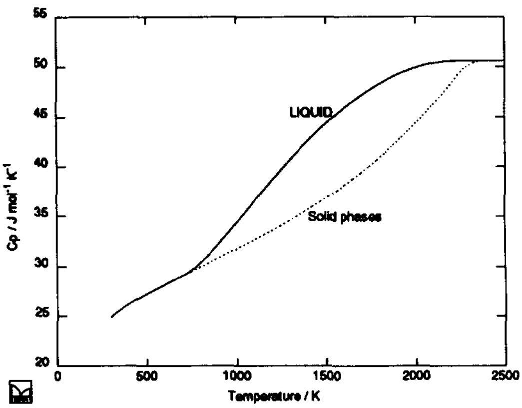
11244.082 + 125.099593 T - 24.0178336 T ln(T) - 3.424186E-3 T^2 - 0.168032E-6 T^3 + 55846 T^{-1} *(298.15 < T < 700.00)*
35898.508 - 147.926418 T + 15.6492377 T ln(T) - 28.665357E-3 T^2 + 2.100572E-6 T^3 - 2638940 T^{-1} *(700.00 < T < 2237.00)*
-18208.54 + 332.974832 T - 50.58456 T ln(T) *(2237.00 < T < 2500.00)*

BCC_A2

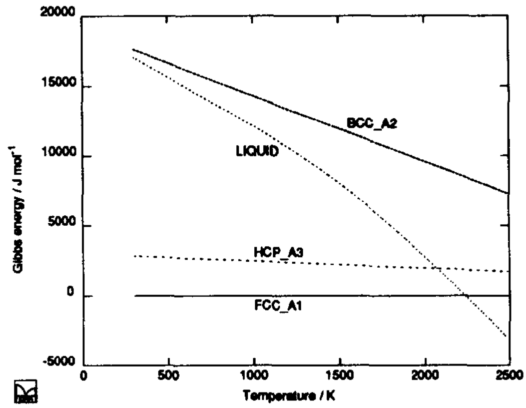
11151.172 + 127.320923 T - 24.0178336 T ln(T) - 3.424186E-3 T^2 - 0.168032E-6 T^3 + 55846 T^{-1} *(298.15 < T < 1200.00)*
-9367.852 + 301.071019 T - 48.3766632 T ln(T) + 9.66345E-3 T^2 - 1.512774E-6 T^3 + 3348162 T^{-1} *(1200.00 < T < 2237.00)*
-6218470.481 + 30146.934226 T - 3874.2105805 T ln(T) + 1049.213607E-3 T^2 - 53.978814E-6 T^3 + 1880362184 T^{-1} *(2237.00 < T < 2450.00)*
-25863.489 + 340.189895 T - 50.58456 T ln(T) *(2450.00 < T < 2500.00)*

HCP_A3

-4848.828 + 131.520923 T - 24.0178336 T ln(T) - 3.424186E-3 T^2 - 0.168032E-6 T^3 + 55846 T^{-1} *(298.15 < T < 1200.00)*
-25367.852 + 305.271019 T - 48.3766632 T ln(T) + 9.66345E-3 T^2 - 1.512774E-6 T^3 + 3348162 T^{-1} *(1200.00 < T < 2237.00)*
-6234470.481 + 30151.134226 T - 3874.2105805 T ln(T) + 1049.213607E-3 T^2 - 53.978814E-6 T^3 + 1880362184 T^{-1} *(2237.00 < T < 2450.00)*
-41863.489 + 344.389895 T - 50.58456 T ln(T) *(2450.00 < T < 2500.00)*



Heat capacity of Rh



Gibbs energy of phases of Rh relative to FCC_A1

Data for Rh relative to FCC_A1

LIQUID

19092.910 - 6.921330 T *(298.15 < T < 700.00)*
43747.336 - 279.947341 T + 39.6670713 T ln(T) - 25.241172E-3 T^2 + 2.268604E-6 T^3 - 2694786 T^{-1} *(700.00 < T < 1200.00)*
64266.360 - 453.697437 T + 64.0259009 T ln(T) - 38.328808E-3 T^2 + 3.613346E-6 T^3 - 5987102 T^{-1} *(1200.00 < T < 2237.00)*
6219261.941 - 29818.659394 T + 3823.6260205 T ln(T) - 1049.213607E-3 T^2 + 53.978814E-6 T^3 - 1880362184 T^{-1} *(2237.00 < T < 2450.00)*
26654.949 - 11.915063 T *(2450.00 < T < 2500.00)*

BCC_A2

19000 - 4.70 T *(298.15 < T < 2500.00)*

HCP_A3

3000 - 0.5 T *(298.15 < T < 2500.00)*

Ru

Source of data: L B Pankratz, Bureau of Mines Bull. 672, revised by M H Rand [HCP_A3, LIQUID]
Saunders et al. [FCC_A1, BCC_A2]

Data for Ru in the form of G-HSER

HCP_A3

$-7561.873 + 127.866233\ T - 22.9143287\ T\ \ln(T) - 4.062566E\text{-}3\ T^2 + 0.17641E\text{-}6\ T^3 + 56377\ T^{-1}$ *(298.15 < T < 1500.00)*
$-59448.103 + 489.516214\ T - 72.3241219\ T\ \ln(T) + 18.726245E\text{-}3\ T^2 - 1.952433E\text{-}6\ T^3 + 11063885\ T^{-1}$
(1500.00 < T < 2607.00)
$-38588773.031 + 168610.517401\ T - 21329.7050475\ T\ \ln(T) + 5221.638997E\text{-}3\ T^2 - 240.245985E\text{-}6\ T^3 + 13082992629\ T^{-1}$
(2607.00 < T < 2740.00)
$-55768.304 + 364.482314\ T - 51.8816\ T\ \ln(T)$ *(2740.00 < T < 4500.00)*

LIQUID

$19918.743 + 119.467485\ T - 22.9143287\ T\ \ln(T) - 4.062566E\text{-}3\ T^2 + 0.17641E\text{-}6\ T^3 + 56377\ T^{-1}$ *(298.15 < T < 800.00)*
$50827.232 - 179.818561\ T + 19.539341\ T\ \ln(T) - 26.524167E\text{-}3\ T^2 + 1.667839E\text{-}6\ T^3 - 3861125\ T^{-1}$
(800.00 < T < 2607.00)
$-17161.807 + 349.673561\ T - 51.8816\ T\ \ln(T)$ *(2607.00 < T < 4500.00)*

BCC_A2

$18938.127 + 121.666233\ T - 22.9143287\ T\ \ln(T) - 4.062566E\text{-}3\ T^2 + 0.17641E\text{-}6\ T^3 + 56377\ T^{-1}$ *(298.15 < T < 1500.00)*
$-32948.103 + 483.316214\ T - 72.3241219\ T\ \ln(T) + 18.726245E\text{-}3\ T^2 - 1.952433E\text{-}6\ T^3 + 11063885\ T^{-1}$
(1500.00 < T < 2607.00)
$-38562273.031 + 168604.317401\ T - 21329.7050475\ T\ \ln(T) + 5221.638997E\text{-}3\ T^2 - 240.245985E\text{-}6\ T^3 + 13082992629\ T^{-1}$
(2607.00 < T < 2740.00)
$-29268.304 + 358.282314\ T - 51.8816\ T\ \ln(T)$ *(2740.00 < T < 4500.00)*

FCC_A1

$4938.127 + 125.466233\ T - 22.9143287\ T\ \ln(T) - 4.062566E\text{-}3\ T^2 + 0.17641E\text{-}6\ T^3 + 56377\ T^{-1}$ *(298.15 < T < 1500.00)*
$-46948.103 + 487.116214\ T - 72.3241219\ T\ \ln(T) + 18.726245E\text{-}3\ T^2 - 1.952433E\text{-}6\ T^3 + 11063885\ T^{-1}$
(1500.00 < T < 2607.00)
$-38576273.031 + 168608.117401\ T - 21329.7050475\ T\ \ln(T) + 5221.638997E\text{-}3\ T^2 - 240.245985E\text{-}6\ T^3 + 13082992629\ T^{-1}$
(2607.00 < T < 2740.00)
$-43268.304 + 362.082314\ T - 51.8816\ T\ \ln(T)$ *(2740.00 < T < 4500.00)*

Data for Ru relative to HCP_A3

LIQUID

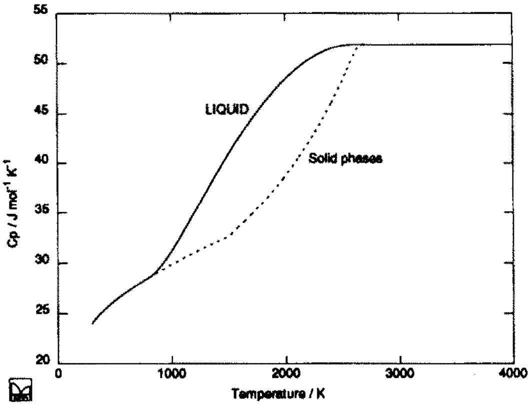
$27480.616 - 8.398748\ T$ *(298.15 < T < 800.00)*
$58389.105 - 307.684793\ T + 42.4536697\ T\ \ln(T) - 22.461602E\text{-}3\ T^2 + 1.491429E\text{-}6\ T^3 - 3917502\ T^{-1}$
(800.00 < T < 1500.00)
$110275.336 - 669.334775\ T + 91.8634629\ T\ \ln(T) - 45.250413E\text{-}3\ T^2 + 3.620272E\text{-}6\ T^3 - 14925010\ T^{-1}$
(1500.00 < T < 2607.00)
$38571611.223 - 168260.84384\ T + 21277.8234475\ T\ \ln(T) - 5221.638997E\text{-}3\ T^2 + 240.245985E\text{-}6\ T^3$
$- 13082992629\ T^{-1}$ *(2607.00 < T < 2740.00)*
$38606.496 - 14.808753\ T$ *(2740.00 < T < 4500.00)*

BCC_A2

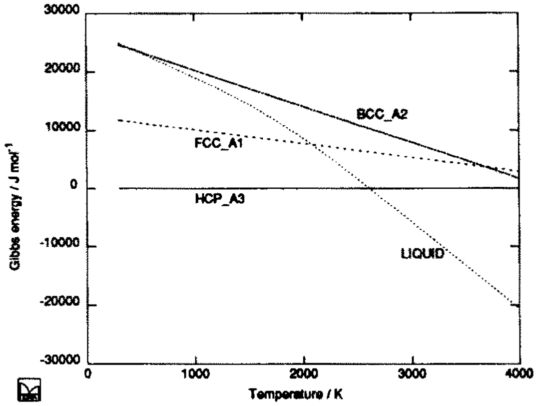
$26500 - 6.20\ T$ *(298.15 < T < 4500.00)*

FCC_A1

$12500 - 2.40\ T$ *(298.15 < T < 4500.00)*



Heat capacity of Ru



Gibbs energy of phases of Ru relative to HCP_A3

S

Source of data: TPIS [ORTHORHOMBIC, MONOCLINIC, LIQUID]
Sundman, (Unpublished work) [FCC_A1, BCC_A2]

Data for S in the form of G-HSER

ORTHORHOMBIC

$-5228.956 + 55.417762\ T - 11.007\ T\ln(T) - 26.529E\text{-}3\ T^2 + 7.754333E\text{-}6\ T^3$ *(298.15 < T < 368.30)*
$-6513.769 + 94.692922\ T - 17.941839\ T\ln(T) - 10.895125E\text{-}3\ T^2 + 1.402558E\text{-}6\ T^3 + 39910\ T^{-1}$ *(368.30 < T < 1300.00)*

MONOCLINIC

$-5701.485 + 89.000772\ T - 17.318\ T\ln(T) - 10.1215E\text{-}3\ T^2$ *(298.15 < T < 388.36)*
$-7435.888 + 114.512564\ T - 21.1094347\ T\ln(T) - 8.604142E\text{-}3\ T^2 + 1.118079E\text{-}6\ T^3 + 120740\ T^{-1}$ *(388.36 < T < 1300.00)*

LIQUID

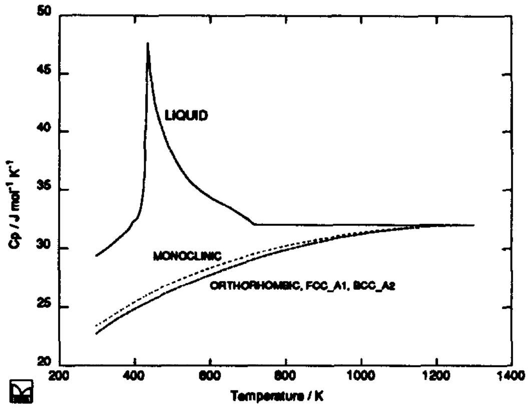
$-4001.549 + 77.905686\ T - 15.504\ T\ln(T) - 18.629E\text{-}3\ T^2 - 0.24942E\text{-}6\ T^3 - 113945\ T^{-1}$ *(298.15 < T < 388.36)*
$-5285183.35 + 118449.601039\ T - 19762.4\ T\ln(T) + 32792.75E\text{-}3\ T^2 - 10221.416667E\text{-}6\ T^3 + 264673500\ T^{-1}$ *(388.36 < T < 428.15)*
$-8174995.226 + 319914.094422\ T - 57607.3\ T\ln(T) + 135304.5E\text{-}3\ T^2 - 52997.333333E\text{-}6\ T^3$ *(428.15 < T < 432.25)*
$-219408.801 + 7758.855935\ T - 1371.85\ T\ln(T) + 2845.035E\text{-}3\ T^2 - 1013.803333E\text{-}6\ T^3$ *(432.25 < T < 453.15)*
$92539.872 - 1336.350272\ T + 202.958\ T\ln(T) - 253.1915E\text{-}3\ T^2 + 51.8835E\text{-}6\ T^3 - 8202200\ T^{-1}$ *(453.15 < T < 717.00)*
$-6889.972 + 176.37082\ T - 32\ T\ln(T)$ *(717.00 < T < 1300.00)*

BCC_A2

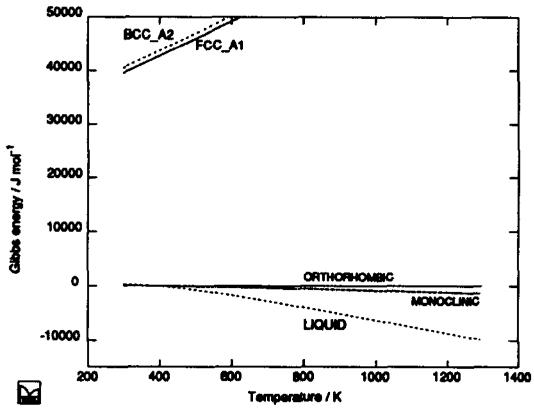
$25771.044 + 87.417762\ T - 11.007\ T\ln(T) - 26.529E\text{-}3\ T^2 + 7.754333E\text{-}6\ T^3$ *(298.15 < T < 368.30)*
$24486.231 + 126.692922\ T - 17.941839\ T\ln(T) - 10.895125E\text{-}3\ T^2 + 1.402558E\text{-}6\ T^3 + 39910\ T^{-1}$ *(368.30 < T < 1300.00)*

FCC_A1

$24771.044 + 87.417762\ T - 11.007\ T\ln(T) - 26.529E\text{-}3\ T^2 + 7.754333E\text{-}6\ T^3$ *(298.15 < T < 368.30)*
$23486.231 + 126.692922\ T - 17.941839\ T\ln(T) - 10.895125E\text{-}3\ T^2 + 1.402558E\text{-}6\ T^3 + 39910\ T^{-1}$ *(368.30 < T < 1300.00)*



Heat capacity of S



Gibbs energy of phases of S relative to ORTHORHOMBIC

Data for S relative to ORTHORHOMBIC

MONOCLINIC

-472.53 + 33.58301 T - 6.311 T ln(T) + 16.4075E-3 T^2 - 7.754333E-6 T^3	*(298.15 < T < 368.30)*
812.283 - 5.692149 T + 0.623839 T ln(T) + 0.773625E-3 T^2 - 1.402558E-6 T^3 - 39910 T^{-1}	*(368.30 < T < 388.36)*
-922.119 + 19.819642 T - 3.1675957 T ln(T) + 2.290983E-3 T^2 - 0.284479E-6 T^3 + 80830 T^{-1}	*(388.36 < T < 1300.00)*

LIQUID

1227.406 + 22.487924 T - 4.497 T ln(T) + 7.9E-3 T^2 - 8.003753E-6 T^3 - 113945 T^{-1}	*(298.15 < T < 368.30)*
2512.219 - 16.787236 T + 2.437839 T ln(T) - 7.733875E-3 T^2 - 1.651978E-6 T^3 - 153855 T^{-1}	*(368.30 < T < 388.36)*
-5278669.581 + 118354.908118 T - 19744.458161 T ln(T) + 32803.645125E-3 T^2 - 10222.819225E-6 T^3 + 264633590 T^{-1}	*(388.36 < T < 428.15)*
-8168481.457 + 319819.4015 T - 57589.358161 T ln(T) + 135315.395125E-3 T^2 - 52998.735892E-6 T^3 - 39910 T^{-1}	*(428.15 < T < 432.25)*
-212895.033 + 7664.163013 T - 1353.908161 T ln(T) + 2855.930125E-3 T^2 - 1015.205892E-6 T^3 - 39910 T^{-1}	*(432.25 < T < 453.15)*
99053.641 - 1431.043194 T + 220.899839 T ln(T) - 242.296375E-3 T^2 + 50.480942E-6 T^3 - 8242110 T^{-1}	*(453.15 < T < 717.00)*
-376.203 + 81.677899 T - 14.058161 T ln(T) + 10.895125E-3 T^2 - 1.402558E-6 T^3 - 39910 T^{-1}	*(717.00 < T < 1300.00)*

BCC_A2

31000 + 32 T	*(298.15 < T < 1300.00)*

FCC_A1

30000 + 32 T	*(298.15 < T < 1300.00)*

Sb

Source of data: Hultgren [RHOMBO_A7, LIQUID]
Saunders et al. [FCC_A1, BCC_A2, HCP_A3]

Data for Sb in the form of G-HSER

RHOMBO_A7

-9242.858 + 156.154689 T - 30.5130752 T ln(T) + 7.748768E-3 T^2 - 3.003415E-6 T^3 + 100625 T^{-1}	*(298.15 < T < 903.78)*
-11738.83 + 169.485872 T - 31.38 T ln(T) + 1.6168E27 T^{-9}	*(903.78 < T < 2000)*

LIQUID

$10579.47 + 134.231525\,T - 30.5130752\,T\ln(T) + 7.748768E\text{-}3\,T^2 - 3.003415E\text{-}6\,T^3 + 100625\,T^{-1} - 1.7485E\text{-}20\,T^7$ *(298.15 < T < 903.78)*

$8175.359 + 147.455986\,T - 31.38\,T\ln(T)$ *(903.78 < T < 2000)*

BCC_A2

$10631.142 + 141.054689\,T - 30.5130752\,T\ln(T) + 7.748768E\text{-}3\,T^2 - 3.003415E\text{-}6\,T^3 + 100625\,T^{-1}$ *(298.15 < T < 903.78)*

$8135.17 + 154.385872\,T - 31.38\,T\ln(T) + 1.6168E27\,T^{-9}$ *(903.78 < T < 2000)*

BCT_A5

$-8242.858 + 156.154689\,T - 30.5130752\,T\ln(T) + 7.748768E\text{-}3\,T^2 - 3.003415E\text{-}6\,T^3 + 100625\,T^{-1}$ *(298.15 < T < 903.78)*

$-10738.83 + 169.485872\,T - 31.38\,T\ln(T) + 1.6168E27\,T^{-9}$ *(903.78 < T < 2000)*

FCC_A1

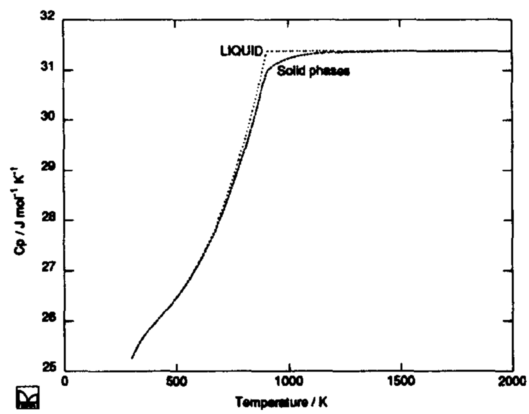
$10631.142 + 142.454689\,T - 30.5130752\,T\ln(T) + 7.748768E\text{-}3\,T^2 - 3.003415E\text{-}6\,T^3 + 100625\,T^{-1}$ *(298.15 < T < 903.78)*

$8135.17 + 155.785872\,T - 31.38\,T\ln(T) + 1.6168E27\,T^{-9}$ *(903.78 < T < 2000)*

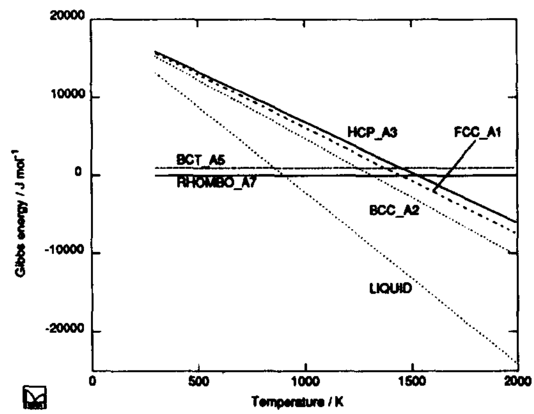
HCP_A3

$10631.142 + 143.154689\,T - 30.5130752\,T\ln(T) + 7.748768E\text{-}3\,T^2 - 3.003415E\text{-}6\,T^3 + 100625\,T^{-1}$ *(298.15 < T < 903.78)*

$8135.17 + 156.485872\,T - 31.38\,T\ln(T) + 1.6168E27\,T^{-9}$ *(903.78 < T < 2000)*



Heat capacity of Sb



Gibbs energy of phases of Sb relative to RHOMBO_A7

Data relative to RHOMBO_A7

LIQUID

$19822.329 - 21.923164\,T - 1.7485E\text{-}20\,T^7$ *(298.15 < T < 903.78)*

$19914.189 - 22.029886\,T - 1.6168E27\,T^{-9}$ *(903.78 < T < 2000)*

BCC_A2

$19874 - 15.1\,T$ *(298.15 < T < 2000)*

BCT_A5

1000 *(298.15 < T < 2000)*

FCC_A1

19874 - 13.7 T *(298.15 < T < 2000)*

HCP_A3

19874 - 13 T *(298.15 < T < 2000)*

Sc

Source of data: Hultgren

Data for Sc in the form of G-HSER

HCP_A3

-8689.547 + 153.48097 T - 28.1882 T ln(T) + 3.21892E-3 T^2 - 1.64531E-6 T^3 + 72177 T^{-1} *(298.15 < T < 800.00)*
-7511.295 + 132.759582 T - 24.9132 T ln(T) - 0.573295E-3 T^2 - 0.859345E-6 T^3 *(800.00 < T < 1608.00)*
261143.04 - 1817.922454 T + 241.4410508 T ln(T) - 117.529396E-3 T^2 + 8.7398E-6 T^3 - 50607159 T^{-1} *(1608.00 < T < 2000.00)*
-30515.246 + 286.474338 T - 44.2249 T ln(T) *(2000.00 < T < 3200.00)*

BCC_A2

-6709.819 + 152.456835 T - 28.1882 T ln(T) + 3.21892E-3 T^2 - 1.64531E-6 T^3 + 72177 T^{-1} *(298.15 < T < 800.00)*
-5531.567 + 131.735447 T - 24.9132 T ln(T) - 0.573295E-3 T^2 - 0.859345E-6 T^3 *(800.00 < T < 1000.00)*
230161.408 - 2004.054685 T + 276.7666402 T ln(T) - 167.120107E-3 T^2 + 15.637371E-6 T^3 - 33783257 T^{-1} *(1000.00 < T < 1608.00)*
-25928.011 + 283.642312 T - 44.2249 T ln(T) *(1608.00 < T < 3200.00)*

LIQUID

6478.66 + 45.427539 T - 10.7967803 T ln(T) - 20.636524E-3 T^2 + 2.13106E-6 T^3 - 158106 T^{-1} *(298.15 < T < 1608.00)*
-11832.111 + 275.871695 T - 44.2249 T ln(T) *(1608.00 < T < 3200.00)*

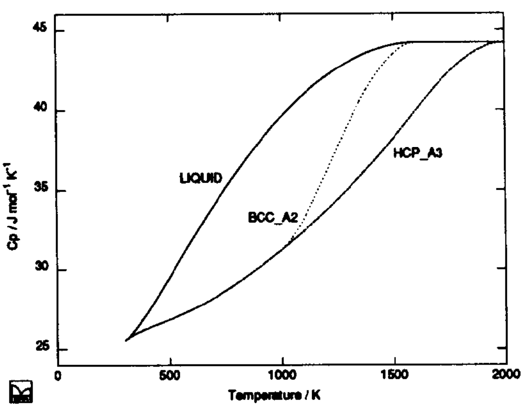
Data for Sc relative to HCP_A3

BCC_A2

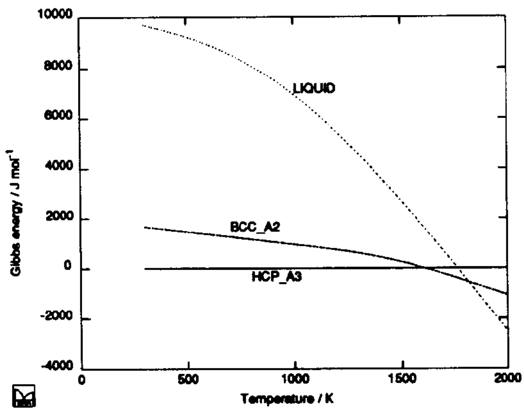
1979.727 - 1.024135 T *(298.15 < T < 1000.00)*
237672.703 - 2136.814267 T + 301.6798402 T ln(T) - 166.546812E-3 T^2 + 16.496716E-6 T^3 - 33783257 T^{-1} *(1000.00 < T < 1608.00)*
-287071.05 + 2101.564766 T - 285.6659508 T ln(T) + 117.529396E-3 T^2 - 8.7398E-6 T^3 + 50607159 T^{-1} *(1608.00 < T < 2000.00)*
4587.235 - 2.832026 T *(2000.00 < T < 3200.00)*

LIQUID

15168.207 - 108.053431 T + 17.3914197 T ln(T) - 23.855444E-3 T^2 + 3.776370E-6 T^3 - 230283 T^{-1} *(298.15 < T < 800.00)*
13989.955 - 87.332043 T + 14.1164197 T ln(T) - 20.063229E-3 T^2 + 2.990405E-6 T^3 - 158106 T^{-1} *(800.00 < T < 1608.00)*
-272975.15 + 2093.794148 T - 285.6659508 T ln(T) + 117.529396E-3 T^2 - 8.7398E-6 T^3 + 50607159 T^{-1} *(1608.00 < T < 2000.00)*
18683.135 - 10.602643 T *(2000.00 < T < 3200.00)*



Heat capacity of Sc



Gibbs energy of phases of Sc relative to HCP_A3

Se

Source of data: Hultgren

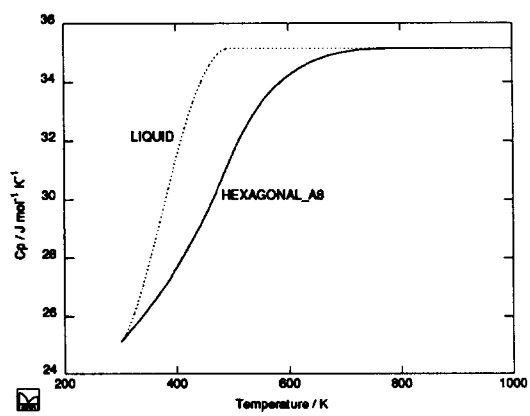
Data for Se in the form of G-HSER

HEXAGONAL_A8

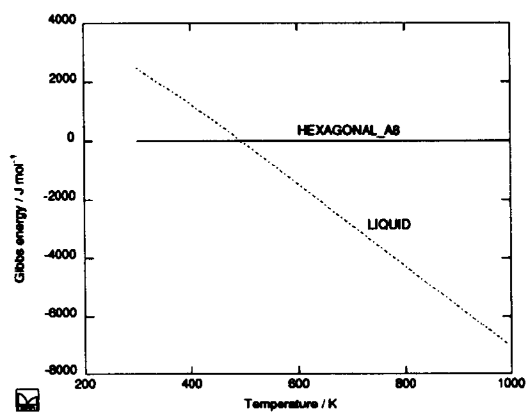
-9376.371 + 174.205877 T - 33.6527 T ln(T) + 24.24314E-3 T^2 - 15.318461E-6 T^3 + 102249 T^{-1} *(298.15 < T < 494.00)*
-37546.134 + 507.111538 T - 81.2006585 T ln(T) + 37.144892E-3 T^2 - 5.611026E-6 T^3 + 2614263 T^{-1}
(494.00 < T < 800.00)
-12193.47 + 197.770166 T - 35.1456 T ln(T) *(800.00 < T < 1000.00)*

LIQUID

50533.347 - 1178.288242 T + 194.1074389 T ln(T) - 390.268991E-3 T^2 + 119.219297E-6 T^3 - 2224398 T^{-1}
(298.15 < T < 494.00)
-5228.304 + 183.72559 T - 35.1456 T ln(T) *(494.00 < T < 1000.00)*



Heat capacity of Se



Gibbs energy of phases of Se relative to HEXAGONAL_A8

Data for Se relative to HEXAGONAL_A8

LIQUID

$59909.718 - 1352.494119\ T + 227.7601389\ T\ ln(T) - 414.512131E\text{-}3\ T^2 + 134.537758E\text{-}6\ T^3 - 2326646\ T^{-1}$ *(298.15 < T < 494.00)*

$32317.830 - 323.385948\ T + 46.0550585\ T\ ln(T) - 37.144892E\text{-}3\ T^2 + 5.611026E\text{-}6\ T^3 - 2614263\ T^{-1}$ *(494.00 < T < 800.00)*

$6965.166 - 14.044576\ T$ *(800.00 < T < 1000.00)*

Si

Source of data: JANAF [DIAMOND_A4, LIQUID]
Saunders et al. [BCC_A2, FCC_A1, HCP_A3]
Kaufman [BCC_A12, CUB_A13]

Data for Si in the form of G-HSER

DIAMOND_A4

$-8162.609 + 137.236859\ T - 22.8317533\ T\ ln(T) - 1.912904E\text{-}3\ T^2 - 0.003552E\text{-}6\ T^3 + 176667\ T^{-1}$ *(298.15 < T < 1687)*
$-9457.642 + 167.281367\ T - 27.196\ T\ ln(T) - 4.2037E30\ T^{-9}$ *(1687 < T < 3600)*

LIQUID

$42533.751 + 107.13742\ T - 22.8317533\ T\ ln(T) - 1.912904E\text{-}3\ T^2 - 0.003552E\text{-}6\ T^3 + 176667\ T^{-1} + 2.0931E\text{-}21\ T^7$ *(298.15 < T < 1687)*
$40370.523 + 137.722298\ T - 27.196\ T\ ln(T)$ *(1687 < T < 3600)*

BCC_A2

$38837.391 + 114.736859\ T - 22.8317533\ T\ ln(T) - 1.912904E\text{-}3\ T^2 - 0.003552E\text{-}6\ T^3 + 176667\ T^{-1}$ *(298.15 < T < 1687)*
$37542.358 + 144.781367\ T - 27.196\ T\ ln(T) - 4.2037E30\ T^{-9}$ *(1687 < T < 3600)*

FCC_A1

$42837.391 + 115.436859\ T - 22.8317533\ T\ ln(T) - 1.912904E\text{-}3\ T^2 - 0.003552E\text{-}6\ T^3 + 176667\ T^{-1}$ *(298.15 < T < 1687)*
$41542.358 + 145.481367\ T - 27.196\ T\ ln(T) - 4.2037E30\ T^{-9}$ *(1687 < T < 3600)*

BCC_A12

$42045.391 + 116.859859\ T - 22.8317533\ T\ ln(T) - 1.912904E\text{-}3\ T^2 - 0.003552E\text{-}6\ T^3 + 176667\ T^{-1}$ *(298.15 < T < 1687)*
$40750.358 + 146.904367\ T - 27.196\ T\ ln(T) - 4.2037E30\ T^{-9}$ *(1687 < T < 3600)*

CUB_A13

$39116.391 + 116.859859\ T - 22.8317533\ T\ ln(T) - 1.912904E\text{-}3\ T^2 - 0.003552E\text{-}6\ T^3 + 176667\ T^{-1}$ *(298.15 < T < 1687)*
$37821.358 + 146.904367\ T - 27.196\ T\ ln(T) - 4.2037E30\ T^{-9}$ *(1687 < T < 3600)*

HCP_A3

$41037.391 + 116.436859\ T - 22.8317533\ T\ ln(T) - 1.912904E\text{-}3\ T^2 - 0.003552E\text{-}6\ T^3 + 176667\ T^{-1}$ *(298.15 < T < 1687)*
$39742.358 + 146.481367\ T - 27.196\ T\ ln(T) - 4.2037E30\ T^{-9}$ *(1687 < T < 3600)*

Data for Si relative to DIAMOND_A4

LIQUID

$50696.36 - 30.099439\ T + 2.0931E\text{-}21\ T^7$ *(298.15 < T < 1687.00)*
$49828.165 - 29.559068\ T + 4.2037E30\ T^{-9}$ *(1687.00 < T < 3600.00)*

FCC_A1

51000 - 21.8 T *(298.15 < T < 3600.00)*

BCC_A2

47000 - 22.5 T *(298.15 < T < 3600.00)*

BCC_A12

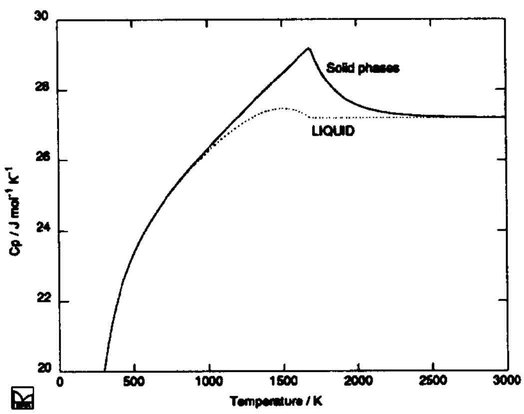
50208 - 20.377 T *(298.15 < T < 3600.00)*

CUB_A13

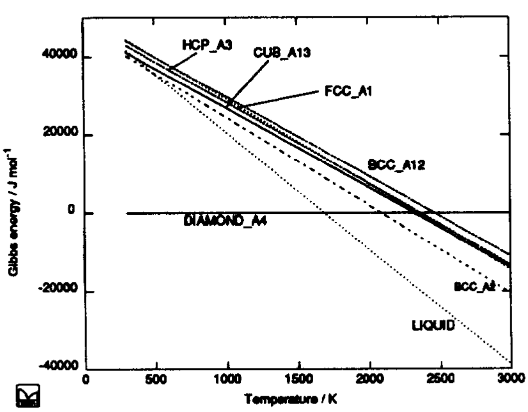
47279 - 20.377 T *(298.15 < T < 3600.00)*

HCP_A3

49200 - 20.8 T *(298.15 < T < 3600.00)*



Heat capacity of Si



Gibbs energy of phases of Si relative to DIAMOND_A4

Sm

Source of data: Hultgren

Data for Sm in the form of G-HSER

RHOMB

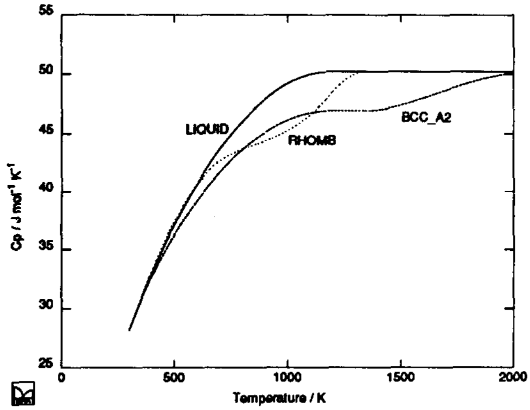
$-3872.013 - 32.10748\,T - 1.6485\,T\ln(T) - 50.254\text{E-}3\,T^2 + 10.10345\text{E-}6\,T^3 - 82168\,T^{-1}$ *(298.15 < T < 700.00)*
$-50078.215 + 627.869894\,T - 102.665\,T\ln(T) + 47.4522\text{E-}3\,T^2 - 7.538383\text{E-}6\,T^3 + 3861770\,T^{-1}$ *(700.00 < T < 1190.00)*
$289719.819 - 2744.509764\,T + 381.4198202\,T\ln(T) - 254.986338\text{E-}3\,T^2 + 27.512152\text{E-}6\,T^3 - 40102102\,T^{-1}$ *(1190.00 < T < 1345.00)*
$-23056.079 + 282.194375\,T - 50.208\,T\ln(T)$ *(1345.00 < T < 2100.00)*

BCC_A2

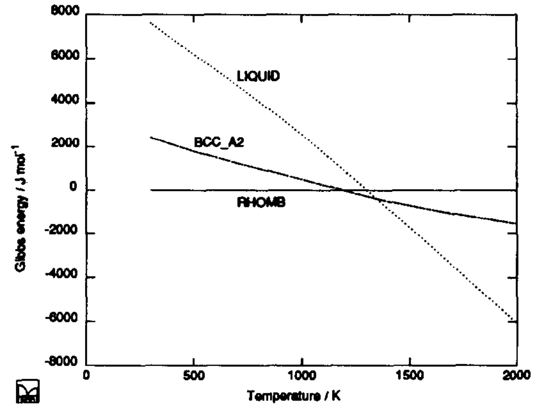
$-4368.72 + 55.972523\,T - 16.9298494\,T\ln(T) - 25.446016\text{E-}3\,T^2 + 3.579527\text{E-}6\,T^3 + 94209\,T^{-1}$ *(298.15 < T < 1190.00)*
$-15957.862 + 253.121044\,T - 46.9445\,T\ln(T)$ *(1190.00 < T < 1345.00)*
$111191.653 - 624.680805\,T + 71.6856914\,T\ln(T) - 47.314968\text{E-}3\,T^2 + 3.329865\text{E-}6\,T^3 - 24870276\,T^{-1}$ *(1345.00 < T < 2100.00)*

LIQUID

3468.783 + 20.117456 T - 11.6968284 T ln(T) - 32.418177E-3 T^2 + 4.544272E-6 T^3 + 23528 T^{-1} *(298.15 < T < 1190.00)*
-11728.229 + 273.487076 T - 50.208 T ln(T) *(1190.00 < T < 2100.00)*



Heat capacity of Sm



Gibbs energy of phases of Sm relative to RHOMB

Data for Sm relative to RHOMB

BCC_A2

-496.707 + 88.080003 T - 15.2813494 T ln(T) + 24.807984E-3 T^2 - 6.523923E-6 T^3 + 176376 T^{-1} *(298.15 < T < 700.00)*
45709.496 - 571.897371 T + 85.7351506 T ln(T) - 72.898216E-3 T^2 + 11.117911E-6 T^3 - 3767561 T^{-1}
(700.00 < T < 1190.00)
-305677.681 + 2997.630808 T - 428.3643202 T ln(T) + 254.986338E-3 T^2 - 27.512152E-6 T^3 + 40102102 T^{-1}
(1190.00 < T < 1345.00)
134247.732 - 906.87518 T + 121.8936914 T ln(T) - 47.314968E-3 T^2 + 3.329865E-6 T^3 - 24870276 T^{-1}
(1345.00 < T < 2100.00)

LIQUID

7340.796 + 52.224935 T - 10.0483284 T ln(T) + 17.835823E-3 T^2 - 5.559178E-6 T^3 + 105696 T^{-1} *(298.15 < T < 700.00)*
53546.998 - 607.752439 T + 90.9681716 T ln(T) - 79.870377E-3 T^2 + 12.082655E-6 T^3 - 3838242 T^{-1}
(700.00 < T < 1190.00)
-301448.048 + 3017.996839 T - 431.6278202 T ln(T) + 254.986338E-3 T^2 - 27.512152E-6 T^3 + 40102102 T^{-1}
(1190.00 < T < 1345.00)
11327.849 - 8.707299 T *(1345.00 < T < 2100.00)*

Sn

Source of data: Hultgren [BCT_A5, DIAMOND_A4, LIQUID]
Saunders et al. [FCC_A1, HCP_A3, BCC_A2]

Data for Sn in the form of G-HSER

BCT_A5

-7958.517 + 122.765451 T - 25.858 T ln(T) + 0.51185E-3 T^2 - 3.192767E-6 T^3 + 18440 T^{-1} *(100 < T < 250)*
-5855.135 + 65.443315 T - 15.961 T ln(T) - 18.8702E-3 T^2 + 3.121167E-6 T^3 - 61960 T^{-1} *(250 < T < 505.078)*
2524.724 + 4.005269 T - 8.2590486 T ln(T) - 16.814429E-3 T^2 + 2.623131E-6 T^3 - 1081244 T^{-1} - 1.2307E25 T^{-9}
(505.078 < T < 800)
-8256.959 + 138.99688 T - 28.4512 T ln(T) - 1.2307E25 T^{-9} *(800 < T < 3000)*

DIAMOND_A4

$-9579.608 + 114.007785\,T - 22.972\,T\ln(T) - 8.13975E{-3}\,T^2 + 2.7288E{-6}\,T^3 + 25615\,T^{-1}$ *(100 < T < 298.15)*
$-9063.001 + 104.84654\,T - 21.5750771\,T\ln(T) - 8.575282E{-3}\,T^2 + 1.784447E{-6}\,T^3 - 2544\,T^{-1}$ *(298.15 < T < 800)*
$-10909.351 + 147.396535\,T - 28.4512\,T\ln(T)$ *(800 < T < 3000)*

LIQUID

$-855.425 + 108.677684\,T - 25.858\,T\ln(T) + 0.51185E{-3}\,T^2 - 3.192767E{-6}\,T^3 + 18440\,T^{-1} + 1.47031E{-18}\,T^7$ *(100 < T < 250)*
$1247.957 + 51.355548\,T - 15.961\,T\ln(T) - 18.8702E{-3}\,T^2 + 3.121167E{-6}\,T^3 - 61960\,T^{-1} + 1.47031E{-18}\,T^7$ *(250 < T < 505.078)*
$9496.31 - 9.809114\,T - 8.2590486\,T\ln(T) - 16.814429E{-3}\,T^2 + 2.623131E{-6}\,T^3 - 1081244\,T^{-1}$ *(505.078 < T < 800)*
$-1285.372 + 125.182498\,T - 28.4512\,T\ln(T)$ *(800 < T < 3000)*

FCC_A1

$-3808.517 + 117.565451\,T - 25.858\,T\ln(T) + 0.51185E{-3}\,T^2 - 3.192767E{-6}\,T^3 + 18440\,T^{-1}$ *(100 < T < 250)*
$-1705.135 + 60.243315\,T - 15.961\,T\ln(T) - 18.8702E{-3}\,T^2 + 3.121167E{-6}\,T^3 - 61960\,T^{-1}$ *(250 < T < 505.078)*
$6674.724 - 1.194731\,T - 8.2590486\,T\ln(T) - 16.814429E{-3}\,T^2 + 2.623131E{-6}\,T^3 - 1081244\,T^{-1} - 1.2307E25\,T^{-9}$ *(505.078 < T < 800)*
$-4106.959 + 133.79688\,T - 28.4512\,T\ln(T) - 1.2307E25\,T^{-9}$ *(800 < T < 3000)*

HCP_A3

$-4058.517 + 118.365451\,T - 25.858\,T\ln(T) + 0.51185E{-3}\,T^2 - 3.192767E{-6}\,T^3 + 18440\,T^{-1}$ *(100 < T < 250)*
$-1955.135 + 61.043315\,T - 15.961\,T\ln(T) - 18.8702E{-3}\,T^2 + 3.121167E{-6}\,T^3 - 61960\,T^{-1}$ *(250 < T < 505.078)*
$6424.724 - 0.394731\,T - 8.2590486\,T\ln(T) - 16.814429E{-3}\,T^2 + 2.623131E{-6}\,T^3 - 1081244\,T^{-1} - 1.2307E25\,T^{-9}$ *(505.078 < T < 800)*
$-4356.959 + 134.59688\,T - 28.4512\,T\ln(T) - 1.2307E25\,T^{-9}$ *(800 < T < 3000)*

RHOMBO_A7

$-5923.517 + 122.765451\,T - 25.858\,T\ln(T) + 0.51185E{-3}\,T^2 - 3.192767E{-6}\,T^3 + 18440\,T^{-1}$ *(100 < T < 250)*
$-3820.135 + 65.443315\,T - 15.961\,T\ln(T) - 18.8702E{-3}\,T^2 + 3.121167E{-6}\,T^3 - 61960\,T^{-1}$ *(250 < T < 505.078)*
$4559.724 + 4.005269\,T - 8.2590486\,T\ln(T) - 16.814429E{-3}\,T^2 + 2.623131E{-6}\,T^3 - 1081244\,T^{-1} - 1.2307E25\,T^{-9}$ *(505.078 < T < 800)*
$-6221.959 + 138.99688\,T - 28.4512\,T\ln(T) - 1.2307E25\,T^{-9}$ *(800 < T < 3000)*

BCC_A2

$-3558.517 + 116.765451\,T - 25.858\,T\ln(T) + 0.51185E{-3}\,T^2 - 3.192767E{-6}\,T^3 + 18440\,T^{-1}$ *(100 < T < 250)*
$-1455.135 + 59.443315\,T - 15.961\,T\ln(T) - 18.8702E{-3}\,T^2 + 3.121167E{-6}\,T^3 - 61960\,T^{-1}$ *(250 < T < 505.078)*
$6924.724 - 1.994731\,T - 8.2590486\,T\ln(T) - 16.814429E{-3}\,T^2 + 2.623131E{-6}\,T^3 - 1081244\,T^{-1} - 1.2307E25\,T^{-9}$ *(505.078 < T < 800)*
$-3856.959 + 132.99688\,T - 28.4512\,T\ln(T) - 1.2307E25\,T^{-9}$ *(800 < T < 3000)*

Data for Sn relative to BCT_A5

DIAMOND_A4

$-1621.091 - 8.757666\,T + 2.886\,T\ln(T) - 8.6516E{-3}\,T^2 + 5.921567E{-6}\,T^3 + 7175\,T^{-1}$ *(100.00 < T < 250.00)*
$-3724.473 + 48.56447\,T - 7.011\,T\ln(T) + 10.73045E{-3}\,T^2 - 0.392367E{-6}\,T^3 + 87575\,T^{-1}$ *(250.00 < T < 298.15)*
$-3207.866 + 39.403225\,T - 5.6140771\,T\ln(T) + 10.294918E{-3}\,T^2 - 1.336719E{-6}\,T^3 + 59416\,T^{-1}$ *(298.15 < T < 505.08)*
$-11587.724 + 100.841271\,T - 13.3160284\,T\ln(T) + 8.239147E{-3}\,T^2 - 0.838684E{-6}\,T^3 + 1078700\,T^{-1} + 1.2307E25\,T^{-9}$ *(505.08 < T < 800.00)*
$-2652.392 + 8.399655\,T + 1.2307E25\,T^{-9}$ *(800.00 < T < 3000.00)*

LIQUID

$7103.092 - 14.087767\,T + 1.47031E{-18}\,T^7$ *(100.00 < T < 505.08)*
$6971.587 - 13.814382\,T + 1.2307E25\,T^{-9}$ *(505.08 < T < 3000.00)*

FCC_A1

4150 - 5.2 T *(298.15 < T < 3000.00)*

HCP_A3

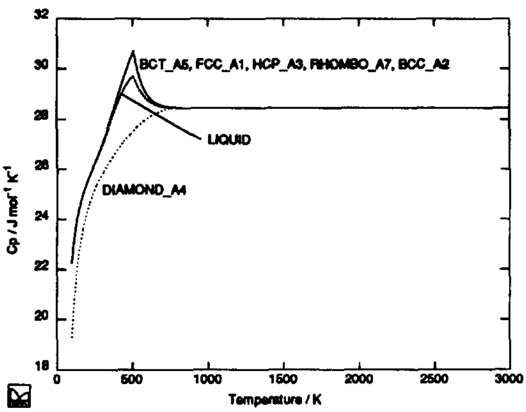
3900 - 4.4 T *(298.15 < T < 3000.00)*

RHOMBO_A7

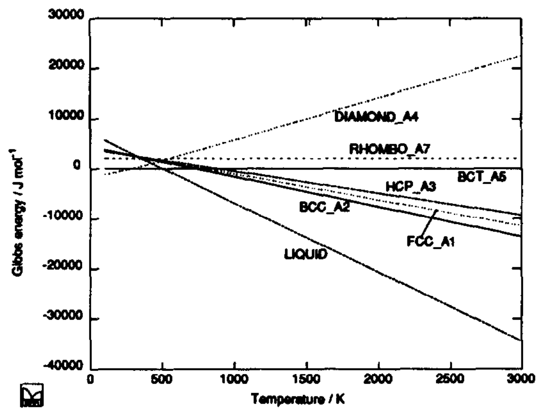
2035 *(298.15 < T < 3000.00)*

BCC_A2

4400 - 6.0 T *(298.15 < T < 3000.00)*



Heat capacity of Sn



Gibbs energy of phases of Sn relative to BCT_A5

Sr

Source of data: JANAF [FCC_A1, BCC_A2, LIQUID]
Saunders et al. [HCP_A3]

FCC_A1

$-7532.367 + 107.183879\ T - 23.905\ T\ \ln(T) - 4.61225E\text{-}3\ T^2 - 0.167477E\text{-}6\ T^3 - 2055\ T^{-1}$ *(298.15 < T < 820.00)*
$-13380.102 + 153.196104\ T - 30.0905432\ T\ \ln(T) - 3.251266E\text{-}3\ T^2 + 0.184189E\text{-}6\ T^3 + 850134\ T^{-1}$ *(820.00 < T < 3000.00)*

BCC_A2

$-6779.234 + 116.583654\ T - 25.6708365\ T\ \ln(T) - 3.126762E\text{-}3\ T^2 + 0.22965E\text{-}6\ T^3 + 27649\ T^{-1}$ *(298.15 < T < 820.00)*
$-6970.594 + 122.067301\ T - 26.57\ T\ \ln(T) - 1.9493E\text{-}3\ T^2 - 0.017895E\text{-}6\ T^3 + 16495\ T^{-1}$ *(820.00 < T < 1050.00)*
$8168.357 + 0.423037\ T - 9.7788593\ T\ \ln(T) - 9.539908E\text{-}3\ T^2 + 0.520221E\text{-}6\ T^3 - 2414794\ T^{-1}$ *(1050.00 < T < 3000.00)*

LIQUID

$2194.997 - 10.118994\ T - 5.0668978\ T\ \ln(T) - 31.840595E\text{-}3\ T^2 + 4.981237E\text{-}6\ T^3 - 265559\ T^{-1}$ *(298.15 < T < 1050.00)*
$-10855.29 + 213.406219\ T - 39.463\ T\ \ln(T)$ *(1050.00 < T < 3000.00)*

HCP_A3

$-7282.367 + 107.883879\ T - 23.905\ T\ \ln(T) - 4.61225E\text{-}3\ T^2 - 0.167477E\text{-}6\ T^3 - 2055\ T^{-1}$ *(298.15 < T < 820.00)*

$-13130.102 + 153.896104\ T - 30.0905432\ T\ln(T) - 3.251266\mathrm{E}{-3}\ T^{2} + 0.184189\mathrm{E}{-6}\ T^{3} + 850134\ T^{-1}$ *(820.00 < T < 3000.00)*

Data for Sr relative to FCC_A1

BCC_A2

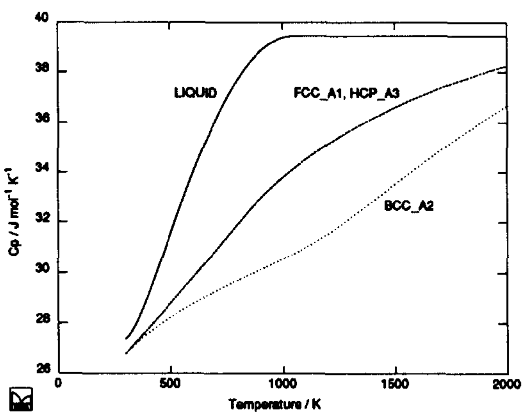
$753.133 + 9.399775\ T - 1.7658365\ T\ln(T) + 1.485488\mathrm{E}{-3}\ T^{2} + 0.397127\mathrm{E}{-6}\ T^{3} + 29704\ T^{-1}$ *(298.15 < T < 820.00)*
$6409.508 - 31.128803\ T + 3.5205432\ T\ln(T) + 1.301966\mathrm{E}{-3}\ T^{2} - 0.202084\mathrm{E}{-6}\ T^{3} - 833639\ T^{-1}$ *(820.00 < T < 1050.00)*
$21548.459 - 152.773067\ T + 20.3116839\ T\ln(T) - 6.288642\mathrm{E}{-3}\ T^{2} + 0.336032\mathrm{E}{-6}\ T^{3} - 3264928\ T^{-1}$ *(1050.00 < T < 3000.00)*

LIQUID

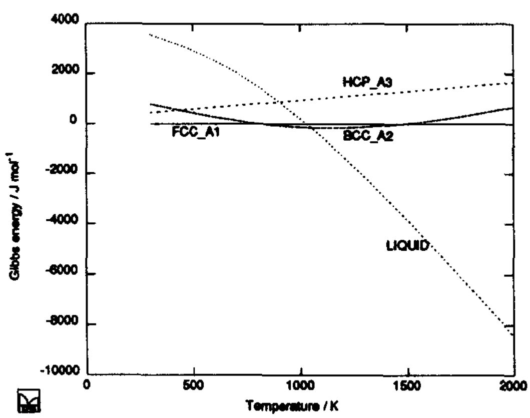
$9727.364 - 117.302874\ T + 18.8381022\ T\ln(T) - 27.228345\mathrm{E}{-3}\ T^{2} + 5.148714\mathrm{E}{-6}\ T^{3} - 263504\ T^{-1}$ *(298.15 < T < 820.00)*
$15575.099 - 163.315098\ T + 25.0236455\ T\ln(T) - 28.589329\mathrm{E}{-3}\ T^{2} + 4.797048\mathrm{E}{-6}\ T^{3} - 1115693\ T^{-1}$ *(820.00 < T < 1050.00)*
$2524.811 + 60.210115\ T - 9.3724568\ T\ln(T) + 3.251266\mathrm{E}{-3}\ T^{2} - 0.184189\mathrm{E}{-6}\ T^{3} - 850134\ T^{-1}$ *(1050.00 < T < 3000.00)*

HCP_A3

$250 + 0.7\ T$ *(298.15 < T < 3000.00)*



Heat capacity of Sr



Gibbs energy of phases of Sr relative to FCC_A1

Ta

Source of data: JANAF [BCC_A2, LIQUID]
A Fernandez Guillermet, W Huang, Z. Metallkde., 1988, 79, 88 [FCC_A1, HCP_A3]

Data for Ta in the form of G-HSER

BCC_A2

$-7285.889 + 119.139857\ T - 23.7592624\ T\ln(T) - 2.623033\mathrm{E}{-3}\ T^{2} + 0.170109\mathrm{E}{-6}\ T^{3} - 3293\ T^{-1}$ *(298.15 < T < 1300)*
$-22389.955 + 243.88676\ T - 41.137088\ T\ln(T) + 6.167572\mathrm{E}{-3}\ T^{2} - 0.655136\mathrm{E}{-6}\ T^{3} + 2429586\ T^{-1}$ *(1300 < T < 2500)*
$229382.886 - 722.59722\ T + 78.5244752\ T\ln(T) - 17.983376\mathrm{E}{-3}\ T^{2} + 0.195033\mathrm{E}{-6}\ T^{3} - 93813648\ T^{-1}$ *(2500 < T < 3290)*
$-1042384.014 + 2985.491246\ T - 362.1591318\ T\ln(T) + 43.117795\mathrm{E}{-3}\ T^{2} - 1.055148\mathrm{E}{-6}\ T^{3} + 554714342\ T^{-1}$ *(3290 < T < 6000)*

LIQUID

$21875.086 + 111.561128\ T - 23.7592624\ T\ln(T) - 2.623033\mathrm{E}{-3}\ T^{2} + 0.170109\mathrm{E}{-6}\ T^{3} - 3293\ T^{-1}$ *(298.15 < T < 1000)*
$43884.339 - 61.981795\ T + 0.0279523\ T\ln(T) - 12.330066\mathrm{E}{-3}\ T^{2} + 0.614599\mathrm{E}{-6}\ T^{3} - 3523338\ T^{-1}$ *(1000 < T < 3290)*
$-6314.543 + 258.110873\ T - 41.84\ T\ln(T)$ *(3290 < T < 6000)*

FCC_A1

8714.111 + 120.839857 T - 23.7592624 T ln(T) - 2.623033E-3 T^2 + 0.170109E-6 T^3 - 3293 T^{-1} *(298.15 < T < 1300)*
-6389.955 + 245.58676 T - 41.137088 T ln(T) + 6.167572E-3 T^2 - 0.655136E-6 T^3 + 2429586 T^{-1} *(1300 < T < 2500)*
245382.886 - 720.89722 T + 78.5244752 T ln(T) - 17.983376E-3 T^2 + 0.195033E-6 T^3 - 93813648 T^{-1} *(2500 < T < 3290)*
-1026384.014 + 2987.191246 T - 362.1591318 T ln(T) + 43.117795E-3 T^2 - 1.055148E-6 T^3+ 554714342 T^{-1} *(3290 < T < 6000)*

HCP_A3

4714.111 + 121.539857 T - 23.7592624 T ln(T) - 2.623033E-3 T^2 + 0.170109E-6 T^3 - 3293 T^{-1} *(298.15 < T < 1300)*
-10389.955 + 246.28676 T - 41.137088 T ln(T) + 6.167572E-3 T^2 - 0.655136E-6 T^3 + 2429586 T^{-1} *(1300 < T < 2500)*
241382.886 - 720.19722 T + 78.5244752 T ln(T) - 17.983376E-3 T^2 + 0.195033E-6 T^3 - 93813648 T^{-1} *(2500 < T < 3290)*
-1030384.014 + 2987.891246 T - 362.1591318 T ln(T) + 43.117795E-3 T^2 - 1.055148E-6 T^3+ 554714342 T^{-1} *(3290 < T < 6000)*

Data relative to BCC_A2

LIQUID

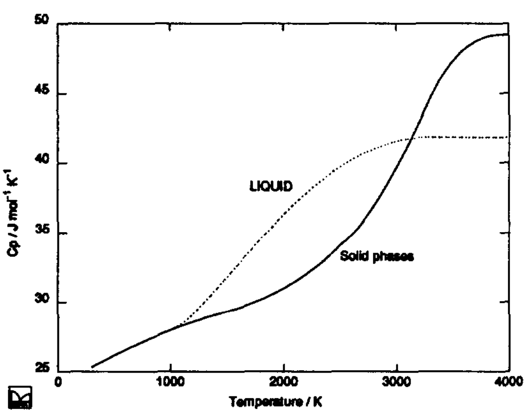
29160.975 - 7.578729 T *(298.15 < T < 1000)*
51170.228 - 181.121652 T + 23.7872147 T ln(T) - 9.707033E-3 T^2 + 0.44449E-6 T^3 - 3520045 T^{-1} *(1000 < T < 1300)*
66274.294 - 305.868555 T + 41.1650403 T ln(T) - 18.497638E-3 T^2 + 1.269735E-6 T^3 - 5952924 T^{-1} *(1300 < T < 2500)*
-185498.547 + 660.615425 T - 78.4965229 T ln(T) + 5.65331E-3 T^2 + 0.419566E-6 T^3 + 90290310 T^{-1} *(2500 < T < 3290)*
1036069.471 - 2727.380373 T + 320.3191318 T ln(T) - 43.117795E-3 T^2 + 1.055148E-6 T^3 - 554714342 T^{-1} *(3290 < T < 6000)*

FCC_A1

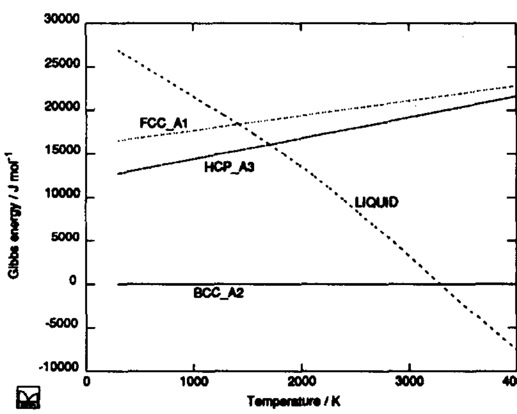
16000 + 1.7 T *(298.15 < T < 6000)*

HCP_A3

12000 + 2.4 T *(298.15 < T < 6000)*



Heat capacity of Ta



Gibbs energy of phases of Ta relative BCC_A2

Tb

Source of data: Hultgren, modified by M H Rand

HCP_A3

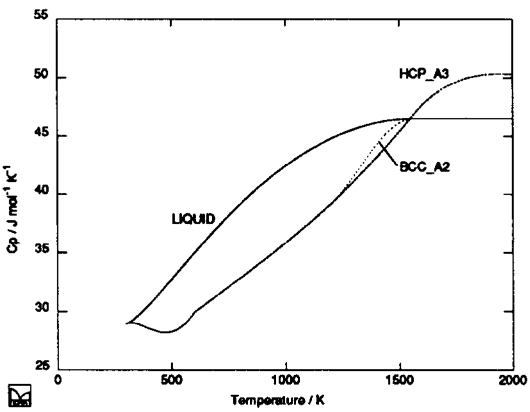
-20842.158 + 409.309555 T - 77.5006 T ln(T) + 83.2265E-3 T^2 - 25.672833E-6 T^3 + 562430 T^{-1} *(298.15 < T < 600.00)*
-8772.606 + 102.61162 T - 25.8659 T ln(T) - 2.757005E-3 T^2 - 0.805838E-6 T^3 + 172355 T^{-1} *(600.00 < T < 1200.00)*
-7944.942 + 101.7776 T - 25.9584 T ln(T) - 1.676335E-3 T^2 - 1.067632E-6 T^3 *(1200.00 < T < 1562.00)*
-265240.309 + 1456.042685 T - 200.2156949 T ln(T) + 41.615159E-3 T^2 - 2.044697E-6 T^3 + 65043790 T^{-1}
(1562.00 < T < 3000.00)

BCC_A2

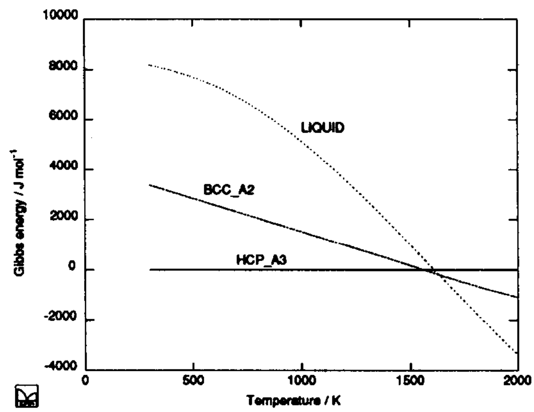
-16674.323 + 406.656848 T - 77.5006 T ln(T) + 83.2265E-3 T^2 - 25.672833E-6 T^3 + 562430 T^{-1} *(298.15 < T < 600.00)*
-4604.771 + 99.958913 T - 25.8659 T ln(T) - 2.757005E-3 T^2 - 0.805838E-6 T^3 + 172355 T^{-1} *(600.00 < T < 1200.00)*
633060.245 - 5157.777795 T + 706.5805957 T ln(T) - 373.763517E-3 T^2 + 34.100235E-6 T^3 - 103233571 T^{-1}
(1200.00 < T < 1562.00)
-23398.029 + 257.388486 T - 46.4842 T ln(T) *(1562.00 < T < 3000.00)*

LIQUID

3945.831 + 29.867521 T - 14.252646 T ln(T) - 20.466105E-3 T^2 + 2.17475E-6 T^3 - 160724 T^{-1} *(298.15 < T < 1562.00)*
-13247.649 + 251.16889 T - 46.4842 T ln(T) *(1562.00 < T < 3000.00)*



Heat capacity of Tb



Gibbs energy of phases of Tb relative to HCP_A3

Data for Tb relative to HCP_A3

BCC_A2

4167.835 - 2.652707 T *(298.15 < T < 1200.00)*
641005.187 - 5259.555395 T + 732.5389957 T ln(T) - 372.087182E-3 T^2 + 35.167867E-6 T^3 - 103233571 T^{-1}
(1200.00 < T < 1562.00)
241842.280 - 1198.654199 T + 153.7314949 T ln(T) - 41.615159E-3 T^2 + 2.044697E-6 T^3 - 65043790 T^{-1}
(1562.00 < T < 3000.00)

LIQUID

24787.989 - 379.442034 T + 63.247954 T ln(T) - 103.692605E-3 T^2 + 27.847583E-6 T^3 - 723154 T^{-1}
(298.15 < T < 600.00)
12718.438 - 72.744099 T + 11.613254 T ln(T) - 17.7091E-3 T^2 + 2.980588E-6 T^3 - 333078 T^{-1} *(600.00 < T < 1200.00)*
11890.773 - 71.910079 T + 11.705754 T ln(T) - 18.78977E-3 T^2 + 3.242382E-6 T^3 - 160724 T^{-1} *(1200.00 < T < 1562.00)*
251992.660 - 1204.873795 T + 153.7314949 T ln(T) - 41.615159E-3 T^2 + 2.044697E-6 T^3 - 65043790 T^{-1}
(1562.00 < T < 3000.00)

Tc

Source of data: A Fernandez Guillermet, G Grimvall, J. Less Common Metals, 1989, 147, 195 [HCP_A3, LIQUID]
Saunders et al. [FCC_A1, BCC_A2]

Data for Tc in the form of G-HSER

HCP_A3

-7947.794 + 132.5101 T - 24.3394 T ln(T) - 2.954747E-3 T^2 + 63855.44 T^{-1} *(298.15 < T < 2430.00)*
-47759.990 + 318.286 T - 47.0 T ln(T) + 6.638289E32 T^{-9} *(2430.00 < T < 4000.00)*

LIQUID

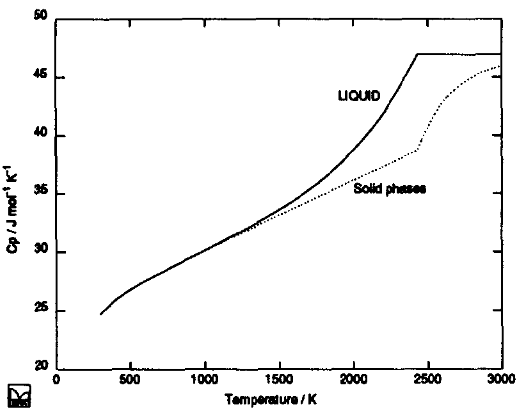
22454.34 + 120.1971 T - 24.3394 T ln(T) - 2.954747E-3 T^2 + 63855.44 T^{-1} - 9.623853E-22 T^7 *(298.15 < T < 2430.00)*
-12221.90 + 303.7538 T - 47.0 T ln(T) *(2430.00 < T < 4000.00)*

FCC_A1

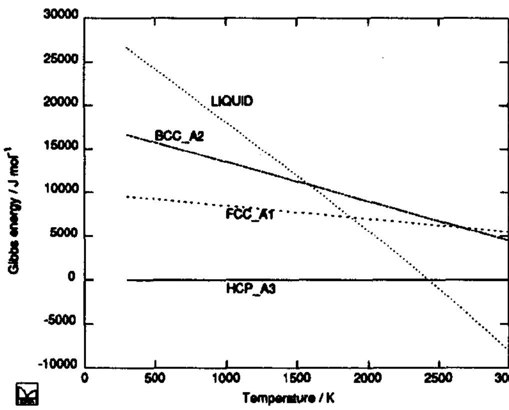
2052.206 + 131.0101 T - 24.3394 T ln(T) - 2.954747E-3 T^2 + 63855.44 T^{-1} *(298.15 < T < 2430.00)*
-37759.990 + 316.786 T - 47.0 T ln(T) + 6.638289E32 T^{-9} *(2430.00 < T < 4000.00)*

BCC_A2

10052.206 + 128.0101 T - 24.3394 T ln(T) - 2.954747E-3 T^2 + 63855.44 T^{-1} *(298.15 < T < 2430.00)*
-29759.990 + 313.786 T - 47.0 T ln(T) + 6.638289E32 T^{-9} *(2430.00 < T < 4000.00)*



Heat capacity of Tc



Gibbs energy of phases of Tc relative to HCP_A3

Data for Tc relative to HCP_A3

LIQUID

30402.134 - 12.313 T - 9.623853E-22 T^7 *(298.15 < T < 2430.00)*
35538.09 - 14.5322 T - 6.638289E32 T^{-9} *(2430.00 < T < 4000.00)*

FCC_A1

10000 - 1.5 T *(298.15 < T < 4000.00)*

BCC_A2

18000 - 4.5 T *(298.15 < T < 4000.00)*

Te

Source of data: Hultgren

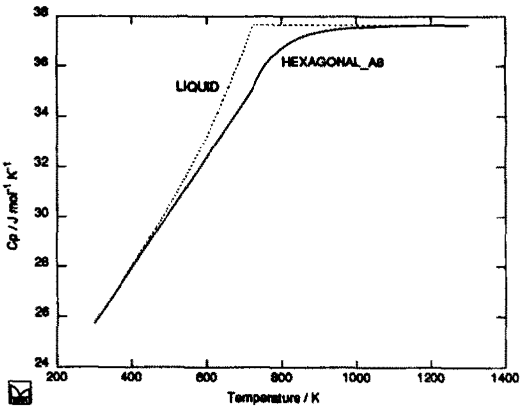
Data for Te in the form of G-HSER

HEXAGONAL_A8

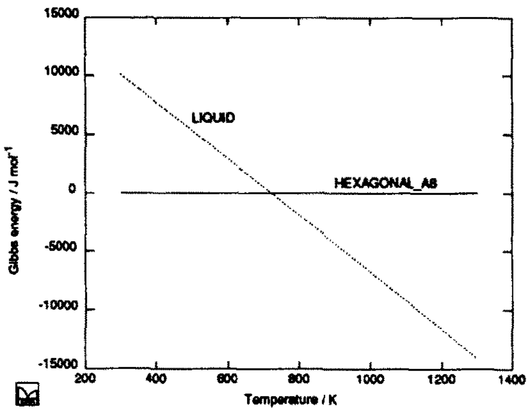
-6677.083 + 85.019049 T - 19.1003366 T ln(T) - 11.050509E-3 T^2	*(298.15 < T < 722.66)*
-14523.024 + 210.012403 T - 37.656 T ln(T) + 1.1154E27 T^{-9}	*(722.66 < T < 1261)*

LIQUID

10545.258 + 61.248705 T - 19.1003366 T ln(T) - 11.050509E-3 T^2 - 4.31979E-19 T^7	*(298.15 < T < 722.66)*
3173.591 + 185.552954 T - 37.656 T ln(T)	*(722.66 < T < 1261)*



Heat capacity of Te



Gibbs energy of phases of Te relative to HEXAGONAL_A8

Data relative to HEXAGONAL_A8

LIQUID

17222.341 - 23.770345 T - 4.31979E-19 T^7	*(298.15 < T < 722.66)*
17696.615 - 24.459449 T - 1.1154E27 T^{-9}	*(722.66 < T < 1261)*

Th

Source of data: M H Rand (Unpublished work)

Data for Th in the form of G-HSER

FCC_A1

-7732.08 + 117.022775 T - 24.841 T ln(T) - 2.36725E-3 T^2 - 0.52883E-6 T^3 + 13010 T^{-1}	*(298.15 < T < 1633)*
-37352.871 + 237.654918 T - 39.107 T ln(T) - 3.58025E-3 T^2 + 0.236893E-6 T^3 + 7981000 T^{-1}	*(1633 < T < 2900)*
-33353.313 + 283.979845 T - 46.024 T ln(T)	*(2900 < T < 4000)*

BCC_A2

-2321.06 + 134.279995 T - 28.244 T ln(T) + 0.43775E-3 T^2 - 0.53048E-6 T^3 + 91190 T^{-1}	*(298.15 < T < 1633)*
-115978.348 + 801.657849 T - 116.453 T ln(T) + 30.98E-3 T^2 - 2.536883E-6 T^3 + 27512600 T^{-1}	*(1633 < T < 2023)*
-33602.796 + 209.523509 T - 35.813 T ln(T) - 3.46655E-3 T^2 + 0.166067E-6 T^3 + 11876950 T^{-1}	*(2023 < T < 3600)*
-34333.615 + 283.930294 T - 46.024 T ln(T)	*(3600 < T < 4000)*

LIQUID

5031.109 + 111.635145 T - 24.987 T ln(T) - 1.68345E-3 T^2 - 0.909067E-6 T^3 + 10865 T^{-1} *(298.15 < T < 1499.8)*
-15602.847 + 128.406516 T - 24.03 T ln(T) - 13.6421E-3 T^2 + 1.210117E-6 T^3 + 7111100 T^{-1} *(1499.8 < T < 2014.5)*
-17273.382 + 275.750074 T - 46.024 T ln(T) *(2014.5 < T < 4000)*

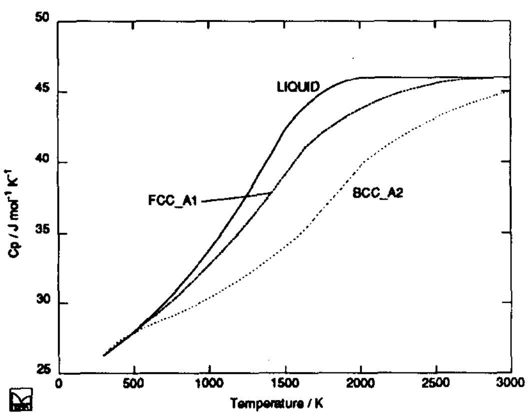
Data for Th relative to FCC_A1

BCC_A2

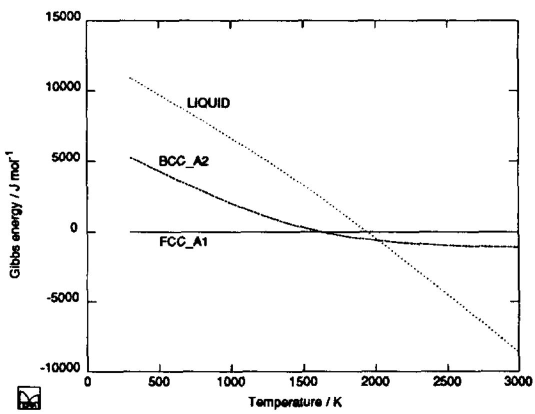
5411.02 + 17.25722 T - 3.403 T ln(T) + 2.805E-3 T^2 - 0.001650E-6 T^3 + 78180 T^{-1} *(298.15 < T < 1633.00)*
-78625.477 + 564.002931 T - 77.346 T ln(T) + 34.56025E-3 T^2 - 2.773777E-6 T^3 + 19531600 T^{-1} *(1633.00 < T < 2023.00)*
3750.075 - 28.131409 T + 3.294 T ln(T) + 0.1137E-3 T^2 - 0.070827E-6 T^3 + 3895950 T^{-1} *(2023.00 < T < 2900.00)*
-249.482 - 74.456336 T + 10.211 T ln(T) - 3.46655E-3 T^2 + 0.166067E-6 T^3 + 11876950 T^{-1} *(2900.00 < T < 3600.00)*
-980.302 - 0.04955 T *(3600.00 < T < 4000.00)*

LIQUID

12763.189 - 5.387629 T - 0.146 T ln(T) + 0.6838E-3 T^2 - 0.380237E-6 T^3 - 2145 T^{-1} *(298.15 < T < 1499.80)*
-7870.766 + 11.383741 T + 0.811 T ln(T) - 11.27485E-3 T^2 + 1.738947E-6 T^3 + 7098090 T^{-1} *(1499.80 < T < 1633.00)*
21750.024 - 109.248401 T + 15.077 T ln(T) - 10.06185E-3 T^2 + 0.973223E-6 T^3 - 869900 T^{-1} *(1633.00 < T < 2014.50)*
20079.489 + 38.095156 T - 6.917 T ln(T) + 3.58025E-3 T^2 - 0.236893E-6 T^3 - 7981000 T^{-1} *(2014.50 < T < 2900.00)*
16079.931 - 8.229771 T *(2900.00 < T < 4000.00)*



Heat capacity of Th



Gibbs energy of phases of Th relative to FCC_A1

Ti

Source of data: A T Dinsdale (Unpublished work) [HCP_A3, BCC_A2, LIQUID]
Saunders et al. [FCC_A1]
Kaufman [BCC_A12, CUB_A13]
M Pajunen (Unpublished work) [DIAMOND_A4]

Data for Ti in the form of G-HSER

HCP_A3

-8059.921 + 133.615208 T - 23.9933 T ln(T) - 4.777975E-3 T^2 + 0.106716E-6 T^3 + 72636 T^{-1} *(298.15 < T < 900)*
-7811.815 + 132.988068 T - 23.9887 T ln(T) - 4.2033E-3 T^2 - 0.090876E-6 T^3 + 42680 T^{-1} *(900 < T < 1155)*
908.837 + 66.976538 T - 14.9466 T ln(T) - 8.1465E-3 T^2 + 0.202715E-6 T^3 - 1477660 T^{-1} *(1155 < T < 1941)*
-124526.786 + 638.806871 T - 87.2182461 T ln(T) + 8.204849E-3 T^2 - 0.304747E-6 T^3 + 36699805 T^{-1} *(1941 < T < 4000)*

BCC_A2

$-1272.064 + 134.71418\ T - 25.5768\ T\ \ln(T) - 0.663845E\text{-}3\ T^2 - 0.278803E\text{-}6\ T^3 + 7208\ T^{-1}$ *(298.15 < T < 1155)*
$6667.385 + 105.366379\ T - 22.3771\ T\ \ln(T) + 1.21707E\text{-}3\ T^2 - 0.84534E\text{-}6\ T^3 - 2002750\ T^{-1}$ *(1155 < T < 1941)*
$26483.26 - 182.426471\ T + 19.0900905\ T\ \ln(T) - 22.00832E\text{-}3\ T^2 + 1.228863E\text{-}6\ T^3 + 1400501\ T^{-1}$ *(1941 < T < 4000)*

LIQUID

$4134.494 + 126.63427\ T - 23.9933\ T\ \ln(T) - 4.777975E\text{-}3\ T^2 + 0.106716E\text{-}6\ T^3 + 72636\ T^{-1}$ *(298.15 < T < 900)*
$4382.601 + 126.00713\ T - 23.9887\ T\ \ln(T) - 4.2033E\text{-}3\ T^2 - 0.090876E\text{-}6\ T^3 + 42680\ T^{-1}$ *(900 < T < 1155)*
$13103.253 + 59.9956\ T - 14.9466\ T\ \ln(T) - 8.1465E\text{-}3\ T^2 + 0.202715E\text{-}6\ T^3 - 1477660\ T^{-1}$ *(1155 < T < 1300)*
$369519.198 - 2554.0225\ T + 342.059267\ T\ \ln(T) - 163.409355E\text{-}3\ T^2 + 12.457117E\text{-}6\ T^3 - 67034516\ T^{-1}$
(1300 < T < 1941)
$-19887.066 + 298.7367\ T - 46.29\ T\ \ln(T)$ *(1941 < T < 4000)*

FCC_A1

$-2059.921 + 133.515208\ T - 23.9933\ T\ \ln(T) - 4.777975E\text{-}3\ T^2 + 0.106716E\text{-}6\ T^3 + 72636\ T^{-1}$ *(298.15 < T < 900)*
$-1811.815 + 132.888068\ T - 23.9887\ T\ \ln(T) - 4.2033E\text{-}3\ T^2 - 0.090876E\text{-}6\ T^3 + 42680\ T^{-1}$ *(900 < T < 1155)*
$6908.837 + 66.876538\ T - 14.9466\ T\ \ln(T) - 8.1465E\text{-}3\ T^2 + 0.202715E\text{-}6\ T^3 - 1477660\ T^{-1}$ *(1155 < T < 1941)*
$-118526.786 + 638.706871\ T - 87.2182461\ T\ \ln(T) + 8.204849E\text{-}3\ T^2 - 0.304747E\text{-}6\ T^3 + 36699805\ T^{-1}$
(1941 < T < 4000)

BCC_A12

$-3457.721 + 133.615208\ T - 23.9933\ T\ \ln(T) - 4.777975E\text{-}3\ T^2 + 0.106716E\text{-}6\ T^3 + 72636\ T^{-1}$ *(298.15 < T < 900)*
$-3209.615 + 132.988068\ T - 23.9887\ T\ \ln(T) - 4.2033E\text{-}3\ T^2 - 0.090876E\text{-}6\ T^3 + 42680\ T^{-1}$ *(900 < T < 1155)*
$5511.037 + 66.976538\ T - 14.9466\ T\ \ln(T) - 8.1465E\text{-}3\ T^2 + 0.202715E\text{-}6\ T^3 - 1477660\ T^{-1}$ *(1155 < T < 1941)*
$-119924.586 + 638.806871\ T - 87.2182461\ T\ \ln(T) + 8.204849E\text{-}3\ T^2 - 0.304747E\text{-}6\ T^3 + 36699805\ T^{-1}$
(1941 < T < 4000)

CUB_A13

$-528.721 + 133.615208\ T - 23.9933\ T\ \ln(T) - 4.777975E\text{-}3\ T^2 + 0.106716E\text{-}6\ T^3 + 72636\ T^{-1}$ *(298.15 < T < 900)*
$-280.615 + 132.988068\ T - 23.9887\ T\ \ln(T) - 4.2033E\text{-}3\ T^2 - 0.090876E\text{-}6\ T^3 + 42680\ T^{-1}$ *(900 < T < 1155)*
$8440.037 + 66.976538\ T - 14.9466\ T\ \ln(T) - 8.1465E\text{-}3\ T^2 + 0.202715E\text{-}6\ T^3 - 1477660\ T^{-1}$ *(1155 < T < 1941)*
$-116995.586 + 638.806871\ T - 87.2182461\ T\ \ln(T) + 8.204849E\text{-}3\ T^2 - 0.304747E\text{-}6\ T^3 + 36699805\ T^{-1}$
(1941 < T < 4000)

DIAMOND_A4

$16940.079 + 133.615208\ T - 23.9933\ T\ \ln(T) - 4.777975E\text{-}3\ T^2 + 0.106716E\text{-}6\ T^3 + 72636\ T^{-1}$ *(298.15 < T < 900)*
$17188.185 + 132.988068\ T - 23.9887\ T\ \ln(T) - 4.2033E\text{-}3\ T^2 - 0.090876E\text{-}6\ T^3 + 42680\ T^{-1}$ *(900 < T < 1155)*
$25908.837 + 66.976538\ T - 14.9466\ T\ \ln(T) - 8.1465E\text{-}3\ T^2 + 0.202715E\text{-}6\ T^3 - 1477660\ T^{-1}$ *(1155 < T < 1941)*
$-99526.786 + 638.806871\ T - 87.2182461\ T\ \ln(T) + 8.204849E\text{-}3\ T^2 - 0.304747E\text{-}6\ T^3 + 36699805\ T^{-1}$
(1941 < T < 4000)

Data for Ti relative to HCP_A3

BCC_A2

$6787.856 + 1.098972\ T - 1.5835\ T\ \ln(T) + 4.11413E\text{-}3\ T^2 - 0.385519E\text{-}6\ T^3 - 65428\ T^{-1}$ *(298.15 < T < 900.00)*
$6539.750 + 1.726111\ T - 1.5881\ T\ \ln(T) + 3.539455E\text{-}3\ T^2 - 0.187927E\text{-}6\ T^3 - 35472\ T^{-1}$ *(900.00 < T < 1155.00)*
$5758.548 + 38.389841\ T - 7.4305\ T\ \ln(T) + 9.363570E\text{-}3\ T^2 - 1.048055E\text{-}6\ T^3 - 525090\ T^{-1}$ *(1155.00 < T < 1941.00)*
$151010.046 - 821.233343\ T + 106.3083366\ T\ \ln(T) - 30.213169E\text{-}3\ T^2 + 1.533611E\text{-}6\ T^3 - 35299304\ T^{-1}$
(1941.00 < T < 4000.00)

LIQUID

$12194.415 - 6.980938\ T$ *(298.15 < T < 1300.00)*
$368610.36 - 2620.999038\ T + 357.005867\ T\ \ln(T) - 155.262855E\text{-}3\ T^2 + 12.254402E\text{-}6\ T^3 - 65556856\ T^{-1}$
(1300.00 < T < 1941.00)
$104639.72 - 340.070171\ T + 40.9282461\ T\ \ln(T) - 8.204849E\text{-}3\ T^2 + 0.304747E\text{-}6\ T^3 - 36699805\ T^{-1}$
(1941.00 < T < 4000.00)

FCC_A1

$6000 - 0.1\,T$ *(298.15 < T < 3000.00)*

CUB_A13

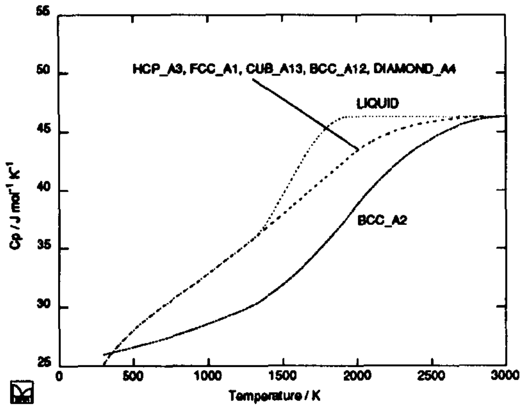
7531.2 *(298.15 < T < 3000.00)*

BCC_A12

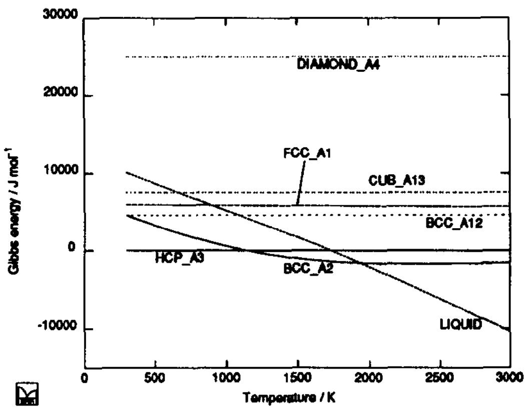
4602.2 *(298.15 < T < 3000.00)*

DIAMOND_A4

25000 *(298.15 < T < 3000.00)*



Heat capacity of Ti



Gibbe energy of phases of Ti relative to HCP_A3

Tl

Source of data: I Ansara and N Saunders (unpublished work) [HCP_A3, BCC_A2]
Hultgren [LIQUID]
Saunders et al. [FCC_A1]

Data for Tl in the form of G-HSER

HCP_A3

$-8104.038 + 107.140405\,T - 25.2274\,T\ln(T) - 3.3063E\text{-}3\,T^2 - 0.121807E\text{-}6\,T^3 + 42058\,T^{-1}$ *(200.00 < T < 577.00)*
$-15406.859 + 196.771926\,T - 38.4130658\,T\ln(T) + 5.228106E\text{-}3\,T^2 - 0.519136E\text{-}6\,T^3 + 729665\,T^{-1}$
(577.00 < T < 1800.00)

BCC_A2

$-9194.493 + 150.019517\,T - 33.0508\,T\ln(T) + 17.2318E\text{-}3\,T^2 - 10.115933E\text{-}6\,T^3 + 82153\,T^{-1}$ *(200.00 < T < 577.00)*
$-41836.403 + 482.633817\,T - 79.2926704\,T\ln(T) + 26.042993E\text{-}3\,T^2 - 2.359101E\text{-}6\,T^3 + 3507810\,T^{-1}$
(577.00 < T < 1800.00)

LIQUID

$-946.623 + 0.755649\,T - 7.44455\,T\ln(T) - 44.350292E\text{-}3\,T^2 + 14.248046E\text{-}6\,T^3 - 54228\,T^{-1}$ *(200.00 < T < 577.00)*
$-614.74 + 98.472609\,T - 25.8437\,T\ln(T) - 0.83662E\text{-}3\,T^2 + 0.000009E\text{-}6\,T^3 - 612570\,T^{-1}$ *(577.00 < T < 1800.00)*

FCC_A1

-7794.038 + 107.140405 T - 25.2274 T ln(T) - 3.3063E-3 T^2 - 0.121807E-6 T^3 + 42058 T^{-1} *(200.00 < T < 577.00)*
-15096.859 + 196.771926 T - 38.4130658 T ln(T) + 5.228106E-3 T^2 - 0.519136E-6 T^3 + 729665 T^{-1}
(577.00 < T < 1800.00)

Data for Tl relative to HCP_A3

BCC_A2

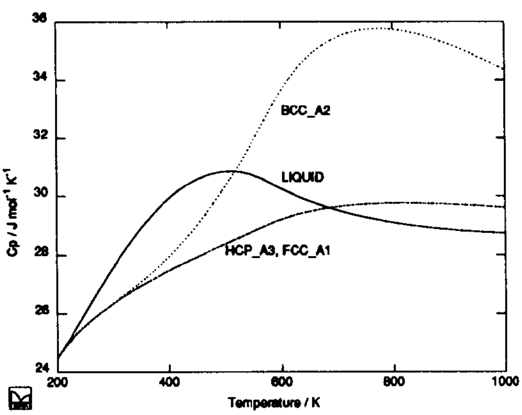
-1090.455 + 42.879112 T - 7.8234 T ln(T) + 20.5381E-3 T^2 - 9.994127E-6 T^3 + 40095 T^{-1} *(200.00 < T < 577.00)*
-26429.544 + 285.861892 T - 40.8796045 T ln(T) + 20.814887E-3 T^2 - 1.839964E-6 T^3 + 2778145 T^{-1}
(577.00 < T < 1800.00)

LIQUID

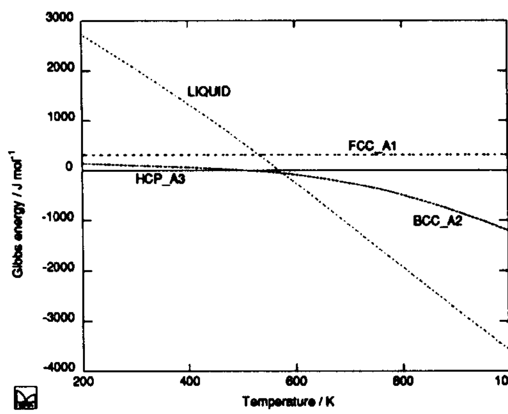
7157.414 - 106.384756 T + 17.78285 T ln(T) - 41.043992E-3 T^2 + 14.369853E-6 T^3 - 96286 T^{-1} *(200.00 < T < 577.00)*
14792.119 - 98.299316 T + 12.5693658 T ln(T) - 6.064726E-3 T^2 + 0.519146E-6 T^3 - 1342235 T^{-1}
(577.00 < T < 1800.00)

FCC_A1

310 *(200.00 < T < 1800.00)*



Heat capacity of Tl



Gibbs energy of phases of Tl relative to HCP_A3

Tm

Source of data: Hultgren

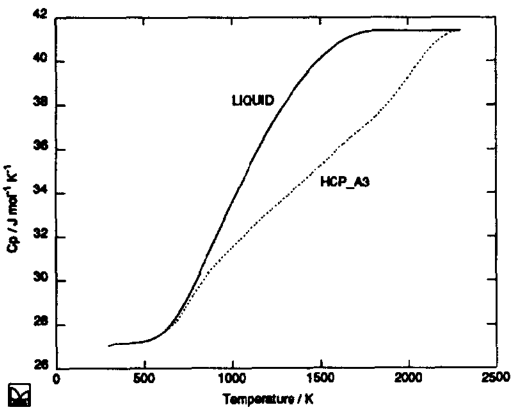
Data for Tm in the form of G-HSER

HCP_A3

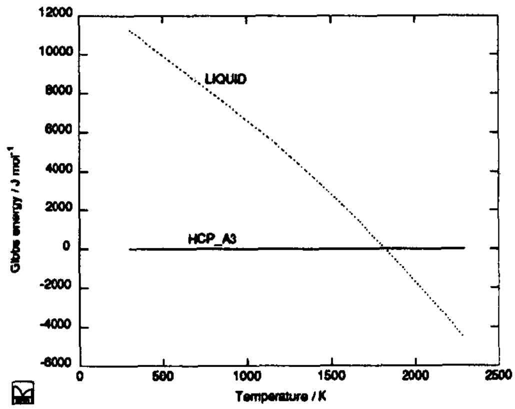
-10016.715 + 151.037648 T - 34.3664974 T ln(T) + 12.110965E-3 T^2 - 3.831156E-6 T^3 + 95982 T^{-1}
(298.15 < T < 700.00)
-14701.965 + 147.957496 T - 32.1951269 T ln(T) + 0.444753E-3 T^2 - 0.396694E-6 T^3 + 1091664 T^{-1}
(700.00 < T < 1600.00)
-8669.227 + 97.98144 T - 25.1816969 T ln(T) - 3.384563E-3 T^2 *(1600.00 < T < 1818.00)*
727125.608 - 4147.400632 T + 534.082763 T ln(T) - 190.93039E-3 T^2 + 11.689185E-6 T^3 - 180382220 T^{-1}
(1818.00 < T < 2300.00)

LIQUID

$3182.534 + 144.479977\ T - 34.3664974\ T\ ln(T) + 12.110965E\text{-}3\ T^2 - 3.831156E\text{-}6\ T^3 + 95982\ T^{-1}$ *(298.15 < T < 600.00)*
$22640.028 - 126.738485\ T + 6.8744933\ T\ ln(T) - 25.487085E\text{-}3\ T^2 + 2.288172E\text{-}6\ T^3 - 1585412\ T^{-1}$
(600.00 < T < 1818.00)
$-10090.305 + 214.184413\ T - 41.37976\ T\ ln(T)$ *(1818.00 < T < 2300.00)*



Heat capacity of Tm



Gibbs energy of phases of Tm relative to HCP_A3

Data for Tm relative to HCP_A3

LIQUID

$13199.249 - 6.557671\ T$ *(298.15 < T < 600.00)*
$32656.744 - 277.776133\ T + 41.2409907\ T\ ln(T) - 37.59805E\text{-}3\ T^2 + 6.119328E\text{-}6\ T^3 - 1681394\ T^{-1}$ *(600.00 < T < 700.00)*
$37341.993 - 274.695982\ T + 39.0696202\ T\ ln(T) - 25.931838E\text{-}3\ T^2 + 2.684866E\text{-}6\ T^3 - 2677077\ T^{-1}$
(700.00 < T < 1600.00)
$31309.256 - 224.719925\ T + 32.0561902\ T\ ln(T) - 22.102522E\text{-}3\ T^2 + 2.288172E\text{-}6\ T^3 - 1585412\ T^{-1}$
(1600.00 < T < 1818.00)
$-737215.914 + 4361.585045\ T - 575.462523\ T\ ln(T) + 190.93039E\text{-}3\ T^2 - 11.689185E\text{-}6\ T^3 + 180382220\ T^{-1}$
(1818.00 < T < 2300.00)

U

Source of data: M H Rand and A T Dinsdale (Unpublished work)

Data for U in the form of G-HSER

ORTHORHOMBIC_A20

$-8407.734 + 130.955151\ T - 26.9182\ T\ ln(T) + 1.25156E\text{-}3\ T^2 - 4.426050E\text{-}6\ T^3 + 38568\ T^{-1}$ *(298.15 < T < 955.00)*
$-22521.8 + 292.121093\ T - 48.66\ T\ ln(T)$ *(955.00 < T < 3000.00)*

TETRAGONAL

$-5156.136 + 106.976316\ T - 22.841\ T\ ln(T) - 10.84475E\text{-}3\ T^2 + 0.027889E\text{-}6\ T^3 + 81944\ T^{-1}$ *(298.15 < T < 941.50)*
$-14327.309 + 244.16802\ T - 42.9278\ T\ ln(T)$ *(941.50 < T < 3000.00)*

BCC_A2

$-752.767 + 131.5381\ T - 27.5152\ T\ ln(T) - 8.35595E\text{-}3\ T^2 + 0.967907E\text{-}6\ T^3 + 204611\ T^{-1}$ *(298.15 < T < 1049.00)*
$-4698.365 + 202.685635\ T - 38.2836\ T\ ln(T)$ *(1049.00 < T < 3000.00)*

LIQUID

$3947.766 + 120.631251\ T - 26.9182\ T\ \ln(T) + 1.25156E\text{-}3\ T^2 - 4.42605E\text{-}6\ T^3 + 38568\ T^{-1}$	*(298.15 < T < 955.00)*
$-10166.3 + 281.797193\ T - 48.66\ T\ \ln(T)$	*(955.00 < T < 3000.00)*

Data for U relative to ORTHORHOMBIC_A20

TETRAGONAL

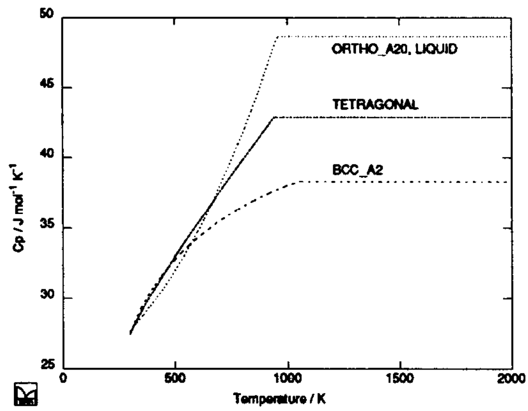
$3251.598 - 23.978835\ T + 4.0772\ T\ \ln(T) - 12.09631E\text{-}3\ T^2 + 4.453939E\text{-}6\ T^3 + 43376\ T^{-1}$	*(298.15 < T < 941.50)*
$-5919.575 + 113.212869\ T - 16.0096\ T\ \ln(T) - 1.25156E\text{-}3\ T^2 + 4.42605E\text{-}6\ T^3 - 38568\ T^{-1}$	*(941.50 < T < 955.00)*
$8194.491 - 47.953074\ T + 5.7322\ T\ \ln(T)$	*(955.00 < T < 3000.00)*

BCC_A2

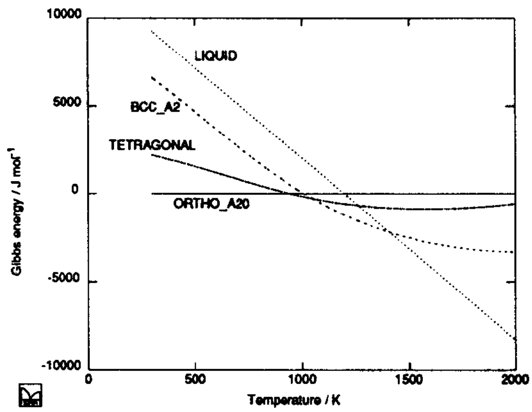
$7654.967 + 0.582949\ T - 0.597\ T\ \ln(T) - 9.60751E\text{-}3\ T^2 + 5.393957E\text{-}6\ T^3 + 166043\ T^{-1}$	*(298.15 < T < 955.00)*
$21769.033 - 160.582993\ T + 21.1448\ T\ \ln(T) - 8.35595E\text{-}3\ T^2 + 0.967907E\text{-}6\ T^3 + 204611\ T^{-1}$	*(955.00 < T < 1049.00)*
$17823.434 - 89.435459\ T + 10.3764\ T\ \ln(T)$	*(1049.00 < T < 3000.00)*

LIQUID

$12355.5 - 10.3239\ T$	*(298.15 < T < 3000.00)*



Heat capacity of U



Gibbs energy of phases of U relative to ORTHORHOMBIC_A20

V

Source of data: J Smith - Bull. Alloy Phase Diag. [BCC_A2, LIQUID]
A Fernandez Guillermet, W Huang, Z. Metallkde., 1988, 79, 88. [FCC_A1, HCP_A3]
Weiming Huang, TRITA-MAC-0439 [BCC_A12, CUB_A13]

Data for V in the form of G-HSER

BCC_A2

$-7930.43 + 133.346053\ T - 24.134\ T\ \ln(T) - 3.098E\text{-}3\ T^2 + 0.12175E\text{-}6\ T^3 + 69460\ T^{-1}$	*(298.15 < T < 790.00)*
$-7967.842 + 143.291093\ T - 25.9\ T\ \ln(T) + 0.0625E\text{-}3\ T^2 - 0.68E\text{-}6\ T^3$	*(790.00 < T < 2183.00)*
$-41689.864 + 321.140783\ T - 47.43\ T\ \ln(T) + 6.4439E31\ T^{-9}$	*(2183.00 < T < 4000.00)*

LIQUID

$12833.687 + 123.890501\ T - 24.134\ T \ln(T) - 3.098E\text{-}3\ T^2 + 0.121750E\text{-}6\ T^3 + 69460\ T^{-1} - 5.19136E\text{-}22\ T^7$ *(298.15 < T < 790.00)*
$12796.275 + 133.835541\ T - 25.9\ T \ln(T) + 0.0625E\text{-}3\ T^2 - 0.68E\text{-}6\ T^3 - 5.19136E\text{-}22\ T^7$ *(790.00 < T < 2183.00)*
$-19617.510 + 311.055983\ T - 47.43\ T \ln(T)$ *(2183.00 < T < 4000.00)*

FCC_A1

$-430.43 + 135.046053\ T - 24.134\ T \ln(T) - 3.098E\text{-}3\ T^2 + 0.12175E\text{-}6\ T^3 + 69460\ T^{-1}$ *(298.15 < T < 790.00)*
$-467.842 + 144.991093\ T - 25.9\ T \ln(T) + 0.0625E\text{-}3\ T^2 - 0.68E\text{-}6\ T^3$ *(790.00 < T < 2183.00)*
$-34189.864 + 322.840783\ T - 47.43\ T \ln(T) + 6.4439E31\ T^{-9}$ *(2183.00 < T < 4000.00)*

HCP_A3

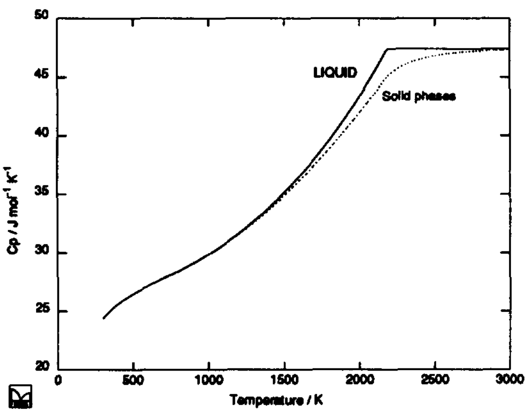
$-3930.43 + 135.746053\ T - 24.134\ T \ln(T) - 3.098E\text{-}3\ T^2 + 0.12175E\text{-}6\ T^3 + 69460\ T^{-1}$ *(298.15 < T < 790.00)*
$-3967.842 + 145.691093\ T - 25.9\ T \ln(T) + 0.0625E\text{-}3\ T^2 - 0.68E\text{-}6\ T^3$ *(790.00 < T < 2183.00)*
$-37689.864 + 323.540783\ T - 47.43\ T \ln(T) + 6.4439E31\ T^{-9}$ *(2183.00 < T < 4000.00)*

BCC_A12

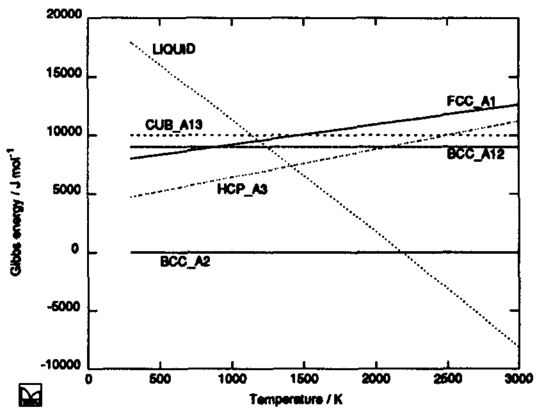
$1069.57 + 133.346053\ T - 24.134\ T \ln(T) - 3.098E\text{-}3\ T^2 + 0.12175E\text{-}6\ T^3 + 69460\ T^{-1}$ *(298.15 < T < 790)*
$1032.158 + 143.291093\ T - 25.9\ T \ln(T) + 0.0625E\text{-}3\ T^2 - 0.68E\text{-}6\ T^3$ *(790 < T < 2183)*
$-32689.864 + 321.140783\ T - 47.43\ T \ln(T) + 6.4439E31\ T^{-9}$ *(2183 < T < 4000)*

CUB_A13

$2069.57 + 133.346053\ T - 24.134\ T \ln(T) - 3.098E\text{-}3\ T^2 + 0.12175E\text{-}6\ T^3 + 69460\ T^{-1}$ *(298.15 < T < 790)*
$2032.158 + 143.291093\ T - 25.9\ T \ln(T) + 0.0625E\text{-}3\ T^2 - 0.68E\text{-}6\ T^3$ *(790 < T < 2183)*
$-31689.864 + 321.140783\ T - 47.43\ T \ln(T) + 6.4439E31\ T^{-9}$ *(2183 < T < 4000)*



Heat capacity of V



Gibbs energy of phases of V relative to BCC_A2

Data for V relative to BCC_A2

LIQUID

$20764.117 - 9.455552\ T - 5.19136E\text{-}22\ T^7$ *(298.15 < T < 2183.00)*
$22072.353 - 10.0848\ T - 6.4439E31\ T^{-9}$ *(2183.00 < T < 4000.00)*

FCC_A1

$7500 + 1.7\ T$ *(298.15 < T < 4000.00)*

HCP_A3

4000 + 2.4 T *(298.15 < T < 4000.00)*

BCC_A12

9000 *(298.15 < T < 4000.00)*

CUB_A13

10000 *(298.15 < T < 4000.00)*

W

Source of data: P Gustafson, Int. J. Thermophys., 1986, **6**, 395-409

Data for W in the form of G-HSER

BCC_A2

A = 9.5168E-6 a_0 = 9.386E-6 a_1 = 5.51E-9
K_0 = 3.1575E-12 K_1 = 1.6E-16 K_2 = 3.1E-20 n = 4

-7646.311 + 130.4 T - 24.1 T ln(T) - 1.936E-3 T^2 + 2.07E-7 T^3 - 5.33E-11 T^4 + 44500 T^{-1} + Gpres *(298.15 < T < 3695.00)*
-82868.801 + 389.362335 T - 54.0 T ln(T) + 1.528621E33 T^{-9} + Gpres *(3695.00 < T < 6000.00)*

LIQUID

A = 10.3E-6 a_0 = 9.386E-6 a_1 = 5.51E-9
K_0 = 3.1575E-12 K_1 = 1.6E-16 K_2 = 3.1E-20 n = 4

44514.273 + 116.29001 T - 24.1 T ln(T) - 1.936E-3 T^2 + 2.07E-7 T^3 - 5.33E-11 T^4 + 44500 T^{-1} - 2.713468E-24 T^7 + Gpres
(298.15 < T < 3695.00)
-30436.051 + 375.175 T - 54.0 T ln(T) + Gpres *(3695.00 < T < 6000.00)*

FCC_A1

A = 9.5168E-6 a_0 = 9.386E-6 a_1 = 5.51E-9
K_0 = 3.1575E-12 K_1 = 1.6E-16 K_2 = 3.1E-20 n = 4

11653.689 + 131.03 T - 24.1 T ln(T) - 1.936E-3 T^2 + 2.07E-7 T^3 - 5.33E-11 T^4 + 44500 T^{-1} + Gpres
(298.15 < T < 3695.00)
-63568.801 + 389.992335 T - 54.0 T ln(T) + 1.528621E33 T^{-9} + Gpres *(3695.00 < T < 6000.00)*

HCP_A3

A = 9.5168E-6 a_0 = 9.386E-6 a_1 = 5.51E-9
K_0 = 3.1575E-12 K_1 = 1.6E-16 K_2 = 3.1E-20 n = 4

7103.689 + 130.4 T - 24.1 T ln(T) - 1.936E-3 T^2 + 2.07E-7 T^3 - 5.33E-11 T^4 + 44500 T^{-1} + Gpres *(298.15 < T < 3695.00)*
-68118.801 + 389.362335 T - 54.0 T ln(T) + 1.528621E33 T^{-9} + Gpres *(3695.00 < T < 6000.00)*

Data for W relative to BCC_A2

BCC_A2

A = 9.5168E-6 a_0 = 9.386E-6 a_1 = 5.51E-9
K_0 = 3.1575E-12 K_1 = 1.6E-16 K_2 = 3.1E-20 n = 4

Gpres *(298.15 < T < 6000.00)*

LIQUID

A = 10.3E-6	a_0 = 9.386E-6	a_1 = 5.51E-9	
K_0 = 3.1575E-12	K_1 = 1.6E-16	K_2 = 3.1E-20	n = 4

52160.584 - 14.10999 T - 2.713468E-24 T^7 + Gpres *(298.15 < T < 3695.00)*
52432.75 - 14.187335 T - 1.528621E33 T^{-9} + Gpres *(3695.00 < T < 6000.00)*

FCC_A1

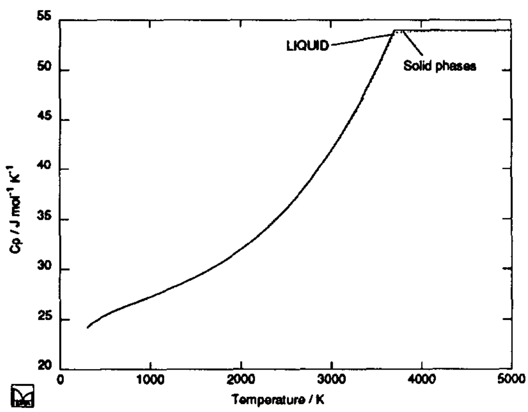
A = 9.5168E-6	a_0 = 9.386E-6	a_1 = 5.51E-9	
K_0 = 3.1575E-12	K_1 = 1.6E-16	K_2 = 3.1E-20	n = 4

19300 + 0.63 T + Gpres *(298.15 < T < 6000.00)*

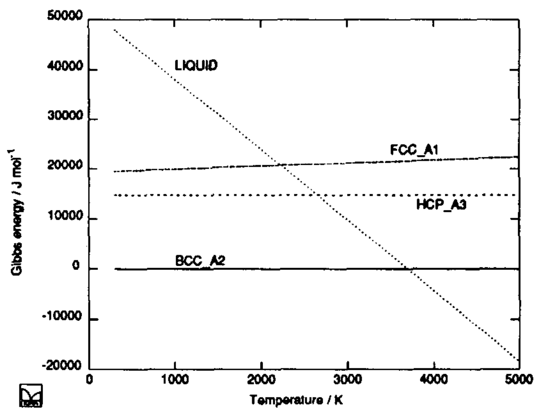
HCP_A3

A = 9.5168E-6	a_0 = 9.386E-6	a_1 = 5.51E-9	
K_0 = 3.1575E-12	K_1 = 1.6E-16	K_2 = 3.1E-20	n = 4

14750 + Gpres *(298.15 < T < 6000.00)*



Heat capacity of W



Gibbs energy of phases of W relative to BCC_A2

Y

Source of data: Hultgren

Data for Y in the form of G-HSER

HCP_A3

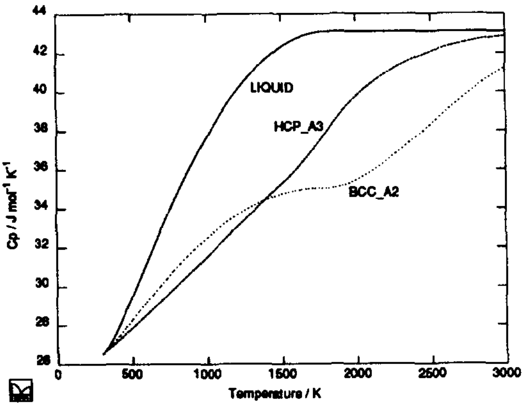
-7347.055 + 117.532124 T - 23.8685 T ln(T) - 3.845475E-3 T^2 + 0.011125E-6 T^3 - 16486 T^{-1} *(298.15 < T < 1500.00)*
-15802.62 + 229.831717 T - 40.2851 T ln(T) + 6.8095E-3 T^2 - 1.14182E-6 T^3 *(1500.00 < T < 1799.00)*
-72946.216 + 393.885821 T - 58.2078433 T ln(T) + 2.436461E-3 T^2 - 0.072627E-6 T^3 + 20866567 T^{-1} *(1799.00 < T < 3700.00)*

BCC_A2

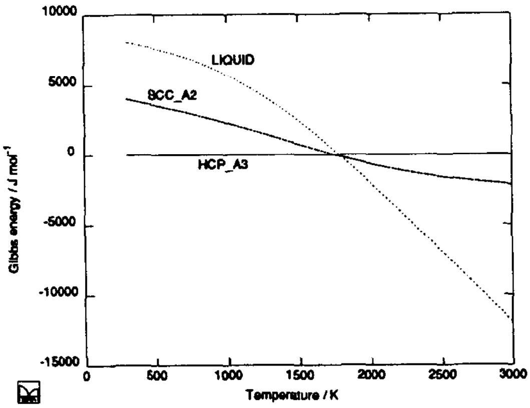
-1861.198 + 97.522398 T - 20.940576 T ln(T) - 7.995833E-3 T^2 + 0.758716E-6 T^3 - 54349 T^{-1} *(298.15 < T < 1752.00)*
-10207.724 + 195.741984 T - 35.0201 T ln(T) *(1752.00 < T < 1799.00)*
104813.954 - 386.167564 T + 39.8075986 T ln(T) - 19.918739E-3 T^2 + 0.841308E-6 T^3 - 31549963 T^{-1} *(1799.00 < T < 3700.00)*

LIQUID

$3934.121 + 59.921688\ T - 14.8146562\ T\ \ln(T) - 15.623487E{-3}\ T^2 + 1.442946E{-6}\ T^3 - 140695\ T^{-1}$ *(298.15 < T < 1799.00)*
$-13337.609 + 258.004539\ T - 43.0952\ T\ \ln(T)$ *(1799.00 < T < 3700.00)*



Heat capacity of Y



Gibbs energy of phases of Y relative to HCP_A3

Data for Y relative to HCP_A3

BCC_A2

$5485.858 - 20.009726\ T + 2.927924\ T\ \ln(T) - 4.150358E{-3}\ T^2 + 0.747591E{-6}\ T^3 - 37863\ T^{-1}$ *(298.15 < T < 1500.00)*
$13941.422 - 132.309319\ T + 19.344524\ T\ \ln(T) - 14.805333E{-3}\ T^2 + 1.900536E{-6}\ T^3 - 54349\ T^{-1}$ *(1500.00 < T < 1752.00)*
$5594.895 - 34.089733\ T + 5.265\ T\ \ln(T) - 6.8095E{-3}\ T^2 + 1.14182E{-6}\ T^3$ *(1752.00 < T < 1799.00)*
$177760.169 - 780.053385\ T + 98.0154419\ T\ \ln(T) - 22.3552E{-3}\ T^2 + 0.913936E{-6}\ T^3 - 52416530\ T^{-1}$
(1799.00 < T < 3700.00)

LIQUID

$11281.176 - 57.610437\ T + 9.0538438\ T\ \ln(T) - 11.778012E{-3}\ T^2 + 1.431821E{-6}\ T^3 - 124210\ T^{-1}$ *(298.15 < T < 1500.00)*
$19736.74 - 169.91003\ T + 25.4704438\ T\ \ln(T) - 22.432987E{-3}\ T^2 + 2.584766E{-6}\ T^3 - 140695\ T^{-1}$ *(1500.00 < T < 1799.00)*
$59608.606 - 135.881282\ T + 15.1126433\ T\ \ln(T) - 2.436461E{-3}\ T^2 + 0.072627E{-6}\ T^3 - 20866567\ T^{-1}$
(1799.00 < T < 3700.00)

Yb

Source of data: Hultgren

Data for Yb in the form of G-HSER

FCC_A1

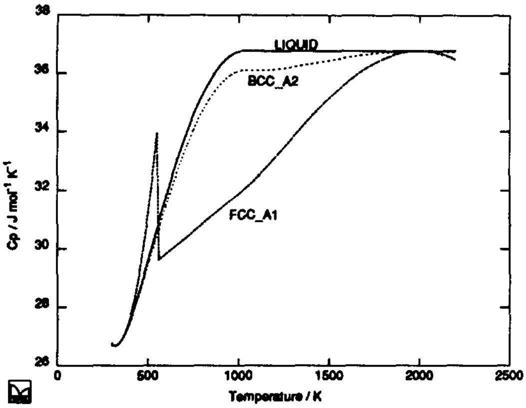
$-9370.941 + 189.327664\ T - 40.0791\ T\ \ln(T) + 42.27115E{-3}\ T^2 - 22.242E{-6}\ T^3$ *(298.15 < T < 553)*
$-8192.154 + 121.065655\ T - 26.7591\ T\ \ln(T) - 2.56065E{-3}\ T^2$ *(553 < T < 1033)*
$16034.89 - 89.478241\ T + 2.7623966\ T\ \ln(T) - 17.961331E{-3}\ T^2 + 1.421719E{-6}\ T^3 - 3631462\ T^{-1}$ *(1033 < T < 2000)*

BCC_A2

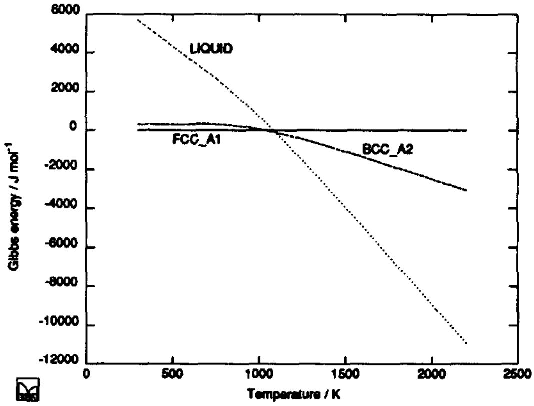
$-965.99 - 21.293677\ T - 3.8534432\ T\ \ln(T) - 30.009694E{-3}\ T^2 + 4.743871E{-6}\ T^3 - 334650\ T^{-1}$ *(298.15 < T < 1033)*
$-13368.113 + 188.313864\ T - 36.1079\ T\ \ln(T)$ *(1033 < T < 1097)*
$-3911.846 + 113.174165\ T - 25.7402233\ T\ \ln(T) - 4.743348E{-3}\ T^2 + 0.363044E{-6}\ T^3 - 1553668\ T^{-1}$ *(1097 < T < 2000)*

LIQUID

$7030.788 - 40.615571\ T - 1.8061816\ T\ \ln(T) - 32.50938E{-3}\ T^2 + 5.136665E{-6}\ T^3 - 370554\ T^{-1}$ *(298.15 < T < 1033)*
$-6445.835 + 186.690399\ T - 36.7774\ T\ \ln(T)$ *(1033 < T < 2000)*



Heat capacity of Yb



Gibbs energy of phases of Yb relative to FCC_A1

Data for Yb relative to FCC_A1

BCC_A2

$8404.952 - 210.621341\,T + 36.2256568\,T\ln(T) - 72.280844E\text{-}3\,T^{2} + 26.985871E\text{-}6\,T^{3} - 334650\,T^{-1}$ *(298.15 < T < 553)*
$7226.165 - 142.359332\,T + 22.9056568\,T\ln(T) - 27.449044E\text{-}3\,T^{2} + 4.743871E\text{-}6\,T^{3} - 334650\,T^{-1}$ *(553 < T < 1033)*
$-29403.003 + 277.792105\,T - 38.8702966\,T\ln(T) + 17.961331E\text{-}3\,T^{2} - 1.421719E\text{-}6\,T^{3} + 3631462\,T^{-1}$ *(1033 < T < 1097)*
$-19946.736 + 202.652406\,T - 28.5026199\,T\ln(T) + 13.217982E\text{-}3\,T^{2} - 1.058675E\text{-}6\,T^{3} + 2077794\,T^{-1}$ *(1097 < T < 2000)*

LIQUID

$16401.729 - 229.943235\,T + 38.2729184\,T\ln(T) - 74.78053E\text{-}3\,T^{2} + 27.378665E\text{-}6\,T^{3} - 370554\,T^{-1}$ *(298.15 < T < 553)*
$15222.942 - 161.681226\,T + 24.9529184\,T\ln(T) - 29.94873E\text{-}3\,T^{2} + 5.136665E\text{-}6\,T^{3} - 370554\,T^{-1}$ *(553 < T < 1033)*
$-22480.725 + 276.168639\,T - 39.5397966\,T\ln(T) + 17.961331E\text{-}3\,T^{2} - 1.421719E\text{-}6\,T^{3} + 3631462\,T^{-1}$ *(1033 < T < 2000)*

Zn

Source of data: Hultgren [HCP_A3, LIQUID]
S an Mey (Unpublished) [FCC_A1]
Kaufman [BCC_A2]

Data for Zn in the form of G-HSER

HCP_A3 (Zn non ideal)

$-7285.787 + 118.470069\,T - 23.701314\,T\ln(T) - 1.712034E\text{-}3\,T^{2} - 1.264963E\text{-}6\,T^{3}$ *(298.15 < T < 692.68)*
$-11070.559 + 172.34566\,T - 31.38\,T\ln(T) + 4.7051E26\,T^{-9}$ *(692.68 < T < 1700)*

LIQUID

$-128.574 + 108.177079\,T - 23.701314\,T\ln(T) - 1.712034E\text{-}3\,T^{2} - 1.264963E\text{-}6\,T^{3} - 3.5896E\text{-}19\,T^{7}$ *(298.15 < T < 692.68)*
$-3620.391 + 161.608594\,T - 31.38\,T\ln(T)$ *(692.68 < T < 1700)*

BCC_A2

$-4398.827 + 115.959669\,T - 23.701314\,T\ln(T) - 1.712034E\text{-}3\,T^{2} - 1.264963E\text{-}6\,T^{3}$ *(298.15 < T < 692.68)*
$-8183.599 + 169.83526\,T - 31.38\,T\ln(T) + 4.7051E26\,T^{-9}$ *(692.68 < T < 1700)*

FCC_A1

$-4315.967 + 116.900389\,T - 23.701314\,T\ln(T) - 1.712034E\text{-}3\,T^{2} - 1.264963E\text{-}6\,T^{3}$ *(298.15 < T < 692.68)*
$-8100.739 + 170.77598\,T - 31.38\,T\ln(T) + 4.7051E26\,T^{-9}$ *(692.68 < T < 1700)*

Data relative to HCP_A3 (Zn non ideal)

LIQUID

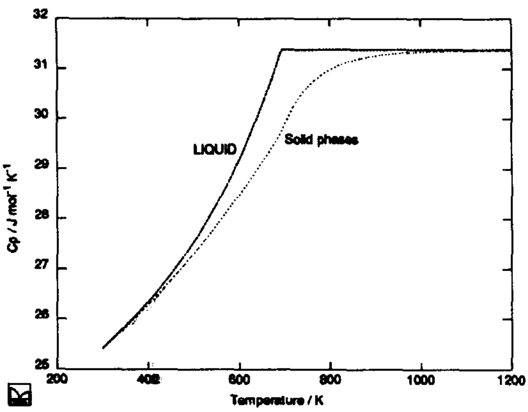
$7157.213 - 10.29299\ T - 3.5896E\text{-}19\ T^{7}$	*(298.15 < T < 692.68)*
$7450.168 - 10.737066\ T - 4.7051E26\ T^{-9}$	*(692.68 < T < 1700)*

BCC_A2

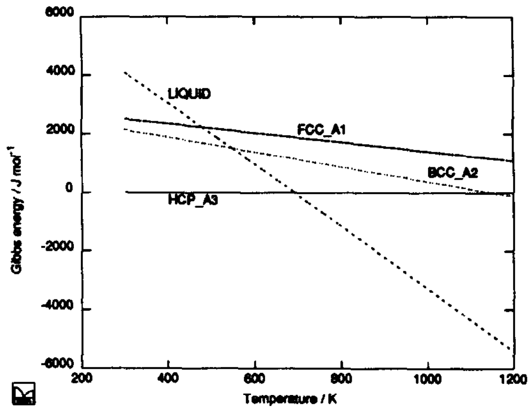
$2886.96 - 2.5104\ T$	*(298.15 < T < 1700)*

FCC_A1

$2969.82 - 1.56968\ T$	*(298.15 < T < 1700)*



Heat capacity of Zn



Gibbs energy of phases of Zn relative to HCP_A3

Zr

Source of data: A Fernandez Guillermet, High Temp. - High Press., 1987, **19**, 119-60 [HCP_A3, BCC_A2, OMEGA, LIQUID]
Saunders et al. [FCC_A1]

Data for Zr in the form of G-HSER

HCP_A3

$A = 13.9567E\text{-}6$	$a_0 = 12.443E\text{-}6$	$a_1 = 14.76E\text{-}9$
$K_0 = 1.0063E\text{-}11$	$K_1 = 1.573E\text{-}15$	$n = 3.006$

$-7827.595 + 125.64905\ T - 24.1618\ T\ln(T) - 4.37791E\text{-}3\ T^{2} + 34971\ T^{-1} + Gpres$	*(130.00 < T < 2128.00)*
$-26085.921 + 262.724183\ T - 42.144\ T\ln(T) - 1.342895E31\ T^{-9} + Gpres$	*(2128.00 < T < 4000.00)*

BCC_A2

$A = 13.7141E\text{-}6$	$a_0 = 3.0381E\text{-}5$	
$K_0 = 1.0063E\text{-}11$	$K_1 = 1.573E\text{-}15$	$n = 3.006$

$-525.539 + 124.9457\ T - 25.607406\ T\ln(T) - 3.40084E\text{-}4\ T^{2} - 9.7289735E\text{-}9\ T^{3} - 7.6142894E\text{-}11\ T^{4} + 25233\ T^{-1} + Gpres$	*(298.15 < T < 2128.00)*
$-30705.955 + 264.284163\ T - 42.144\ T\ln(T) + 1.276058E32\ T^{-9} + Gpres$	*(2128.00 < T < 4000.00)*

OMEGA

$A = 1.37115E\text{-}5$ $a_0 = 3.0381E\text{-}5$
$K_0 = 1.0063E\text{-}11$ $K_1 = 1.573E\text{-}15$ $n = 3.006$

$-8878.082 + 144.432234\,T - 26.8556\,T\ln(T) - 2.7994455E\text{-}3\,T^2 + 38376\,T^{-1} + Gpres$ *(298.15 < T < 2128.00)*
$-29500.524 + 265.290858\,T - 42.144\,T\ln(T) + 7.17444982E31\,T^{-9} + Gpres$ *(2128.00 < T < 4000.00)*

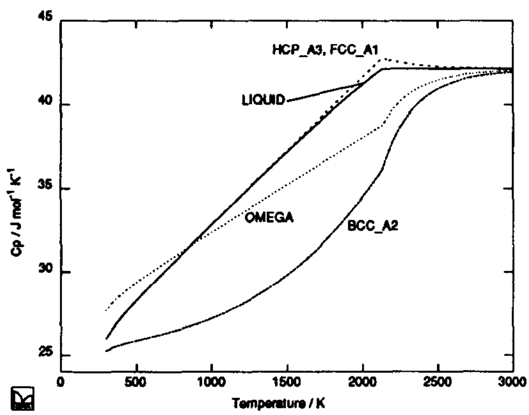
LIQUID

$A = 1.44092E\text{-}5$ $a_0 = 3.0381E\text{-}5$
$K_0 = 1.0063E\text{-}11$ $K_1 = 1.573E\text{-}15$ $n = 3.006$

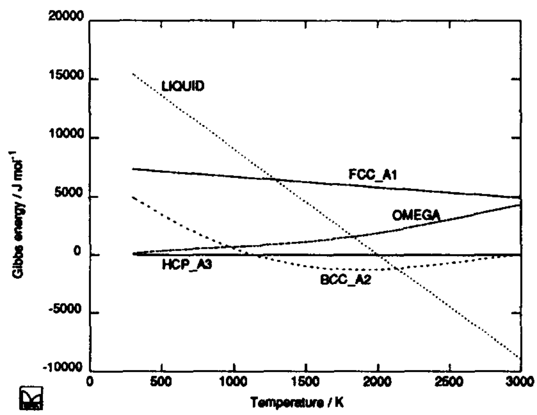
$10320.095 + 116.568238\,T - 24.1618\,T\ln(T) - 4.37791E\text{-}3\,T^2 + 34971\,T^{-1} + 1.6275E\text{-}22\,T^7 + Gpres$
(298.15 < T < 2128.00)
$-8281.26 + 253.812609\,T - 42.144\,T\ln(T) + Gpres$ *(2128.00 < T < 4000.00)*

FCC_A1

$-227.595 + 124.74905\,T - 24.1618\,T\ln(T) - 4.37791E\text{-}3\,T^2 + 34971\,T^{-1} + Gpres$ *(298.15 < T < 2128.00)*
$-18485.921 + 261.824183\,T - 42.144\,T\ln(T) - 1.342895E31\,T^{-9} + Gpres$ *(2128.00 < T < 4000.00)*



Heat capacity of Zr



Gibbs energy of phases of Zr relative to HCP_A3

Data for Zr relative to HCP_A3

HCP_A3

$A = 13.9567E\text{-}6$ $a_0 = 12.443E\text{-}6$ $a_1 = 14.76E\text{-}9$
$K_0 = 1.0063E\text{-}11$ $K_1 = 1.573E\text{-}15$ $n = 3.006$

Gpres *(130.00 < T < 4000.00)*

BCC_A2

$A = 13.7141E\text{-}6$ $a_0 = 3.0381E\text{-}5$
$K_0 = 1.0063E\text{-}11$ $K_1 = 1.573E\text{-}15$ $n = 3.006$

$7302.056 - 0.70335\,T - 1.445606\,T\ln(T) + 4.037826E\text{-}3\,T^2 - 9.7289735E\text{-}9\,T^3 - 7.6142894E\text{-}11\,T^4 - 9737\,T^{-1} + Gpres$
(298.15 < T < 2128.00)
$-4620.034 + 1.55998\,T + 1.41035E32\,T^{-9} + Gpres$ *(2128.00 < T < 4000.00)*

OMEGA

$A = 1.37115E\text{-}5$ $a_0 = 3.0381E\text{-}5$
$K_0 = 1.0063E\text{-}11$ $K_1 = 1.573E\text{-}15$ $n = 3.006$

$-1050.487 + 18.783184\ T - 2.6938\ T \ln(T) + 1.5784645E\text{-}3\ T^2 + 3406\ T^{-1} + Gpres$ *(298.15 < T < 2128.00)*
$-3414.603 + 2.566675\ T + 8.517345E31\ T^{-9} + Gpres$ *(2128.00 < T < 4000.00)*

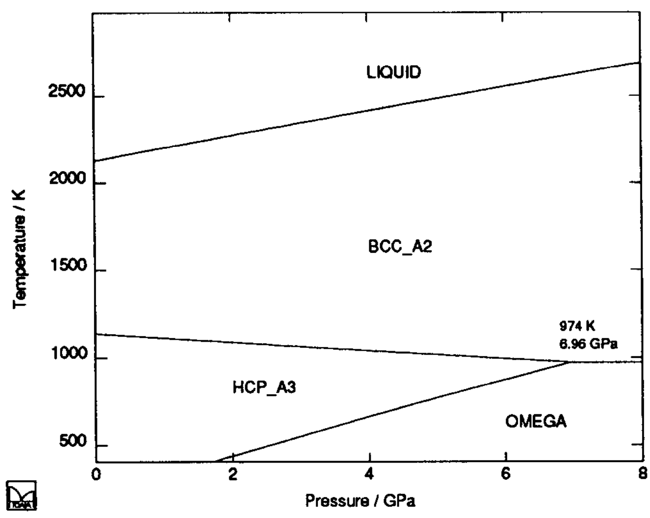
LIQUID

$A = 1.44092E\text{-}5$ $a_0 = 3.0381E\text{-}5$
$K_0 = 1.0063E\text{-}11$ $K_1 = 1.573E\text{-}15$ $n = 3.006$

$18147.69 - 9.080812\ T + 1.6275E\text{-}22\ T^7 + Gpres$ *(298.15 < T < 2128.00)*
$17804.661 - 8.911574\ T + 1.342895E31\ T^{-9} + Gpres$ *(2128.00 < T < 4000.00)*

FCC_A1

$7600 - 0.9\ T$ *(298.15 < T < 4000.00)*



P-T phase diagram for Zr