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Calculation of phase diagrams of the actinides

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Abstract

The prediction of phase diagrams of actinides is difficult because, in addition to the use of s, p and d electrons, the use of f electrons in binding by the metals from Pa to Cf must be considered. Also, the actinides have an unusual number of electronic configurations of comparable stability considering promotion energies and bonding energies. The availability of different configurations with different sizes also makes it possible to achieve higher densities than one would expect for close-packed structures. Calculations of the thermodynamic stabilities of various structures for all pure actinides will be published shortly. We are calculating the thermodynamics and phase diagrams of the binary systems. In the space available here, I will discuss only systems with no intermediate phases using a modification of the regular-solution model which is normally expressed in terms of energies of vaporization from the condensed phase to the gaseous atom in the ground electronic state, which is appropriate for organic compounds for which the energy of vaporization is a measure of the van der Waals bonding. For most metals, the energy of vaporization is not a proper measurement of bonding energy as the electronic configuration in the condensed phase is different from that of the ground state of the gaseous atom. The correct bonding energy is the difference between the energy of the condensed phase and the energy of the gaseous atom with the same electronic configuration as the condensed phase. As an example, the $\Delta H_{298}/R$ value of 33.4 kK for the sublimation of b.c.c. Am to the gaseous ground state (f^7s^2) must be increased by 29.5 kK, the promotion energy to f^6d^2s, to obtain the bonding energy of 62.9 kK. Of this total bonding energy, 23.8 kK is due to the s electron, 35 kK is due to the two d electrons and 4.2 kK is the contribution due to f electron bonding. Examples will be given of the use of the modified regular-solution model for calculation of phase diagrams.

1. Introduction

A paper will be published [1] later this year that presents the calibrations of the bonding capabilities of electrons in 4s to 7s, 4p to 7p, 3d to 6d, and 4f to 5f orbitals in pure metals. The promotion energies of the various electronic configurations are presented so that the stabilities of various structures can be calculated. The next step is the extension to bonding energies when these orbitals are shared by two different metals so that binary phase diagrams can be calculated and ultimately, multicomponent mixtures of any metals can be treated. Although the actinides are only a small portion of this project, it was originally initiated 50 years ago when I was given the job in the Manhattan Project of predicting the properties of the actinides and their compounds and I have maintained special interest in the actinides.

The actinides pose special problems owing to contributions to bonding by f electrons for some of the actinides and especially because of the unusual number of electronic configurations that can contribute to bonding. This is illustrated by Table 1 that lists for some of the actinides the ground electronic configurations and excited electronic configurations that can play a role in bonding. Values are given for all the actinides from Ac to Lr in ref. 1. The promotion energies $\Delta E/R$ (kK), are given for the lowest electronic level of each configuration. The values of the bonding energies [1] per electron are given (Table 2) for the 7s and 7p electrons and for the 6d electrons depending on how many d orbitals are used. For the 5f electrons, the total bonding energy for all f electrons present is given as a function of the number of f orbitals occupied. The enthalpies of the b.c.c., h.c.p. and c.c.p. structures relative to the stable structure at 298 K have been calculated for most metals [1]. The values for the actinides are given in Table 3. The values in parentheses are predicted values. The other values are experimental values listed in refs. 2 and 3.

When atoms of different sizes are mixed, it is possible to obtain structures with coordination numbers and densities higher than for the close-packed structures. These dense structures can be obtained for pure actinides from Pa to Pu since they have three or more configurations for which their bonding will yield similar stabilities. With their high densities, the stability ranges of these structures are increased by pressure. Pressure

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TABLE 1. Promotion energies $\Delta E/R$ (kK) of actinide atoms

	Ac		Th		Pa		U		Np	
Ground state	ds^2		d^2s^2		f^2ds^2		f^3ds^2		f^4ds^2	
b.c.c.										
d^2s	d^2s	13.26			f^2d^2s	10.07	f^3d^2s	8.991	f^4d^2s	10.223
d^3s			d^3s	8.00	fd^3s	10.91	f^2d^3s	(24.36)	f^3d^3s	(35.2) ± 3
d^4s							fd^4s	(32.0) ± 7	f^2d^4s	(50.4) ± 4
h.c.p.										
dsp	dsp	19.73			f^2dsp	20.71	f^3dsp	21.069	f^4dsp	20.631
d^2sp			d^2sp	20.81	fd^2sp	21.67	f^2d^2sp	34.5	f^3d^2sp	(48.20) ± 2
									f^2d^3sp	59.0 ± 9
c.c.p.										
sp^2			fsp^2	(33.0) ± 9	f^2sp^2	(24.0) ± 9	f^3sp^2	(27.0) ± 7	f^4sp^2	(32.0) ± 7
dsp^2			dsp^2	(18.0) ± 14	$fdsp^2$	(27.0) ± 15				
	Pu		Am		Cm		Bk		Cf	
Ground state	f^6s^2		f^7s^2		f^7ds^2		f^9s^2		$f^{10}s^2$	
b.c.c.										
ds			f^7ds	20.87			f^9ds	24.72	$f^{10}ds$	28.84
d^2s	f^5d^2s	21.45	f^6d^2s	29.53	f^7d^2s	14.60	f^8d^2s	30.94	f^9d^2s	(45.3)
h.c.p.										
sp	f^6sp	22.23	f^7sp	22.46			f^9sp	24.34	$f^{10}sp$	25.12
dsp	f^5dsp	29.97	f^6dsp	37.23	f^7dsp	21.95	f^8dsp	35.47	f^9dsp	48.85
c.c.p.										
sp^2	f^5sp^2	(34.0) ± 7	f^6sp^2	(41.5) ± 6	f^7sp^2	(28.5)	f^8sp^2	(40.0) ± 7	f^9sp^2	(54.0) ± 4

TABLE 2. s, p electron and d electron bonding $\Delta H_{298}/R$ (kK electron^{-1}) for the actinides and total bonding in kilokelvins for n electrons for f^n configurations

	s, p bonding	d bonding per electron as function of the following numbers of d orbitals used			
		1	2	3	4
Ac	23.5	19.0	18.0		
Th	23.1	20.0	19.0	18.7	
Pa	23.2	18.0	17.0	16.5	
U	23.3	18.5	17.5	17.0	16.6
Np	23.3	17.5	16.8	16.0	
Pu	23.3	17.5	16.8		
Am	23.8	18.8	17.6		
Cm	24.0	18.0	17.0		
Bk	24.5	20.0	19.0		
Cf	25.0	20.0	19.0		
Es	25.5	19.0	18.0		
Lr	(26.0)	(24.0)	(22.0)		

Number of f orbitals	1	2	3	4	5	6	7	8	9	10
Total bonding (kK)	5.0	8.0	9.0	8.0	5.0	4.2	3.0	3.0	2.5	0

For the actinides from Fm to No using only two non-f electrons in bonding, the s, p bonding is 22 kK per electron and the d bonding enthalpy per electron is 19 kK if one d orbital is used and 20 kK for 0.5 d orbitals. The 5f orbitals are too localized to contribute significantly to bonding for configurations with 10 to 14 f electrons. For Es, at the transition point to divalent bonding, the same enthalpies of sublimation are calculated for b.c.c. and h.c.p. structures using the f^{11} configurations with the divalent bonding enthalpies listed for Fm to No or using the f^{10} configurations with the trivalent bonding enthalpies listed in the table above.

TABLE 3. $\Delta H_{298}/R$ (kK) of the metastable structures of the actinides at 298 K

	Metastable structure and $\Delta H_{298}/R$ (kK)							References	Stable structure 298 K
Ac	b.c.c.	(3.0)	h.c.p.	(3.0)					c.c.p.
Th	b.c.c.	0.43	h.c.p.	(6.0) ± 2				2, 3	c.c.p.
Pa	b.c.c.	(2.0) ± 2	h.c.p.	(3.0) ± 2	c.c.p.	0.8		3	α-Pa
U	b.c.c.	0.9	h.c.p.	(8.0) ± 3	c.c.p.	(12.0) ± 7	β 0.3	2, 3	α-U
Np	b.c.c	1.3	h.c.p.	(4.0) ± 2	c.c.p.	(10.0) ± 7	β 0.67	2	α-Np
Pu	b.c.c.	1.04	h.c.p.	(2.0)	c.c.p.	0.66	β 0.45	2	α-Pu
Am	b.c.c.	0.8			c.c.p.	0.11		2	d.h.c.p.
Cm	b.c.c.	(2.0) ± 2			c.c.p.	0.33		3	d.h.c.p.
Bk	b.c.c.	(2.0) ± 2			c.c.p.	0.44		2	d.h.c.p.
Cf	b.c.c.	(3.0)			c.c.p.	0.3		2	d.h.c.p.
Es	b.c.c.	(3.0) ± 2							h.c.p.
Fm	b.c.c.	(4.0) ± 2							h.c.p.
Md	b.c.c.	(5.0) ± 3							h.c.p.
No	b.c.c.	(5.0) ± 3							h.c.p.
Lr	b.c.c.	(9.0) ± 3			c.c.p.	(2.0)			h.c.p.

also improves the overlap of d and f orbitals, resulting in increased stability of the b.c.c. structure, the structure with the fewest p electrons and therefore the most 6d and 5f electrons, as compared with the close-packed structures.

2. Modification of regular-solution theory

Only the simplest binary phase diagrams with no intermediate phases will be discussed here. The regular-solution theory is based on the internal pressure $\Delta E/V$, where ΔE is the energy of vaporization and V is the molal volume for each component. For materials such as organic molecules held together by van der Waals' interactions, there is no change in electronic configuration between the condensed phase and the gas. However, for most metals the electronic configuration of the ground state of the gaseous atom is different from the electronic configuration of the condensed phase. The internal pressure term of the regular solution theory must be replaced by a term using the energy of vaporization from the condensed phase to the gaseous state that has the same electronic configuration as the condensed phase. The b.c.c. phase of Am can be taken as an example. The Hume-Rothery rules restrict the electronic configuration for the b.c.c. phase to have less than 1.5 s, p electrons. Am has two electronic configurations with one outer-shell electron (Table 1). Although f^7ds has a lower promotion energy, the f^6d^2s configuration will be more important in the solid as the additional d electron will increase the bonding by 2(17.6) − 18.8 kK or 16.4 kK and the use of only 6f orbitals improves the bonding by 1.2 kK resulting in an increased stability of 16.4 + 1.2 − 8.66 kK or 8.9 kK for the f^6d^2s configuration over the f^7ds configuration. The configurations containing sp electrons have higher promotion energies but their replacement of one d by one p electron compared with the b.c.c. configurations makes the h.c.p. structure more stable at low temperatures. Because of the higher heat capacity and entropy of the b.c.c. phase which has a lower coordination number and thus lower vibrational frequencies, the b.c.c. structure will become stable at higher temperatures. However, because of the closeness of stability of the two structures, the b.c.c. phase will mix the s and sp configurations up to the limit of the Hume-Rothery rule of 1.5 s, p electrons. One can calculate accurately the mix of competing configurations [1]. The energy $\Delta E/R$ of vaporization to the ground electronic state must be increased by 33 kK to obtain the correct measure of the bonding energy to be used to calculate the internal pressure. For the h.c.p. or d.h.c.p. structure of Am, the consideration of the promotion energies (Table 1) and the bonding values (Table 2) indicates that the configuration will be predominantly f^6dsp even though f^7sp has a lower promotion energy by 14.77 kK since the replacement of an f electron by a d electron increases the bonding by 20 kK. For the sublimation of d.h.c.p. Am, $\Delta H_{298}/R$ is 34.2 ± 1 kK. For the sublimation to the valence state, $\Delta H^*_{298}/R$ is 71.4 ± 1 kK. However, if a transition metal including lanthanides and actinides is dissolved in a non-transition metal that cannot provide orbitals to overlap effectively with d orbitals, d bonding is greatly reduced and the f^7ds and f^7sp configurations will predominate over the f^6d^2s and f^6dsp configurations.

3. Regular-solution calculations for liquid actinides

Although the solubility limits of solid phases are of interest, it is particularly difficult to obtain liquid solubilities and the ability to make predictions is important.

Three quantities are needed for the appropriate internal pressure values. The enthalpy of sublimation at 298 K must be converted to the enthalpy of sublimation at the melting point. The enthalpy of fusion must then be subtracted to obtain the enthalpy of vaporization of the liquid to the ground electronic state of the gaseous atom. The enthalpy of vaporization must be converted to the energy of vaporization by subtracting $\Delta PV/R$. As the volume of the liquid is negligible compared with the volume of the gas, $\Delta PV/R$ is close to T or $T/1000$ in kilokelvins. Finally the promotion energies must be added to obtain the vaporization to the valence state. The results of the first steps of this procedure are illustrated in Table 4 where the energy of vaporization of the liquid to the ground electronic state is tabulated for all the elements of interest. Also, molal volumes are tabulated.

It is not easy to find reliable values of molal volumes of metallic liquids as it is a difficult measurement. Fortunately, Crawley [4] provided critically evaluated values of the reported experimental values or supplied estimates for the elements Ag, Al, As, Au, B, Be, Bi, Cd, Co, Cu, Fe, Ge, Hf, Hg, In, Ir, K, La, Li, Mg, Mn, Mo, Na, Nd, Ni, Os, Pb, Pd, Pt, Pu, Rb, Re, Rh, Ru, Si, Sn, Ta, Te, Ti, Tl, U, V, W, Zn, and Zr. Lamoreaux [5] provided estimates for Ac, Am, Bk, Cf, Cm, Es, Fm, Fr, Gd, Ho, Lr, Lu, Md, No, Np, Pa, Pm, Po, Ra, Sm, Tb, Tc, Tm, and Y. A few recent measurements were obtained from the compilation of Lang [6] for Ba, Ca, Ce, Cr, Cs, Dy, Er, Eu, Ga, Nb, Pr, Sb. Lamoreaux [5] also cited values for C[7], Sr and Th [8], and Yb [9].

For thermodynamic data over a range of temperatures, the tables of Hultgren *et al.* [10] are still the best source for many of the elements. Where they overlap, the *JANEF* tables [11] and the tables of Glushko *et al.* [12] were in good agreement with Hultgren *et al.* However, in a few instances the latter tables were used as they did have access to data that were slightly different. Desai [13, 14], who was part of the Hultgren group, has updated data for Al, Fe, Mn, Mo, Ni, Ti, and V. Alcock *et al.* [15] have presented a recent review of data for the alkaline earth metals from Be to Ba. Gurvich *et al.* [16] have provided a recent review for the fourth group elements from C to Pb. Data for the actinides from Th to Es are presented by Ward *et al.* [2]. The recent reviews of Guillermet and coworkers [17] for Co, Fe, Mn, Mo, and Zr were useful. Stull and Sinke [18] provided estimates for Ac, Fr, Pm, Po, and Ra. Lamoreaux [5] provided estimates for the actinides from Fm to Lr. The review of thermodynamic data for the condensed phases of the elements by Dinsdale [19] was useful in providing recent data or even data not yet published. Although the enthalpy

TABLE 4. Molal volume and energy of vaporization of liquid

V_ℓ	$cm^3\ mol^{-1}$	Molal Volume of Liquid
$\Delta E^o_g/R$	kK	Energy of Vaporization of Liquid to Ground State Atom at melting point

Li 13.5 18.2											Be 5.33 34.8	B 5.2 58.2	C (7.46) 66.0	N	O	F	Ne
Na 24.2 12.2											Mg 15.3 15.2	Al 11.3 36.85	Si 11.13 46.0	P	S	Cl	Ar
K 47.18 10.0	Ca 29.5 18.2	Sc 16,1 39.0	Ti 11.57 50.6	V 9.50 54.3	Cr 8.21 39.2	Mn 9.55 28.0	Fe 7.94 43.2	Co 7.75 44.5	Ni 7.44 45.54	Cu 7.91 36.75	Zn 9.98 13.80	Ga 11.52 31.7	Ge 13.23 38.0	As 14.35 30.0	Se 19.8 27.1	Br	Kr
Rb 58.42 9.14	Sr 36.97 16.8	Y (21.0) 45.0	Zr 15.92 65.4	Nb (12.0) 79.0	Mo (10.47) 67.5	Tc (9.6) 70.0	Ru (9.27) 67.4	Rh (9.27) 58.0	Pd 10.14 40.0	Ag 11.56 30.85	Cd 14.06 11.86	In 16.37 28.3	Sn 17.02 34.7	Sb 18.94 28.4	Te 21.93 22.0	I	Xe
Cs 72.0 8.6	Ba 41.4 19.9	La 23.31 48.6	Hf (14.87) 65.0	Ta (12.06) 82.5	W (10.51) 87.0	Re (9.96) 78.0	Os (9.46) 81.2	Ir (9.61) 69.0	Pt 10.32 61.1	Au 11.36 40.6	Hg 14.66 7.08	Tl 18.21 20.4	Pb 19.57 22.0	Bi 20.83 23.1	Po (24.1) 15.2	At	Rn
Fr (82.) (9.0)	Ra (44.8) 16.0	Ac (27.4) 44.0															
			Ce 20.98 46.7	Pr 21.38 39.0	Nd 21.46 35.0	Pm (21.0) 33.6	Sm 21.0 19.5	Eu 31.2 18.0	Gd 21.3 42.9	Tb 20.7 41.0	Dy 19.8 29.3	Ho 19.78 30.0	Er 19.4 31.4	Tm 18.8 22.1	Yb 27.8 15.4	Lu 18.8 45.6	
			Th (21.8) 65.0	Pa (21.0) 60.0	U 13.8 58.3	Np (14.2) 52.0	Pu 14.5 38.4	Am (19.0) 29.0	Cm (18.9) 41.0	Bk (18.0) 33.0	Cf (18.0) 20.0	Es (18.0) 13.0	Fm (16.9) (12.0)	Md (25.5) (11.0)	No (25.0) (10.0)	Lr (16.1) (31.0)	

TABLE 5. Regular-solution parameter $\left[\frac{(\Delta E^*/R)}{V}\right]^{1/2}$ (kK$^{1/2}$ cm$^{-3/2}$) of liquid at melting point

Li s 1.16											Be sp 3.5	B sp^2 4.4	C sp^3 3.61	N	O	F	Ne
Na s 0.71											Mg sp 1.75	Al sp^2 2.64	Si sp^3 2.91	P	S	Cl	Ar
K s 0.46	Ca (c) 1.22	Sc (c) 1.9	Ti (c) 2.4	V (c) 2.67	Cr (c) 2.64	Mn (c) 2.37	Fe (c) 2.80	Co (f) 3.42	Ni (f) 3.57	Cu (f) 3.61	Zn sp 2.458	Ga sp^2 2.74	Ge sp^3 2.74	As s^2p^3 1.45	Se s^2p^4 1.17	Br	Kr
Rb s 0.396	Sr (c) 1.04	Y (c) 1.74	Zr (b) 2.20	Nb (a) 2.57	Mo (a) 2.54	Tc (d) 3.0	Ru (d) 3.16	Rh (f) 3.6	Pd (f) 3.4	Ag (f) 3.16	Cd sp 1.981	In sp^2 2.19	Sn sp^3 2.32	Sb s^2p^3 1.225	Te s^2p^4 1.00	I	Xe
Cs s 0.346	Ba ds 0.89	La (c) 1.61	Hf (c) 2.44	Ta (c) 2.91	W (a) 2.95	Re (e) 3.25	Os (e) 3.47	Ir (f) 3.6	Pt (f) 3.44	Au (f) 3.2	Hg sp 2.044	Tl sp^2 2.17	Pb ---	Bi s^2p^3 1.05	Po s^2p^4 0.79	At	Rn
Fr s 0.33	Ra (c) 0.89	Ac dsp 1.5															

$d^{n-1}s$	(a)
$d^{n-1.3}sp^{0.3}$	(b)
$d^{n-1.5}sp^{0.5}$	(c)
$d^{n-1.7}sp^{0.7}$	(d)
$d^{n-2}sp$	(e)
$d^{n-2.5}sp^{1.5}$	(f)
$f^{n-3}d^{1.5}sp^{0.5}$	(g)
$f^{n-3}dsp$	(h)

Ce (g) 1.664	Pr (g) 1.631	Nd (g) 1.614	Pm (g) 1.6	Sm (g) 1.61	Eu f^7ds 1.08	Gd (g) 1.64	Tb (g) 1.67	Dy (g) 1.73	Ho (h) 1.81	Er (h) 1.82	Tm (h) 1.85	Yb (c) 1.28	Lu (h) 1.94
Th (c) 1.9	Pa $fdsp^2$ 2.0	U (g) 2.6	Np (g) 2.7	Pu (g) 2.1	Am (h) 1.9	Cm (h) 1.8	Bk (h) 1.9	Cf $f^{10}sp$ 1.6	Es $f^{11}sp$ 1.5	Fm $f^{12}sp$ 1.55	Md $f^{13}sp$ 1.3	No sp 1.3	Lr dsp 2.1

increases from 298 K to the melting point were used from the above sources, the ΔH_{298} enthalpies of vaporization were replaced by values from Brewer [20] for many of the elements.

Table 5 indicates the electron configurations of the liquid that were taken as a first approximation to be the same as for the solid in equilibrium with the liquid. This is reasonable for most of the metals, but not for Pa to Pu. As noted above, these elements can form a mixture of configurations that would be likely for the liquid that does not have a controlling lattice distribution of the atoms. In subsequent uses of Table 5, the internal pressure figures will be modified. There is the additional complication that the electron configurations of most metals can change depending on what is added. An example is given below. In addition, the regular-solution procedure is not applicable if generalized Lewis acid–base reactions are taking place as for example when platinum group metals are added to actinides, lanthanides or left-hand transition metals. Thus even though the procedures outlined here and additional procedures that will be published in the future will provide useful predictions of phase diagrams. One has to consider carefully the chemistry of the interactions taking place in the solution and the resulting changes in electron configurations.

4. Calculation of phase diagrams

When two elements are mixed, the comparison of internal pressures or regular-solution parameters allows one to predict the general character of the diagram as has been illustrated for the actinides [21–23]. When the internal pressures are close, the liquids will be miscible. With a substantial difference, the diagram will consist of two liquids for which the concentrations can be readily calculated by equating the partial molal Gibbs energies of each component in the two phases. The usual regular-solution equations assume that the interaction between the two components is the geometric mean of the interactions in the pure liquids. With the modification of using the energies of vaporization to the excited valence state, an empirical modification was made [24] with $\epsilon_{AB} = (1/4)[\epsilon_{AA}^{1/2} + \epsilon_{BB}^{1/2}]^2$. Following the usual regular-solution procedure of expansion of the volume fraction in a power series and dropping terms beyond the cubic term, $\Delta\bar{G}^{E}{}_{A}/R = bx_B{}^2 + cx_B{}^3$ and $\Delta\bar{G}^{E}{}_{B}/R = (b + 1.5c)x_A{}^2 - cx_A{}^3$ where $b + c = (V_A/2)$-$[(\Delta E^*A/RV_A)^{1/2} - (\Delta E^*{}_B/RV_B)^{1/2}]^2$ and $(b + c)/(b + c/2) = V_A/V_B$. If the mole fractions are expressed as $x_A = 1 - y$ and $x_B = y$ in the A-rich phase and $x_A = x$ and $x_B = 1 - x$ in the B-rich phase and the $\Delta\bar{G}/RT$ of each component are equated for the two phases, one obtains

$$\ln x + (b/T)(1 - x)^2 + (c/T)(1 - x)^3$$
$$= \ln(1 - y) + (b/T)y^2 + (c/T)y^3$$

$$\ln y + (b/T + 1.5c/T)(1 - y)^2 - (c/T)(1 - y)^3$$
$$= \ln(1 - x) + (b/T + 1.5c/T)x^2 - (c/T)x^3$$

For a given value of T, the simultaneous solution of these two equations for x and y can be carried out by a simple iterative solution using the secant method. As an example, the data for Am and Ba in Tables 4 and 5 yield, at 1500 K, $b = 13.1$ and $c = -0.52$ kK. The internal pressure difference is so large that the solubilities are very small and one can solve the two equations separately assuming as the first approximation that the solubilities are zero. As the molal volumes are closely the same, the phase diagram is close to symmetrical and one calculates an activity coefficient for Am in Ba of 4.4×10^3 yielding $x = 2.3 \times 10^{-4}$ for the solubility of f^6dsp Am in ds Ba and for Ba in Am. As an example of the need to change the internal pressure parameters of Table 5 depending on the metals added, compare the calculations for Am in ds Ba with those for Am in sp Mg. Since Mg has no d orbitals to overlap with the Am d orbitals, the f^7sp configuration of Am will be more stable for Am dissolved in Mg than the f^6dsp configuration. Using the f^7sp promotion energy of 22.46 kK from Table 1 with the energy of vaporization from Table 4, a change in the regular-solution parameter of Table 5 from 1.9 to 1.65 is calculated. With the parameter value of Mg of 1.75, one calculates an activity coefficient for Am in Mg at 1500 K of 0.88. Thus the liquids are miscible and form an almost ideal solution. Lack of time and space does not allow a wider range of examples, but complete results for the binary diagrams of all the elements with one another will be available in the near future. The calculations of the phase diagrams of all the actinides with Mo are available [24].

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