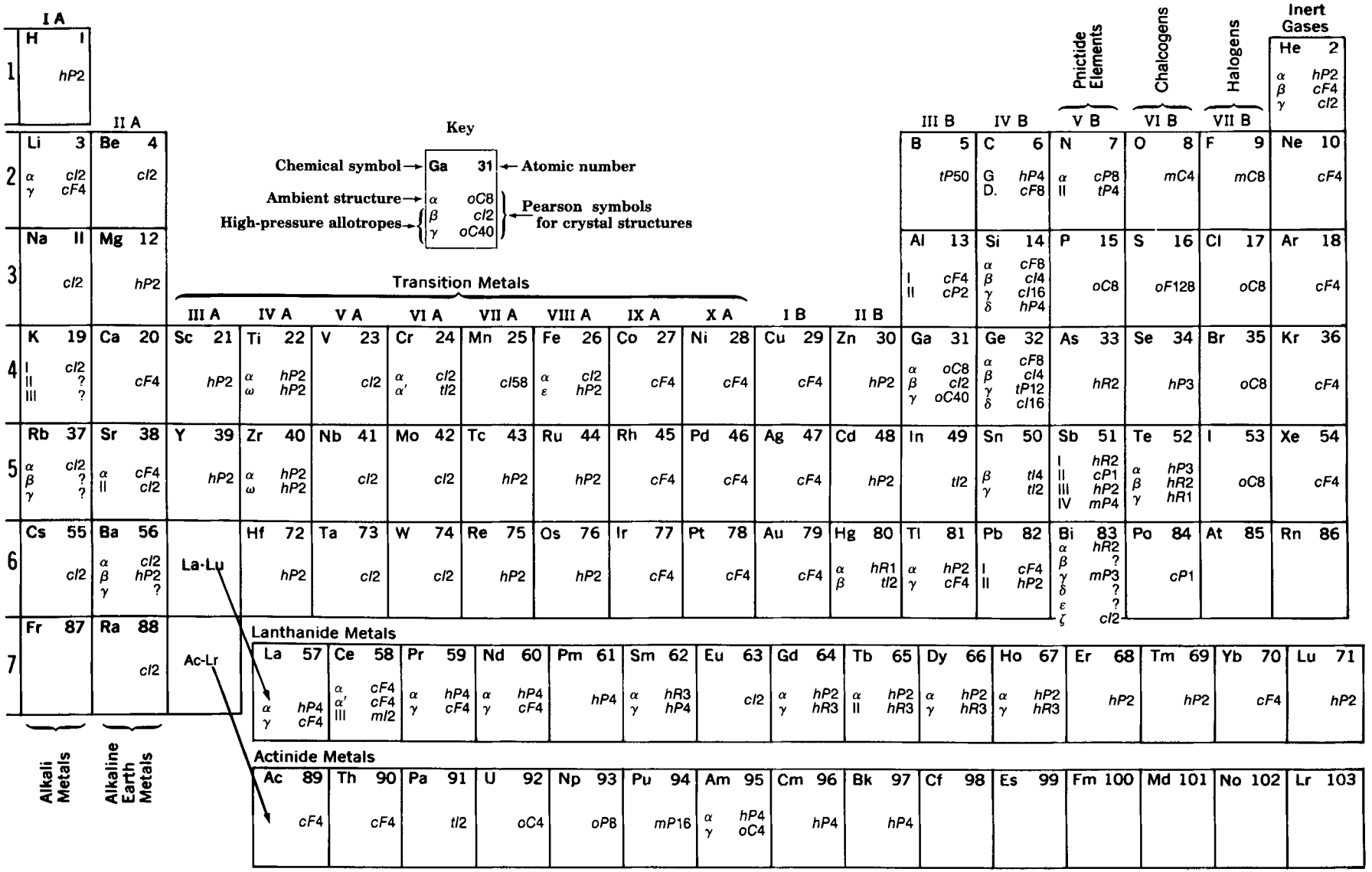
Pressure-Dependent Allotropic Structures of the Elements

See reverse for explanation



Pressure-Dependent Allotropic Structures of the Elements

By H. W. King
Technical University of Nova Scotia

The allotropic structures of the elements listed below and on the reverse side of this tear-out sheet are presented using the Pearson symbol [*Bull. Alloy Phase Diagrams, 2*(2), 153-157 (1981)]. The lattice parameters of the unit cells are given in nanometers. Earlier data reported in kX units were converted to nm by multiplying the original kX by 0.100202. The accuracy of the data presented in the table is considered to be reliable to ±2 in the last reported digit. Ambient condition data (RTP) refer to 25 °C and atmospheric pressure using the structural data reported in an earlier volume in this series [H. W. King, *Bull. Alloy Phase Diagrams, 2*(3), 401-402 (1981)]. High-pressure data refer to pressures within ±1 of the last reported digit in kilobars.

The nomenclature for the various allotropes may at times appear to be inconsistent, with some missing structures. This compilation is complementary to the temperature-dependent allotropic structural data given in an earlier issue of the *Bulletin* [H. W. King, *Bull. Alloy Phase Diagrams, 3*(2), 275-276 (1982)]. The missing allotropes will thus be found to be temperature-dependent structures.

Sources

The lattice parameter values are based on data published in *A Handbook of Lattice Spacings and Structures of Metals and Alloys*, W. B. Pearson, Ed., Vol. 1 (1958), Vol. 2 (1967), Pergamon Press, NY; "The Structure of the Pure Metals", H. W. King in *Physical Metallurgy*, 2nd ed., R. W. Cahn, Ed., North-Holland, Amsterdam (1970); *The Structure of the Pure Elements*, J. Donohue, John Wiley and Sons, NY (1974); *Handbook on the Physics and Chemistry of Rare Earths*, Vol. 1-*Metals*, K. A. Gschneidner and L. R. Eyring, Ed., North-Holland, Amsterdam (1978); and data from "Structure Reports", compilations made available by Dr. L. Calvert, National Research Council, Ottawa.

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Element and allotrope	Pearson symbol	Lattice parameters, nm a	b	c	c/a or α or β	Stability range
Al-I	*cF4*	0.40496	···	···	···	RTP
Al-II	*hP2*	0.2693	···	0.4398	1.633	>205 kB
αAm	*hP4*	0.3468	···	1.1241	2 × 1.621	RTP
γAm	*oC4*	0.3063	0.5968	0.5169	···	>150 kB
αBa	*cI2*	0.5023	···	···	···	RTP
βBa	*hP2*	0.3901	···	0.6154	1.578	>53 3 kB
γBa	?	···	···	···	···	>230 kB
αBi	*hR2*	0.4760	···	···	α = 57.23°	RTP
βBi	?	···	···	···	···	>28 kB
γBi	*mP3*	0.605	0.420	0.465	β = 85.33°	>30 kB
δBi	?	···	···	···	···	>43 kB
εBi	?	···	···	···	···	>65 kB
ζBi	*cI2*	3.800	···	···	···	>90 kB
C (graph)	*hP4*	0.24612	···	0.67090	2.7259	RTP
C (dia)	*cF8*	0.35669	···	···	···	600 kB
αCe	*cF4*	0.51610	···	···	···	RTP
α'Ce	*cF4*	0 482	···	···	···	>15 kB
Ce-III	*mI2*	0.4762	0.3170	0.3169	β = 91.7°	>51 kB
αCr	*cI2*	0.28847	···	···	···	RTP
α'Cr	*tI2*	0.2882	···	0.2887	1.002	HP
Cs-I	*cI2*	0 6141	···	···	···	RTP
Cs-II	*cF4*	0.5984	···	···	···	>23.7 kB
Cs-III	*cF4*	0.5800	···	···	···	>42 2 kB
αDy	*hP2*	0.35915	···	0 56501	1.5731	RTP
γDy	*hR3*	0.3436	···	2.4830	4.5 × 1.606	>75 kB
αFe	*cI2*	0 28665	···	···	···	RTP
εFe	*hP2*	0.2485	···	0.3990	1.606	>130 kB
αGa	*oC8*	0.45192	0.76586	0.45258	···	RTP
βGa	*tI2*	0.2808	···	0.4458	1.587	>12 kB
γGa	*oC40*	1.0593	1.3523	0.5203	···	>30 kB; 220 K
αGd	*hP2*	0 36336	···	0 57810	1.5910	RTP
γGd	*hR3*	0.361	···	2.603	4.5 × 1.60	>30 kB
αGe	*cF8*	0.56574	···	···	···	RTP
βGe	*tI4*	0.4884	···	0.2692	0.551	>120 kB
γGe	*tP12*	0.593	···	0.698	0 18	(Decompressed βGe)
δGe	*cI16*	0.692	···	···	···	>120 kB
αHe	*hP2*	0.3577	···	0.5842	1.633	4.2 K
βHe	*cF4*	4.240	···	···	···	1.25 kB; 1.6 K
γHe	*cI2*	4.110	···	···	···	0.3 kB; 1.73 K
αHg	*hR1*	0.3005	···	···	α = 70.53°	227 K
βHg	*tI2*	0.3995	···	0.2825	0.707	HP; 77 K
αHo	*hP2*	0.35778	···	0.56178	1.5702	RTP
γHo	*hR3*	0.334	···	2.45	4.5 × 1.63	>40 kB

Element and allotrope	Pearson symbol	Lattice parameters, nm a	b	c	c/a or α or β	Stability range
K-I	*cI2*	0 5321	···	···	···	RTP
K-II	?	···	···	···	···	280 kB, 77 K
K-III	?	···	···	···	···	360 kB; 77 K
αLa	*hP4*	0 37740	···	1.2171	2 × 1.6125	RTP
β'La	*cF4*	0.517	···	···	···	>20 kB
αLi	*cI2*	0.35093	···	···	···	RTP
γLi	*cF4*	0.4388	···	···	···	CW at <72 K
αN	*cP8*	0.5659	···	···	···	4.2 K
N-II	*tP4*	0.3957	···	5.101	1.289	>33 kB; 20 K
αNd	*hP4*	0.36582	···	1 17966	2 × 1 6124	RTP
γNd	*cF4*	0.480	···	···	···	>50 kB
Pb-I	*cF4*	0.49502	···	···	···	RTP
Pb-II	*hP2*	0 3265	···	0.5387	1 653	>103 kB
αPr	*hP4*	0.36721	···	1 18326	2 × 1 6111	RTP
γPr	*cF4*	0.488	···	···	···	>40 kB
αRb	*cI2*	0 5703	···	···	···	RTP
βRb	?	···	···	···	···	>10.8 kB
γRb	?	···	···	···	···	>20.5 kB
Sb-I	*hR2*	0.45065	···	···	α = 57.11°	RTP
Sb-II	*cP1*	0.2992	···	···	···	>50 kB
Sb-III	*hP2*	0.3376	···	0.5341	1.582	>75 kB
Sb-IV	*mP4*	0.556	0 404	0.422	β = 86.0°	>140 kB
αSi	*cF8*	0.54306	···	···	···	RTP
βSi	*tI4*	0 4686	···	0 2585	0.551	>95 kB
γSi	*cI16*	0.636	···	···	···	>160 kB
δSi	*hP4*	0.380	···	0.628	1.635	Decompressed βSi
αSm	*hR3*	0 36290	···	2 607	4 5 × 1 6048	RTP
γSm	*hP4*	0.3618	···	1 166	2 × 1.611	>40 kB
βSn	*tI4*	0.58316	···	0.31815	0.5456	RTP
γSn	*tI2*	0 370	···	0.337	0.911	>90 kB
αSr	*cF4*	0.6084	···	···	···	RTP
Sr-II	*cI2*	0.4437	···	···	···	>35 kB
αTb	*cP2*	0.36055	···	0.56966	1.5800	RTP
Tb-II	*hR3*	0.341	···	2.45	4 5 × 1 60	>60 kB
αTe	*hP3*	0.44561	···	0.59271	1.3301	RTP
βTe	*hR2*	0.469	···	···	α = 53.30°	>30 kB
γTe	*hR1*	0 3002	···	···	α = 103.3°	>70 kB
αTi	*hP2*	0.34563	···	0 55263	1.5989	RTP
ωTi	*hP2*	0.4625	···	0.2813	0.608	Decompressed
αTl	*hP2*	0 34563	···	0.55540	1 5700	RTP
γTl	*cF4*	···	···	···	···	HP
αZr	*hP2*	0.32217	···	0.51476	1 5928	RTP
ωZr	*hP2*	0.506	···	0.3109	0.617	Decompressed