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Crystallography of the Chemical Elements

As Tabulated by William Hume-Rothery
in "The Structure of Metals and Alloys," Monograph No. 1, British Institute of Metals.

Emendations (by H. C. Vacher) Represent Values that Have Appeared in the Literature from 1936 to 1940 Inclusive.

Element Atomic No.	Electron Arrangement in Free Atoms	Crystal Structure (Note a)	Axial Ratio c÷a	Coordination No.	Lattice Constant a	Lattice Constant c	Interatomic Distance d_1	Interatomic Distance d_2	Atomic Diameter Coordination No. 12 (Note f)	Reference (g)
Group IV A in Periodic Sequence										
22, Titanium	[2][8][10]2	α=○	1.601	6,6	2.953	4.729	2.915	2.953	2.93	—
(slightly over 900°C.)		β=□	—	8	3.32	—	2.875	—	2.96	2
40, Zirconium	[2][8][18][10]2	α=○	1.589	6,6	3.223	5.123	3.166	3.223	3.19	—
(data for 867°C.)		β=□	—	8	3.61	—	3.126	—	—	—
72, Hafnium	[2][8][18][32][10]2	○	1.587	6,6	3.200	5.077	3.139	3.200	3.17	—
90, Thorium	[2][8][18][32][18][10]2	⊡	—	12	5.077 or 5.091	—	3.590 or 3.600	—	—	—
Group IV B, Including Carbon and Silicon										
6, Carbon, diamond	[2]4	◇	—	4	3.5606	—	1.5113	—	—	—
graphite		○ (b)	2.75	6	2.46	6.78	1.42	2.46	—	—
14, Silicon	[2][8]4	◇	—	4	5.4173±5	—	2.3457	—	—	1
32, Germanium	[2][8][18]4	◇	—	4	5.647	—	2.445	—	2.788	—
50, Tin, gray	[2][8][18][18]4	◇	—	4	6.46	—	—	—	3.164	—
white		△	0.5456	4,2	5.8194	3.1753	3.0161	3.1753	—	—
82, Lead	[2][8][18][32][18]4	⊡	—	12	4.9389	—	3.492s	—	3.494	—
Group V A in Periodic Sequence										
23, Vanadium	[2][8][11]2	□	—	8	3.038	—	2.627 4	—	2.69	1
41, Columbium	[2][8][18][12]1	□	—	8	3.294±1	—	2.853	—	2.94	—
73, Tantalium	[2][8][18][32][11]2	□	—	8	3.295 9±3	—	2.854 4	—	2.94	1
91, Protoactinium	[2][8][18][32][18][11]2	—	—	—	—	—	—	—	—	—
Group V B										
7, Nitrogen	[2]5	α=cubic	—	—	5.66	—	1.06	—	—	—
		β=hex.	1.633	—	4.034±9	6.587±15	—	—	—	1
15, Phosphorus, metallic	[2][8]5	▯	a÷b÷c = 1:1.32:3.17		3.31	b=4.38 10.50	2.17	2.20	—	1
33, Arsenic	[2][8][18]5	▱	α=54°7.5′	3,3	4.13 5±6	—	2.507	3.139	—	1
51, Antimony	[2][8][18][18]5	▱	α=57°6.5′	3,3	4.497 6±2	—	2.879 5	3.378 4	3.228	1
83, Bismuth	[2][8][18][32][18]5	▱	α=57°14.2′	3,3	4.735 6±6	—	3.103 6	3.472 8	3.64	1
Group VI A in Periodic Sequence										
24, Chromium	[2][8][13]1	α=□	—	8	2.878 6	—	2.492 9	—	2.57	—
		β=○	1.626	6,6	2.717	4.418	2.709	2.717	2.71	—
42, Molybdenum	[2][8][18][13]1	□	—	8	3.140 3	—	2.719 6	—	2.80	—
74, Tungsten	[2][8][18][32][12]2	α=□	—	8	3.158 3	—	2.735 2	—	2.82	—
		β=cubic (c) 8 atoms in unit cell			5.038	—	2.519	2.816	—	—
92, Uranium	[2][8][18][32][13][12]2	▯	4 atoms in unit cell, a:b:c = 1:2.056:1.734,		2.852	4.945 b=5.865	2.76	2.85	—	9
Group VI B										
8, Oxygen	[2]6	α=▯	4 atoms in unit cell a:b:c=1:0.691:0.625,		5.50	3.44 b=3.82	—	—	—	1
		β=▱	α=99.1°; 12 atoms in unit cell		6.19	—	—	—	—	1
		γ=cube	16 atoms in unit cell		6.83	—	—	—	—	1
16, Sulphur	[2][8]6	α=▯	128 atoms in unit cell a:b:c = 1:1.233:2.343;		10.48	24.55 b=12.92	2.12	3.36	—	1
at 103°C.		(d) mono-clinic	a:b:c = 1:1.011:1.006 ; β=83°16′;		10.90	10.96 b=11.02	—	—	—	2
34, Selenium	[2][8][18]6	○ (e)	1.140	2,4	4.337	4.945	2.316	3.457	—	—
		monoclinic (α)	a:b:c = 1:0.998:1.281 32 atoms in unit cell; β=91°34′;		8.992	11.52 b=8.973	—	—	—	1
		monoclinic (β)	a:b:c = 1:6.311:7.261 32 atoms in unit cell; β=93°4′;		12.74	9.25 b=8.04	—	—	—	1
52, Tellurium	[2][8][18][18]6	○ (e)	1.33	2,4	4.445	5.912	2.858	3.46	—	—
84, Polonium	[2][8][18][32][18]6	pseudo hexagonal	3 atoms in pseudocell		4.25	20.6 or 14.12	—	—	—	6
		probably monoclinic	a:b:c = 1:0.578:1.900 12 atoms in unit cell; β=92°;		7.42	14.10 b=4.29	3.4	4.0	—	6

Notes: (a) ⊡ is body-centered cubic; ⊡ is face-centered cubic; ○ is close packed hexagonal except as noted; ◇ is diamond; △ is tetragonal; ▱ is rhombohedral, and ▯ is orthorhombic.

(b) Graphite is hexagonal, not close packed, with four atoms per unit cell.

(c) Cubic structure; two positions distinguishable, X and Y. Each atom X has 12 Y at 2.816 Å; each atom Y has 2 Y at 2.519, and 4 X at 2.816 Å.

(d) Unit cell contains 48 S or 6 S8.

(e) Hexagonal, not close packed; each atom has 2 neighbors at d_1 and 4 at d_2.

(f) Atomic diameters for new values have been computed by following Hume-Rothery's procedure whenever possible.

(g) See Page 580, Metal Progress, May 1941.