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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 VII A in Periodic Sequence										
25, Manganese	[2][8][13]2	α = cubic (note b)	—	—	8.894	—	—	—	—	—
		β = cubic (note c)		12	6.300	—	—	—	—	—
		γ = △	0.934	—	3.774	3.526	2.582	2.669	—	—
43, Masurium	[2][8][18][14] 1	—	—	—	—	—	—	—	—	—
75, Rhenium	[2][8][18][32][18]2	○	1.6148	—	2.7553	4.4493	2.7349	2.7553	2.75	—
Group VII B										
9, Fluorine	[2]7	—	—	—	—	—	—	—	—	—
17, Chlorine	[2][8]7	△	0.715	—	8.56	6.12	1.88 (note e)	—	—	4
			16 atoms in unit cell							
35, Bromine	[2][8][18]7	□	a:b:c = 1:1.49:1.95		4.48	8.72	2.27	noted	—	5
			8 atoms in unit cell; b = 6.67							
53, Iodine	[2][8][18][18]7	□	a:b:c = 1:1.51:2.04		4.795	9.780	2.70	noted	—	—
			8 atoms in unit cell; b = 7.255							
85, Alabamine	[2][8][18][32][18]7	—	—	—	—	—	—	—	—	—
Group VIII in Periodic Sequence										
26, Iron	[2][8][14]2	α = ⧈	—	—	2.861	—	2.477	—	—	—
		β = ⊡	—	—	3.64 at 900°C.	—	2.58	—	2.52	—
27, Cobalt	[2][8][15]2	α = ○	1.624	—	2.507	4.072	2.499	2.507	2.50	—
		β = ⊡	—	—	3.545	—	2.507	—	2.507	—
28, Nickel	[2][8][16]2	α = ○	1.64	—	2.49	4.08	2.49	2.49	2.49	—
		β = ⊡	—	—	3.517	—	2.486	—	2.487	—
44, Ruthenium	[2][8][18][15]1	○	1.583	—	2.6984	4.273	2.644	2.698	2.67	8
45, Rhodium	[2][8][18][16]1	⊡	—	—	3.795	—	2.683	—	2.684	—
46, Palladium	[2][8][18][18]	⊡	—	—	3.882	—	2.745	—	2.745	—
76, Osmium	[2][8][18][32][14]2	○	1.579	—	2.7298	4.3104	2.670	2.730	2.70	8
77, Iridium	[2][8][18][32][15]2	⊡	—	—	3.831	—	2.709	—	2.709	—
78, Platinum	[2][8][18][32][16]2	⊡	—	—	3.915	—	2.768	—	2.769	—
Rare Earth Group										
58, Cerium	[2][8][18][19][9]2	α = ○	1.62	6,6	3.65	5.91	3.63	3.65	3.64	—
		β = ⊡	—	12	5.143	—	3.637	—	3.637	—
59, Praseodymium	[2][8][18][20][9]2	○	1.620	6,6	3.657	5.924	3.638	3.657	3.65	—
60, Neodymium	[2][8][18][21][9]2	○	1.608	6,6	3.657	5.88	3.619	3.657	3.64	—
67, Holmium	[2][8][18][28][9]2	○	1.580	6,6	3.557±3	5.620±5	3.480	3.557	3.52	11
68, Erbium	[2][8][18][29][9]2	○	1.63	6,6	3.74	6.09	3.73	3.74	3.73	—

Notes: (a) ⧈ is body-centered cubic; ⊡ is face-centered cubic; ○ is close packed hexagonal; □ is orthorhombic; △ is tetragonal.

(b) Approximates ⧈ where each lattice point is a cluster of 29 atoms; 1 type X, 4 type A, 12 type D_2 and 12 type D_1. The X atoms occupy the largest volume and the D_2 the smallest. Interatomic distances of neighboring atoms are as follows:

X atoms have: 12 D_2 at 2.71; 4 A at 2.82

A atoms have: 1 X at 2.82; 3 D_1 at 2.49 and 3 at 2.96; 3 D_2 at 2.69 and 3 at 2.89

D_2 atoms have: 1 X at 2.71; 2 A at 2.69 and 1 at 2.89; 1 D_2 at 2.24 and 2 at 2.38; 1 D_1 at 2.45, 2 at 2.51 and 2 at 2.66

D_1 atoms have: 1 A at 2.49 and 1 at 2.96; 1 D_2 at 2.45, 2 at 2.51 and 2 at 2.66; 6 D_1 at 2.67

(c) Complicated structure with 20 atoms of two kinds in unit cell. Each atom of the first kind has:

3 neighbors at 2.365
3 -"- -"- 2.530
3 -"- -"- 2.671
3 -"- -"- 2.675

Each atom of the second kind has: 2 neighbors at 2.530
2 -"- -"- 2.615
4 -"- -"- 2.659
2 -"- -"- 2.671
2 -"- -"- 2.675

(d) Atoms arranged in pairs so that each one has one close neighbor at a distance d_1

(e) The authors give 1.99 as the closest approach to a neighboring atom, however, they did not indicate clearly the space group. If the space group is D_{4h}^{16} with 16 atoms to a unit cell and the X, Y, and Z parameters are 0.125, 0.167 and 0.102, respectively, then $d_1 = 1.88$.

(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.