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RESEARCH MEMORANDUM

CRYSTAL STRUCTURES AND ATOMIC VOLUMES OF THE ELEMENTS

W. G. McMillan

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The following table is a compilation of the available data[1] on the crystal structures of the common modifications of the elements at zero pressure. From the lattice parameters the volume per atom ("$v_{x\text{-}ray}$") was calculated as the ratio of the volume of the unit cell to the number of atoms per unit cell, and compared with that ("v_{dens}") calculated from the bulk density. Also given is the radius r_o of the equivalent sphere, i.e., having the atomic volume. Where known, the experimental temperatures are given for the lattice parameter determinations; "RT" means room temperature. Temperatures of the experimental density measurements are 300 $\pm$ 10°K, unless otherwise specified.

Although these calculations are exceedingly trivial, the frequent reference to the old manuscript copy appeared to indicate that a wider circulation might prove useful.

I have to thank Mr. D. C. MacNeilage for numerical assistance.

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[1] The principal source of this data was the compilation by J. G. Albright in the Handbook of Physics and Chemistry, 35th ed. Where necessary this was supplemented with data from Wyckoff, The Structure of Crystals (looseleaf) and Barrett, Structure of Metals, 2nd ed., McGraw-Hill (1952). Data for plutonium (Z=94) were taken from R. R. Jette, "Some Physical Properties of Plutonium Metal," J. Chem. Phys., 23, 365 (1955).

Z	A Mol.Wt.	Phase	Structure Type	Sym	Temp	Lattice Parameters a	b/a	c	Atoms /Cell	$v_{x\text{-}ray}$	r_o	Expt'l Density	$v_{density}$
					°K	Å	Å/deg.	Å		Å^3	Å	gm/cm^3	Å^3
1 H	1.00813	(s) (l)	hex		2	3.75		6.11	4	18.60	1.644	0.070 (21°K)	23.9
D	2.011471												
T	3.01695												
2 He	4.003	(s) (l)	cph	A3	2	3.57		5.83	2	32.17	1.973	0.147 (2.4°K)	45.2
3 Li	6.940		bcc	A2	RT	3.5093			2	21.6038	1.7279	0.534	21.58
		cold worked	fcc	A1	78	4.41			4	21.44	1.723		
4 Be	9.013	a	cph	A3	291	2.28105		3.57714	2	8.05945	1.2438	1.84	8.13
			hex			5.12		15.77	44 ?	8.14 ?	1.248 ?		
5 B	10.82		hex			11.98		9.54	180	6.587	1.103		
			tetr			8.57		8.13	78	7.655	1.223	3.33	5.39
			monocl										
6 C	12.010	diamond	cub	A4	291	3.56665-3.56723			8	5.67141-5.67419	1.1063-1.1065	3.52	5.66
		a-graphite	hex	A9	293	2.4611		6.7077	4	8.7964	1.2806		
		β-graphite	rhbdr			3.635	α=39°30'		2 ?	8.746 ?	1.2781 ?		
		"graphite"	cub									2.25	8.86
		amorphous, blk										1.8-2.1	11.1-9.5
7 N	14.008	a(s)	cub		21	5.66			$4N_2$	22.67	1.756	1.026 (20.7°K)	22.67

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Z	A Mol.Wt.	Phase	Structure Type	Sym	Temp	Lattice Parameters a	b/c	c	Atoms /Cell	$V_{x\text{-ray}}$	r_o	Expt'l Density	$V_{density}$
					°K	Å	Å/deg.	Å		$Å^3$	Å	gm/cm^3	$Å^3$
8 O	16.000	α(s)	orthrb		21	5.50	b:3.82	3.44	4	18.07	1.628		
		β(s)	rhbdr		35	6.19	α:99.1°		6	37.85*	2.083		
		γ(s)	cub		50	6.83			8	39.83	2.119		
		(s)	hex									1.426 (20.7°K)	18.63
9 F	19.00	(ℓ)										1.108 (86°K)	28.47
10 Ne	20.183	(s)	f.c.c.	A1	20	4.52			4	23.09	1.766		
		(ℓ)										1.204 (27.3°K)	27.83
11 Na	22.997		b.c.c.	A2	293	4.2820			2	39.2563	2.1083	0.9712	39.315*
12 Mg	24.32		c.p.h.	A3	298	3.20280		5.19983	2	23.0967	1.7667	1.741	23.19
13 Al	26.98		f.c.c.	A1	298	4.04145			4	16.5026	1.5794	2.699	16.597
14 Si	28.09		dia.cub.	A4	298	5.43048			8	20.0182	1.6844	2.42	19.27
		stabilized by CaF_2	hex.		high	6.86		10.29	20 ?	20.97 ?	1.711?		
15 P	30.975	met.	hex,rhbdr			5.14	α:34°07'		2	19.04	1.657		
		"	rhbdr., f.c.			5.96	α:60°47'		8	19.04	1.657		
		blk	orthrb	A16	R.T.	3.31	b:4.38	10.50	8	19.03	1.656	2.70	19.05
		white	cub.		238	7.17			$4P_4$	23.04	1.765*		
		yellow	cub.									1.82	28.3
		red	cub.									2.20	23.4
		violet	monocl.									2.36	21.79

Z	A Mol.Wt.	Phase	Structure Type	Sym	Temp	Lattice Parameters a	b/c	c	Atoms /Cell	$V_{x\text{-ray}}$	r_o	Expt'l Density	$V_{density}$
					°K	Å	Å/deg.	Å		Å^3	Å	gm/cm^3	Å^3
16 S	±0.003 32.066	α	orthrb	A17	293	10.48	b=12.92	24.55	128	25.97	1.837	2.07	25.7
		β	monocl		376	10.90	b=11.02 m=83°16'	10.96	48	27.24	1.866	1.96	27.2
			plastic, str. ?			26.4	b= 9.26 m=79°15'	12.32	112	?			
			rhombic pseudocell ?			8.90	b=10.61 m=92°44'	8.90	32	?			
		γ-amorphous										1.92	27.7
17 Cl	35.457	(α) (ε)	tetr		88	8.56		6.12	8	56.05	2.374	1.507 (239.6°K)	39.06
18 A	39.944	(α)	fcc	A1	20	5.43			4	40.03	2.122	1.65 (40°K)	40.2
19 K	39.100		bcc	A2	123	5.20			2	70.3	2.560	0.87	74.6
20 Ca	40.08	α	fcc	A1	193	5.565			4	43.086	2.1768	1.54	43.2
		γ	cph	A3	723	3.98		6.52	2	44.7	2.202		
21 Sc	44.96	α	fcc	A1	293	4.532			4	23.271	1.7711		
		β	cph	A3	RT	3.302		5.245	2	24.763	1.3082		
												2.5	30.
22 Ti	47.90	α	cph	A3	298	2.92		4.67	2	17.24	1.603	4.5	17.7
		β	bcc	A2	>1173	3.32			2	18.30	1.635		
23 V	50.95		bcc	A2	293	3.0338			2	13.9615	1.4938	5.96	14.19

Z	A Mol.Wt.	Phase	Structure Type	Structure Sym	Temp °K	Lattice Parameters a Å	Lattice Parameters b/c Å/deg.	Lattice Parameters c Å	Atoms /Cell	$V_{x\text{-ray}}$ Å^3	r_o Å	Expt'l Density gm/cm^3	$V_{density}$ Å^3
24 Cr	52.01	α	b.c.c.	A2	291	2.8796			2	11.9390	1.4178	7.20	11.99
		β	c.p.h.	A3		2.717		4.418	2	14.122	1.4995		
		γ	b.c.c.	A2		8.717			58	11.420	1.3970		
25 Mn	54.93	α	cub	A12	293	8.894			58	12.130	1.4254		
		β	cub	A13	R.T.	6.300			20	12.502	1.4398		
		γ	tetr.,f.c. cub. or tetr.	A6	R.T.	3.774		3.526	4	12.555*	1.4418	7.20	12.29
26 Fe	55.85	α	b.c.c.	A2	293	2.86635			2	11.7749	1.4113	7.86	11.80
		β	b.c.c.	A2	1073	2.90			2	12.19	1.428		
		γ	f.c.c.	A1	1373	3.63			4	11.96	1.419		
		δ	b.c.c.	A2	1698	2.93			2	12.58	1.443		
		gray cast										7.03-13	13.19-01
		white cast										7.58-73	12.23-00
27 Co	58.94	α	c.p.h.	A3	293	2.5017		4.0629	2	11.0105	1.3801		
		β	f.c.c.	A1	R.T.	3.554			4	11.223	1.3889	8.9	11.0
28 Ni	58.69	α	c.p.h.	A3	443	2.65		4.32	2	13.14	1.464		
		β	f.c.c.	A1	298	3.51684			4	10.8742	1.3744	8.90	10.95
29 Cu	63.54	compressed	f.c.c. cub	A1	291	3.6073			4	11.7351	1.4097	8.9376	11.804
30 Zn	65.38	wrought	c.p.h. hex.	A3	298	2.65949		4.93685	2	15.1198	1.5340	7.19	15.10

Z	A Mol.Wt.	Phase	Structure Type	Sym	Temp	Lattice Parameters a	b/ω	c	Atoms /Cell	$V_{x\text{-ray}}$	r_o	Expt'l Density	$V_{density}$
					°K	Å	Å/deg.	Å		Å³	Å	gm/cm³	Å³
31 Ga	69.72		tetr (simple) orthrb rhombic			4.51 4.5107	b:4.5167	7.51 7.6448	8 8 ?	19.09 19.4689 ?	1.658 1.6689 ?	5.903	19.610
32 Ge	72.60		dia cub	A4	293	5.62			8	22.19	1.743	5.46	22.08
33 As	74.91		rhbdr rhbdr,fc	A7	293	4.123 5.599	ω:54°10' ω:84°18'		2 8	21.405* 21.635	1.7224 1.7286		
		met amorphous,brwn-blk yellow	hex cub									5.727 3.70 2.0	21.718 33.62 62.
34 Se	78.96	α-red metastable	monocl.I		RT	8.992	b:8.973 ω:91°34'	11.52	32 (Se₈)	29.04	1.907	4.46	29.39
		β-red metastable	monocl.II		RT	12.74	b:8.04 ω:93°04'	9.25	32	29.57	1.918		
		stable gray-met.	hex	A8	293	4.337		4.944	3	26.845*	1.8575*		
		amorphous red-powder vitreous, dark brwn-blk gray met.	trig									4.82 4.14 4.79	27.20 31.67 27.37
35 Br	79.916	(s) (ℓ)	orthrb		123	4.48	b:6.67	8.72	8	32.57	1.981	3.12	42.5

Z	A Mol.Wt.	Phase	Structure Type	Sym	Temp	Lattice Parameters a	b/c	c	Atoms /Cell	$V_{x\text{-ray}}$	r_o	Expt'l Density	$V_{density}$
					°K	Å	Å/deg.	Å		Å^3	Å	gm/cm^3	Å^3
36 Kr	83.8	(s) (ℓ)	f.c.c.	A1	89	5.694			4	46.152	2.2252	2.155 (120.3°K)	64.56
37 Rb	85.48		b.c.c.	A2	292	5.709			2	93.04	2.8110	1.532	92.64
38 Sr	87.63		f.c.c.	A1	293	6.049			4	55.334	2.3639	2.50-58	58.2-564
39 Y	88.92		c.p.h.	A3		3.629		5.750	2	32.790	1.9856	5.51	26.79
40 Zr	91.22	α β	c.p.h. b.c.c.	A3 A2	1123	3.23 3.61		5.14	2 2	23.22 23.52	1.770 1.777	6.44	23.52
41 Nb	92.91		b.c.c. rhombic	A2		3.2941			2	17.8723	1.6219	8.55	18.04
42 Mo	95.95		b.c.c.	A2	298	3.14103			2	15.4948	1.5466	10.2	15.6
43 Tc	(99)*		c.p.h.	A3		2.735		4.388	2	14.213	1.5027		
44 Ru	101.7	α gray white br-mst. blk porous	c.p.h. hex.	A3	293	2.69844		4.27305	2	13.4730	1.4761	12.063 12.6	14.00 13.4
45 Rh	102.91	β	f.c.e.	A1	291	3.79559			4	13.6703	1.4833	12.44	13.74
46 Pd	106.7		f.c.e.	A1	291	3.88238			4	14.6297	1.5172	11.40	15.54

* Most stable isotope

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Z	A Mol.Wt.	Phase	Structure Type	Sym	Temp	Lattice Parameters a	b/a	c	Atoms /Cell	$V_{x\text{-}ray}$	r_o	Expt'l Density	$V_{density}$
					°K	Å	Å/deg.	Å		Å^3	Å	gm/cm^3	Å^3
47 Ag	107.880	compressed	fcc cub	A1	298	4.07787			4	16.9527	1.5936	10.503	17.054
48 Cd	112.41	vacuo-distilled	cph hex	A3	298	2.97311		5.60694	2	21.4610	1.7239	8.648	21.582
49 In	114.76		tetr,fc	A6	293	4.583		4.963	4	26.060	1.8392	7.28	26.17
50 Sn	118.70	α-gray β-white γ-br-white	dia.cub tetr rhombic	A4 A5	291 293	6.46 5.818		3.174	8 4	33.70 26.859	2.004 1.8578	5.75 7.28 6.52-56	34.28 27.07 30.23-04
51 Sb	121.76		rhbdr rhbdr,fc hex	A7	298	4.49762 5.226	α:57°06.6' α:87°24'		2 8	30.0242 30.077	1.9281 1.9292	6.684	30.246
52 Te	127.61	sil-wh-met crystal br-blk amorphous	hex rhbdr	A8	293	4.495		5.912	3	34.483	2.0192	6.25 6.00	33.90 35.31
53 I	126.91		orthrb rhombic		291	4.7761	b:7.2501	9.7711	8	42.2932	2.1614	4.94	42.65*
54 Xe	131.3	(s) (ℓ)	fcc	A1	88	6.24			4	60.74	2.439	3.52 (164°K)	61.9

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Z	A Mol.Wt.	Phase	Structure Type	Structure Sym	Temp	Lattice Parameters a	Lattice Parameters b/a	Lattice Parameters c	Atoms /Cell	$V_{x\text{-ray}}$	r_o	Expt'l Density	$V_{density}$
					°K	Å	Å/deg.	Å		Å³	Å	gm/cm³	Å³
55 Cs	132.91		bcc hex	A2	88	6.05			2	110.7	2.979	1.873	117.82
56 Ba	137.36		bcc	A2	293	5.009			2	62.84	2.4663	3.78	60.3
57 La	138.92	α β	cph fcc	A3 A1	293 RT	3.75 5.294		6.06	2 4	36.90 37.093	2.065* 2.0689	6.15	37.50
58 Ce	140.13	α β at ca 12,450 atmos.	cph fcc fcc	A3 A1 A1	 RT RT	3.65 5.140 4.84		5.96	2 4 4	34.38 33.949 28.34	2.017 2.0087 1.891	6.7 6.90	34.7 33.72
59 Pr	140.92	α β	cph fcc	A3 A1	293 RT	3.662 5.151		5.908	2 4	34.307 34.168	2.0157 2.0130	6.475	36.135*
60 Nd	144.27		cph	A3	293	3.650		5.890	2	33.978	2.0093	6.96	34.42
61 Pm	(145)												
62 Sm	150.43		hex									7.7-8	32.4-0
63 Eu	152.0		bcc	A2	293	4.573			2	47.82	2.2516		
64 Gd	156.9		cph	A3	293	3.622		5.748	2	32.652	1.9828		
65 Tb	159.2		cph	A3	293	3.585		5.662	2	31.510	1.9594		

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Z	A Mol.Wt.	Phase	Structure Type	Structure Sym	Temp	Lattice Parameters a	Lattice Parameters b/c	Lattice Parameters c	Atoms /Cell	$V_{x\text{-}ray}$	r_o	Expt'l Density	$V_{density}$
					°K	Å	Å/deg.	Å		Å^3	Å	gm/cm^3	Å^3
66 Dy	162.46		cph	A3	293	3.578		5.648	2	31.310	1.9552		
67 Ho	164.94		cph	A3	293	3.557		5.620	2	30.790	1.9443		
68 Er	167.2		cph	A3	293	3.532		5.589	2	30.191	1.9317	4.77 ?	58.2 ?
69 Tm	169.4		cph	A3	293	3.523		5.564	2	29.903	1.9255		
70 Yb	173.04		fcc	A1		5.468			4	40.872	2.1369		
71 Lu	174.99		cph	A3	293	3.509		5.559 ?	2	29.639 ?	1.9198?		
72 Hf	178.6	gray	cph	A3	293	3.32		5.46	2	26.06	1.839	13.3	22.3
73 Ta	180.88	gray-blk metal blk powder	bcc cub	A2	293	3.2959			2	17.9017	1.6228	16.6 14.491	18.1 20.725
74 W	183.92	α	bcc	A2	298	3.15837			2	15.7528	1.5551	19.3	15.82
		β-unstable	cub	A15	293	5.04			8	16.00	1.563		
75 Re	186.31		cph	A3	293	2.7353		4.4493	2	14.6262	1.5171	20.53	15.068
76 Os	190.2		cph	A3	293	2.72980		4.3104	2	13.9085	1.4919	22.48	14.048
77 Ir	193.1		fcc	A1	291	3.8312			4	14.0587	1.4972	22.421	14.300
78 Pt	195.23		fcc	A1	291	3.91580			4	15.0107	1.5303	21.45	15.112

Z	A Mol.Wt.	Phase	Structure Type	Sym	Temp	Lattice Parameters a	b/a	c	Atoms /Cell	$V_{x\text{-ray}}$	r_o	Expt'l Density	$V_{density}$
					°K	Å	Å/deg.	Å		Å^3	Å	gm/cm^3	Å^3
79 Au	197.2	cold rolled	f.c.c.	A1 cub.	298	4.07042			4	16.8600	1.5907	19.296	16.968
80 Hg	200.61	(s)	rhbdr		227	2.997	α=70°32'		1	23.170	1.7685	14.383 (85°K)	23.158
		(s)	rhbdr.f.c.		227	4.578	α=98°13'		4	23.168	1.7685		
81 Tl	204.39	α	c.p.h.	A3	R.T.	3.4496		5.5137	2	28.4106	1.8929		
		β	f.c.c.	A1	>303	4.841			4	28.362	1.8918		
			b.c.c.	A2		3.874			2	29.070	1.9074	11.86	28.61
			tetr.										
82 Pb	207.21		f.c.c.	A1	298	4.9408			4	30.1530	1.9308	11.3437	30.329
83 Bi	209.00		rhbdr.	A7	298	4.7364	α=57°14.5'		2	35.1800	2.0327		
		vacuo-distilled	rhbdr.f.c. hex.			6.578	α=87°34'		8	35.486	2.0386	9.781	35.478
84 Po	210	α	cub(simple)		263	3.34			1	37.3	2.072		
			monoel.			7.42	b:4.29 α=92° ?	14.10	12 ?	37.4 ?	2.07 ?		
85 At	(210)												
86 Rn	222	(f)										4.4 (211°K)	84.
87 Fr	(223)												
88 Ra	226.05											5. ?	80. ?

Z	A Mol.Wt.	Phase	Structure Type	Sym	Temp	Lattice Parameters a	b/a	c	Atoms /Cell	$V_{x\text{-ray}}$	r_o	Expt'l Density	$V_{density}$
					K°	Å	Å/deg.	Å		Å^3	Å^3	gm/cm	Å^3
89 Ac	227												
90 Th	232.12		f.c.c.	A1	293	5.04			4	32.01	1.970	11.3-7	34.1-32.9
91 Pa	231												
92 U	238.07	α	orthrb.	A20	293	2.852	b:5.865	4.945	4	20.679	1.7027		
		γ	b.c.c.	A2	1073	3.474			2	20.963	1.7105	18.7	21.1
			monocl.			2.829	b:4.887	3.308	2	?			
							a: ?						
93 Np	(237)												
94 Pu	239	α										19.737 (298°K)	20.11
		β										17.65 (423°K)	22.48
		γ	orthrb.,	fc.	483	3.1603	b:5.7624	10.141	8	23.085	1.7664	17.19 (483°K)	23.08
		δ	f.c.c.		593	4.6370			4	24.9259	1.8121	15.92 (593°K)	24.9
		δ'	tetr.,	f.c.	738	4.701		4.489	4	24.801	1.8091	15.99 (738°K)	24.8
		ε	b.c.c.		773	3.638			2	24.075	1.7912	16.48 (773°K)	24.1
95 Am	(243)												
96 Cm	(243)												
97 Bk	(245)												
98 Cf	(246)												

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END