

NEW DATA ON ATOMIC DIMENSIONS

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In a review of a paper by V. M. Goldschmidt¹ attention was called to the fact that new values for atomic dimensions are coming to be accepted, and a summary of some recent work along this line may be worth publishing here. By means of X-rays it is possible to measure with a high degree of accuracy the distances between the centers of layers of atoms in crystals, and, whenever the arrangements of atoms in these layers can be worked out, the distances between the centers of adjacent atoms can be calculated. Until recently, however, there has been a considerable difference of opinion as to what fraction of the distance is assignable to each member of the pair of atoms. In halite, for example, the distance between Na and Cl centers is known with precision to be 2.814 am. units,² but what proportion of this length may be regarded as representing the radius of the sodium, and what the chlorine, remains to be determined.

On the basis of some reasonable though admittedly empirical assumptions as to the refractive powers of atoms, Goldschmidt³ has calculated effective radii of a large number of atoms in variously charged conditions, and Pauling,⁴ on the basis of modern wave-mechanics theories of electron arrangement, has presented theoretical values for most of the same elements, the two series of data agreeing well in many cases. The radius values deduced in these studies, with a few from other sources, are listed in table 1. The elements are arranged in the order of their atomic numbers and data are given for three different conditions, namely positively charged, neutral, and negatively charged (the first and last being

¹ *Am. Mineral.*, 12, 28-31 (1927).

² Atomic dimensions are commonly stated in units of 10^{-8} cm., often called ångström units; as, however, the initial character in this word is difficult to get set in type and to pronounce, in this country, I prefer to substitute the symbol *am.*, which may be regarded as an abbreviation of "atom-meter."

³ *Geochemische Verteilungsgesetze der Elemente. VII. Die Gesetze der Krystallochemie. Skr. Norske Vidensk. Akad. Oslo I. Mat.-Nat. Kl. No. 2*, 117 pages, 1926. This paper, together with the other members of the series, I to VIII, represents the most important contribution to chemical crystallography and geochemistry of recent years.

⁴ *J. Am. Chem. Soc.*, 49, 765-790 (1927).

termed ions). In many instances the radii for each condition given by different methods of calculation or by measurements on different classes of compounds show some divergence, so instead of a single value a range is stated. The theoretical wave-mechanics values are placed in bold-face type, and the values considered non-typical are surrounded by parentheses. For example, the 14th line in the table reads: 14 Si^{+4} (0.22—) 0.39—**0.41**. Si° (1.12—) 1.18. Si^{-4} (1.98); **2.71**. This signifies first, that the element with atomic number 14, silicon, when carrying 4 positive charges, has an apparent radius of between 0.22 and 0.41, but that the lower values are obtained from compounds in which the atoms appear to be deformed or otherwise abnormal, so Goldschmidt gives 0.39 as most significant, while wave-mechanics theory yields 0.41. Second, when neutral this atom's radius ranges from 1.12, in abnormal compounds, to 1.18 in those regarded as typical. And third, when carrying 4 negative charges, the value is 1.98, according to calculations deemed faulty, but 2.71 according to the theory.

In applying the data of table 1 to the study of replacements in minerals and of similar problems, it should be borne in mind that in halides and oxides the atoms are usually ionized, so that the values in the outer columns apply. Thus in fluorite the value for Ca^{+2} should be added to that for F^{-1} , giving between 2.32 and 2.42, depending on which ends of the range are used, or 2.37 as a mean; and the observed Ca—F distance in the crystal is 2.36 am. Again, in rutile, Ti^{+4} added to O^{-2} gives 1.96–2.08, mean 2.02, and the observed Ti—O distance is 1.98 am. In the remaining types of compounds, on the other hand, the atoms appear to be largely neutral, so the values in the central column are to be used. In sphalerite, for example, the mean of the sum of the radii of Zn° and S° is 2.36, and the observed Zn—S distance 2.35. The relations in the silicates remain to be worked out—it being possible that in them some atoms are ionized and others not—but it may be noted in passing that in this set of radius values, sodium and calcium lie very close together, and barium and potassium even closer, in both positive ion and neutral columns, lending support to the view that atomic size has something to do with the replaceability observed in these element-pairs.

TABLE I. EFFECTIVE RADII OF ATOMS, IN AM. UNITS.

1			H ⁻¹ (1.27); 2.08.
2		He ⁰ (0.93).	
3	Li ⁺¹ 0.60-0.78(-0.82).	Li ⁰ (1.50-)-1.56.	
4	Be ⁺² 0.31-0.34.	Be ⁰ 1.05(-1.15).	
5	B ⁺³ 0.20.		
6	C ⁺⁴ 0.15.	C ⁰ (0.45-)-0.77.	C ⁻⁴ 2.60.
7	N ⁺⁵ 0.11.	N ⁰ (0.65-)-0.71.	N ⁻³ 1.71.
8	O ⁺⁶ 0.09.	O ⁰ 0.60(-0.65).	O ⁻² 1.32-1.40.
9	F ⁺⁷ 0.07.	F ⁰ 0.67.	F ⁻¹ 1.33-1.36.
10		Ne ⁰ (1.12).	
11	Na ⁺¹ 0.95-0.98(-1.09).	Na ⁰ (1.77-)-1.86.	
12	Mg ⁺² 0.65-0.78(-0.85).	Mg ⁰ (1.42-)-1.62.	
13	Al ⁺³ 0.50-0.57(-0.66).	Al ⁰ (1.16-)-1.43.	
14	Si ⁺⁴ (0.22-)-0.39-0.41.	Si ⁰ (1.12-)-1.18.	Si ⁻⁴ (1.98); 2.71.
15	P ⁺⁵ 0.34.	P ⁰ 0.93	P ⁻³ 2.12.
16	S ⁺⁶ 0.29-0.34.	S ⁰ 1.02-1.04.	S ⁻² 1.74-1.84.
17	Cl ⁺⁷ 0.26.	Cl ⁰ 1.05-1.07.	Cl ⁻¹ 1.81.
18		Ar ⁰ (1.54).	
19	K ⁺¹ 1.33(-1.84).	K ⁰ (2.07-)-2.23.	
20	Ca ⁺² 0.99-1.06(-1.50).	Ca ⁰ (1.70-)-1.97.	
21	Sc ⁺³ 0.81-0.83.	Sc ⁰ 1.51.	
22	Ti ⁺⁴ (0.58-)-0.64-0.68.	Ti ⁰ (1.40-)-1.49(-1.53).	
23	V ⁺⁵ 0.59.		
	V ⁺⁴ 0.59-0.61.	V ⁰ 1.32(-1.43).	
24	Cr ⁺⁶ 0.52-0.65.	Cr ⁰ (1.17-)-1.25(-1.54).	
25	Mn ⁺⁷ 0.46.		
	Mn ⁺⁴ 0.50-0.52.		
	Mn ⁺² 0.80-0.91.	Mn ⁰ (1.17-)-1.29(-1.59).	
26	Fe ⁺³ (0.49-)-0.67.		
	Fe ⁺² 0.75-0.83.	Fe ⁰ (1.21-)-1.26(-1.45).	
27	Co ⁺³ 0.29-0.47.		
	Co ⁺² 0.72-0.82.	Co ⁰ 1.26(-1.39).	
28	Ni ⁺³ 0.35.		
	Ni ⁺² 0.69-0.78	Ni ⁰ 1.24(-1.39).	
29	Cu ⁺² 0.70.		
	Cu ⁺¹ (0.58-)-0.96.	Cu ⁰ (1.22-)-1.27(-1.37).	
30	Zn ⁺² 0.74-0.83.	Zn ⁰ 1.31-1.34.	
31	Ga ⁺³ 0.62.	Ga ⁰ (1.28-)-1.33(-1.45).	
32	Ge ⁺⁴ 0.44-0.53.	Ge ⁰ 1.22.	Ge ⁻⁴ 2.72.
33	As ⁺⁵ 0.47.		
	As ⁺³ 0.69.	As ⁰ (1.04-)-1.16(-1.26).	As ⁻³ 2.22.
34	Se ⁺⁶ 0.42.	Se ⁰ 1.13-1.17.	Se ⁻² 1.91-1.98.
35	Br ⁺⁷ 0.39.	Br ⁰ 1.19.	Br ⁻¹ 1.95-1.96.
36		Kr ⁰ (1.69).	
37	Rb ⁺¹ 1.48-1.49(-1.88).	Rb ⁰ (2.25-)-2.36.	
38	Sr ⁺² 1.13-1.27(-1.45).	Sr ⁰ 1.95.	
39	Y ⁺³ 0.93-1.06.		

40	Zr ⁺⁴	(0.68-)0.80-0.89.	Zr°	1.60-1.62.	
41	Cb ⁺⁵	0.69-0.70.			
	Cb ⁺⁴	0.67-0.69.	Cb°	1.43(-1.50).	
42	Mo ⁺⁶	0.62.			
	Mo ⁺⁴	0.66(-0.83).	Mo°	1.36.	
43	—				
44	Ru ⁺⁴	0.63-0.65.	Ru°	1.27-1.34.	
45	Rh ⁺³	0.69.	Rh°	1.34-1.35.	
46			Pd°	1.37.	
47	Ag ⁺¹	(0.79-)1.13-1.26.	Ag°	(1.17-)1.44.	
48	Cd ⁺²	(0.78-)0.97-1.03.	Cd°	(1.47-)1.49(-1.60).	
49	In ⁺³	0.81-0.92.	In°	1.45-1.62.	
50	Sn ⁺⁴	(0.64-)0.71(-0.81).	Sn°	(1.27-)1.40.	Sn ⁻⁴ (2.15); 2.94.
51	Sb ⁺⁵	0.62.			
	Sb ⁺³	0.90.	Sb°	(1.22)1.34(-1.44).	Sb ⁻³ 2.45.
52	Te ⁺⁶	0.56.			
	Te ⁺⁴	0.81-0.89.	Te°	1.33-1.43.	Te ⁻² 2.03-2.21.
53	I ⁺⁷	0.50.			
	I ⁺⁵	0.94.	I°	1.36-1.40.	I ⁻¹ 2.16-2.20.
54			Xe°	(1.90).	
55	Cs ⁺¹	1.65-1.69(-1.75).	Cs°	(2.37-)2.55.	
56	Ba ⁺²	1.35-1.43(-1.49).	Ba°	2.10.	
57	La ⁺³	1.15-1.22.			
58	Ce ⁺⁴	1.01-1.02.			
	Ce ⁺³	1.18.	Ce°	1.82-1.83.	
59	Pr ⁺⁴	0.92-1.00.			
	Pr ⁺³	1.16.			
60	Nd ⁺³	1.15.			
61	—				
62	Sm ⁺³	1.13.			
63	Eu ⁺³	1.13.			
64	Gd ⁺³	1.11.			
65	Tb ⁺³	1.09.			
66	Dy ⁺³	1.07.			
67	Ho ⁺³	1.05.			
68	Er ⁺³	1.04.			
69	Tm ⁺³	1.04.			
70	Yb ⁺³	1.00.			
71	—				
72			Hf°	1.66.	
73			Ta°	1.42-1.44.	
74	W ⁺⁶	0.88.			
	W ⁺⁴	0.66-0.68.	W°	1.37.	
75	—				
76	Os ⁺⁴	0.65-0.67.	Os°	1.30-1.34.	
77	Ir ⁺⁴	0.64.-0.66.	Ir°	1.35.	
78			Pt°	1.38(-1.43).	
79	Au ⁺¹	1.37.	Au°	1.40-1.44.	

80 Hg ⁺²	1.10-1.12.	Hg [°]	1.46-1.49.	
81 Tl ⁺³	0.95-1.05.			
Tl ⁺¹	1.44-1.51.	Tl [°]	(1.71-)1.99(-2.25).	
82 Pb ⁺⁴	0.84.			
Pb ⁺²	(0.98-)1.21-1.32.	Pb [°]	1.74(-1.90).	Pb ⁻⁴ 2.15.
83 Bi ⁺⁵	0.74.	Bi [°]	(1.34-)1.46(1.55).	
84 to 89	—			
90 Th ⁺⁴	1.02-1.10.	Th [°]	1.80-1.82.	
91	—			
92 U ⁺⁴	0.97-1.05.			
— NH ₄ ⁺¹	1.42-1.59.			