Ionic radius

Ionic radius, r_{ion} , is the radius ascribed to an atom's ion. Although neither atoms nor ions have sharp boundaries, it is useful to treat them as if they are hard spheres with radii such that the sum of ionic radii of the cation and anion gives the distance between the ions in a crystal lattice. Ionic radii are typically given in units of either picometers (pm) or Angstroms (Å), with 1 Å = 100 pm. Typical values range from 30 pm (0.3 Å) to over 200 pm (2 Å).

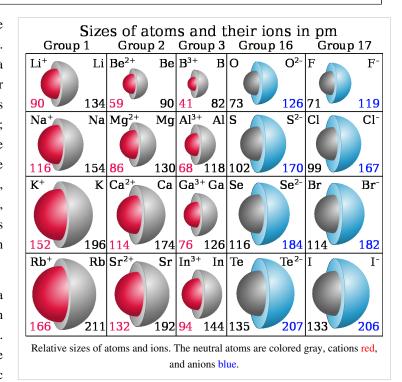
Trends in ionic radii

X ⁻	NaX	AgX
F	464	492
Cl	564	555
Br	598	577
Unit cell parameters (in pm, equal to two M–X	ζ bond lengths) for sodium and silver halides. A	ll compounds crystallize in the NaCl structure.

Ions may be larger or smaller than the neutral atom, depending on the ion's charge. When an atom loses an electron to form a the lost electron contributes to shielding the other electrons from charge of the the nucleus; consequently, the other electrons are more strongly attracted to the nucleus, and the radius of the atom gets smaller. Likewise, when an electron is added to an atom, forming an anion, the added electron shields the other electrons from the nucleus, with

The ionic radius is not a fixed property of a given ion, but varies with coordination number, spin state and other parameters. Nevertheless, ionic radius values are sufficiently transferable to allow periodic trends to be recognized. As with other types

the result that the size of the atom increases.



of atomic radius, ionic radii increase on descending a group. Ionic size (for the same ion) also increases with increasing coordination number, and an ion in a high-spin state will be larger than the same ion in a low-spin state. In general, ionic radius decreases with increasing positive charge and increases with increasing negative charge.

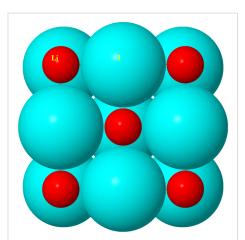
An "anomalous" ionic radius in a crystal is often a sign of significant covalent character in the bonding. No bond is *completely* ionic, and some supposedly "ionic" compounds, especially of the transition metals, are particularly covalent in character. This is illustrated by the unit cell parameters for sodium and silver halides in the table. On the basis of the fluorides, one would say that Ag^+ is larger than Na^+ , but on the basis of the chlorides and bromides the opposite appears to be true. [1] This is because the greater covalent character of the bonds in AgCl and AgBr reduces the bond length and hence the apparent ionic radius of Ag^+ , an effect which is not present in the halides of the more electropositive sodium, nor in silver fluoride in which the fluoride ion is relatively unpolarizable.

Determination of ionic radii

The distance between two ions in an ionic crystal can be determined by X-ray crystallography, which gives the lengths of the sides of the unit cell of a crystal. For example, the length of each edge of the unit cell of sodium chloride is found to be 564.02 pm. Each edge of the unit cell of sodium chloride may be considered to have the atoms arranged as Na⁺•••Cl⁻•••Na⁺, so the edge is twice the Na-Cl separation. Therefore, the distance between the Na⁺ and Cl⁻ ions is half of 564.02 pm, which is 282.01 pm. However, although X-ray crystallography gives the distance between ions, it doesn't indicate where the boundary is between those ions, so it doesn't directly give ionic radii.

Landé^[2] estimated ionic radii by considering crystals in which the anion and cation have a large difference in size, such as LiI. The lithium ions are so much smaller than the iodide ions that the lithium fits into holes within the crystal lattice, allowing the iodide ions to touch. That is, the distance between two neighboring iodides in the crystal is assumed to be twice the radius of the iodide ion, which was deduced to be 214 pm. This value can be used to determine other radii. For example, the inter-ionic distance in RbI is 356 pm, giving 142 pm for the ionic radius of Rb⁺. In this way values for the radii of 8 ions were determined.

Wasastjerna estimated ionic radii by considering the relative volumes of ions as determined from electrical polarizability as determined by measurements of refractive index.^[3] These results were extended by Victor Goldschmidt^[4] Both Wasastjerna and Goldschmidt used a value of 132 pm for the O²⁻ ion.



Front view of the unit cell of a LiI crystal, using Shannon's crystal data (Li⁺ = 90 pm; Γ = 206 pm). The iodide ions nearly touch (but don't quite), indicating that Landé's assumption is fairly good.

Pauling used effective nuclear charge to proportion the distance between ions into anionic and a cationic radii. ^[5] His data gives the O²⁻ ion a radius of 140 pm.

A major review of crystallographic data led to the publication of revised ionic radii by Shannon. [6] Shannon gives different radii for different coordination numbers, and for high and low spin states of the ions. To be consistent with Pauling's radii, Shannon has used a value of $r_{\text{ion}}(O^{2-}) = 140 \text{ pm}$; data using that value are referred to as "effective" ionic radii. However, Shannon also includes data based on $r_{\text{ion}}(O^{2-}) = 126 \text{ pm}$; data using that value are referred to as "Crystal" ionic radii. Shannon states that "it is felt that crystal radii correspond more closely to the physical size of ions in a solid." [6] The two sets of data are listed in the two tables below.

Crystal ionic radii in pm of elements in function of ionic charge and spin (ls = low spin, hs = high spin).

Ions are 6-coordinate unless indicated differently in parentheses (e.g. 146 (4) for 4-coordinate N^{3-}).^[6]

Number	Name	Symbol	3–	2-	1-	1+	2+	3+	4+	5+	6+	7+	8+
3	Lithium	Li				90							
4	Beryllium	Ве					59						
5	Boron	В						41					
6	Carbon	С							30				
7	Nitrogen	N	132 (4)					30		27			
8	Oxygen	О		126									

9	Fluorine	F		119							22	
11	Sodium	Na			116							
12	Magnesium	Mg				86						
13	Aluminum	Al					67.5					
14	Silicon	Si						54				
15	Phosphorus	P					58		52			
16	Sulfur	S	170					51		43		
17	Chlorine	Cl		167					26 (3py)		41	
19	Potassium	K			152							
20	Calcium	Ca				114						
21	Scandium	Sc					88.5					
22	Titanium	Ti				100	81	74.5				
23	Vanadium	v				93	78	72	68			
24	Chromium	Cr				87 ls; 94 hs	75.5	69	63	58		
25	Manganese	Mn				81 <i>ls</i> ; 97 <i>hs</i>	72 ls; 78.5 hs	67	47 (4)	39.5 (4)	60	
26	Iron	Fe				75 ls; 92 hs	69 ls; 78.5 hs	72.5		39 (4)		
27	Cobalt	Co				79 ls; 88.5 hs	68.5 ls; 75 hs	67 hs				
28	Nickel	Ni				83	70 ls; 74 hs	62 ls				
29	Copper	Cu			91	87	68 <i>ls</i>					
30	Zinc	Zn				88						
31	Gallium	Ga					76					
32	Germanium	Ge				87		67				
33	Arsenic	As					72		60			
34	Selenium	Se	184					64		56		
35	Bromine	Br		182			73 (4sq)		45 (3py)		53	
37	Rubidium	Rb			166							
38	Strontium	Sr				132						
39	Yttrium	Y					104					
40	Zirconium	Zr						86				
41	Niobium	Nb					86	82	78			
42	Molybdenum	Мо					83	79	75	73		
43	Technetium	Тс						78.5	74		70	
44	Ruthenium	Ru					82	76	70.5		52 (4)	50 (4)
45	Rhodium	Rh					80.5	74	69			
46	Palladium	Pd			73 (2)	100	90	75.5				
47	Silver	Ag			129	108	89					
48	Cadmium	Cd				109						
49	Indium	In					94					
50	Tin	Sn						83				

51	Antimony	Sb					90		76			
52	Tellurium	Те	207					111		70		
53	Iodine	I		206					109		67	
54	Xenon	Xe									-	62
55	Caesium	Cs			181							-
56	Barium	Ba				149						
57	Lanthanum	La					117.2					
58	Cerium	Ce					115	101				
59	Praseodymium						113	99				
60	Neodymium	Nd				143 (8)	112.3					
61	Promethium	Pm					111					
62	Samarium	Sm				136 (7)	109.8					
63	Europium	Eu				131	108.7					
64	Gadolinium	Gd					107.5					
65	Terbium	Tb					106.3	90				
66	Dysprosium	Dy				121	105.2					
67	Holmium	Но					104.1					
68	Erbium	Er					103					
69	Thulium	Tm				117	102					
70	Ytterbium	Yb				116	100.8					
71	Lutetium	Lu					100.1					
72	Hafnium	Hf						85				
73	Tantalum	Та					86	82	78			
74	Tungsten	W						80	76	74		
75	Rhenium	Re						77	72	69	67	
76	Osmium	Os						77	71.5	68.5	66.5	53 (4)
77	Iridium	Ir					82	76.5	71			
78	Platinum	Pt				94		76.5	71			
79	Gold	Au			151		99		71			
80	Mercury	Hg			133	116						
81	Thallium	Tl			164		102.5					
82	Lead	Pb				133		91.5				
83	Bismuth	Bi					117		90			
84	Polonium	Po						108		81		
85	Astatine	At									76	
87	Francium	Fr			194							
88	Radium	Ra				162 (8)						
89	Actinium	Ac					126					
90	Thorium	Th						108				

91	Protactinium	Pa				116	104	92			
92	Uranium	U				116.5	103	90	87		
93	Neptunium	Np			124	115	101	89	86	85	
94	Plutonium	Pu				114	100	88	85		
95	Americium	Am			140 (8)	111.5	99				
96	Curium	Cm				111	99				
97	Berkelium	Bk				110	97				
98	Californium	Cf				109	96.1				

Effective ionic radii in pm of elements in function of ionic charge and spin (ls = low spin, hs = high spin).

Ions are 6-coordinate unless indicated differently in parentheses (e.g. 146 (4) for 4-coordinate N^{3-}). [6]

Number	Name	Symbol	3–	2–	1-	1+	2+	3+	4+	5+	6+	7+	8+
3	Lithium	Li				76							
4	Beryllium	Be					45						
5	Boron	В						27					
6	Carbon	С							16				
7	Nitrogen	N	146 (4)					16		13			
8	Oxygen	О		140									
9	Fluorine	F			133							8	
11	Sodium	Na				102							
12	Magnesium	Mg					72						
13	Aluminum	Al						53.5					
14	Silicon	Si							40				
15	Phosphorus	P						44		38			
16	Sulfur	S		184					37		29		
17	Chlorine	Cl			181					12 (3py)		27	
19	Potassium	K				138							
20	Calcium	Ca					100						
21	Scandium	Sc						74.5					
22	Titanium	Ti					86	67	60.5				
23	Vanadium	V					79	64	58	54			
24	Chromium	Cr					73 ls; 80 hs	61.5	55	49	44		
25	Manganese	Mn					67 ls; 83 hs	58 ls; 64.5 hs	53	33 (4)	25.5 (4)	46	
26	Iron	Fe					61 ls; 78 hs	55 ls; 64.5 hs	58.5		25 (4)		
27	Cobalt	Co					65 ls; 74.5 hs	54.5 ls; 61 hs	53 hs				
28	Nickel	Ni					69	56 ls; 60 hs	48 <i>ls</i>				
29	Copper	Cu				77	73	54 <i>ls</i>					

	1							1	1	1		
30	Zinc	Zn				74						
31	Gallium	Ga					62					
32	Germanium	Ge				73		53				
33	Arsenic	As					58		46			
34	Selenium	Se	198					50		42		
35	Bromine	Br		196			59 (4sq)		31 (3py)		39	
37	Rubidium	Rb			152							
38	Strontium	Sr				118						
39	Yttrium	Y					90					
40	Zirconium	Zr						72				
41	Niobium	Nb					72	68	64			
42	Molybdenum	Мо					69	65	61	59		
43	Technetium	Тс						64.5	60		56	
44	Ruthenium	Ru					68	62	56.5		38 (4)	36 (4)
45	Rhodium	Rh					66.5	60	55			
46	Palladium	Pd			59 (2)	86	76	61.5				
47	Silver	Ag			115	94	75					
48	Cadmium	Cd				95						
49	Indium	In					80					
50	Tin	Sn						69				
51	Antimony	Sb					76		60			
52	Tellurium	Те	221					97		56		
53	Iodine	I		220					95		53	
54	Xenon	Xe										48
55	Caesium	Cs			167							
56	Barium	Ba				135						
57	Lanthanum	La					103.2					
58	Cerium	Ce					101	87				
59	Praseodymium	Pr					99	85				
60	Neodymium	Nd				129 (8)	98.3					
61	Promethium	Pm					97					
62	Samarium	Sm				122 (8)	95.8					
63	Europium	Eu				117	94.7					
64	Gadolinium	Gd					93.5					
65	Terbium	Tb					92.3	76				
66	Dysprosium	Dy				107	91.2					
67	Holmium	Но					90.1					
68	Erbium	Er					89					
69	Thulium	Tm				103	88					
L												

70	Ytterbium	Yb		102	86.8					
71	Lutetium	Lu			86.1					
72	Hafnium	Hf				71				
73	Tantalum	Та			72	68	64			
74	Tungsten	W				66	62	60		
75	Rhenium	Re				63	58	55	53	
76	Osmium	Os				63	57.5	54.5	52.5	39 (4)
77	Iridium	Ir			68	62.5	57			
78	Platinum	Pt		80		62.5	57			
79	Gold	Au	137	,	85		57			
80	Mercury	Hg	119	102						
81	Thallium	Tl	150)	88.5					
82	Lead	Pb		119		77.5				
83	Bismuth	Bi			103		76			
84	Polonium	Po				94		67		
85	Astatine	At							62	
87	Francium	Fr	180)						
88	Radium	Ra		148 (8)						
89	Actinium	Ac			112					
90	Thorium	Th				94				
91	Protactinium	Pa			104	90	78			
92	Uranium	U			102.5	89	76	73		
93	Neptunium	Np		110	101	87	75	72	71	
94	Plutonium	Pu			100	86	74	71		
95	Americium	Am		126 (8)	97.5	85				
96	Curium	Cm			97	85				
97	Berkelium	Bk			96	83				
98	Californium	Cf			95	82.1				

Non-spherical Ions

The concept of ionic radii is based on the assumption of a spherical ion shape. However, from a group-theoretical point of view the assumption is only justified for ions that reside on high-symmetry crystal lattice sites like Na and Cl in halite or Zn and S in sphalerite. A clear distinction can be made, when the point symmetry group of the respective lattice site is considered, which are the cubic groups O_h and T_d in NaCl and ZnS. For ions on lower-symmetry sites significant deviations of their electron density from a spherical shape may occur. This holds in particular for ions on lattice sites of polar symmetry, which are the crystallographic point groups C_1 , C_{1h} , C_n or C_{nv} , $c_n = 2$, $c_n =$

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- [1] On the basis of conventional ionic radii, Ag^{+} (129 pm) is indeed larger than Na^{+} (116 pm)
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