Covalent radius

The **covalent radius**, r_{cov} , is a measure of the size of an <u>atom</u> that forms part of one <u>covalent bond</u>. It is usually measured either in <u>picometres</u> (pm) or angstroms (Å), with 1 Å = 100 pm.

In principle, the sum of the two co equal the covalent <u>bond length</u> between two atoms, R(AB) = r(A) + r(B). Moreover, different radii can be introduced for single, double and triple bonds (r_1 , r_2 and r_3 below), in a purely operational sense. These relationships are certainly not exact because the size of an atom is not constant but depends on its chemical environment. For <u>heteroatomic</u> A—B bonds, ionic terms may enter. Often the <u>polar covalent bonds</u> are shorter than would be expected on the basis of the sum of covalent radii. Tabulated values of covalent radii are either average or idealized values, which nevertheless show a certain transferability between different situations, which makes them useful.

The bond lengths R(AB) are measured by X-ray diffraction (more rarely, neutron diffraction on molecular crystals). Rotational spectroscopy can also give extremely accurate values of bond lengths. For homonuclear A-A bonds, Linus Pauling took the covalent radius to be half the single-bond length in the element, e.g. R(H-H), in H_2 = 74.14 pm so $r_{cov}(H)$ = 37.07 pm: in practice, it is usual to obtain an average value from a variety of covalent compounds, although the difference is usually small. Sanderson has published a recent set of non-polar covalent radii for the main-group elements, [1] but the availability of large collections of bond lengths, which are more transferable, from the Cambridge Crystallographic Database [2][3] has rendered covalent radii obsolete in many situations.

Contents

Average radii Radii for multiple bonds See also References

Average radii

The values in the table below are based on a statistical analysis of more than 228,000 experimental bond lengths from the Cambridge Structural Database.^[4] For carbon, values are given for the different hybridisations of the orbitals.

| Covalent radii in pm from analysis of the Cambridge Structural Database, which contains about 1,030,000 crystal structures ^[4] | | | | | | | | | | | | | | | | |
|---|---------|-----------------------------|---|--------|--------|----------------------------|-------------------------------|----------------------------|--------|---------|--------|--------|-----------------------|---------|--------|------|
| Н | | | | | | | | | | | | | | | | |
| 1 | | | | | | | | | | | | | | | | |
| 31(5) | .(5) | | | | | | | | | | | | | | | |
| Li | Be | | | В | С | Ν | Ο | F | | | | | | | | |
| 3 | 4 | | 5 | 6 | 7 | 8 | 9 | | | | | | | | | |
| 128(7) | 96(3) | | | | | | | | | | | 84(3) | sp ³ 76(1) | 71(1) | 66(2) | 57(|
| | | | | | | | | | | | | | sp ² 73(2) | | | |
| | | | | | | | | | | | | Al | sp 69(1) | _ | _ | |
| Na | Mg | | | | | | | | | | | | Si 14 | P | S | Cl |
| 11 | | 12 | | | | | | | | | | | | 15 | 16 | 17 |
| 166(9) | 141(7) | _ | | | _ | | _ | _ | | _ | _ | 121(4) | 111(2) | 107(3) | 105(3) | 102(|
| K | Ca | Sc | Ti | V | Cr | Mn | Fe | Co | Ni | Cu | Zn | Ga | Ge | As | Se | Br |
| 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 | 30 | 31 | 32 | 33 | 34 | 35 |
| 203(12) | 176(10) | 170(7) | 160(8) | 153(8) | | l.s. 139(5) h.s. 161(8) | l.s. 132(3) h.s. 152(6) | l.s. 126(3) h.s. 150(7) | 124(4) | 132(4) | 122(4) | 122(3) | 120(4) | 119(4) | 120(4) | 120(|
| Rb | Sr | Υ | Zr | Nb | Mo | Tc | Ru | Rh | Pd | Ag | Cd | In | Sn | Sb | Te | - 1 |
| 37 | 38 | 39 | 40 | 41 | 42 | 43 | 44 | 45 | 46 | 47 | 48 | 49 | 50 | 51 | 52 | 53 |
| 220(9) | 195(10) | 190(7) | (7) 175(7) 164(6) 154(5) 147(7) 146(7) 142(7) 139 | | | | | | | 145(5) | 144(9) | 142(5) | 139(4) | 139(5) | 138(4) | 139(|
| Cs | Ba | La Hf | Ta | W | Re | Os | Ir | Pt | Au | Hg | TI | Pb | Bi | Po | At | Rr |
| 55 | 56 | 72 | 73 | 74 | 75 | 76 | 77 | 78 | 79 | 80 | 81 | 82 | 83 | 84 | 85 | 86 |
| 244(11) | 215(11) | 187(8) | 170(8) | 162(7) | 151(7) | 144(4) | 141(6) | 136(5) | 136(6) | 132(5) | 145(7) | 146(5) | 148(4) | 140(4) | 150 | 150 |
| Fr | Ra | Ac | | | | | | | | | | | | | | |
| 87 | 88 | | | | | | | | | | | | | | | |
| 260 | 221(2) | | | | | | | | | | | | | | | |
| | | | La | Ce | Pr | Nd | Pm | Sm | Eu | Gd | Tb | Dy | Но | Er | Tm | Yţ |
| | | | 57 | 58 | 59 | 60 | 61 | 62 | 63 | 64 | 65 | 66 | 67 | 68 | 69 | 7C |
| | | 207(8) 204(9) 203(7) 201(6) | | | | 199 | 198(8) 198(6) 196(6) 194(5) 1 | | | | | 192(7) | | 190(10) | | |
| | | Ac Th Pa U Np Pu Am Cm | | | | | | | | _5 .(5) | ===(.) | (·) | _55(5) | _30(_0) | | |
| | | | 89 | 90 | 91 | 92 | 93 | 94 | 95 | 96 | | | | | | |
| | | | 215 | 206(6) | 200 | 196(7) | 190(1) | 187(1) | 180(6) | | | | | | | |
| | | | | _00(0) | | | | | _55(5) | _55(5) | | | | | | |

Radii for multiple bonds

A different approach is to make a self-consistent fit for all elements in a smaller set of molecules. This was done separately for single, [6] double, [6] and triple bonds [7] up to superheavy elements. Both experimental and computational data were used. The single-bond results are often similar to those of Cordero et al. [4] When they are different, the <u>coordination numbers</u> used can be different. This is notably the case for most (d and f) transition metals. Normally one expects that $r_1 > r_2 > r_3$. Deviations may occur for weak multiple bonds, if the differences of the ligand are larger than the differences of R in the data used.

Note that elements up to <u>atomic number</u> 118 (<u>oganesson</u>) have now been experimentally produced and that there are chemical studies on an increasing number of them. The same, self-consistent approach was used to fit tetrahedral covalent radii for 30 elements in 48 crystals with subpicometer accuracy.^[8]

Single-,^[5] double-,^[6] and triple-bond^[7] covalent radii, determined using typically 400 experimental or calculated primary distances, *R*, per set.

| H | | | | | | | | | | | | | | | | |
|------------|------------|-------------|----------------------------|-------------------|-------------------|-------------------|-------------------|------------|------------|-------------------|------------|--------------|------------|------------|------------|------------|
| 1 32 | | | | | | | | | | | | | | | | |
| - | | | | | | | | | | | | | | | | |
| Li | Ве | | | | | | | | | | | В | С | N | 0 | F |
| 3 133 | 4 102 | | | | | Radius / | | | | | | 5 85 | 6 75 | 7 71 | 8 63 | 9 64 |
| 124 | 90 | double-bond | single-bond double-bond | | | | | | | | | 78 73 | 67 | 60 | 57 | 59 |
| - | 85 | triple-bond | | | | | | | | | | | 60 | 54 | 53 | 53 |
| No | Ma | inplo sonia | | | | | | | | | | A. I. | C: | Б | | CI |
| Na 11 | Mg 12 | | | | | | | | | | | Al 13 | Si 14 | P 15 | S 16 | CI 17 |
| 155 | 139 | | | | | | | | | | | 126 | 116 | 111 | 103 | 99 |
| 160 | 132 127 | | | | | | | | | | | 113 111 | 107 102 | 102 94 | 94 95 | 95 93 |
| K | Ca | Sc | Ti | V | Cr | Mn | Fe | Со | Ni | Cu | Zn | Ga | Ge | 94 As | Se | 93 Br |
| 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 | 30 | 31 | 32 | 33 | 34 | 35 |
| 196 | 171 | 148 | 136 | 134 | 122 | 119 | 116 | 111 | 110 | 112 | 118 | 124 | 121 | 121 | 116 | 114 |
| 193 - | 147 133 | 116 114 | 117 108 | 112 106 | 111 103 | 105 103 | 109 102 | 103 96 | 101 101 | 115 120 | 120 | 117 121 | 111 114 | 114 106 | 107 107 | 10! 11(|
| Rb | Sr | Υ | Zr | Nb | Мо | Tc | Ru | Rh | Pd | Ag | Cd | In | Sn | Sb | Te | 1 |
| 37 | 38 | 39 | 40 | 41 | 42 | 43 | 44 | 45 | 46 | 47 | 48 | 49 | 50 | 51 | 52 | 53 |
| 210 202 | 185 157 | 163 130 | 154 127 | 147 125 | 138 121 | 128 120 | 125 114 | 125 110 | 120 117 | 128 139 | 136 144 | 142 136 | 140 130 | 140 133 | 136 128 | 13: 12! |
| - | 139 | 124 | 121 | 116 | 113 | 110 | 103 | 106 | 112 | 137 | - | 146 | 132 | 127 | 121 | 12! |
| Cs | Ва | La-Lu | Hf | Ta | W | Re | Os | Ir | Pt | Au | Hg | TI | Pb | Bi | Po | At |
| 55 | 56 | | 72 | 73 | 74 | 75 101 | 76 | 77 | 78 | 79 | 80 | 81 | 82 | 83 | 84 | 85 |
| 232 209 | 196 161 | | 152 128 | 146 126 | 137 120 | 131 119 | 129 116 | 122 115 | 123 112 | 124 121 | 133 142 | 144 142 | 144 135 | 151 141 | 145 135 | 14 13 |
| - | 149 | | 122 | 119 | 115 | 110 | 109 | 107 | 110 | 123 | - | 150 | 137 | 135 | 129 | 138 |
| Fr | Ra | Ac-Lr | Rf | Db | Sg | Bh | Hs | Mt | Ds | Rg | Cn | Nh | FI | Mc | Lv | Ts |
| 87 223 | 88 201 | | 104 157 | 105 149 | 106 143 | 107 141 | 108 134 | 109 129 | 110 128 | 111 121 | 112 122 | 113 136 | 114 143 | 115 162 | 116 175 | 11 16! |
| 218 | 173 | | 140 | 136 | 128 | 128 | 125 | 125 | 116 | 116 | 137 | - | - | - | - | - |
| - | 159 | | 131 | 126 | 121 | 119 | 118 | 113 | 112 | 118 | 130 | - | - | - | - | - |
| | | | La | Ce | Pr | Nd | Pm | Sm | Eu | Gd | Tb | Dy | Но | Er | Tm | Yb |
| | | | 57 | 58 | 59 | 60 | 61 | 62 | 63 | 64 | 65 | 66 | 67 | 68 | 69 | 70 |
| | | | 180 139 139 | 163 137 131 | 176 138 128 | 174 137 | 173 135 | 172 134 | 168 134 | 169 135 132 | 168 135 | 167 133 | 166 133 | 165 133 | 164 131 | 17(12! |
| | | | Ac | Th | Pa | U | Np | Pu | Am | Cm | Bk | Cf | Es | Fm | Md | Nc |
| | | | 89 | 90 | 91 | 92 | 93 | 94 | 95 | 96 | 97 | 98 | 99 | 100 | 101 | 10: |
| | | | 186 153 140 | 175 143 136 | 169 138 129 | 170 134 118 | 171 136 116 | 172 135 | 166 135 | 166 136 | 168 139 | 168 140 | 165 140 | 167 | 173 139 | 17(|

See also

Atomic radii of the elements (data page)

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