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Van der Waals radii of elements from the data of structural inorganic chemistry

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Van der Waals radii of elements were determined from the data of the structural inorganic chemistry: from intersitial distances in CdX_2- and graphite-type structures, bond lengths in van der Waals molecules, molar volumes of A_2-type substances, refractometry data, and from quantum chemical and correlation ratios. The recommended values of van der Waals radii of elements are tabulated.

Key words: molecules, anions; van der Waals radii; structure; molar volume; polarizability.

The known systems of van der Waals radii[1—7] were created mainly on the basis of data of structural organic chemistry. Therefore, they contain little information about typical metals, and the data available are rather approximate and are often based on correlation ratios or calculations. As a result, the published tables of van der Waals radii of elements are limited and incomplete.

In several works,[8—11] the authors have tried to compensate for this deficiency, especially as the problem of the determination of van der Waals radii of metals has become rather urgent due to the development of inorganic and organometallic chemistry.

This work is devoted to a discussion of experimental and theoretical data of structural inorganic chemistry that make it possible to determine van der Waals radii of various elements by different methods.

Van der Waals radii of elements in layered crystal structures. It is known that $CdCl_2$- and CdI_2-type structures are layers of atoms ...XCdX...XCdX... between which van der Waals forces act. Therefore, the X...X distances are equal to the twice van der Waals radius (r_w) of the X atom. The values of r_w of the hydroxyl group in metal hydroxides and the halogens in the $CdCl_2$ and CdI_2 structures are presented in Table 1 (see Refs. 12—15). The radii of chalcogenides calculated from the geometric parameters of CdI_2-type structures (see Refs. 15—17) are listed in Table 2.

The structures of the crystalline compounds Ca_2N and Sr_2N are of the anti-$CdCl_2$-type (see Refs. 18 and 19), *i.e.*, van der Waals forces act between the layers of metal atoms in these compounds. The van der Waals radii of Ca and Sr in these structures are 2.174 and 2.363 Å, respectively.

Tl_2S has a distorted anti-CdI_2-type structure (see Ref. 12). The average distance between the layers of Tl atoms corresponds to two r_w and is equal to 1.92 Å.

The hexagonal phases of graphite and boron nitride are also layered structures. In these structures the intersi-

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Table 1. Van der Waals radii (r_w) of hydroxyl groups and halogens

M (in $M(OH)_2$)	$r_w(OH)$/Å	M (in MCl_2)	$r_w(Cl)$/Å	M (in MBr_2)	$r_w(Br)$/Å	M (in MI_2)	$r_w(I)$/Å
Mg	1.499	Mg	1.817	Mg	1.913	Mg	2.094
Ca	1.603	Cd	1.832	Zn	1.932	Ca	2.168
Cd	1.548	Ti	1.792	Cd	1.947	Zn	2.170
Mn	1.520	Mn	1.816	Ti	1.932	Cd	2.102
Fe	1.486	Fe	1.795	V	1.889	Y	2.168
Co	1.478	Co	1.776	Mn	1.900	Ti	2.077
Ni	1.459	Ni	1.765	Fe	1.883	Ge	2.074
	$\bar{r}_w = 1.51$		$\bar{r}_w = 1.80$	Co	1.863	Pb	2.167
				Ni	1.865	V	2.028
					$\bar{r}_w = 1.90$	Mn	2.086
						Fe	2.051
						Co	2.017
						Ni	2.044
						Th	2.122
							$\bar{r}_w = 2.10$

Table 2. Van der Waals radii (r_w) of chalcogens

M (in MS_2)	$r_w(S)$ /Å	M (in MSe_2)	$r_w(Se)$ /Å	M (in MTe_2)	$r_w(Te)$ /Å
Ti	1.731	Ti	1.816	Si	2.083
Zr	1.804	Zr	1.897	Ti	1.956
Hf	1.804	Hf	1.897	Zr	2.012
Sn	1.808	V	1.814	Hf	2.016
Pb	1.856	Mo	1.830		$\bar{r}_w = 2.02$
Ta	1.838		$\bar{r}_w = 1.85$		
Mo	1.745				
	$\bar{r}_w = 1.80$				

tial distances (3.354 and 3.330 Å, respectively[15,20]) are the sum of the van der Waals radii of C or B and N atoms. Thus, we can immediately obtain $r_w(C) = 1.677$ Å and $r_w(B) = 3.330 - r_w(N)$ Å (B and N atoms are arranged above one another in parallel lattices[21]).

It should be noted in the conclusion of this Section that the van der Waals radii of nonmetals in layered structures of polar inorganic compounds are similar to the analogous radii determined from the structures of covalent organic molecules, because the negative charge on the atom does not distort the result due to the similarity of van der Waals and anionic radii.[2] In structures of the anti-CdX_2-type, the van der Waals radii of metals are understated due to the positive charges on the atoms, which causes them to approach the values of the radii of the corresponding cations.

Van der Waals radii of metals in molecular structures. M_2-type molecules of group II metals resemble van der Waals molecules in many respects, because atoms of these metals have stable s^2 electronic configurations in the external shells and do not tend to form normal chemical bonds. The dissociation energies and half-lengths of bonds of these molecules are presented in Table 3.

As can be seen from the data of Table 3, the van der Waals radii of Ca and Sr are close to the values of r_w determined above for the M_2N structures, although they are somewhat lower, which is explained by the comparatively high strength of the bonds in the Ca_2 and Sr_2 molecules.

M^+RM^- structures (where M is an alkali metal and R is an organic moiety), in which the metals are bonded to the H atoms of adjacent molecules by van der Waals forces, have been recently studied.[28] Subtracting the hydrogen radius (1.2 Å) from the M...H bond length, we obtain the following average values of the radii of negatively charged atoms of alkali metals: $r(Na^-) = 2.76$ Å, $r(K^-) = 3.13$ Å, $r(Rb^-) = 3.17$ Å, and $r(Cs^-) = 3.48$ Å. Taking into account the fact that the radii of anions are equal to the values of r_w of the same elements,[2] the values presented characterize the van der Waals radii only of atoms of alkali metals.

Van der Waals radii of several metals have previously been determined[29] from the values of bond lengths in gaseous molecules of the MIg-type, where Ig is an atom of an inert gas. The van der Waals radii obtained in this work are presented in Table 4 as well as the value of r_w for Tl calculated by the same method.[30,31]

Finally, a structural study[32] of the molecular crystal of OsO_4 made it possible for the van der Waals radius of Os to be directly determined: $r_w(Os) = 2.26$ Å.

Table 3. Energies (D_e) and bond lengths (r_e) in M_2 molecules

M_2	D_e/kJ	Reference	$\frac{1}{2}r_e$/Å	Reference
Mg_2	5.2	22	1.94	24
Ca_2	13.1	22	2.14	24
Sr_2	15.2	22	2.22	25
Zn_2	3.3	23	2.2±0.2	23,26
Cd_2	3.9	23	2.3±0.2	23,26
Hg_2	4.2	23	1.9±0.1	23,27

Table 4. Van der Waals radii (r_w) of metals in MIg molecules

M	r_w(M)/Å	M	r_w(M)/Å	M	r_w(M)/Å
Li	2.7	Ag	2.0	B	1.7
Na	2.8	Mg	2.5	Al	1.7
K	2.9	Zn	2.2	In	1.9
Rb	3.0	Cd	2.3	Tl	2.2
Cs	3.1	Hg	2.0	Si	2.0

Van der Waals radii of elements in the structures of simple molecules. The atomic structures of elements of subgroups V—VIIB are substantially anisotropic and, hence, their van der Waals radii strongly depend on direction. Therefore, in this case, intermolecular contacts cannot be characterized by a single value of the van der Waals radius.

Thus, in the α-F_2 structure the intermolecular distances are equal to 3.18, 3.20, 3.26, 3.28, and 3.38 Å inside the layer and 2.82 and 2.87 Å between the layers of molecules. In the β-F_2 structure, each F atom, in addition to those atoms directly bonded to it, is surrounded by two atoms of the closest molecules spaced at 3.34 Å, four atoms spaced at 3.73 Å, and eight atoms spaced at 4.08 Å.[33]

The crystal structures of other halogens are similar to the α-F_2 structure considered above: the van der Waals distances between atoms of different molecules in the same layer are shorter than the distances between molecules of adjacent layers[33] (Table 5).

In the α-O_2 crystal structure, each O atom is surrounded by four atoms of adjacent molecules spaced at 3.20 Å, two O atoms spaced at 3.25 Å, one O atom spaced at 3.35 Å, four O atoms spaced at 3.40 Å, and two O atoms spaced at 3.43 Å.[33]

There are atoms of two crystallographic types (1 and 2) in the α-N_2 structure: the first are spaced at 3.470, 3.584, and 3.742 Å from the nearest atoms of the other molecules, and the second are spaced at 3.470, 3.736, and 3.742 Å, respectively. Two types of van der Waals distances, 3.448 and 3.725 Å, can also be seen in the γ-N_2 structure.[33]

It follows from the data presented that the van der Waals radii in the molecular structures considered are grouped around two values: a minimum value (r_{w1}) and a maximum value (r_{w2}). These radii are presented in Table 6; the van der Waals radii in structures of liquid halogens are also given for comparison.[34]

Table 5. Van der Waals radii (r_w) in structures of halogens

A_2	r_w/Å			
	A...A	in the layer	A...A	between layers
Cl_2	3.32	3.82	3.74	3.84, 3.97
Br_2	3.31	3.79	3.99	4.02, 4.14
I_2	3.57	4.05	4.39	4.35, 4.50

Table 6. Van der Waals radii (r_w) in molecular structures of elements

A_2	Crystal		Liquid:
	r_{w1}/Å	r_{w2}/Å	r_w/Å
F_2	1.42	1.62	1.54
Cl_2	1.66	1.92	1.89
Br_2	1.66	1.99	2.03
I_2	1.78	2.16	2.23
O_2	1.63	1.71	
N_2	1.73	1.85	

In the chain and cyclic structures of chalcogens, the van der Waals radii depend less on the crystallographic direction than in the structures of halogens. During the further polymerization the van der Waals distances become rigidly fixed in the α-structures of P, As, Sb, and Bi[33] (Table 7).

In structures of Si, Ge, and Sn, the distances to the next (after the closest) atoms are, in fact, van der Waals distances, because they characterize the contacts between atoms with closed eight-electron shells.[35] Thus, the van der Waals radii for Si, Ge, and Sn are equal to 1.92, 2.00, and 2.29 Å, respectively.

Determination of van der Waals radii from molar volumes. Since in the crystal structures of simple molecules, as shown above, the van der Waals radii are vector values, and not scalar, it is expedient to use such averaged parameters as molar volumes (V_m) for the estimation of average values of $\bar{r}_w$.

If it is assumed that the packing of A_2 molecules in space is the tightest possible, *i.e.*, the density of the packing $\rho = 0.74$, then, knowing the A—A bond length, one can easily calculate the radius of the van der Waals sphere of an atom.

The necessary experimental data[36] and the results of the calculations of r_w are presented in Table 8 for molecules of hydrogen, halogens, oxygen, and nitrogen. For H_2 and N_2, the adduced molar volumes corresponding to the completely ordered crystalline phase are presented, not the experimental values. The real volumes of these substances correspond to spherically symmetric (due to rotation) H_2 and N_2 molecules; in the first case all molecules rotate,[2] while in the case of γ-N_2 only 25 % of their total number rotate.[37] It is evident that the radii of spherically symmetric molecules are equal to $r(A—A)/2 + r_w$.

Table 7. Van der Waals radii (r_w) of elements of subgroups V and VIB

Element	r_w /Å	Element	r_w /Å
S_8	1.74	P(black)	1.80
Se_8	1.90	α-As	1.56
α-Se	1.72	α-Sb	1.68
α-Te	1.75	α-Bi	1.76

Table 8. Van der Waals radii (r_w) of elements determined from molar volumes

A	V_m/cm^3	$\frac{r(\text{A—A})}{2}$/Å	r_w /Å
H	4.425	0.371	1.217
F	9.664	0.745	1.500
Cl	16.58	0.997	1.770
Br	19.20	1.150	1.838
I	24.63	1.358	1.978
O	10.45	0.604	1.584
S	15.51	1.030	1.770
Se	16.42	1.187	1.783
Te	20.48	1.433	1.866
N	9.79	0.549	1.563
P	11.44	1.115	1.562
As	12.97	1.258	1.580
Sb	18.20	1.454	1.752
Bi	21.33	1.536	1.847

The data on molar volumes also allow one to calculate r_w of atoms in heteronuclear molecules, *e.g.*, HX, which also have spherical symmetry (except HF) due to rotation in the crystalline space. In this case, the diameter of the sphere is equal to $r_w(\text{H}) + r_w(\text{X}) + r(\text{H—X})$. Using the values of r_w for halogens (see Table 8), one can calculate the van der Waals radius of H in these molecules, assuming $\rho = 0.74$.

As can be seen from the data in Table 8, the values of the $r_w(\text{H})$ radius in HX molecules are lower than that in the H_2 molecule, and the order of the decrease in r_w correlates with the increase in bond polarity in the series HCl, HBr, and HI (see Ref. 38).

The method described can be applied to any molecules for which the density of packing in their crystal structures is known. For example, in ice[39] the O atoms are packed according to the law of the diamond, *i.e.*, $\rho = 0.34$, and the H atoms occupy holes between them, *i.e.*, they have $\rho = 1$. In this case, the configuration of the O atom is a van der Waals sphere with two segments cut off at the distance of the covalent radius of oxygen, and the configuration of the H atom is a van der Waals sphere with one segment cut off at the distance of the covalent radius of hydrogen. The length of the real O—H bond (1.013 Å) is somewhat less than the sum of the covalent radii of the O and H atoms (1.106 Å), and this shortening (by 8.4 %) can be introduced as a correction to the values of the distances at which segments are cut off from the van der Waals spheres of oxygen and hydrogen. It is found by varying the $r_w(\text{H})$ value that $r_w(\text{H}) = 0.836$ Å corresponds to the experimental molar volume of ice (I) $V_m = 19.95$ cm^3.

Van der Waals radii of chalcogens and elements of subgroup VB with cyclic, chain (S, Se, and Te), or framework (P, As, Sb, and Bi) structures are calculated analogously. Taking into account that the closest packing of atoms is hindered due to the directed character of covalent bonds, let us accept $\rho = 0.7$ for these structures according to the literature data.[40] Two or three segments are cut off from van der Waals spheres at the distances of covalent radii of these elements (with respect to the valent bonds) in the calculations of r_w by the method described. The values of van der Waals radii thus obtained are presented in Table 8.

Determination of van der Waals radii from polarizabilities. Sizes of atoms and ions were calculated from their polarizabilities (α) about 70 years ago.[41] These calculations are based on the Mossotti—Clausius theory, according to which $\alpha = r^3$. Many attempts to improve this theory[41,42] made it possible to add several refinements concerning the contribution of different electronic shells to the total polarizability; however, the classic formula provides quite appropriate results for the estimation of external radii of isolated atoms from experimental integral polarizabilities.

The experimental values of electronic polarizabilities of isolated atoms and the corresponding values of radii calculated as $\alpha^{1/3}$ are presented in Table 9.

Calculated values of van der Waals radii. In several cases, computational methods allow one to obtain information about values of van der Waals radii of elements. For example, quantum chemical calculations of radii of isolated atoms of group II elements[43] give the sizes of the s^2 electronic shell and, therefore, must be close to $r_w(\text{M})$/Å: 1.99 for Be, 2.31 for Mg, 2.79 for Ca, 2.99 for Sr, 2.10 for Zn, and 2.27 for Cd.

The radii of negatively charged atoms have been previously[44,45] calculated. In the case of halogens, the results obtained are similar to the empirical radii of the anions. Therefore, the theoretical radii of mono- and trivalent negatively charged metals may characterize the van der Waals radii of these metals (Table 10).

Beginning from the works of Pauling,[2] Slater,[46] and Bondi,[3] the van der Waals radii of metals have been calculated by correlations of the $r_w = r_c + a$ type, where r_c is the covalent radius and $a = 0.8\pm0.05$ Å. However, the determination of covalent radii of metals is a special problem that is often difficult, because it is necessary to

Table 9. Van der Waals radii (r_w) of elements determined from polarizabilities

A	Polarizability, α/Å^3	$\bar{\alpha}$/Å^3	r_w /Å
Li	21.8[42], 24.30[43], 22[44]	22.7	2.83
Na	23.8[42], 24.14[43], 24[44]	24.0	2.88
K	43.6[42], 42.45[43], 45[44]	43.7	3.52
Rb	47.6[42], 49[44]	48.3	3.64
Cs	59.5[42], 63[44]	61.2	3.94
Mg	10.6[42], 11.2[45]	10.9	2.22
Ca	25.0[42], 23.9[45]	24.5	2.90
Sr	27.6[42], 29.7[45]	28.6	3.06
Ba	39.7[42], 36.1[45]	37.9	3.36
Al	6.8[46]	6.8	1.89
In	10.2[47]	10.2	2.17
Tl	7.6[48]	7.6	1.97
I	5.0[49]	5.0	1.71

Table 10. "Quantum mechanical" radii (r_{calc}) of negatively charged atoms

A^-	r_{calc}/Å	A^-	r_{calc}/Å	A^-	r_{calc}/Å	A^-	r_{calc}/Å
Li^-	2.59	Cs^-	3.53	Sc^-	2.87	Al^-	2.45
Na^-	2.69	Cu^-	1.89	Y^-	2.86	Ga^-	2.37
K^-	3.19	Ag^-	2.03	La^-	3.06	In^-	2.51
Rb^-	3.33	Au^-	1.92	B^-	1.76	Tl^-	2.54

Table 11. "Structural chemical" radii (r_{str}) of negatively charged atoms

A^-	r_{str}/Å	A^-	r_{str}/Å	A^-	r_{str}/Å	A^-	r_{str}/Å
Li^-	2.38	Cs^-	3.49	Be^{2-}	1.78	Ba^{2-}	2.93
Na^-	2.45	Cu^-	1.96	Mg^{2-}	2.31	Zn^{2-}	1.92
K^-	2.99	Ag^-	2.02	Ca^{2-}	2.61	Cd^{2-}	2.03
Rb^-	3.13	Au^-	1.99	Sr^{2-}	2.86	Hg^{2-}	1.98

know *a priori* the valent states of the atoms. Therefore, the previously suggested method[47] for the calculation of the radius of a negatively charged metal atom by subtracting the radius of the cation from the interatomic distance in the structure of a metal (this is equivalent to the representation of the M—M covalent bond as an M^+M^- ion pair in which the electronic pair oscillates between two positions[48]) seems rather promising.

At the same time, it should be noted that the wave function of the valent electrons of the M—M bond should be presented as the superposition of ionic and covalent terms, and disregarding the latter results in the deviation of the calculated values of the radii of the anions from the van der Waals radii. This can be immediately seen by comparing the data of Table 11 with the empirical van der Waals radii of the same elements.

Table 11 presents the differences in bond lengths in M_2 molecules and the values of molecular ionic radii (M^+) from the literature data[8] as well as the differences in interatomic distances in the structures of group II metals[2] and the corresponding crystal ionic radii for the coordination numbers these metals have in the structures (see Ref. 49). The calculation of $r(M^-)$ for other metals cannot be performed sufficiently correctly due to the indeterminacy of the valent state of the atom in the structure of the metal and/or the absence of the known value of the radius of the cation for the coordination number corresponding to the structure of the metal.

* * *

The data presented above make it possible to tabulate the recommended values of van der Waals radii of elements (Table 12).

What are the areas of application of these parameters? A detailed review on this topic has previously been published.[7] Van der Waals radii are traditionally used for calculations of packing of molecules and their conformations, and for descriptions of chemical reactions depending on steric factors. We would also like to point out the use of the notion and values of these radii for the interpretation of phase transformations of inorganic substances at high pressures.

Thus, the structural studies of halogens, chalcogens, and elements of subgroup VB show that their polymorphic transformations involve shortening intermolecular distances and lengthening intramolecular distances, *i.e.*, they are accompanied by equalization of all interatomic distances.[50—52] This corresponds to the transformation of a molecular substance to the structure of the monoatomic metal, whose radius is intermediate between the initial extreme values. It is clear from this that information about the pressure at which a molecular substance is transformed to the metallic state can be obtained from the difference between the values of r_c and r_w.

It is known that the compression of molecules at first results only in a decrease in van der Waals distances,[51,52] and then r_c increases as r_w further decreases. From the viewpoint of crystal chemistry, this change in the structure of the solid state is quite understandable: isomorphic compression of the crystal occurs to the volume at which normal chemical bonds can be formed between atoms of adjacent molecules, *i.e.*, the coordination number of the atom becomes greater than 1. This moment signifies the beginning of the phase transition.

The physical reason for the polymorphic transformation that occurs when the body is compressed to a certain (critical, for this structure) volume is that there is such a rapid increase in repulsion forces as the atoms

Table 12. Recommended values of van der Waals radii (r_w) of elements

A	r_w/Å	A	r_w/Å	A	r_w/Å	A	r_w/Å	A	r_w/Å
Li	2.6	Be	1.9	B	1.7	N	1.55	Te	2.0
Na	2.8	Mg	2.2	Al	1.8	P	1.7	OH	1.5
K	3.0	Ca	2.5	In	1.9	As	1.7	F	1.5
Rb	3.2	Sr	2.7	Tl	2.2	Sb	1.75	Cl	1.8
Cs	3.5	Ba	3.1	C	1.7	Bi	1.8	Br	1.9
Cu	1.9	Zn	2.2	Si	1.9	O	1.6	I	2.1
Ag	2.0	Cd	2.3	Ge	2.0	S	1.8	Os	2.3
Au	1.9	Hg	2.0	Sn	2.3	Se	1.85		

progressively isomorphically approach to distances smaller than the equilibrium distances that the initial structure becomes energetically unfavorable, resulting in the rearrangement of the atoms to increase the coordination number and the corresponding interatomic distances.

It seems natural that the changes in van der Waals radii that occur as a molecular substance is compressed should be within the same limits within which these radii vary in real structures, *i.e.*, ±10 %, as shown above. It is interesting that the variation in interatomic distances in crystals due to heat vibrations occurs within the same limits.[53] This specific feature can be taken as a basis for the theoretical estimation of the pressure of phase transitions in molecular substances.

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