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Van der Waals Radii of Elements

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Abstract—The available data on the van der Waals radii of atoms in molecules and crystals are summarized. The nature of the continuous variation in interatomic distances from van der Waals to covalent values and the mechanisms of transformations between these types of chemical bonding are discussed.

INTRODUCTION

The notion that an interatomic distance can be thought of as the sum of atomic radii was among the most important generalizations in structural chemistry, treating crystals and molecules as systems of interacting atoms (Bragg, 1920). The next step forward in this area was taken by Mack [1] and Magat [2], who introduced the concept of nonvalent radius (R) for an atom situated at the periphery of a molecule and called it *the atomic domain radius* [1] or *Wirkungsradius* [2], implying that this radius determines intermolecular distances. Later, Pauling [3] proposed to call it *the van der Waals radius*, because it characterizes van der Waals interactions between atoms. He also showed that the van der Waals radii of nonmetals coincide with their ionic radii and exceed their covalent radii (r), typically by 0.8 Å.

Initially, only x-ray diffraction (XRD) data, molar volume measurements, and crystal-chemical considerations were used to determine R. Later studies extended the range of experimental approaches and culminated in a complete system of the van der Waals radii of free and bound atoms. Comparison of the results obtained by various physical methods made it possible to assess the accuracy and locate the applicability limits of the van der Waals radii and to reconcile the concept of van der Waals radius with the quantum-mechanical requirement that the electron density vary continuously at the periphery of atoms.

In this review, the van der Waals radii of atoms evaluated from XRD data, molar volumes, physical properties, and crystal-chemical considerations are used to develop a universal system of van der Waals radii.

ISOTROPIC CRYSTALLOGRAPHIC VAN DER WAALS RADII

Kitaigorodskii [4, 5] was the first to formulate the principle of close packing of molecules in crystalline phases. He assumed that the van der Waals areas of peripheral atoms in neighboring molecules are in contact but do not overlap (rigid-atom model), because the repulsive forces between closed electron shells rise sharply with decreasing intermolecular distance. He made up a system of van der Waals radii as consistent as possible with the intermolecular distances in organic compounds. His radii differed little from Pauling's (Table 1).

The system of van der Waals radii was further refined by Bondi [6, 7]. His detailed tables were very popular among chemists, even though the values of R were criticized in a number of works [8]. Bondi not

Table 1. Crystallographic van der Waals radii of nonmetals

Author, year	R, Å								
	H	F	Cl	Br	I	O	S	N	C
Pauling, 1939	1.2	1.35	1.80	1.95	2.15	1.40	1.85	1.5	1.70
Bondi, 1964	1.20	1.47	1.75	1.85	1.98	1.52	1.80	1.55	1.70
Zefirov, 1974	1.16	1.40	1.90	1.97	2.14	1.29	1.84	1.50	1.71
Gavezzotti, 1983–1999	1.17	1.35	1.80	1.95	2.10	1.40	1.85	1.50	1.70
Batsanov, 1995			1.80	1.90	2.10	1.51	1.80		1.68
Wieberg, 1995		1.5	1.8	1.9	2.1	1.5	1.8	1.6	1.7
Rowland, 1996	1.10	1.46	1.76	1.87	2.03	1.58	1.81	1.64	1.77

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