UNITED JOURNAL OF CHEMISTRY
Rapid Publication | Fully Refereed | Open Access | Double Blind Peer Reviewed
ISSN: 2581-7760

Investigating Diatomic Homonuclear Molecules

Article Type: Research Article

Article publication history: Article Received on: 29-Jun-25 Article Accepted on: 27-Jul-25 Article Published on:

Article review details:
1st Reviewer: Dr. Shivendra Shukla
2nd Reviewer: Dr. Amit Bhatt
Final Recommendation By : Prof. Jay Kushwaha

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Abstract

This study presents a novel theoretical approach and model, along with an equation for diatomic homonuclear molecules that contains a new molecular constant connecting the number of shared electrons and their circumference to determine their covalent radii. All diatomic homonuclear molecules consist of two atoms of the same element with certain geometrical shape held together by covalent bond. It is found that the homogenous distribution of electrons in the diatomic homonuclear molecules for their numbers and radii give a molecular constant value to be (5.4×10^{9} m^{-1}) . The covalent radii can be calculated by using the main physical parameters (number of sharing electrons & constant of molecules). The calculations and results of covalent radii are in good agreement (95 %) with known experimentally determined values and there are only 5 % from 118 elements are deviated.

Keywords: Molecule, Homonuclear, Constant, Radius, Bond.

Introduction

Molecules are a collection of two or more atoms held together by a chemical bond. Molecules may be homonuclear, contain atoms of one chemical element, such as two atoms in the oxygen molecule, or they may be heteronuclear, consisting of more than one chemical element, such as a molecule of water since it has two different atoms. A covalent bond is a chemical bond that contains the sharing of electron pairs between atoms.

A chemical bond is a collection of atoms or ions that constitute molecules and crystals. The chemical bond may be attributed to the electric force between charged ions with opposite signs, as in ionic bonds, or by the sharing of electrons, as in covalent bonds. The polarity, directionality and the strength of bonds can be determined through octet rule, theory of Valence Shell Electron Pair Repulsion (VSEPR), and the theory of Valence Bond (VB), which contains

orbital hybridization, resonance and molecular orbital theory, which comprises a linear combination of ligand field theory and atomic orbitals [1- 6].

Covalent radius is the smallest distance between two atoms bonded together with sharing of electrons. It is the distance between two atoms approaching each other without interfering. The sum of the two covalent radii is equal to the covalent bond length between two atoms. The bond lengths are measured by neutron diffraction on molecular crystals or X-ray diffraction. Rotational spectroscopy gives precise values of bond lengths [7 – 10].

Small systems such as atoms and molecules have constant values because of the homogenous distribution of their constituents. It is found that the atom as a nucleus and electrons at certain distances are contained in a certain area with a certain uniform distribution forming a certain system (atom) with a certain constant (1.1 X 10^8 m^2/Kg) [11]. The same result with certain constant (5.4 X 10^9 m^{-1}) is found for homonuclear molecules as a sharing of electron pairs between two similar atoms with uniform distribution to form certain covalent chemical bonds.

Materials and Methods

Physical relations and laws can be expressed regarding the main physical parameters responsible for their origin. The shared electrons between two atoms forms a covalent bond with a certain uniform distribution, producing a certain uniform system (molecule).

The main goal of collective covalent radii is to estimate approximately as given in equation (1), the length of a bond as the sum of two atomic radii

$$R_{AB=}\ r_A + r_B \qquad (1)$$

The origin for these covalent radii for single bonds is found in [12]. The list of metallic bonding and VCH periodic table is reported in [13,14]. In simple terms, a single bond corresponds to an electron pair in a bonding molecular orbital.

The covalent radii in pure-bred shape are determined by bisecting a homonuclear bond, as shown in the following equation (2).

$$r(E) = R(E - E)/2 \qquad (2)$$

The new group of single bond covalent radii for the elements 1 – 96, based on enormous data mining from the Cambridge Structural Data Base (CSD) and estimating the carbon radii (separately for the three familiar hybridizations), nitrogen and oxygen is found in [15].

The present scheme and method to determine the covalent radii are different. We considered diatomic homonuclear molecules as equal in their spherical geometrical shape. All covalent radii are then obtained self-consistently by using a simple equation connecting the radius, which represents the covalent radius and several sharing electrons. Our approach

confirms that the diatomic homonuclear molecules have spherical shape and its mathematical relation can be used to calculate covalent radii and confirm certain constant (5.4 X 10^9 m^{-1})

Results and Discussions

Density Functional Theory (DFT) is a powerful method utilized in both physics and chemistry to investigate the electronic structure (especially the ground state) for atoms and molecules. Using this theory, the characteristics of a many-electron arrangement can be estimated. In spite of late improvements, there are some difficulties in using DFT to describe intermolecular interactions such as realizing chemical reactions, particularly van der Waals forces [16-17].

Molecular Orbital (MO) theory provides a method to describe the electronic structure of molecules by using molecular quantum mechanics or quantum chemistry. MO theory treating the states of bonded electrons – the molecular orbitals – as Linear Combination of Atomic Orbitals (LCAO) by using the models of Density Functional Theory (DFT) to the Schrodinger equation. These are represented by three kinds (bonding, antibonding, non – bonding). A bonding orbital intensifies electron density in the area between a particular couple of atoms, consequently its electron density will tend to pull each of the two nuclei toward the other and hold the two atoms together [18 – 19].

The participation of electrons between two atoms to form covalent bonds leads to the formation of particular molecules. Diatomic homonuclear molecules are formed with certain geometrical shape (spherical) with a certain circumference for each molecule. It is found that the covalent radii of this type of molecules behave linearly as a result of increasing atomic number in periodic table. The model is based on the number of sharing electrons and the circumference and both of them are increasing with increasing atomic number.

It is found that the proportionality between cubic root of the number of shared electrons and circumference for diatomic homonuclear molecules gives the accurate results with experimental values equations as shown in equations (3 & 4 & 5)

$$\sqrt[3]{n} \propto 2 \times \pi \times r \quad \textbf{(3)}$$

$$\sqrt[3]{n} = cons \times 2 \times \pi \times r \quad \textbf{(4)}$$

$$\text{cons} = \frac{\sqrt[3]{n}}{2 \times \pi \times r} = (5.4 \times 10^9\ m^{-1}) \quad \textbf{(5)}$$

From which the following equation can be deduced

$$r = \frac{\sqrt[3]{n}}{2 \times \pi \times cons} \qquad (6)$$

The calculated covalent radius of homonuclear molecules by using equation (6) is consistent and in good agreement with experimentally determined radii values [20] as indicated in Table 1

where

n is the number of electrons of two atoms

r is the covalent radius

cons. is constant value for molecules

All calculations confirmed that there is a constant value (5.4 X 10^9 m^{-1}) for molecules formed by covalent bonds relating to the cubic root of the number of electrons and their circumference. Table (1) lists the constant value of similar molecules consisting of one chemical element by using equation (5).

A comparison of the present calculations and results for the covalent radius of diatomic homonuclear molecules with the available experimental values shows a good agreement between them [8].

The physical meaning of the constant of diatomic homonuclear molecules represents the number of sharing electrons to form certain covalent bond and radius of spherical geometrical shape of this type of molecules.

There are only seven calculated covalent radii approximately 5 % from 118 molecules by using equation (3) are deviated from the experimental determined values for the elements (Lithium, Beryllium, Sodium, Magnesium, Aluminium, Silicon, Phosphorus). The difference may be referred to the deviation of these molecules from spherical geometrical shape.

Table 1. List the experimental and new covalent radii.

Atomic Number	Symbol	Name	Experimental Covalent Radius picometer (pm)	New Covalent Radius picometer (pm)	Constant
1	H	Hydrogen	32	37	5.4 X 10^9
2	He	Helium	46	47	5.4 X 10^9
3	Li	Lithium	133	54	5.4 X 10^9

4	Be	Beryllium	102	59	5.4 X 10^9
5	B	Boron	85	63	5.4 X 10^9
6	C	Carbon	75	67	5.4 X 10^9
7	N	Nitrogen	71	71	5.4 X 10^9
8	O	Oxygen	63	74	5.4 X 10^9
9	F	Fluorine	64	77	5.4 X 10^9
10	Ne	Neon	67	80	5.4 X 10^9
11	Na	Sodium	155	82	5.4 X 10^9
12	Mg	Magnesium	139	85	5.4 X 10^9
13	Al	Aluminium	126	87	5.4 X 10^9
14	Si	Silicon	116	90	5.4 X 10^9
15	P	Phosphorus	111	92	5.4 X 10^9
16	S	Sulfur	103	94	5.4 X 10^9
17	Cl	Chlorine	99	96	5.4 X 10^9
18	Ar	Argon	96	98	5.4 X 10^9
19	K	Potassium	196	99	5.4 X 10^9
20	Ca	Calcium	171	101	5.4 X 10^9
21	Sc	Scandium	148	103	5.4 X 10^9
22	Ti	Titanium	136	104	5.4 X 10^9
23	V	Vanadium	134	105	5.4 X 10^9
24	Cr	Chromium	122	106	5.4 X 10^9
25	Mn	Manganese	119	108	5.4 X 10^9
26	Fe	Iron	116	110	5.4 X 10^9
27	Co	Cobalt	111	111	5.4 X 10^9
28	Ni	Nickel	110	112	5.4 X 10^9
29	Cu	Copper	112	114	5.4 X 10^9
30	Zn	Zinc	118	115	5.4 X 10^9
31	Ga	Gallium	124	116	5.4 X 10^9
32	Ge	Germanium	121	117	5.4 X 10^9
33	As	Arsenic	121	118	5.4 X 10^9
34	Se	Selenium	116	119	5.4 X 10^9
35	Br	Bromine	114	121	5.4 X 10^9
36	Kr	Krypton	117	122	5.4 X 10^9
37	Rb	Rubidium	210	123	5.4 X 10^9
38	Sr	Strontium	185	125	5.4 X 10^9
39	Y	Yttrium	163	126	5.4 X 10^9

40	Zr	Zirconium	154	127	5.4 X 10^9
41	Nb	Niobium	147	128	5.4 X 10^9
42	Mo	Molybdenum	138	129	5.4 X 10^9
43	Tc	Technetium	128	130	5.4 X 10^9
44	Ru	Ruthenium	125	131	5.4 X 10^9
45	Rh	Rhodium	125	132	5.4 X 10^9
46	Pd	Palladium	120	132	5.4 X 10^9
47	Ag	Silver	128	133	5.4 X 10^9
48	Cd	Cadmium	136	134	5.4 X 10^9
49	In	Indium	142	135	5.4 X 10^9
50	Sn	Tin	140	136	5.4 X 10^9
51	Sb	Antimony	140	137	5.4 X 10^9
52	Te	Tellurium	136	138	5.4 X 10^9
53	I	Iodine	133	139	5.4 X 10^9
54	Xe	Xenon	131	140	5.4 X 10^9
55	Cs	Cesium	232	141	5.4 X 10^9
56	Ba	Barium	196	142	5.4 X 10^9
57	La	Lanthanum	180	143	5.4 X 10^9
58	Ce	Cerium	163	144	5.4 X 10^9
59	Pr	Praseodymium	176	144	5.4 X 10^9
60	Nd	Neodymium	174	145	5.4 X 10^9
61	Pm	Promethium	173	145	5.4 X 10^9
62	Sm	Samarium	172	146	5.4 X 10^9
63	Eu	Europium	168	147	5.4 X 10^9
64	Gd	Gadolinium	169	148	5.4 X 10^9
65	Tb	Terbium	168	149	5.4 X 10^9
66	Dy	Dysprosium	167	149	5.4 X 10^9
67	Ho	Holmium	166	150	5.4 X 10^9
68	Er	Erbium	165	150	5.4 X 10^9
69	Tm	Thulium	164	151	5.4 X 10^9
70	Yb	Ytterbium	170	152	5.4 X 10^9
71	Lu	Lutetium	162	153	5.4 X 10^9
72	Hf	Hafnium	152	153	5.4 X 10^9
73	Ta	Tantalum	146	154	5.4 X 10^9
74	W	Tungsten	137	155	5.4 X 10^9

75	Re	Rhenium	131	156	5.4 X 10^9
76	Os	Osmium	129	156	5.4 X 10^9
77	Ir	Iridium	122	157	5.4 X 10^9
78	Pt	Platinum	123	157	5.4 X 10^9
79	Au	Gold	124	158	5.4 X 10^9
80	Hg	Mercury	133	159	5.4 X 10^9
81	Tl	Thallium	144	159	5.4 X 10^9
82	Pb	Lead	144	160	5.4 X 10^9
83	Bi	Bismuth	151	161	5.4 X 10^9
84	Po	Polonium	145	161	5.4 X 10^9
85	At	Astatine	147	162	5.4 X 10^9
86	Rn	Radon	142	162	5.4 X 10^9
87	Fr	Francium		163	5.4 X 10^9
88	Ra	Radium	201	164	5.4 X 10^9
89	Ac	Actinium	186	165	5.4 X 10^9
90	Th	Thorium	175	165	5.4 X 10^9
91	Pa	Protactinium	169	166	5.4 X 10^9
92	U	Uranium	170	167	5.4 X 10^9
93	Np	Neptunium	171	168	5.4 X 10^9
94	Pu	Plutonium	172	169	5.4 X 10^9
95	Am	Americium	166	170	5.4 X 10^9
96	Cm	Curium	166	170	5.4 X 10^9
97	Bk	Berkelium	168	170	5.4 X 10^9
98	Cf	Californium	168	171	5.4 X 10^9
99	Es	Einsteinium	165	171	5.4 X 10^9
100	Fm	Fermium	167	171	5.4 X 10^9
101	Md	Mendelevium	173	172	5.4 X 10^9
102	No	Nobelium	176	172	5.4 X 10^9
103	Lr	Lawrencium	161	173	5.4 X 10^9
104	Rf	Rutherfordium	157	173	5.4 X 10^9
105	Db	Dubnium	149	175	5.4 X 10^9
106	Sg	Seaborgium	143	175	5.4 X 10^9
107	Bh	Bohrium	141	176	5.4 X 10^9
108	Hs	Hassium	134	176	5.4 X 10^9
109	Mt	Meitnerium	129	176	5.4 X 10^9
110	Ds	Darmstadtium	128	176	5.4 X 10^9

111	Rg	Roentgenium	121	177	5.4×10^9
112	Cn	Copernicium	122	178	5.4×10^9
113	Nh	Nihonium	136	179	5.4×10^9
114	Fi	Flerovium	143	179	5.4×10^9
115	Mc	Moscovium	162	180	5.4×10^9
116	Lv	Livermorium	175	180	5.4×10^9
117	Ts	Tennessine	165	181	5.4×10^9
118	Og	Oganesson	157	181	5.4×10^9

It is noticed that all homonuclear molecules have the same value (5.4×10^9 m^{-1}) This means and indicates that all molecules have the same constant value relating to the cubic root of the number of electrons and their circumference.

Conclusion

The homogenous distribution of participating or sharing electrons for diatomic homonuclear molecules formed by covalent bonds with a certain number and certain circumference leads to the existence of a common constant for all diatomic homonuclear molecules. The cubic root of the number of sharing electrons and their circumference gives constant value with calculations and results of covalent radii in good agreement with experimental determinations.

Acknowledgement

“The author would like to express his sincere appreciation and deepest gratitude to the anonymous referee and all the staff of the **United Journal of Chemistry** whose contribution and support have greatly enhanced the quality, accuracy and publication of this research”

Conflict of interest

The author declares no conflicts of interest.

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