

# Bond Lengths in Carbon Dioxide, Carbon Monoxide and Carbonic Acid as Sums of the Atomic, Ionic and Bohr Radii

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\*Dedicated to Joseph Black (April 1728 - December 1799)

**Abstract:** Joseph Black is known for his pioneering work on "fixed air" which we know as carbon dioxide. This paper accounts for the different carbon to oxygen distances in carbon dioxide, carbon monoxide and carbonic acid in terms of the atomic, ionic and Bohr radii of the atoms, which are all related by the Golden ratio. The results confirm the author's work on the additivity of the appropriate radii of adjacent atoms or ions in the structures of small as well as big molecules.

**Keywords:** CO bond lengths, Atomic radii, Bohr radii, Golden ratio, Additivity of radii in bond lengths, Carbon dioxide, Carbon monoxide, Carbonic acid.

## 1. Introduction

### 1.1. General

Joseph Black<sup>1</sup> (16 April 1728 – 6 December 1799), a Scottish physician chemist and a fascinating personality, is known for his pioneering work on "fixed air" or carbon-dioxide. He was one of the founding pillars of the School of Chemistry of the University of Edinburgh, which is celebrating the tercentenary this year.

His predecessor, Jan Baptist van Helmont<sup>2</sup> (12 January 1580 – 30 December 1644) named the gas given off by burning charcoal as "gas sylvestre" (wood gas). Joseph Black made more fundamental studies of this gas by incinerating chalk and called it "fixed air". Antoine-Laurent de Lavoisier<sup>3</sup> (26 August 1743 – 8 May 1794) investigated further the "fixed air" and discovered the importance of oxygen in combustion, and the gas has since been known as an oxide of carbon.

Carbon dioxide<sup>4</sup> is an important respiratory gas and a fire extinguisher since it does not support fire. Its presence in the atmosphere keeps the Earth warm, but in larger concentrations it contributes to global warming along with other green house gases<sup>5,6</sup>.

Here, the carbon to oxygen bond lengths and structures of carbon dioxide, carbon monoxide and carbonic acid are shown to be sums of the appropriate covalent atomic radii<sup>7</sup>, Golden ratio based ionic radii<sup>8,9</sup> and Bohr radii<sup>10,11</sup> from first ionization potentials.

### 1.2. Bohr radius and its Golden sections

The ground state Bohr radius ( $a_{B,A}$ ) of atom A was calculated<sup>8-11</sup> from its first ionization potential ( $I_{1,A}$ ) as in the case of hydrogen<sup>8,9</sup>,

$$a_{B,A} = (e/2\kappa I_{1,A}) = a_{B,e} + a_{B,n+}; a_{B,n+} = a_{B,A}/\phi^2 < a_{B,e} = a_{B,A}/\phi \quad (1)$$

where  $e$  is the charge,  $\kappa$  is the electrical permittivity of vacuum,  $e/2\kappa = 7.1998 \text{ \AA.eV}$ ,  $\phi = (1+5^{1/2})/2 = 1.618$  is the Golden ratio, also known as The Divine Ratio<sup>12</sup>,  $a_{B,e}$  and  $a_{B,n+}$  are the two Golden sections of the Bohr radius pertaining to the electron and the nucleus, respectively<sup>8-11</sup>. This gives the nucleus and the outer electron their own apportioned distances in the ground state Bohr radius of every atom.

### 1.3. Covalent bond length and its Golden sections

It was also shown in<sup>8,9</sup> that the covalent bond length  $d(AA)$  between two atoms (A) of the same kind are the sums of the cationic ( $R_{A+}$ ) and anionic ( $R_{A-}$ ) radii of the atom, which are the two Golden sections of the bond length,  $d(AA)$ ,

$$d(AA) = 2R_A = R_{A+} + R_{A-}; R_{A+} = d(AA)/\phi^2 < R_A < R_{A-} = d(AA)/\phi \quad (2)$$

where,  $R_A = d(A) = d(AA)/2$ , the covalent radius<sup>7</sup> is half the bond length,  $d(AA)$ .

### 1.4. Covalent and Bohr radii of atoms and structures of molecules

In another paper<sup>13</sup>, many radii of atoms, like van der Waals radii, valence shell radii and covalent radii were all shown to be linearly dependent on their Bohr radii,  $a_{B,A}$  obtained from the first ionization potentials



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( $I_{1,A}$ ). Thus, the ground state Bohr radius can be considered as a yard stick for the different radii of atoms. Further, it has been shown<sup>10, 11</sup> that the covalent radii of all atoms are proportional to their respective Bohr radii, with the constant of proportionality ( $K_\phi$ ) as simple functions of the Golden ratio,

$$d(A) = R_A = K_\phi a_{B,A} \quad (3)$$

where  $a_{B,A} = a_{B,e^-} + a_{B,n^+}$  (see Eq. 1) and  $2d(A) = (R_{A^+} + R_A)/2$  (see Eq. 2).

The values of the Bohr radii, covalent radii, their Golden sections and the constant,  $K_\phi$  in terms of the Golden ratio have all been tabulated in<sup>11</sup> for all the elements of the Periodic Table. Here, the data from<sup>11</sup> for the various radii of hydrogen, carbon, oxygen are given in **Table 1**. For carbon and oxygen,  $K_\phi = (\phi^2 + 1)/2\phi = 1.118$

The bond lengths, bond angles and structures of some simple molecules like  $H_2^+$ ,  $O_2$ ,  $O_3$ ,  $H_2O$ ,  $SO_2$ ,  $NO_2$  and  $CO_2$  have been explained in terms of the appropriate Bohr radii, covalent and ionic radii in<sup>14</sup>.

### 2.1. Bond length and structure of carbon dioxide

The molecule of carbon dioxide is known to be linear<sup>4,7</sup> with both carbon to oxygen bonds of lengths of 1.16 Å. The covalent atomic radius of carbon obtained as half the interatomic distance,  $d(CC)/2 = R_C$ , has the following values<sup>7</sup> for the single bond (sb), and double bond (db):

$$\begin{aligned} d(CC)_{sb}/2 &= R_{C,sb} = 0.77 \text{ \AA} & (4a) \\ d(CC)_{db}/2 &= R_{C,db} = 0.67 \text{ \AA} = (3^{1/2}/2) R_{C,sb} & (4b) \end{aligned}$$

It was shown in<sup>15</sup> that these radii correspond to different distances in a tetrahedron. The graphitic/graphene radius<sup>15</sup> (0.71 Å) of carbon,  $C_{gr}$  is nearly the mean of the single and double radii, which Pauling<sup>7</sup> notes as 1.5 bond character. All the above different radii of the atom are demonstrated in Fig. 1 for  $C_{gr}$  as an example. The covalent single and double bond atomic radii of oxygen are  $d(OO)_{sb}/2 = R_{O,sb} = 0.67 \text{ \AA}$  and  $d(OO)_{db}/2 = R_{O,db} = 0.60 \text{ \AA}$ .

It can be seen from the above radii that the bond length  $d(CO)_{db} = 1.16 \text{ \AA}$  in carbon dioxide is not a sum of the double bond atomic radii of carbon and oxygen,  $0.67 + 0.60 = 1.27 \text{ \AA}$ .

The Bohr radii of C and O, using the first ionization potentials for C (11.260 eV) and O (13.618 eV) from<sup>16</sup> and their sum have the values,

$$a_{B,C} = (e/2kI_{1,C}) = 0.639 \text{ \AA} \quad (5)$$

$$a_{B,O} = (e/2kI_{1,O}) = 0.529 \text{ \AA} \quad (6)$$

$$a_{B,C} + a_{B,O} = 1.168 \text{ \AA} = d(CO) \quad (7)$$

Eq. (7) accounts for the CO bond length in carbon dioxide, as shown in<sup>14</sup>. Fig. 2 a) shows the linear molecule drawn to scale.

### 2.2. Bond length and structure of carbon monoxide

For CO, the bond length has been found<sup>7,17</sup> to be  $d(CO) = 1.13 \text{ \AA}$ . In this case, the radii of carbon and oxygen and their sum are given by,

$$\begin{aligned} R_{C,db} &= 0.67 \text{ \AA} & (8) \\ R_{O^+} &= 0.46 \text{ \AA} & (9) \\ R_{C,db} + R_{O^+} &= 1.13 \text{ \AA} = d(CO) & (10) \end{aligned}$$

This explains the partial ionic character of the CO bond<sup>7</sup> as due to  $O^+$ . This molecule is shown in Fig. 2 b).

### 2.3. Bond length and structure of carbonic acid

In carbonic acid<sup>7,18</sup>,  $H_2CO_3$ , all three CO bonds are of equal length<sup>7</sup>, 1.30 Å. This is accounted for by the radii sum,

$$\begin{aligned} R_{C,sb} &= 0.77 \text{ \AA} & (11) \\ a_{B,O} &= 0.53 \text{ \AA} & (12) \\ R_{C,sb} + a_{B,O} &= 1.30 \text{ \AA} = d(CO) & (13) \end{aligned}$$

Fig. 2 c) shows the structure and bond lengths in this molecule.

Thus, the bond lengths in all the three compounds have been accounted for by the sums of the appropriate radii of the adjacent atoms.

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**Table 1.** Ionization potential ( $I_1$  in eV), Bohr radius ( $a_{B,A}$ ) and its sections,  $a_{B,e^-}$  and  $a_{B,n^+}$ , covalent radius,  $d(A)$ , ionic radii,  $d(A^-)$  and  $d(A^+)$ , the constant  $K_\phi$  and  $d(A)_{cal}$ ; (in Å)

Gp.	Atom	$I_1$	$a_{B,A}$	$a_{e^-}$	$a_{n^+}$	$d(A)$	$d(A^-)$	$d(A^+)$	$K_\phi$	$K_\phi =$ (value)	$d(A)_{cal} =$ $K_\phi a_{B,A}$
1A	H	13.598	0.53	0.33	0.20	0.37	0.46	0.28	$1/2^{1/2}$	0.707	0.37
4A	C	11.260	0.64	0.40	0.24	0.71	0.88	0.54	$(\phi^2+1)/2\phi$	1.118	0.71
6A	O	13.618	0.53	0.33	0.20	0.60	0.75	0.46	$(\phi^2+1)/2\phi$	1.118	0.59

**Figure legends.**

Figure 1. Atomic, ionic and Bohr radii of  $C_{gr}$  (drawn to scale), see<sup>14</sup>.

Figure 2. Structures at the atomic level of a) carbon dioxide<sup>14</sup>, b) carbon monoxide and c) carbonic acid, with bond lengths based on additivity of the appropriate radii of atoms.

Figure 1

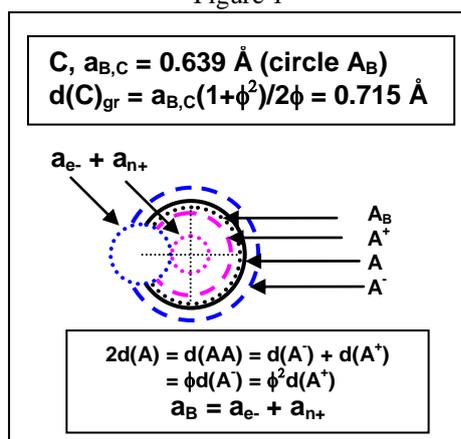


Figure 2

