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Bond Lengths, Bond Angles and Bohr Radii from Ionization Potentials Related via the Golden Ratio for H_2^+, O_2, O_3, H_2O, SO_2, NO_2 and CO_2

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Abstract: In a recent paper, it was shown that the atomic radii of main Group elements are directly proportional to their ground state Bohr radii obtained from the first ionization potentials, with the proportionality constant involving the Golden ratio. It was demonstrated in earlier articles that atomic and Golden ratio based ionic radii are additive in chemical bond lengths. Here the bond lengths and angles are interpreted in terms of the respective Bohr radii and the Golden ratio. Simple molecules present on our Earth and in the environment, which are of importance to our lives have been chosen here as examples.

Keywords: Bond lengths, Bond angles, Bohr radii, Golden ratio, Water molecule, Ozone, Atmospheric molecules.

1. Introduction

In a recent publication[1], it was shown that the radii, d(A) of atoms (A) are directly proportional to their Bohr radii ($a_{B,A}$) obtained from the first ionization potentials (I_1) by the simple relation,

$$d(A) = d(AA)/2 = K_\phi a_{B,A} \quad (1)$$

where d(AA) is the bond length between two atoms of the same kind and K_ϕ is a constant depending on the Golden ratio, $\phi = (1 + 5^{1/2})/2$. The Bohr radius is given by,

$$a_{B,A} = (e/2\kappa I_1) = a_{e-} + a_{n+} \quad (2a)$$

$$(a_{e-}/a_{n+}) = \phi,\ a_{n+} = (a_{B,A}/\phi^2) \text{ and } a_{e-} = (a_{B,A}/\phi) = \phi a_{n+} \quad (2b\text{-}d)$$

where e is the charge, κ is the electrical permittivity of vacuum, e/2κ = 7.1998 Å.eV, a_{e-} and a_{n+} are the Golden sections of $a_{B,A}$, representing the radius of the electron and of the nucleus A_{n+} of atom, A, respectively.

It was shown earlier[1-3] that the Golden ratio based ionic radii of the resonance forms[4], A^- and A^+ of the atom A are related as follows,

$$d(AA) = d(A^-) + d(A^+), \quad (3a)$$

$$d(AA)/d(A^-) = d(A^-)/d(A^+) = \phi \quad (3b)$$

In Table 1 in ref.[1] the values for all the above radii and other quantities have been tabulated for atoms of elements of Groups 1A - 8A. In Fig. 1 here are shown the various radii in the H_2 molecule. The bond length d(HH) = $2^{1/2}a_{B,H}$ = 0.748 Å. Fig. 2 shows the various radii for C. The details can be found in the legends for Figures.

2. Bond lengths, bond angles and Bohr radii related via the Golden ratio.

In this article, the bond lengths and bond angles in the simple molecules mentioned in the title are expressed as simple Golden ratio multiples of the Bohr radii. The data on the various radii of the atoms in the molecules described below can be found in Table 1 in[1]. For the atoms of C, N, O and S, the ratios of atomic covalent radii to Bohr radii are given by (see Table 1 in[1]),

$$d(O)/a_{B,O} = d(N)/a_{B,N} = d(C)/a_{B,C} = K_\phi = (\phi^2+1)/2\phi = 1.118 \quad (4)$$

$$d(S)/a_{B,S} = K_\phi = (\phi^2+1)/\phi^2 = 1.382 \quad (5)$$

a) H_2^+: The bond length in this molecule has been found[4] to be 1.06 Å. This is exactly given[2] by,

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$d(HH^+) = 2a_{B,H} = 2(a_{p+} + a_{e-}) = 1.060$ (6)

where $a_{B,H} = 0.530$ Å. Fig. 3 a) shows the diagram for this molecule.

b) O_2: The bond length in this life-sustaining molecule is given[5] as 1.207 Å. The following equation gives nearly this value,

$d(OO) = 2d(O) = a_{B,O}(\phi^2+1)/\phi = 2.236a_{B,O} = 5^{1/2}a_{B,O} = 1.183$ Å (7)

where $a_{B,O} = 0.529$ Å, (which is very close to the Bohr radius for H). Fig 3 b) shows the oxygen molecule along with the Bohr radius and its Golden sections.

c) O_3: For this molecule, associated with the 'ozone hole', electron diffraction gives the bond length, $d(OO)_{oz} = 1.26$ Å and the angle, θ = OOO = 116° 45, as reported in[6]. Here, it is shown in Fig. 3 c) that the above value is the exact sum,

$d(OO)_{oz} = a_{B,O} + d(O^-) = 0.529 + 0.731 = a_{B,O}(2\phi^2+1)/\phi^2 = 2.382a_{B,O} = 1.260$ Å (8)

where $d(O^-) = d(OO)/\phi = 0.731$ Å. The angle, θ = O^-OO^- is close to that from the cosine ratio of the sides with lengths, $2a_{e-}$ (= $2a_{B,O}/\phi$) and $d(OO)_{oz}$,

$\cos(\theta/2) = 2a_{e-}/d(OO)_{oz} = 2\phi/(2\phi^2+1) = 0.518$; θ = 117.48° (9)

d) H_2O: The life-sustaining water molecule has been the subject of many investigations. The values for the bond length d(OH) have been reported[4,7] to be 0.96 Å, 0.958 Å and the angle, θ = HOH = 104.45°, 104.474°, respectively. Here it can be seen from Fig. 3 d) that the above values are reproduced very closely by the equations for d(OH), and the angle θ = HOH,

$d(OH) = d(O) + d(H) = 0.591 + 0.374 = a_{B,O}(\phi^2+1)/2\phi + a_{B,H}/2^{1//2} = 0.965$ Å (10)
$\cos(\theta/2) = d(O)/d(OH) = 0.591/0.965 = [a_{B,O}(\phi^2+1)/2\phi]/[a_{B,O}(\phi^2+1)/2\phi + a_{B,H}/2^{1//2}] = 0.612$; θ = HOH = 104.47° (11)

Note that $\cos(\theta/2) = 0.612$ is close to $0.618 = 1/\phi$.

e) SO_2: In this atmospheric pollutant molecule, the distance d(SO) is[4,8] 1.43 Å and the angle θ = OSO is[4,8] 119.54°, 116° respectively. This molecule is drawn in Fig. 3e, where $a_{B,S} = 0.695$ Å, and the above bond length d(SO) and the angle θ = O^-SO^- are reproduced by the equations,

$d(SO) = a_{B,S} + d(O^-) = 0.695 + 0.731 = a_{B,S} + a_{B,O}(\phi^2+1)/\phi^2 = 1.426$ Å (12)
$\cos(\theta/2) = d(O^-)/d(SO) = [a_{B,O}(\phi^2+1)/\phi^2]/[a_{B,S} + a_{B,O}(\phi^2+1)/\phi^2] = 0.731/1.426 = 0.513$;
θ = O^-SO^- = 118.32° (13)

f) NO_2: This is another pollutant of the atmosphere. The reported[9] bond length for d(NO) and the angle, ONO are around 1.20 Å and 132° respectively. This molecule is shown in Fig. 3f and the above bond length d(NO) is explained by,

$d(NO) = a_{B,O} + d(N^-) = a_{B,O} + a_{B,N}(\phi^2+1)/\phi^2 = a_{B,O} + 1.382a_{B,N} = 1.214$ Å (14)

where $d(N^-) = d(NN)/\phi = a_{B,N}(\phi^2+1)/\phi^2 = 1.382a_{B,N} = 0.685$, where $a_{B,N} = 0.495$ Å. The angle θ = ON^-O is obtained from the cosine of the sides (see Fig. 3f) as,

$\cos(\theta/2) = a_{B,N}/d(NO) = 0.495/1.214 = a_{B,N}/[a_{B,O} + a_{B,N}(\phi^2+1)/\phi^2] = 0.408$;
θ = ON^-O = 131.87° (15)

g) CO_2: This important gas is also responsible for the 'green house effect'. This linear molecule has[4,10] a bond length, d(CO) = 1.16 Å. It is shown in Fig. 3g, and it accounts for this bond length exactly by the sum of the Bohr radii for the two atoms,

$d(CO) = a_{B,O} + a_{B,C} = 0.529 + 0.639 = 1.168$ Å (16)

It is thus concluded here that the Bohr radii from ionization potentials of elements and the Golden ratio give quantitative measures of the atomic and ionic radii and of bond lengths and bond angles.

References

[1] Heyrovska, R. Atomic and Ionic Radii of Elements and Bohr Radii from Ionization Potentials are Linked Through the Golden Ratio. *International J. Sciences.*, **2**, 82-92, (2013). http://www.ijsciences.com/pub/pdf/V2-201303-19.pdf

[2] Heyrovska, R. The Golden ratio, ionic and atomic radii and bond lengths. *Molecular Physics*, 103, 877 - 882 (2005); and the literature therein.

[3] Heyrovska, R. The Golden ratio in the

creations of Nature arises in the architecture of atoms and ions. Chapter 12 in Book: *Innovations in Chemical Biology*, Editor: Bilge Sener, Springer.com, (2009).
[4] Pauling, L. *The Nature of the Chemical Bond*, Cornell Univ. Press, NY, (1960).
[5] http://www.webelements.com/oxygen/atom_sizes.html
[6] Hughes, R. H. Structure of Ozone from the Microwave Spectrum between 9000 and 45 000 Mc**.** *J. Chem. Phys*., **24**, 131 (1956).
[7] Hasted, J. B. Liquid water: Dielectric properties, in *Water, A comprehensive treatise*, Vol 1, Ed. F. Franks (Plenum Press, New York, 1972) pp. 255-309; (from: http://www.lsbu.ac.uk/water/molecule.html#be
[8] Gillespie, R. J., Robinson, E. A. The sulphur-oxygen bond in sulphuryl and thionyl compounds: correlation of stretching frequencies and force constants with bond lengths, bond angles and bond orders. *Canad. J. Chem*. **41,** 2074-2085 (1963).
[9] Claesson, S., Donohue, J., Schomaker, V. The Molecular Structure of Nitrogen Dioxide. A Reinvestigation by Electron Diffraction. *J. Chem. Phys.* **16,** 207 (1948).
[10] Harris, J. G., Yung, K. H. Carbon Dioxide's Liquid-Vapor Coexistence Curve And Critical Properties as Predicted by a Simple Molecular Model. *J. Phys. Chem.*, **99,** 12021–12024 (1995).

Figure legends

Figure 1. Bohr radius (a_B), its Golden sections, (a_{e-}) and (a_{n+}) and the covalent bond (HH) in the H_2 molecule. $\phi = (1+5^{1/2})/2 = 1.618$ is the Golden ratio. Radius d(H) = d(HH)/2 = $a_{B,H}/2^{1/2}$.

Figure 2. Bohr radius ($a_{B,C}$) for carbon, its Golden sections, (a_{e-}) and (a_{n+}), and covalent atomic radius, d(C_{gr}) for graphite/graphene (subscript: gr). The atomic radius, d(A), and the Golden sections, d(A^-) and d(A^+) of the bond length d(AA), are related as shown: 2d(A) = d(AA) = ϕd(A^-) = ϕ^2d(A^+). Also, d(A) = $K_\phi a_{B,A}$, where $a_{B,A}$, is the Bohr radius for atom A, and K_ϕ is a constant depending on the Golden ratio. Atomic radius, d(C_{gr}) = $a_{B,C}(1+\phi^2)/2\phi$.

Figure 3. Bond lengths and bond angles related to Bohr radii and the Golden ratio. **a)** H_2^+: d(HH^+) = $2a_{B,H}$; **b)** O_2: d(OO) = $a_{B,O}(\phi^2+1)/\phi$; **c)** O_3: θ = O^-OO^-; $d(OO)_{oz} = a_{B,O}$ + d(O^-); **d)** H_2O: θ = HOH; d(OH) = d(O) + d(H); (blank white circle shows one O atom of O_2 replaced by the two H atoms) **e)** SO_2: θ = O^-SO^- ; d(SO) = $a_{B,S}$ + d(O^-); **f)** NO_2: θ = ON^-O; d(NO) = $a_{B,O}$ + d(N^-) and **g)** CO_2: d(CO) = $a_{B,O} + a_{B,C}$.

Figure 1

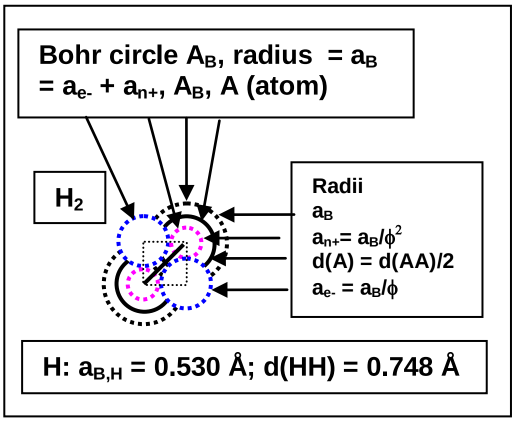


Figure 2

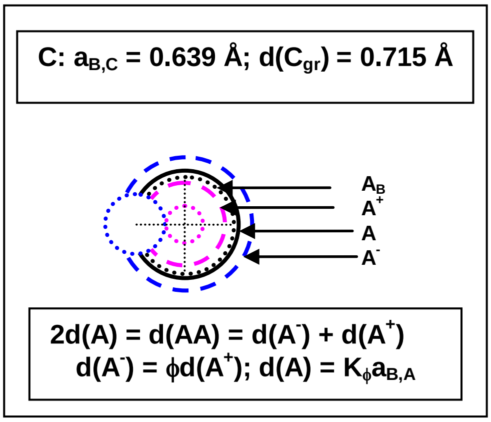
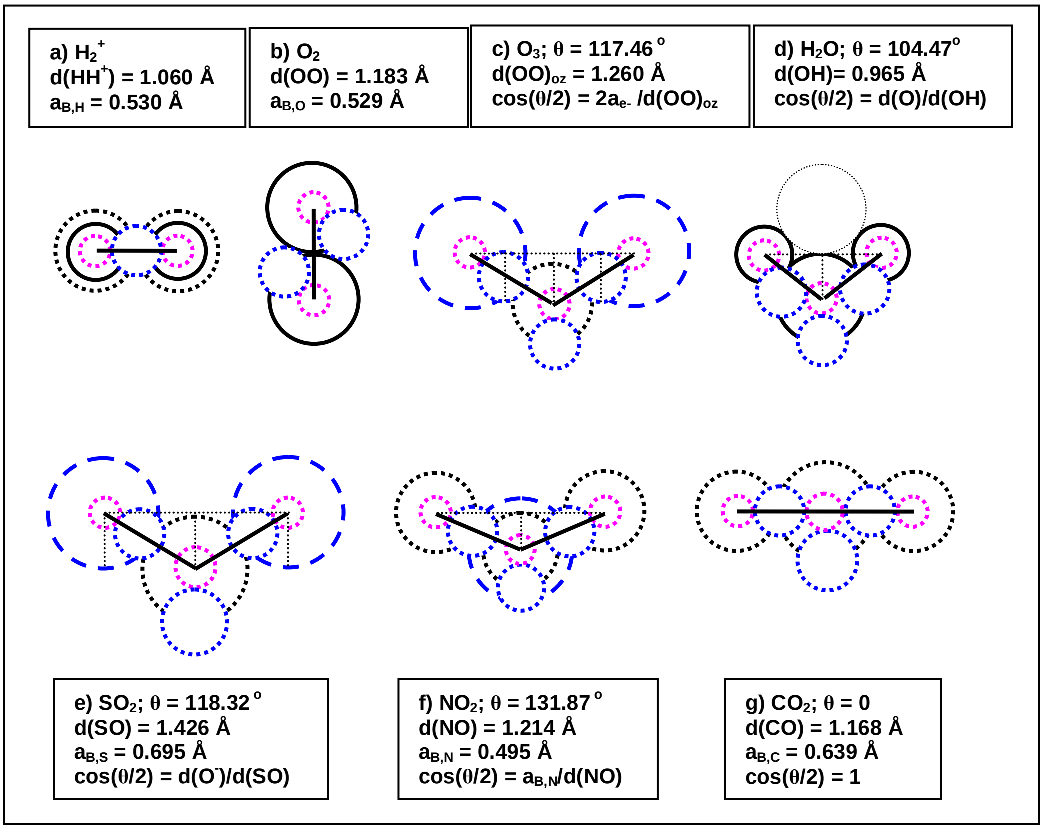


Figure 3


a) H_2^+
d(HH^+) = 1.060 Å
$a_{B,H}$ = 0.530 Å
b) O_2
d(OO) = 1.183 Å
$a_{B,O}$ = 0.529 Å
c) O_3; $\theta = 117.46^o$
$d(OO)_{oz}$ = 1.260 Å
$\cos(\theta/2) = 2a_{e-} / d(OO)_{oz}$
d) H_2O; $\theta = 104.47^o$
d(OH)= 0.965 Å
$\cos(\theta/2) = d(O)/d(OH)$
e) SO_2; $\theta = 118.32^o$
d(SO) = 1.426 Å
$a_{B,S}$ = 0.695 Å
$\cos(\theta/2) = d(O^-)/d(SO)$
f) NO_2; $\theta = 131.87^o$
d(NO) = 1.214 Å
$a_{B,N}$ = 0.495 Å
$\cos(\theta/2) = a_{B,N}/d(NO)$
g) CO_2; $\theta = 0$
d(CO) = 1.168 Å
$a_{B,C}$ = 0.639 Å
$\cos(\theta/2) = 1$