

Simple and Exact Additivity of Atomic and Ionic Radii in Various Types of Bonds in Small as Well as Large Molecules

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Abstract

The nature of the chemical bond has intrigued many a mind. Bohr's theory of the hydrogen atom, which celebrated its centennial recently, gave the correct value but a negative sign for the energy. As this would imply that the energy of the Universe, which consists of 70% hydrogen, is negative, the author was dissatisfied with it. So she proposed a modified approach to the problem, which showed that the energy is positive. Moreover, she found that the Bohr radius is divided into two Golden sections pertaining to the electron and proton. This idea cascaded into the finding that all bond lengths in small as well as large molecules are simply exact sums of the appropriate atomic and or Golden ratio based ionic radii of adjacent atoms or ions. Over the years, this has proved to be correct for various types of bonds, including hydrogen bonds, bonds in graphite and in benzene dimers.

Keywords: Energy of hydrogen atom; Additivity of radii; Bond lengths; Bohr radius; Golden ratio; Ionic radii; Hydrogen bond

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Introduction

Bohr's theory of the hydrogen atom [1] celebrated recently its centennial. It gave the correct magnitude for the ground state energy (E_H),

$$E_H = eI_H = - (1/2)(e^2/\kappa a_B) \quad 1$$

where, I_H is the ionization potential, e is the unit of charge and κ is the electric permittivity constant and a_B is the Bohr radius (distance of the electron from the proton). However, the negative sign has irked the author's conscience, since this implies that the energy of our Universe, which consists of more than 70% hydrogen, is negative. To quote from Gamov [2] about 'False sign': "All the theories expire or bring disappointment, The Sign is forever the fly in your ointment....".

As regards bond lengths, although Pauling [3] suggested that covalent radii are additive, he could not account for many chemical bonds, especially the partially and completely ionic types and had to postulate many theories, concepts and correction factors. However, as correction factors do not explain exact science, the nature of the chemical bond became a theoretical speculation

of many kinds. On re-investigating the Bohr's equation (1), the author arrived at the surprising result that the Bohr radius is divided at the point of electrical neutrality into two Golden sections pertaining to the electron and proton. For an introduction to the Golden ratio, see [4]. This made a breakthrough in the interpretation of bond lengths as simple sums of the radii of the adjacent atoms and or ions [5-9]. The section below gives a brief account of this finding, and the interpretation over the years of existing bond length data in various molecules are listed in the references [5-19].

Additivity of Atomic and Ionic Radii in Bond Lengths and Structures of Molecules at the Atomic Level

For the same magnitude of energy as given by equation (1) of Bohr's theory, the author [5,6] proposed a new interpretation of the ionization potential, I_H , of the hydrogen atom as the difference in potential between that of the proton (p^+), ($=e/\kappa a_p$) and of the electron (e^-), ($=-e/\kappa a_e$) at a mutual distance of the Bohr radius,

$$a_B (=a_p + a_e) = 0.529 \text{ \AA} \text{ from each other, [20-27],}$$

$$I_H = (1/2)(e/ka_B) = (1/2)[(e/ka_p) - (e/ka_e)] \quad 2$$

The ionization energy, $E_H = eI_H = (1/2)(e/ka_B)$ can be interpreted as the electromagnetic energy of an atomic condenser [5-9], with ka_B as the capacitance. As the electron and proton are charged particles with magnetic momenta, this interpretation seems meaningful. From the above equation (2) and the equality, $a_B (= a_p + a_e)$, one obtains for the ratio [28-36],

$$a_e/a_p = a_B/a_e = (1+5^{1/2})/2 = \phi \quad 3$$

where ϕ , a mathematical constant, is the Golden ratio [4]. This surprising result shows that the Golden ratio which manifests in the geometry of many creations in the Universe [4] is right in core of the atom! Thus, the ratio of the electrostatic radii of the electron and proton in the hydrogen atom is the Golden ratio, and an atom is a unique construction of Nature [37-49]. On finding that the covalent bond length $d(HH)$ between the two hydrogen atoms in the molecule H_2 is the diagonal of a square with the Bohr radius as a side, and since the latter is divided into two Golden sections, $a_e = a_B/\phi$ and $a_p = a_B/\phi^2$, pertaining to the electron and proton, $d(HH)$ is actually the sum,

$$d(HH) = 2^{1/2}(a_B) = d(H^-) + d(H^+) \quad 4$$

where $d(H^-) = d(HH)/\phi$ and $d(H^+) = d(HH)/\phi^2$ are the anionic and cationic radii of H. Note that H^- and H^+ are the ionic resonance

forms of H in the hydrogen molecule, suggested by Pauling [3]. For more details, see [9].

On subtracting the cationic radius, $d(H^+)$ from the bond length of partially ionic alkali metal hydrides and hydrogen halides, it was found that the alkali metal cations are Golden sections of the respective interatomic distances in the metal lattice and the halogens have their covalent radii (which are half the covalent bond length).

Further, on subtracting the Golden ratio based cationic radius of the alkali metals from the interionic distance in alkali halides, the Golden ratio based radii of the halogen ions were obtained. See for all details, Ref. [50-59]. Thus, it could be generalized that the covalent bond length between two atoms of the same kind, $d(AA) = d(A^-) + d(A^+)$, the sum of their Golden ratio based cationic and anionic radii (which are similar to the ionic resonance forms of hydrogen in H_2). This finding paved the way to interpret the experimental bond lengths as simple sums of the appropriate radii of the adjacent atoms and or ions and thereby establish the precise structures at the atomic level of simple as well as complex molecules. References [50-59] below give the work from 2004-2016. For a chapter in a book, a pdf of full poster and a review talk in power point, see Ref. [28,31,52].

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