Bond Lengths in Helium Hydrides as Sums of the Relevant Radii of He and H

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Abstract. The latest astrophysical discovery for the first time of HeH^+ inspired the author to look into its bond length. Using the previously calculated values of the various radii of He and H, it is shown here that the reported inter-nuclear distance in HeH+ is the sum of the radii of He- and the section of the Bohr radius pertaining to the proton. Interpreted here also is the inter-nuclear distance of the He..H bond in $He..H..He^+$, as the sum of the covalent radius of He and the Bohr radius of H. Both cases support the rule of additivity of radii of adjacent atoms and or ions in bond lengths established by the author over the years.

1. Introduction

The author has shown over the years (see for collected papers [1]) that inter-atomic distances are sums of the radii of adjacent atoms or ions, whether the bond is completely or partially covalent or ionic. The covalent inter-atomic distance, d(AA) between two atoms (A) of the same kind was shown to be the sum of the radii of its cation and anion (Pauling's resonance forms), R_{A+} and R_{A-} respectively,

$$d(AA) = 2R_A = R_{A+} + R_{A-} \qquad (1)$$

where R_A is the covalent radius of A. The ionic radii are the Golden sections of d(AA) given by,

$$R_{A+} = d(AA)/\phi^2 \text{ and } R_{A-} = d(AA)/\phi \qquad (2)$$

where ϕ is the Golden ratio [1]. It was shown [1] that the Golden ratio divides the ground state Bohr radius, a_{BA} of an atom A (calculated from its first ionization potential, I_1) into two sections, $a_{B,e-}$ and $a_{B,n+}$ pertaining to the outer electron (e^-) and the nucleus (n^+) as follows,

$a_{B,n+} = a_{B,A}/\phi^2$ and $a_{B,e-} = a_{B,A}/\phi$ (3)

The above radii have been tabulated for all the elements of The Periodic Table in [2,3]. This report pertains to the bond in helium hydride HeH^+, [4-6] which has roused great interest recently [4] and also to He..H in $He..HHe^+$reported earlier [5]. For an introduction and review of research on HeH^+, see [7].

2. Interpretation of the observed inter-nuclear distance, d(HeH^+)

The observed distance d(HeH^+) as reported in [4-6] is 0.77 Å. The various radii for H and He copied from [2,3] are given here in Table 1. See the Figures in [2] for the radii of H and He.

Table 1. The various radii in Å for **H and He, data from [2,3].**

A	I_1 (ev)	$a_{B,A}$	a_{e-}	a_{p+}	R_A	R_{A-}	R_{A+}	$R_A/a_{B,A}$	
H	13.598	0.53	0.33	0.20	0.37	0.46	0.28	$1/2^{1/2}$	= 0.707
He	24.587	0.29	0.18	0.11	0.46	0.57	0.35	ϕ	= 1.618

From the data in Table 1, the observed distance [4], d(HeH+) = 0.77Å is interpreted here as the sum of radii,

$d(He..H^+) = R_{He-} + a_{p+} = 0.57 + 0.20 = 0.77$ Å (4)

3. Interpretation of the observed [6] inter-nuclear distance, d(He..H) in $He..H..He^+$

The reported [6] inter-nuclear distance, d(He..H) = 0.95Å in $He..HH^+$ corresponds to the sum,

$d(He..H) = R_{He} + a_{B.H} = 0.46 + 0.53 = 0.96$Å (5)

Thus, additivity of atomic and or ionic radii found [1] for chemical bonds in small as well as large molecules holds for the bond distances in HeH^+ and in He..H as well.

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