New Simple Relations Connecting Bond Lengths, Lattice Parameters and Bohr Radii for the Biologically Important Elements, C, N, O, P and S

– Dedicated to Sir J.J. Thomson ((18 Dec 1856 - 30 Aug 1940) to commemorate his 160th Birth Anniversary

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Abstract

This paper presents some new simple relations connecting bond lengths between two same atoms, their Bohr radii obtained from first ionization potentials and their lattice parameters. The biologically important elements, C, N, O, P and S are chosen as examples.

1. Introduction

The author has shown in her previous work the simple relations between the covalent atomic radii of elements and their Bohr radii obtained from their first ionization potentials. These data have been tabulated for all the Group A & B elements in [1,2]. In the work [3] on the atomic structures of graphene and graphite, it was found that the interatomic distance, d(CC) was related to the lattice parameter of the hcp carbon structure. Here, results are presented for all the main biologically important elements, C, N, O, P and S. For detailed introduction with figures and data, see [1-9].

2. Results

a) Carbon

The CC bond length in graphene and graphite (subscript: g.b.), $d(CC)_{gb}$ = 1.42 (+/- 0.01) Å [1-4], Bohr radius, a_B = 0.639 Å and the lattice parameter, a, are related as follows:

$$d(CC)_{g.b.} = (5^{1/2})a_B = (a/2)/(3^{1/2}/2) = 2.84 \quad (1)$$

where a = 2.464 Å is the lattice constant (hcp) [10].

The CC triple bond, double bond and single bond lengths of C are related by [5],

$$d(CC)_{t.b.} = 2a_B\cos 18^0 = [2d(CC)_{g.b.}/5^{1/2}]\cos 18^o = 1.21 \quad (2)$$

$$d(CC)_{s.b.} = \varphi^{1/2}\, d(CC)_{t.b.} = 1.545 \quad (3)$$

$$d(CC)_{d.b.} = d(CC)_{s.b.}(3^{1/2}/2) = 1.341 \quad (4)$$

where $\varphi = (1 + 5^{1/2})/2 = 1.618..$ the Golden ratio [1,2] and $\cos 36^o = \varphi/2$. These bond lengths agree well with those (1.20, 1.34 and 1.54 Å respectively) in [11,12].

b) Nitrogen

The bond length $d(NN)_{t.b.}$ = 1.10 Å in the nitrogen molecule [1,2] is related to its Bohr radius, $a_{B,A}$ = 0.495 Å [1,2] and the lattice parameter (hcp), a = b = 3.861 Å [10] as follows:

$$d(NN)_{t.b.} = a_{B,A}(5^{1/2}) = 0.495*2.236 = 1.107 \quad (5)$$

$$d(NN)_{d.b.} = d(NN)_{t.b.}(\phi^2/2)(3^{1/2}/2) = d(NN)_{s.b.}(3^{1/2}/2) = 1.255 \quad (6)$$

$d(NN)_{s.b.} = d(NN)_{d.b.}(2/3^{1/2}) = d(NN)_{t.b.}(\phi^2/2) = (a/2)(3/4) = (3.861/2)*3/4 = 1.449$ (7)

These values agree with those (1.45, 1.25 and 1.10 Å) in [12].

c) Oxygen

In this case, the various lengths and the lattice parameter, b [11], are as follows:

$a_B = 0.529$ Å; $b = 3.429$ Å (8)

$d(OO)_{d.b.} = 2a_B (5^{1/2}/2) = 1.183$ Å (9)

$d(OO)_{s.b.} = d(OO)_{d.b.}(5^{1/2}/2) = 2a_B (5^{1/2}/2) (5^{1/2}/2) = b(1/\phi^2) = 1.31$ Å (10)

The double bond and single bond lengths (1.20 and 1.32 Å in [12] are close to the above.

d) Phosphorus

The relations in this case are,

$a_B = 0.686$ Å (11)

$d(PP) = 2a_B \phi$ (=2.22 Å) $= b/(5/2) = 2.20$ Å (12)

where the lattice parameter, $b = 5.503$ Å. The value, $d(PP) = 2.21$ Å [10,12] is well reproduced in Eq. (12).

e) Sulphur

The various relations are as follows:

$a_B = 0.695$ Å (13)

$d(SS) = 3a_B = b(\phi/10) = 2.08$ (14)

where, the lattice constant, b = 12.845 Å. Eq. (14) explains the value d(SS) = 2.08 in [10,12].

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