Atomic and Ionic Radii of Elements and Bohr Radii from Ionization Potentials are Linked Through the Golden Ratio

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Abstract: In an earlier article, Bohr radius of hydrogen was shown to be the sum of two Golden sections pertaining to the electron and proton. This led to discovering that all bond lengths between same two atoms are sums of two Golden sections representing the radii of the anion and cation, and that the radii of adjacent atoms and or ions in chemical bonds are additive. Subsequently, atomic radii were shown to vary linearly with their Bohr radii obtained from the first ionization potentials. Reported here is a new finding mentioned in the title, for elements of Groups 1A - 8A. The electron is found to occupy a space of its own in the atoms, in support of works on solvated electrons and electrides.

Keywords: Bond lengths, Covalent Radii, Ionic radii, Bohr radii, Golden sections, Main group elements, radii of electrons, Nuclear radii, Golden ratio

1. Introduction
1.1. Golden sections of the ground state Bohr radius of hydrogen

In this introductory section, the present author's work so far on the Golden ratio in atomic and ionic radii is described briefly. She arrived at a new interpretation[1] of the ground state Bohr radius, a_B of hydrogen (H) atom, by considering the ground state ionization potential (I_H) as the difference between the potentials of the proton (p^+) and the electron (e^-). This led to the discovery[1] that a_B, which is the distance between the proton and electron, is divided at the point of electrical neutrality (P_{el}), the Golden point, into two Golden sections, a_{e^-} and a_{p^+} pertaining to the electron and proton, respectively. The latter distances were obtained[1] through the relations:

$$a_B = (e/2\kappa I_H) = a_{e^-} + a_{p^+} \tag{1a}$$
$$(e/2\kappa)(1/a_B) = I_H = (1/2\kappa)[(e/a_{p^+}) - (e/a_{e^-})] \tag{1b}$$
$$(a_{e^-}/a_{p^+})^2 - (a_{e^-}/a_{p^+}) - 1 = 0, \quad (a_{e^-}/a_{p^+}) = \phi \tag{1c,d}$$
$$a_{p^+} = (a_B/\phi^2) \text{ and } a_{e^-} = (a_B/\phi) = \phi a_{p^+} \tag{1e,f}$$

where e is the charge, κ is the electrical permittivity of vacuum $e/2\kappa$ = 7.1998 Å.eV. The measured ionization potential is composed of the two components, $I_{p^+} = (e/\kappa a_{p^+})$ and $I_{e^-} = (-e/\kappa a_{e^-})$ in equation (1b). On combining equations (1a) and (1b), one obtains the Golden quadratic equation (1c), whose +ve root (see equation 1d) is the Golden ratio, (a_{e^-}/a_{p^+}) = $(1 + 5^{1/2})/2)$ = ϕ = 1.618. This ratio appears in the geometrical features of microscopic as well as macroscopic world and is called[2] The Divine Ratio. Thus, it was shown that the Golden ratio arises due to electrostatic reasons right in the core of atoms[1,3].

In the case of hydrogen, a_B = 0.53 Å and the covalent bond length (0.74 Å) in the hydrogen molecule[4], d(HH) = 2d(H) = $2^{1/2} a_B$ = $2^{1/2}(a_{e^-} + a_{p^+})$ = d(H$^-$) + d(H$^+$) is the sum of two Golden sections[1,3] of d(HH). The ionic forms, H$^+$ and H$^-$ correspond to the resonance forms of the molecule[4]. The atomic radius considered[5] as half the bond length, also called the covalent radius[4], d(H) = $a_B/2^{1/2}$ = 0.37Å, and the ionic radii, d(H$^+$) = d(HH)/ϕ^2) = 0.74/2.618 = 0.28 Å and d(H$^-$) = d(HH)/ϕ) 0.74/1.618 = 0.46 Å. (*Note*: the symbol d is used here for radii since they are apportioned distances.) These three values exactly account for the bond

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lengths of completely or partially covalent and or ionic bonds of about forty hydrides[6] and also the lengths of hydrogen bonds[7] in many inorganic and biochemical compounds. Golden ratio was also observed in the hydrogen bonds of borates[8].

1.2 The Golden ratio based ionic radii of alkali metals and halogens

In the case of the partially ionic bonds in alkali metal hydrides, it was shown[1,3] that the difference, $d(MH) - d(H^+) = d(M^+) = d(MM)/\phi^2$, where $d(MM)$ is the bond length of between the edge atoms in the metal lattice. On subtracting the above value of $d(M^+)$ from the crystal ionic distance, $d(M^+X^-)$ in the alkali halide, the radius $d(X^-)$ of the halogen anion, $(X^-) = d(XX)/\phi$, was obtained. These results showed that $d(MM) = d(M^+) + d(M^-)$ and $d(XX) = d(X^+) + d(X^-)$ are sums of two Golden sections representing the anionic and cationic radii. Thus it was found[1] that the distances, $d(M^+X^-)$ in all alkali halides are sums of the Golden ratio based ionic radii as shown,

$$d(M^+) = d(MM)/\phi^2, \quad d(X^-) = d(XX)/\phi \quad \text{and} \quad d(MX) = d(M^+) + d(X^-) \tag{2a-c}$$

where the inter-metallic bond length, $d(MM) = a$, the lattice parameter for the bcc lattice of the alkali metals and $d(XX)$ is the bond length in the diatomic halogen molecules.

1.3 Atomic radii and Golden ratio based ionic radii and additivity of radii in chemical bonds

The above led to the general finding[1,3,6] that the bond length $d(AA)$ between two atoms (A) of the same kind is divided at the Golden point into two Golden sections, $d(A^-)$ and $d(A^+)$, which form the anionic (A^-) and cationic (A^+) radii of atoms as shown below,

$$d(AA) = 2d(A) = d(A^-) + d(A^+) \tag{3a}$$
$$d(A^+) = d(AA)/\phi^2 = (2/\phi^2)d(A) \quad \text{and} \quad d(A^-) = d(AA)/\phi = (2/\phi)d(A) \tag{3b,c}$$
$$d(A^+) < d(A) < d(A^-) = (2/\phi^2) < 1 < (2/\phi) = 0.764 < 1 < 1.236 \tag{3d}$$

where the atomic radius, $d(A) = d(AA)/2$ is defined[4] as the covalent radius. The radii increase, as pointed out[4] in the order shown in equation (3d).

Soon the general additivity rule of covalent radii and or the Golden ratio based ionic radii was established for bond lengths between two different atoms, $d(AB)$, in many inorganic, organic and biological molecules, see e.g.,[9] (a full list of publications is in http://www.jh-inst.cas.cz/~rheyrovs).

The Golden ratio was also observed in the sizes of ions and ion-water distances in aqueous solutions[10,11].

1.4. More on ionization potentials, correlation with aqueous redox potentials and dependence of various atomic radii on Bohr radii.

Further, linear relations between gaseous ionization potentials and aqueous redox potentials helped to establish the absolute $a_B = e/2\kappa I_1$

aqueous redox potentials of elements[12,13] and to obtain Golden ratio dependent radii of redox components in solutions[14]. In another paper[15], linear correlations between Bohr radii, a_B obtained from the first ionization potentials (I_1) of the atoms and various radii of atoms, including the covalent atomic radii, $d(A)$ obtained from lattice constants and bond lengths $d(AA)$, were demonstrated.

2. Present work: atomic and ionic radii of elements related to Bohr radii through the Golden ratio.

Here, another fundamental observation is reported connecting two different properties, namely the atomic radii obtained from lattice parameters and bond lengths with the Bohr radii obtained[15] from the first ionization potentials, as in the case of hydrogen, from the equation,

$$\tag{4}$$

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The Golden sections of the Bohr radii of atoms are related as follows,

$$a_B = a_{e^-} + a_{n+}, \quad a_{e^-} = a_B/\phi \quad \text{and} \quad a_{n+} = a_B/\phi^2 \qquad \text{(5a-c)}$$
$$a_{e^-} = \phi a_{n+} \quad \text{and} \quad a_B = \phi a_{e^-} = \phi^2 a_{n+} \qquad \text{(5d,e)}$$

where a_{e^-} and a_{n+} are the Golden sections of a_B, representing the radius of the electron and of the nucleus A_{n+}. These distances are shown as the radii of the corresponding circles in Fig. 1a for Li.

On comparing them with the covalent, anionic and cationic radii, $d(A)$, $d(A^-)$ and $d(A^+)$ respectively, one finds that the Golden ratio connects them all, as shown in Fig. 1b for Li. It is interesting to note that the nucleus with radius, a_{n+} and electron of radius a_{e^-} exactly fit the square with the edge atoms of the bcc lattice of Li. Thus the electron corresponding to the first ionization potential of the atom (A) is found to have its own space identity in the lattice.

The above finding was found to hold also for other members of the Group 1A elements. The radii $d(A)$ in Table 1 were obtained using bond lengths and lattice parameters from[1,16], and the Bohr radii calculated from the data[17] on first ionization potentials are also given in Table 1. Figs. 2 show the dependences of the atomic, ionic and Bohr radii (data in Table 1) on the Golden ratio for elements of Group 1A. In all these cases, the atomic radii were found to be directly proportional to their Bohr radii as shown by the simple equation,

$$d(A) = d(AA)/2 = K_\phi a_B \qquad \text{(6)}$$

where K_ϕ is a constant (see Fig. 2 and Table 1) depending on the Golden ratio.

On investigating further the dependence of the atomic and ionic radii of the elements of Groups 2A - 8A, similar results were obtained. Fig. 2 shows the atomic, ionic and Bohr radii for all these elements. Corresponding data are given in Table 1. The values of $d(A)$, $d(A^-)$ or $d(A^+)$, coincide with a_B, $a_B\phi$, or other Golden ratio multiples of a_B, and these values are underlined in Table 1. It can be seen that in every case K_ϕ is a simple function of the Golden ratio and that each group of elements show some trends. The last column in Table 1 gives the values of $d(A)_{cal}$ calculated as per equation (6). Fig. 3 shows a plot of $d(A)_{cal}$ vs $d(A)$ for the atoms of all the Groups 1A - 8A elements. The least square line shows the good correspondence with equation (6) and thereby it can be seen that the atomic, ionic and Bohr radii are all linked in a simple way through the Golden ratio. Fig. 4 shows a graph of $d(A)$ vs a_B for the various values of K_ϕ.

The observation here that the electron is an entity of its own kind supports similar views in the work on solvated electrons[18] and on electrides[19]. Most notable works on the Golden ratio in molecular structures is the work by Shechtman[20] and by Coldea[21]. The structures of the compounds in the latter work with Golden ratio based ionic radii can be seen in[22].

Thus, it can be concluded that the Golden ratio connects lattice parameters, bond lengths and atomic and ionic radii with the Bohr radii of atoms and is therefore a fundamental geometrical constant in atomic structure and physics.

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Figure legends

Figure 1. a) The Bohr circle of radius, $a_B = (e/2\kappa I_1)$ for Li and its Golden sections, a_{e^-} and a_{n+} pertaining to the electron and nucleus, respectively, b) the four edge atoms in Li (bcc). Bond length $d(AA)$, and its Golden sections, $d(A^+)$, and $d(A^-)$ pertaining to the (resonance forms, A^+, A^-) cation and anion respectively.

Figure 2: **Groups 1A - 8A.** Comparison of atomic and ionic radii with the Bohr radii for elements. The circles A^+ (pink dashes), A (black full line) and A^- (blue dashes) have cationic, covalent and anionic radii, $d(A^+)$, $d(A)$ and $d(A^-)$ respectively. The circles e^- (blue dots), A_B (black dots) and A_{n+} (pink dots) have radii, $a_{e^-} = a_B/\phi$, a_B (Bohr radius) and $a_{n+} = a_B/\phi^2$. All are drawn to scale.

Figure 3. Linear correlation of calculated values of atomic radii, $d(A)_{cal}$ with the observed values, $d(A) = d(AA)/2$.

Figure. 4. Linear graphs of atomic radii, $d(A)$ vs Bohr radii, a_B, for elements of Groups 1A- 8A for various values of K_ϕ

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Figure 1

b) Li (bcc, 4 edge atoms): $a_B = 1.34$ Ǎ, d(A) = 1.75 Ǎ,
$d(A^+) = a_B$; $d(A^-) = a_B + a_{e-} = a_B\phi$; $d(AA) = d(A^+) + d(A^-) = a_B\phi^2$

d(A⁻) $P_{el,B}$ $P_{el,A}$ a_B d(A⁺)

a) Bohr circle, A_B
(a_{e-}, P_{el}, a_{n+}, A_B)

$a_{e-} + a_{n+} = a_B$

$a_{e-} = a_B/\phi$
$a_{n+} = a_B/\phi^2$
$\phi = (1+5^{1/2})/2$
$= 1.618$

d(AA) = 2d(A)

Figure 2 Group 1A

Group 1A: a) H, (d(A) = 0.37 Å) b) Li, (1.75), c) Na (1.83), d) K (2.26), e) Rb (2.79), f) Cs (3.02)

Bohr circle A_B, radius = a_B = a_{e-} + a_{n+}, A_B, A

A_B, A^+, A, A^-

H_2

a) H, d(A) = d(AA)/2 = $a_B/2^{1/2}$, b) Li, d(A) = $(\phi^2/2)a_B$

c) Na, d(A) = $(\phi^2/2)a_B$

d) K, d(A) = $(1+1/\phi^2)a_B$

e) Rb, d(A) = ϕa_B

f) Cs, d(A) = ϕa_B

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Figure 2 Group 2A

Group 2A: a) Be (d(A) = 1.11 Å), b) Mg (1.60), c) Ca (1.98), d) Sr (2.15), e) Ba (2.51)

a) Be, d(A) = $(1+1/\phi^2)a_B$, b) Mg, d(A) = ϕa_B c) Ca, d(A) = ϕa_B

d) Sr, d(A) = ϕa_B, e) Ba, d(A) = $(\phi^2+1)a_B/2$

Figure 2 Groups 3A and 4A

Group 3A: a) B (d(A) = 0.89 Å), b) Al (2.02), c) Ga (1.60), d) In (1.63), e) Tl (1.22)

a) B, d(A) = a_B, b) Al, d(A) = ϕa_B, c) Ga, d(A) = $(\phi^2/2)a_B$

d) In, d(A) = $(\phi^2/2)a_B$, e) Tl, d(A) = a_B

Group 4A: a) C (0.71 Å), b) Si (1.18 Å), c) Ge (1.23 Å), d) Sn(1.41 Å)

a) C, d(A) = $a_B(1+\phi^2)/2\phi$, b) Si, d(A) = $(\phi^2/2)a_B$, c) Ge and d) Sn, d(A) = $(1+1/\phi^2)a_B$

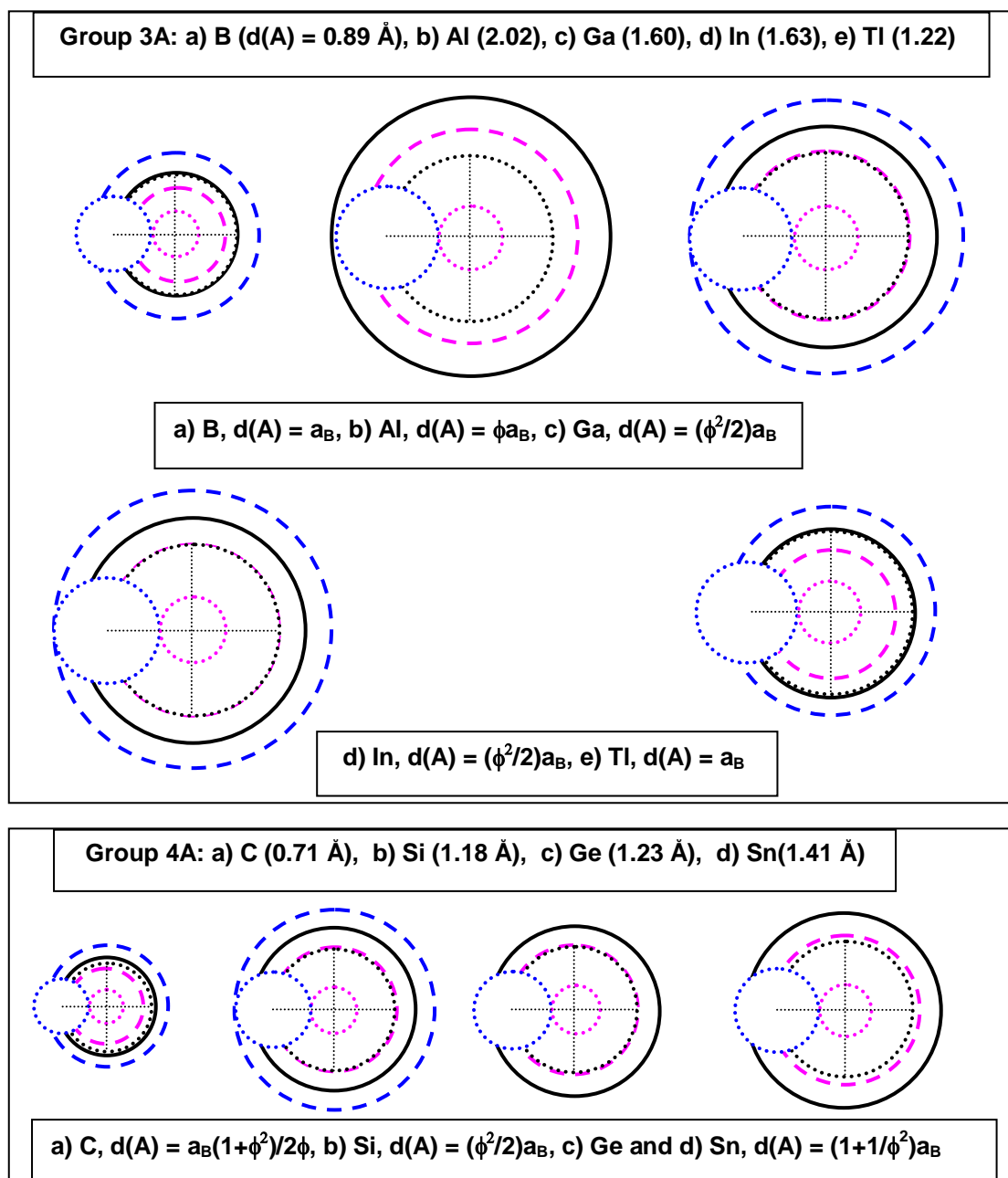**Figure 2 Groups 5A, 6A, 7A and 8A**

Group 5A: a) N (0.55 Ǎ), b) P (1.11 Ǎ), c) As (1.25 Ǎ), d) Sb (1.45 Ǎ)

a) N, d(A) = $a_B(1+\phi^2)/2\phi$, b) P and c) As, d(A) = ϕa_B, d) Sb, d(A) = $(\phi^2+1)a_B/2$

Group 6A: a) O (d(A) = 0.60 Ǎ), b) S (1.03 Ǎ), c) Se (1.16 Ǎ), d) Te (1.43 Ǎ), e) Po (1.68 Ǎ)

a) O, d(A) = $a_B(1+\phi^2)/2\phi$, b) S, d(A) = $(1+1/\phi^2)a_B$, c) Se and d) Te, d(A) = $(\phi^2+1)a_B/2$, e) Po, d(A) = $2a_B$

Group 7A: a) F (d(AA) = 0.71 Ǎ), b) Cl (0.99 Ǎ), c) Br (1.11 Ǎ), d) I (1.28 Ǎ)

a) F, b) Cl, c) Br and d) I, d(A) = $(\phi^2+1)a_B/2$

Group 8A: a) He (0.46 Ǎ), b) Ne (0.67 Ǎ), c) Ar (0.96 Ǎ), d) Kr (1.17 Ǎ), e) Xe (1.31 Ǎ)

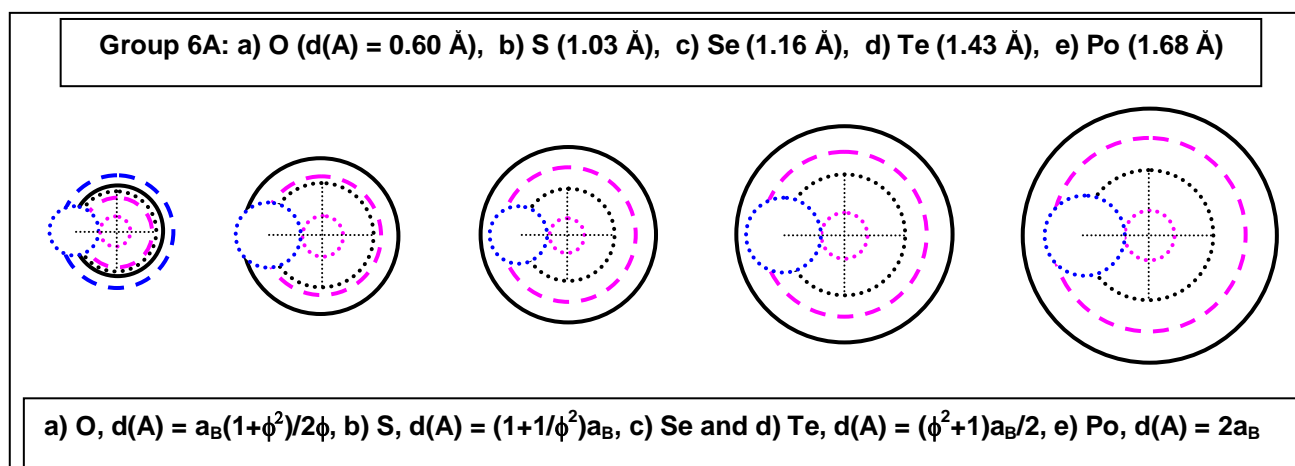a) He, d(A) = ϕa_B, b) Ne, c) Ar, d) Kr and e) Xe, d(A) = $\phi^3 a_B/2$
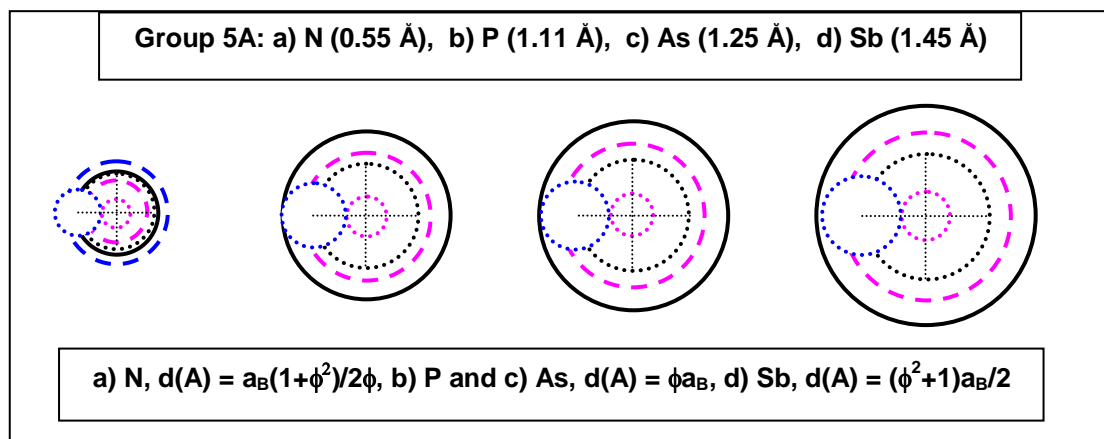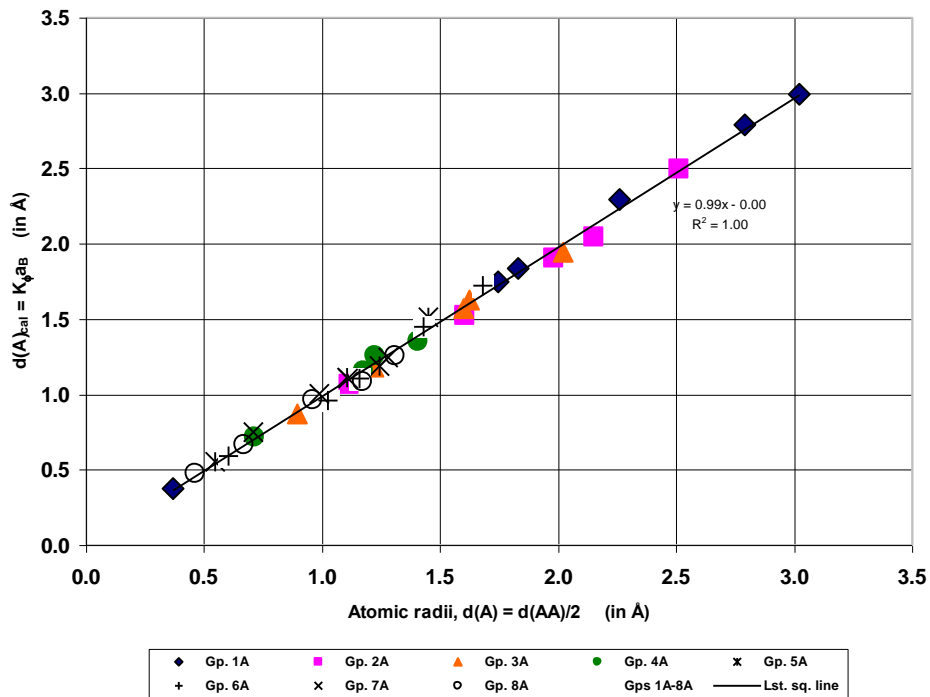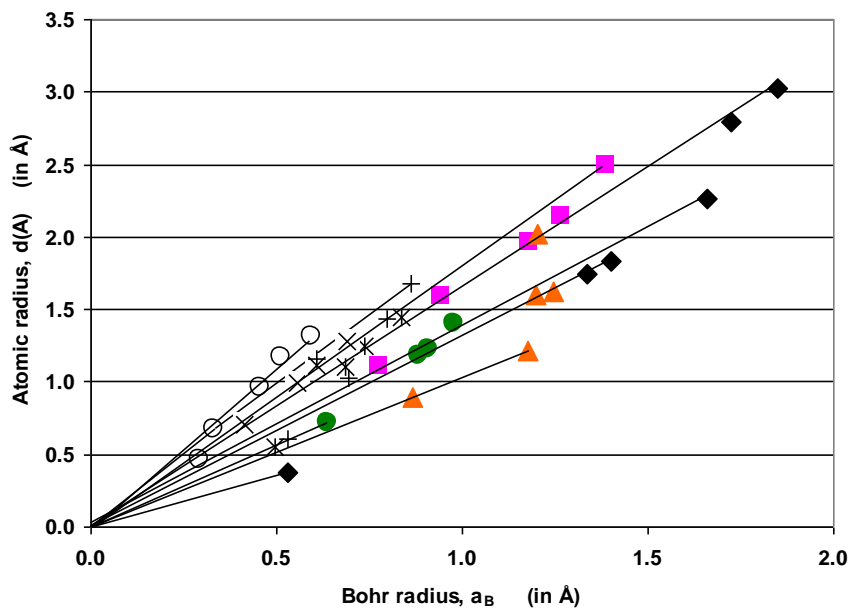
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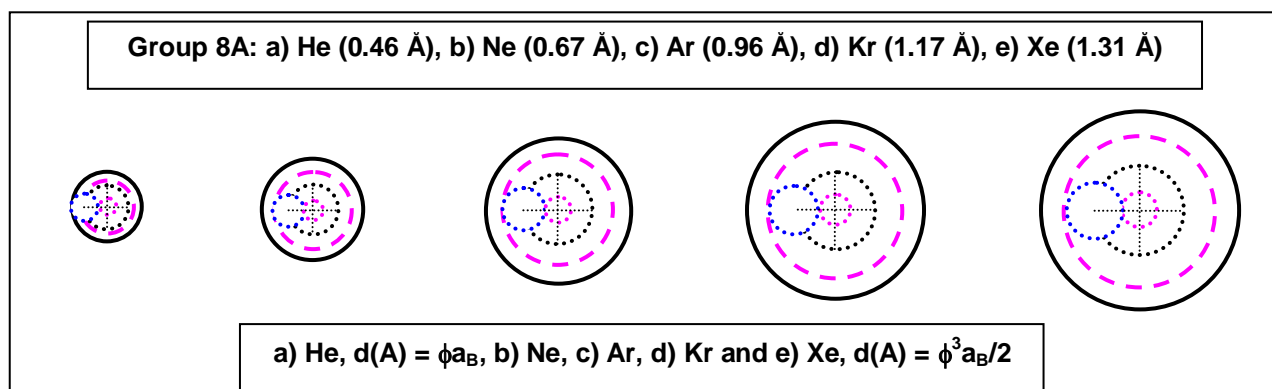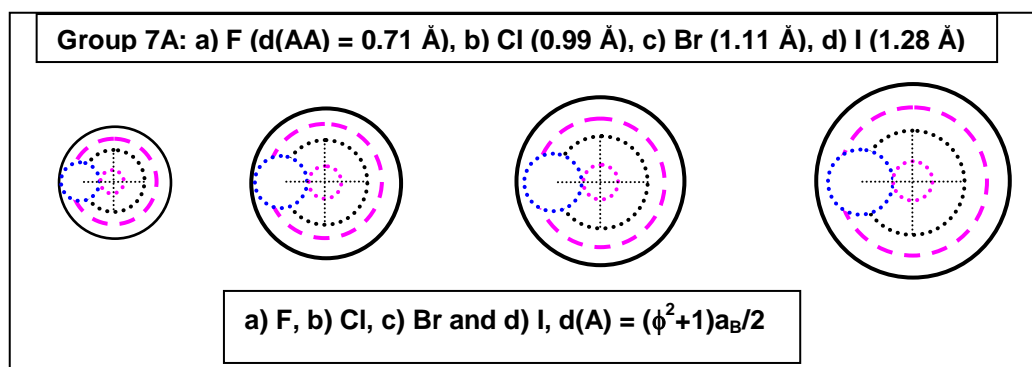
Figure 3

Figure 4

Table 1. Covalent radii, d(A) = d(AA)/2 of atoms (A) of elements of Groups 1A - 8A, related to Bohr radii (a_B) obtained from 1st ionization potentials, I_1, through the Golden ratio, ϕ (= 1.618). Ionic radii, $d(A^-)$ = d(AA)/ϕ and $d(A^+)$ = d(AA)/ϕ^2. $d(A)_{cal}$ = $K_\phi a_B$. Bohr radius, a_B = (e/2κI_1), radius a_{e^-} = a_B/ϕ of the electron (e⁻) and a_{n+} = a_B/ϕ^2 of the nucleus (A_{n+}) of A. All radii in Å.

Gp. 1A	I_1	a_B	d(A)	d(A⁻)	d(A⁺)	a_{e-}	a_{n+}	$a_B(1+1/\phi)$	$a_B(1+1/\phi^2)$	K_ϕ	K_ϕ	$d(A)_{cal}$
H	13.598	0.53	**0.37**	0.46	0.28	0.33	0.20	0.86	0.73	$1/2^{1/2}$	0.707	**0.37**
Li	5.392	1.34	**1.75**	2.16	1.33	0.83	0.51	2.16	1.85	$\phi^2/2$	1.309	**1.75**
Na	5.139	1.40	**1.83**	2.26	1.40	0.87	0.54	2.27	1.94	$\phi^2/2$	1.309	**1.84**
K	4.341	1.66	**2.26**	2.80	1.73	1.03	0.63	2.68	2.29	$(\phi^2+1)/\phi^2$	1.382	**2.29**
Rb	4.177	1.72	**2.79**	3.45	2.13	1.07	0.66	2.79	2.38	ϕ	1.618	**2.79**
Cs	3.894	1.85	**3.02**	3.74	2.31	1.14	0.71	2.99	2.56	ϕ	1.618	**2.99**
Gp. 2A												
Be	9.323	0.77	**1.11**	1.38	0.85	0.48	0.29	1.25	1.07	$(\phi^2+1)/\phi^2$	1.382	**1.07**
Mg	7.646	0.94	**1.60**	1.98	1.23	0.58	0.36	1.52	1.30	ϕ	1.618	**1.52**
Ca	6.113	1.18	**1.98**	2.45	1.51	0.73	0.45	1.91	1.63	ϕ	1.618	**1.91**
Sr	5.695	1.26	**2.15**	2.66	1.64	0.78	0.48	2.05	1.75	ϕ	1.618	**2.05**
Ba	5.212	1.38	**2.51**	3.10	1.92	0.85	0.53	2.24	1.91	$(\phi^2+1)/2$	1.809	**2.50**
Gp. 3A												
B	8.298	0.87	**0.89**	1.11	0.68	0.54	0.33	1.40	1.20	1.00	1	**0.87**
Al	5.986	1.20	**2.02**	2.50	1.55	0.74	0.46	1.95	1.66	ϕ	1.618	**1.95**
Ga	5.999	1.20	**1.60**	1.98	1.22	0.74	0.46	1.94	1.66	$\phi^2/2$	1.309	**1.57**
In	5.786	1.24	**1.63**	2.01	1.24	0.77	0.48	2.01	1.72	$\phi^2/2$	1.309	**1.63**
Tl	6.108	1.18	**1.22**	1.51	0.93	0.73	0.45	1.91	1.63	1.00	1	**1.18**
Gp. 4A												
C	11.260	0.64	**0.71**	0.88	0.54	0.40	0.24	1.03	0.88	$(\phi^2+1)/2\phi$	1.118	**0.72**
Si	8.152	0.88	**1.18**	1.45	0.90	0.55	0.34	1.43	1.22	$\phi^2/2$	1.309	**1.16**
Ge	7.899	0.91	**1.23**	1.51	0.94	0.56	0.35	1.47	1.26	$(\phi^2+1)/\phi^2$	1.382	**1.26**
Sn	7.344	0.98	**1.41**	1.74	1.07	0.61	0.37	1.59	1.35	$(\phi^2+1)/\phi^2$	1.382	**1.35**
Gp. 5A												
N	14.534	0.50	**0.55**	0.68	0.42	0.31	0.19	0.80	0.68	$(\phi^2+1)/2\phi$	1.118	**0.55**
P	10.487	0.69	**1.11**	1.37	0.84	0.42	0.26	1.11	0.95	ϕ	1.618	**1.11**
As	9.789	0.74	**1.25**	1.54	0.95	0.45	0.28	1.19	1.02	ϕ	1.618	**1.19**
Sb	8.608	0.84	**1.45**	1.79	1.11	0.52	0.32	1.35	1.16	$(\phi^2+1)/2$	1.809	**1.51**
Gp. 6A												
O	13.618	0.53	**0.60**	0.75	0.46	0.33	0.20	0.86	0.73	$(\phi^2+1)/2\phi$	1.118	**0.59**
S	10.360	0.69	**1.03**	1.27	0.78	0.43	0.27	1.12	0.96	$(\phi^2+1)/\phi^2$	1.382	**0.96**
Se	11.814	0.61	**1.16**	1.43	0.89	0.38	0.23	0.99	0.84	$(\phi^2+1)/2$	1.809	**1.10**
Te	9.010	0.80	**1.43**	1.77	1.09	0.49	0.31	1.29	1.10	$(\phi^2+1)/2$	1.809	**1.45**
Po	8.414	0.86	**1.68**	2.08	1.28	0.53	0.33	1.39	1.19	2.00	2	**1.72**
Gp. 7A												
F	17.423	0.41	**0.71**	0.88	0.54	0.26	0.16	0.67	0.57	$(\phi^2+1)/2$	1.809	**0.75**
Cl	12.968	0.56	**0.99**	1.22	0.76	0.34	0.21	0.90	0.77	$(\phi^2+1)/2$	1.809	**1.00**
Br	11.814	0.61	**1.11**	1.37	0.85	0.38	0.23	0.99	0.84	$(\phi^2+1)/2$	1.809	**1.10**
I	10.451	0.69	**1.28**	1.58	0.98	0.43	0.26	1.11	0.95	$(\phi^2+1)/2$	1.809	**1.25**
Gp. 8A												
He	24.587	0.29	**0.46**	0.57	0.35	0.18	0.11	0.47	0.40	ϕ	1.618	**0.47**
Ne	21.565	**0.33**	**0.67**	0.83	0.51	0.21	0.13	0.54	0.46	$\phi^3/2$	2	**0.67**
Ar	15.760	0.46	**0.96**	1.19	0.73	0.28	0.17	0.74	0.63	$\phi^3/2$	2.118	**0.97**
Kr	14.000	0.51	**1.17**	1.45	0.89	0.32	0.20	0.83	0.71	$\phi^3/2$	2.118	**1.09**
Xe	12.130	0.59	**1.31**	1.62	1.00	0.37	0.23	0.96	0.82	$\phi^3/2$	2.118	**1.26**