Bohr Radius as the Sum of Golden Sections Pertaining to the Electron and Proton, Covalent Bond Lengths Between Same Two Atoms as Exact Sums of Their Cationic and Anionic Radii and Additivity of Atomic and or Ionic Radii in Bond Lengths

– Collected work dedicated to Johannes Kepler (1571 - 1630).

Raji Heyrovska

Private Research Scientist (present), Academy of Sciences of the Czech Republic (past).

E-mail: rheyrovs@hotmail.com

Abstract.

The author has shown over a decade ago that the energy of the hydrogen atom is actually positive (not negative as per Bohr). In Bohr's treatment, the energy amounts to half the Coulombic energy between an electron and a proton, and hence is negative. The present author considered an alternate approach: the ionization potential as the difference in the potentials of the electron and proton at a distance of the Bohr radius. This makes the energy positive and it has the same magnitude as given by Bohr's equation. Moreover, Bohr radius was found to be divided into two Golden sections pertaining to the proton and electron. Further, all covalent bond lengths amounted to exact sums of the Golden ratio based cationic and anionic radii. Bond lengths were shown to be simple sums of atomic and ionic radii. This article is a collection of the author's work.

1. Introduction

The author sent a copy of her first publication on the Golden ratio [1] right in the core of the atom to a renowned scientist (Prof. D.R. Herschbach), the reply came back saying that ‘Kepler will be pleased.’ So this collected work is dedicated to Johannes Kepler: *”Geometry has two great treasures: one is the theorem of Pythagoras, the other the division of a line into mean and extreme ratio. The first we may compare to a mass of gold, the second we may call a precious jewel.” - On the Golden ratio, by J. Kepler*.

The negative sign for the energy of hydrogen atom in the Bohr’s model [2] has been irking the author’s conscience for long as well as other’s [3]. While working on electrode potentials, which are considered as the difference between the potentials of the anode (+ve) and the cathode (-ve), it occurred to the author to treat the ionization potential of hydrogen in a similar way. Thus, on dividing the ionization potential into two parts, one pertaining to the proton (+ve) and the other to the electron (-ve), a surprising result was obtained. It was found that the ionization energy is actually positive and that the Bohr radius has two Golden sections. This gave rise to amazing simplicity in the interpretation of ionic radii and bond lengths in general in small as well as large molecules [4 - 8]. This is explained briefly below and the author’s work confirming this approach for various molecules can be found in [4 - 43].

2. Bohr’s model modified

In the Bohr’s model [2], the ground state energy (E_H) of the hydrogen atom, considered as the sum of the kinetic energy and potential energy (Coulombic energy), is given by

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

which is half the Coulombic energy, $-e^2/\kappa a_B$ of two opposite charges at a distance, a_B (= Bohr radius) where e is the electric charge and κ is the electric constant. This energy is negative, since the Coulombic energy is negative.

The ground state energy (E_H), ionization potential (I_H) and Bohr radius are related by the equation,

$$E_H = eI_H \text{ where } E_H/e = I_H = (1/2)(e/\kappa a_B) \qquad (2)$$

The negative sign in Eq (1) for the energy of hydrogen implies that the energy of the Universe which consists of more than 70% hydrogen is negative! This bothered the author's conscience and therefore the author considered [37] an alternate approach to the ionization energy: as the energy needed to pull apart the proton and electron from each other. The ionization potential (I_H) could thus be expressed as the absolute difference between those of the proton (I_p) and the electron (I_e). Thus, on dividing the Bohr radius into two segments a_p and a_e pertaining to the proton and electron respectively, where $a_B = a_p + a_e$, the following relations were obtained:

$$I_H = e/(2\kappa a_B) = (e/2\kappa a_p) – (e/2\kappa a_e) \qquad (3)$$

$$I_p = (e/2\kappa a_p) \text{ and } I_e = (-e/2\kappa a_e) \qquad (4a,b)$$

$$1/a_B = 1/(a_p + a_e) = (1/a_p) – (1/a_e) \qquad (5)$$

On rewriting Eq. 5 in terms of the ratio (a_e/a_p), one gets the Golden quadratic,

$$(a_e/a_p)^2 - (a_e/a_p) - 1 = 0 \qquad (6)$$

$$(a_e/a_p) = (1+5^{1/2})/2 = \phi = 1.618..\ \text{(Golden ratio!)} \qquad (7)$$

$$a_e = a_B/\phi \ \&\ a_p = a_B/\phi^2 \ \text{(Golden sections.)} \qquad (8a,b)$$

whose solution is ϕ, the Golden ratio, a mathematical constant, found in the geometry of many spontaneous creations in the Universe [1]! Thus, it was found that ***Bohr radius has two Golden sections pertaining to p^+ & e^-***!

The ionization energy, $E_H = eI_H = (1/2)(e^2/\kappa a_B)$ as given by Eq. (2) can also be interpreted as the electromagnetic energy of a condenser with two unit charges of opposite sign at a distance of the Bohr radius from each other and with κa_B as the capacity. Note also from Eq. (3) that the ground state energy, $E_H = eI_H$ is the difference between two terms, as found in spectroscopy [8].

3. **Golden ratio based ionic radii and the Golden cascade**

3.1. Bohr radius:

$$a_B = (a_B/\phi) + (a_B/\phi^2) = \text{Bohr radius (Hydrogen atom)} \qquad (9)$$

3.2. Hydrogen molecule:

$$d(HH)_{obs} = 0.74Å = 2^{1/2}a_B = 2^{1/2}(a_B/\phi + a_B/\phi^2) = R_{H+} + R_{H-}; \quad (10)$$

$$R_{H+} = 2^{1/2} a_B/\phi^2 = 0.28Å; R_{H-} = 2^{1/2} a_B/\phi = 0.74 - 0.28 = 0.46Å \quad (11a,b)$$

This (0.28Å) is amazingly exactly the value Pauling [44] suggests empirically for H in hydrogen halides, HX (!). So actually it is the Golden ratio based radius of the cation, H^+, which Pauling was not aware of.

3.3. Hydrogen halides: **HX**

$$d(HX)_{obs} - R_{H+} = d(XX)/2 = R_X \text{ (= the covalent radii of X in HX)} \quad (12)$$

$$d(HX)_{obs} = R_{H+} + R_X ; \quad (13)$$

Therefore, the 'partial ionic character' [44] of HX bond is due to H^+. Also note that ionic and atomic covalent radii are additive!

3.4. Alkali metal hydrides: **MH**

$$d(MH)_{obs} - R_{H+} = R_{M+} = L(MM)/\phi^2 = d(MM)/\phi^2 \quad (14)$$

which is the Golden ratio based cationic radii of alkali metals (M), where L is the edge length of the metal cubic lattice. Therefore, the 'ionic character' [44] of MH bonds is due to M^+ & H^+.

3.5. Alkali halides: MX

$$d(MX)_{obs} - R_{M+} = R_{X-} = d(XX)/\phi \quad (15)$$

which is the Golden ratio based anionic radii of X in alkali halides, MX

$$d(MX)_{obs} = d(MX)_{cal} = R_{M+} + R_{X-} \quad (16)$$

Therefore, note that Pauling's 'radius ratio corrections' are not needed to account for the observed crystal ionic distances, d(MX)! When the author found to her surprise more than a decade ago the two sections of the Bohr radius in the Golden ratio, a mathematical constant right in the architecture of the atom (!), she couldn't believe it and did not publish it till she could explain the crystal ionic distances in all the alkali halides. See the perfect additivity of radii for all alkali halides in Figs. in [8, 37] and in the power point slides in [35].

3.6. Bond length between atoms of the same kind: d(AA)

$$d(AA) = 2R_A = R_{A+} + R_{A-}; \quad (17)$$

$$R_{A+} = d(AA)/\phi^2 = 0.764d(A) \text{ and } R_{A-} = d(AA)/\phi = 1.236\delta(A) \quad (18a,b)$$

$$R_{A+} : R_A : R_{A+} = 0.382 : 1 : 0.618 \quad (19)$$

where R_A is the covalent radius and R_{A+} and R_{A-} are the Golden ratio based ionic radii of the ionic resonance forms (Pauling, [44]) of A.

3.7. All bond lengths d(AB) are exact sums of the atomic and or Golden ratio based ionic radii, R_A, R_{A+}, R_{A-}, R_B, R_{B+} and R_{B-}

These are described for many molecules and bonds including hydrogen bonds in [4-43]. Pauling pointed out that covalent radii are additive but was not aware that covalent radii of different valence are also additive. Therefore he failed to explain many covalent bond lengths. A review of the author's work is in the power point lecture in [35].

References:

1. M. Livio, M. *The Golden Ratio, the story of phi, the world's most astonishing number*. Broadway Books, New York, 2002.

2. https://en.wikipedia.org/wiki/Bohr_model

3. E. A. Moelwyn Hughes, *Physical Chemistry*, Pergamon Press, London New York, 1957.

4. R. Heyrovska, Hydrogen as an atomic condenser.
35th Meeting of DAMOP, APS, Tucson, AZ, May 2004, Poster, Abstract: P-132.
http://flux.aps.org/meetings/YR04/DAMOP04/baps/abs/S400132.html

5. R. Heyrovska, The decisive role of the Golden ratio in atomic dimensions.
35th Meeting of DAMOP, APS, Tucson, AZ, May 2004, Poster, Abstract P-133.
http://flux.aps.org/meetings/YR04/DAMOP04/baps/abs/S400133.html

6. R. Heyrovska,The Golden ratio, atomic, ionic and molecular capacities and bonding distances in hydrides.

2004 International Joint meeting of ECS, USA and Japanese, Korean and Australian Societies, Honolulu, Hawaii, October 2004, Vol. 2004 - 2, Extended. Abs. C2-0551.

http://www.electrochem.org/dl/ma/206/pdfs/0551.pdf

7. R. Heyrovska, Exploring the atomic properties using ionization potential and the Golden ratio.

V pracovního setkání fyzikálních chemiků a elektrochemiků, Masarykova univerzita v Brně, Unor, 8, 2005 (Vth Working Meeting of Physical Chemists and Electrochemists, Masaryk University, Brno, February 2005), Book of Abstracts, p. 32-33. (In English),

http://cheminfo.chemi.muni.cz/ktfch/Setkani05/Sbornik2005.pdf;

8. R. Heyrovska, The Golden ratio, ionic and atomic radii and bond lengths.

Special Issue of Molecular Physics, 103 (2005) 877 - 882.

9. R. Heyrovska and S. Narayan, Fine structure constant, anomalous magnetic moment, relativity factor and the Golden ratio that divides the Bohr radius

arXiv:physics/0509207 [pdf] (2005).

10. R. Heyrovska, Dependence of ion-water distances on covalent radii, ionic radii in water and distances of oxygen and hydrogen of water from ion/water boundaries.

Chemical Physics Letters, 429 (2006) 600 - 605.

11. R. Heyrovska, Dependence of the length of the hydrogen bond on the covalent and cationic radii of hydrogen, and additivity of bonding distances.

Chemical Physics Letters, 432 (2006) 348 - 351.

12. R. Heyrovska, Dependences of molar volumes in solids, partial molal and hydrated ionic volumes of alkali halides on covalent and ionic radii and the Golden ratio. *Chemical Physics Letters*, 436 (2007) 287 - 293.

13. R. Heyrovska and S. Narayan, Atomic structures of molecules based on additivity of atomic and/or ionic radii.

AIP Conference Proceedings 1119 (2009) 216; Editor(s): Beverly Karplus Hartline, Renee K. Horton, Catherine M. Kaicher.3rd IUPAP International Conference on Women In Physics 2008, Seoul, South Korea, 7th -10th of October, 2008;

Nature Precedings http://precedings.nature.com/documents/3292/version/1 (2009).

14. R. Heyrovska, Various carbon to carbon bond lengths inter-related via the Golden ratio, and their linear dependence on bond energies.

arXiv:0809.1957 [pdf] (2008)

15. R. Heyrovska, The Golden ratio in the creations of Nature arises in the architecture of atoms and ions.

Proceedings of the 9th Eurasia Conference on Chemical Sciences, Antalya, Turkey, September 2006: Chapter 12 in Book: *"Innovations in Chemical Biology"*, Editor: Bilge Sener, Springer.com, January 2009: (Full text of Invited Lecture)

16. R. Heyrovska, Golden sections of interatomic distances as exact ionic radii and additivity of atomic and ionic radii in chemical bonds.

arXiv:0902.1184 [pdf] (2009)

17. R. Heyrovska, Golden sections of inter-atomic distances as exact ionic radii of atoms.

Nature Precedings, http://precedings.nature.com/documents/2929/version/1 (2009). See also the ref. above.

18. R. Heyrovska, Bonding distances as exact sums of the radii of the constituent atoms in nanomaterials - Boron Nitride and Coronene.

arXiv:1004.2667 [pdf] (2010); http://arxiv.org/abs/1004.2667v2

19. R. Heyrovska, L. Atchison, S. Narayan, Precise atomic structures of three novel nanomaterials in nanotechnology, biomedicine and cosmology: Graphene, Boron Nitride and Coronene.

The Nanomaterials Symposium, 19 April, 2010, JHU/APL Kossiakoff Center, MD. (Poster);

Nature Precedings (2010) http://precedings.nature.com/documents/4357/version/1;

http://dx.doi.org/10.1038/npre.2010.4357

20. R. Heyrovska, L. Atchison and S. Narayan, Precise atomic structures of two important molecules in biochemistry: Ascorbic acid (vitamin C) and aspirin (acetyl salicylic acid)

International Year of Chemistry 2011, ACS Spring Meeting March 2011, Anaheim, CA, USA. (Poster)

Nature Precedings (2011) http://precedings.nature.com/documents/5966/version/1;

21. R. Heyrovska, Atomic and molecular structures of positronium, dipositronium and positronium hydride

Nature Precedings (2011) http://precedings.nature.com/documents/6290/version/1

http://dx.doi.org/10.1038/npre.2011.5966.1

22. R. Heyrovska, Precise molecular structures of Cysteine, Cystine, Hydrogen-Bonded Dicysteine, Cysteine Dipeptide, Glutathione and Acetyl Cysteine based on additivity of atomic radii.

Nature Precedings (2011) http://precedings.nature.com/documents/6692/version/1

23. R. Heyrovska, Structures at the atomic level of Cobalt, Zinc and Lead Niobates (with an Appendix: Atomic structure of cobalt niobate crystal).

Nature Precedings <http://hdl.handle.net/10101/npre.2011.6059.2> (2011)

24. R. Heyrovska and S. Narayan, Structures of molecules at the atomic level: Caffeine and related compounds

Philippine Journal of Science, 140(2): 119-124, 2011 (Full paper in English)

25. R. Heyrovska, New insight into DNA damage by cisplatin at the atomic scale

Nature Precedings (2012) http://precedings.nature.com/documents/6891/version/1

Invited talk: The 12th Eurasia Conference on Chemical Sciences, Corfu, Greece, April 16-21, 2012. Abstract in:

http://eurasia12.uoi.gr/Abstracts_pdf/%281%29%20Bioinorganic/S1%20ORAL/OP8_Abstract_Heyrovska_Eurasia12.pdf

Photo: http://eurasia12.uoi.gr/images/photos/conf/P4162678.JPG

26. R. Heyrovska, Atomic and ionic radii of elements and Bohr radii from ionization potentials are linked through the Golden ratio.

International J. Sciences., Vol 2, 82-92, Issue-Mar-2013.

http://www.ijsciences.com/pub/pdf/V2-201303-19.pdf

27. R. Heyrovska, 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, NO2 and CO_2

International J. Sciences., Vol 2, 1-4, Issue-Apr-2013,

http://www.ijsciences.com/pub/pdf/V2-201304-08.pdf

28. R. Heyrovska, Atomic, ionic and Bohr radii linked via the Golden ratio for Elements including Lanthanides and Actinides.

International J. Sciences., Vol 2, 63-68, Issue-Apr-2013,

http://www.ijsciences.com/pub/pdf/V2-201304-18.pdf

29. R. Heyrovska, Atomic, ionic and Bohr radii linked via the Golden ratio for the elements in DNA: C, N, O, P and H

"XIII. Meeting of physical chemists and electrochemists "and" VII. Electrochemical Summer School", Mendel University, Brno, May 2013. Theme: "60 years DNA: 1953 - 2013 "

30. R. Heyrovska, Golden ratio based Fine structure constant and Rydberg constant for Hydrogen spectra.

International J. Sciences., Vol 2, 28-31, Issue-May-2013,

http://www.ijsciences.com/pub/pdf/V2-201305-08.pdf

31. R. Heyrovska, Bond lengths in Carbon Dioxide, Carbon Monoxide and Carbonic Acid as sums of atomic, ionic and Bohr radii. - *Dedicated to Joseph Black (April 1728 - December 1799)*

International J. Sciences., Vol 2, 30-32, Issue-Dec-2013,

http://www.ijsciences.com/pub/pdf/V220131214.pdf

32. R. Heyrovska, The Golden ratio in atomic architecture (Keynote talk)

"Shechtman International Symposium, Cancun, Mexico, 29 June - 3 July 2014";

http://www.flogen.org/ShechtmanSymposium/plenary_abst.php?page=2&p=Raji_Heyrovska&e=rheyrovs@hotmail.com&pi=124

33. R. Heyrovska, Bond lengths as exact sums of the radii of adjacent atoms and or Ions in the structures of molecules (Lead Lecture)

13th Eurasia Conference on Chemical Sciences, 14-18 December, 2014, I.I.Sc., Bangalore, India: Lead Lecture: 17th December 2014, Abstract number 165.

http://eurasia13.org/abstract-file/abstract/CTC/IL/1.pdf

34. R. Heyrovska, New interpretation of the structure and formation of ozone based on the atomic and Golden ratio based ionic radii of Oxygen

http://viXra.org/abs/1503.0269, http://vixra.org/pdf/1503.0269v1.pdf

35. R. Heyrovska, The Golden ratio, a key geometrical constant in atomic architecture (Invited talk), 113th Statistical Mechanics Conference, Rutgers University, Hill Center, May 10-12, 2015, Program of Conference, Abstract B2, p 22. Power point presentation in: https://www.researchgate.net/publication/281270357

36. R. Heyrovska, Structural insights at the atomic level of important materials: Al and Mn as special examples in honor of D. Shechtman.

http://vixra.org/abs/1506.0003; http://vixra.org/pdf/1506.0003v2.pdf

37. R. Heyrovska, Sorry Bohr, ground state energy of hydrogen atom is not negative.

http://vixra.org/abs/1506.0064; http://vixra.org/pdf/1506.0064v3.pdf

38. R. Heyrovska, Simple interpretation of the bond lengths and bond angles in stratospheric chlorine monoxide and peroxide based on atomic and ionic radii.

http://vixra.org/abs/1507.0190 ; http://vixra.org/pdf/1507.0190v1.pdf

39. R. Heyrovska, The Coulombic nature of the van der Waals bond connecting conducting graphene layers in graphite.
http://vixra.org/abs/1601.0273?ref=8736553; http://vixra.org/pdf/1601.0273v2.pdf

40. R. Heyrovska, A simple and precise interpretation of the bond lengths and angles in diborane in terms of atomic and ionic radii. - *Dedicated to Dmitri Mendeleev (8 Feb.1834 - 2 Feb 1907) on his birth anniversary.*
http://www.vixra.org/abs/1602.0091; http://www.vixra.org/pdf/1602.0091v1.pdf

41. R. Heyrovska, The Coulombic nature of the van der Waals bond connecting conducting graphene layers in graphite. - *Dedicated to geo-carbon expert, Prof. Gustaf Arrhenius, of Scripps Institution of Oceanography, CA.* (Full article)
Graphene, 5, 35-38, 2016, http://dx.doi.org/10.4236/graphene.2016.52004
Journal Cover photo in *Graphene* April 2016 issue:
http://file.scirp.org/pdf/Graphene_05_02_Content_2016022615134040.pdf

42. R. Heyrovska, Linear dependence on covalent radii of atomic and ionic radii of elements calculated by Rahm, Hoffmann and Ashcroft – *Dedicated to Alfred B. Nobel (21 Oct.1833 – 10 Dec.1896) to commemorate the 120th Anniversary of his demise*
http://vixra.org/abs/1612.0173 ; http://vixra.org/pdf/1612.0173v1.pdf

43. R. Heyrovska, 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*
http://vixra.org/abs/1612.0290 (abstract); http://vixra.org/pdf/1612.0290v1.pdf

44. L. Pauling, *The Nature of the Chemical Bond*, Cornell Univ. Press, Ithaca, 1960.