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

- Collected work dedicated to John Dalton (1766 – 1844) in commemoration of his 250th birth anniversary

Raji Heyrovska[$]

Private Research Scientist, Praha, Czech Republic. Email: rheyrovs@hotmail.com

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 bonds.

[$]Academy of Sciences of the Czech Republic (former)

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),

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

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 [5-59].

2. Additivity of atomic and ionic radii in bond lengths and structures of molecules at the atomic level [5-59]

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 Å from each other,

$$I_H = (1/2)(e/\kappa a_B) = (1/2)[(e/\kappa a_p) - (e/\kappa a_e)] \qquad (2)$$

The ionization energy, $E_H = eI_H = (1/2)(e/\kappa a_B)$ can be interpreted as the electromagnetic energy of an atomic condenser [5-9], with κa_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 [5-9],

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

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!*

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,

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

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, [5-9].

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 [5 – 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 [28], [31] and [52] respectively.

References:

1. Bohr, N. a) https://en.wikipedia.org/wiki/Niels_Bohr,

b) https://en.wikipedia.org/wiki/Bohr_model

2. Gamow, G. Thirty Years That Shook Physics. Dover, NY, 1966, p.204.

3. Pauling, L. The Nature of the Chemical Bond. Cornell Univ. Press, NY, 1960.

4. Livio, M. The Golden Ratio, the story of phi, the world's most astonishing number. Broadway Books, NY, 2002.

5. Heyrovska, R. Hydrogen as an atomic condenser

5th Meeting of DAMOP, APS, Tucson, AZ, May 2004, Poster, Abstract: P-132;

http://flux.aps.org/meetings/YR04/DAMOP04/baps/abs/S400132.html

6. Heyrovska, R. 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

7. Heyrovska, R. 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

8. Heyrovska, R. 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, pp. 32-33. (In English) http://cheminfo.chemi.muni.cz/ktfch/Setkani05/Sbornik2005.pdf

9. Heyrovska, R. The Golden ratio, ionic and atomic radii and bond lengths Molecular Physics, 103 (2005) 877 - 882. Special Issue of in honor of Nicholas Handy (Full invited paper)

10. Heyrovska, R. and Narayan, S. A New Contribution for WYP 2005: The Golden Ratio, Bohr Radius, Planck's Constant, Fine-structure Constant, and g-Factors 2nd IUPAP International Conference on Women in Physics, Rio de Janeiro, Brazil, May 2005, (Poster). Short abstract in:
http://www.sbf1.sbfisica.org.br/eventos/wp/ii/sys/resumos/R0100-2.pdf
AIP Conference Proceedings 795 (2005) 205; (Short abstract)
"WOMEN IN PHYSICS: Second IUPAP International Conference on Women in Physics", Rio de Janeiro, Brazil, 23-25 May 2005, Eds.Beverly Karplus Hartline and Ariel Michelman-Ribeiro; Published November 2005; ISBN 0-7354-0278-7.
http://proceedings.aip.org/proceedings/confproceed/795.jsp

11. Heyrovska, R. and Narayan, S. Fine-structure Constant, Anomalous Magnetic Moment, Relativity Factor and the Golden Ratio that Divides the Bohr Radius http://arxiv.org/ftp/physics/papers/0509/0509207.pdf (2005, Full paper)

12. Heyrovska, R. Linear relation between the ionic radii of alkali and halogen ions in the crystal (based on the Golden ratio and in aqueous solutions)
VI pracovního setkání fyzikálních chemiků a elektrochemiků, Masarykova univerzita v Brně, Unor, 7, 2006 (VIth Working Meeting of Physical Chemists and

Electrochemists, Masaryk University, Brno, February 2006), Book of Abstracts, pp. 38-39. http://cheminfo.chemi.muni.cz/ktfch/Setkani06/PROGRAM_2006.pdf

13. Heyrovska, R. The Golden ratio in the creations of Nature arises in the architecture of atoms and ions.
9th Eurasia Conference on Chemical Sciences, Antalya, Turkey, September 2006, Book of Abstracts, p. 37. (Invited Lecture)

14. Heyrovska, R. Dependence of the length of the hydrogen bond on the covalent and cationic radii of hydrogen, and additivity of bonding distances
Chem. Phys. Lett. 432 (2006) 348 - 351; doi:10.1016/j.cplett.2006.10.037

15. Heyrovska, R. Dependences of molar volumes in solids, partial molal and hydrated ionic volumes of alkali halides on covalent and ionic radii and the Golden ratio.
Chem. Phys. Lett. 436 (2007) 287 - 293.

16. Heyrovska, R. Linear Dependencies of Van Der Waals, Covalent and Valence Shell Radii of Atoms of Groups 1a - 8a on their Bohr Radii
http://arxiv.org/ftp/arxiv/papers/0708/0708.1108.pdf (v1)

17. Heyrovska, R. Atomic Structures of the Molecular Components in DNA and RNA based on Bond Lengths as Sums of Atomic Radii
http://arxiv.org/abs/0708.1271v1

18. Heyrovska, R. and Narayan, S. Structures of molecules at the atomic level: Caffeine and related compounds
10th Eurasia Conference on Chemical Sciences, Manila, Phillipines, 7 - 11 January 2008, Book of Abstracts, Published by the Kapisanag Kimika ng Pilipinas (Chemical Society of the Philippines, Inc.), ISBN: 978-971-93848-1-6, Abstract number O-11, page 330. (Poster).

http://eurasiachem10.philippinechem.org/assets/EuAsC2S-10FINAL.doc

http://arxiv.org/ftp/arxiv/papers/0801/0801.4261.pdf

19. Heyrovska, R. Direct dependence of covalent, van der Waals and valence shell radii of atoms on their Bohr radii for elements of Groups 1A - 8A
10th Eurasia Conference on Chemical Sciences, Manila, Phillipines, 7 - 11 January 2008, Ohtaki Memorial Lecture: Book of Abstracts, Published by the Kapisanag Kimika ng Pilipinas (Chemical Society of the Philippines, Inc.), ISBN: 978-971-93848-1-6, Abstract number OC-4-3, page 82. (Invited lecture)
http://eurasiachem10.philippinechem.org/assets/EuAsC2S-10FINAL.doc
(v2) in: http://arxiv.org/ftp/arxiv/papers/0708/0708.1108.pdf

20. Heyrovska, R. Structures of the Molecular Components in DNA and RNA with Bond Lengths Interpreted as Sums of Atomic Covalent Radii
The Open Structural Biology Journal, 2 (2008) 1 - 7;
http://www.bentham.org/open/articles.htm; (Full paper)
http://www.bentham.org/open/tosbj/openaccess2.htm (Full downloadable text); doi: 10.2174/1874199100802010001; http://arxiv.org/abs/0708.1271v4

21. Heyrovska, R. Atomic Structures of all the Twenty Essential Amino Acids and a Tripeptide, with Bond Lengths as Sums of Atomic Covalent Radii
(v2) in: http://arxiv.org/ftp/arxiv/papers/0804/0804.2488.pdf

22. Heyrovska, R. Atomic Structures of Graphene, Benzene and Methane with Bond Lengths as Sums of the Single, Double and Resonance Bond Radii of carbon
(v1) in: http://arxiv.org/ftp/arxiv/papers/0804/0804.4086.pdf

23. Heyrovska, R. Atomic Structures of Riboflavin (Vitamin B2) and its Reduced Form with Bond Lengths Based on Additivity of Atomic Radii
Full text in (v1): http://arxiv.org/ftp/arxiv/papers/0806/0806.3462.pdf

24. Heyrovska, R. Atomic Structure of Benzene Which Accounts for Resonance Energy

http://arxiv.org/ftp/arxiv/papers/0806/0806.4502.pdf

25. Heyrovska, R. Bond Energy Sums in Benzene, Cyclohexatriene and Cyclohexane Prove Resonance Unnecessary

http://arxiv.org/ftp/arxiv/papers/0807/0807.4140.pdf

26. Heyrovska, R. Various Carbon to Carbon Bond Lengths Inter-related via the Golden Ratio, and their Linear Dependence on Bond Energies

http://arxiv.org/ftp/arxiv/papers/0809/0809.1957.pdf

27. Heyrovska, R. Direct depnedence of covalent, van der Waals and valence shell radii of atoms on their Bohr radii for elements of Groups 1A - 8A

Philippine Journal of Science, 137 (2): 133-139, December 2008, ISSN 0031 - 7683; (see also Ref. 15 above); (Full paper)

http://www.stii.dost.gov.ph/pjsweb/vol137no2/Direct%20dependence%20of%20covalent.html

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

Chapter 12 in: "Innovations in Chemical Biology", Editor: Bilge Sener, Springer.com, January 2009; ISBN-10: 1402069545, ISBN-13: 978-1402069543 (Proceedings of the 9th EurasiaConference on Chemical Sciences, Antalya, Turkey, September 2006; Invited Lecture).

29. Heyrovska, R. Golden Sections of Interatomic Distances as Exact Ionic Radii and Additivity of Atomic and Ionic Radii in Chemical Bonds

arXiv:0902.1184 [pdf]; http://arxiv.org/ftp/arxiv/papers/0902/0902.1184.pdf

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

Nature Precedings http://precedings.nature.com/documents/2929/version/1 (2009).

31. Heyrovska, R. and Narayan, S. 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.

"WOMEN IN PHYSICS: Third IUPAP International Conference on Women in Physics"; DOI:10.1063/1.3137724; (Short abstract). Nature Precedings http://precedings.nature.com/documents/3292/version/1 (2009), (poster in pdf).

32. Heyrovska, R. Aqueous Redox Potentials Found to be Inversely Proportional to the Bohr Radius

216th ECS Meeting, Vienna, Austria, October 2009: Electrochem. Soc. 902, 3067, 2009. (Abstract)

Electrochem. Soc. Trans., 25, (2010) 159-163. (Full text)

33. Heyrovska, R. Radii of redox components from absolute redox potentials compared with covalent and aqueous ionic radii

Electroanalysis, 22, (2010) 903 - 907, Published online; 4 March 2010. (Full text)

34. Heyrovska, R. Bonding distances as Exact Sums of the Radii of the Constituent Atoms in Nanomaterials - Boron Nitride and Coronene.

http://arxiv.org/abs/1004.2667v2 (2010) (Full paper)

35. Heyrovska, R., Atchison, L. and Narayan, S.

Precise Atomic Structures of Three Novel Nanomaterials in Nanotechnology, Biomedicine and Cosmology: Graphene, Boron Nitride and Coronene

The Nanomaterials Symposium, April 19, 2010, JHU/APL Kossiakoff Center, MD, Nature Precedings http://precedings.nature.com/documents/4357/version/1 (poster)

36. Heyrovska, R. Gender discrimination is a drawback for the progress of science

Author: R. Heyrovska

Symposium: International Women in Science, Challenges and Triumphs,

International Year of Chemistry 2011

ACS Spring Meeting March 2011, Anaheim, CA, USA. (Invited talk)

http://www.chemistry2011.org/participate/activities/show?id=153

http://www.softconference.com/ACSchem/player.asp?PVQ=HGFE&fVQ=FIDDGM&hVQ (Full .ppt text with audio, includes Golden ratio based ionic radii, etc)

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

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

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

Nature Precedings http://precedings.nature.com/documents/6059/version/1 (Full text)

http://precedings.nature.com/documents/6059/version/2 ; (2011) (Full text)

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

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

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

Philippine Journal of Science, 140(2): 119-124, 2011.

41. Heyrovska, R. Precise Molecular Structures of Cysteine, Cystine, Hydrogen-Bonded Dicysteine, Cysteine Dipeptide,Glutathione and Acetyl Cysteine Based on Additivity of Atomic Radii

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

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

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

Presented at: the 12th Eurasia Conference on Chemical Sciences, Corfu, Greece, April 16-21, 2012. (Invited talk) Abstract in:

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

43. Heyrovska, R. Precise Atomic Structures of L-DOPA, Dopamine, Noradrenaline, Adrenaline, Isoprenaline, 5-HTP, Serotonin and Histamine with Bond Lengths as Exact Sums of Adjacent Atomic Radii.

International J. Sci., Vol 1, 1-9, Issue: Nov-2012.

http://www.ijsciences.com/pub/pdf/V1-201211-16.pdf [Research Article (ISSN 2305-3925)]

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

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

http://www.ijsciences.com/pub/pdf/V2-201303-19.pdf [Research Article (ISSN 2305-3925)]

45. Heyrovska, R. 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, NO_2 and CO_2

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

http://www.ijsciences.com/pub/pdf/V2-201304-08.pdf [Research Article (ISSN 2305-3925)]

46. Heyrovska, R. Atomic, Ionic and Bohr Radii Linked via the Golden Ratio for Elements Including Lanthanides and Actinides

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

http://www.ijsciences.com/pub/pdf/V2-201304-18.pdf [Research Article (ISSN 2305-3925)]

47. Heyrovska, R. 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"

48. Heyrovska, R. Golden Ratio Based Fine Structure Constant and Rydberg Constant for Hydrogen Spectra

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

http://www.ijsciences.com/pub/pdf/V2-201305-08.pdf [Research Article (ISSN 2305-3925)]

49. Heyrovska, R. 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

50. Heyrovska, R. 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

51. Heyrovska, R. 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

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

53. Heyrovska, R. 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
http://www.flogen.org/sips2015/cv.php?page=2&p=Raji_Heyrovska&e=rheyrovs@hotmail.com&pi=308

54. Heyrovska, R. Sorry Bohr, Ground State Energy of Hydrogen Atom is Not Negative.
http://vixra.org/abs/1506.0064; http://vixra.org/pdf/1506.0064v1.pdf

55. Heyrovska, R. 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

56. Heyrovska, R. 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

57. Heyrovska, R. 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

58. Heyrovska, R. 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, (see Ref. 54, preprint)

59. Heyrovska, R. A Simple and Exact Interpretation of the Bond Lengths and Stacking Distances in Benzene and its Dimers in Terms of Atomic Covalent Radii - *Dedicated to organic chemist, Prof. P.R. Ayyar, I.I.Sc., on the 50th anniversary of his demise*.
http://vixra.org/abs/1602.0348?ref=8776956
http://vixra.org/pdf/1602.0348v2.pdf