

Interpretation of the Longest C-C Bond Reported by Ishigaki et al

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Abstract. The recently observed longest C-C bond of length 1.806 Å has been interpreted in this short article in terms of the Bohr radii of C and O, just when the hydroxyl groups break away from C by reduction with Zn. A figure drawn to scale has been presented.

Introduction. Recently, Ishigaki et al [1] have reported (see [2]) the longest C-C bond of length, $d(C_1C_2) = 1.806 = \text{Å}$. In this article the author provides an interpretation of this bond length, based on the earlier success of similar explanation of the long O-O bond [3]. Various radii of atoms and many bond lengths and bond angles have previously been quantitatively related to the respective Bohr radii obtained from the first ionization potentials [4-9]. The long C-C bond is explained here in terms of the Bohr radii (a_B) of C and O.

Present work. The longest observed C-C bond length, $d(C_1-C_2)$, is shown in Fig. 1. The various radii are clearly described in the left column in the Fig. 1. The Figure shows the oxygen atoms of the hydroxyl groups just before Zn breaks them off from C_1 and C_2 .

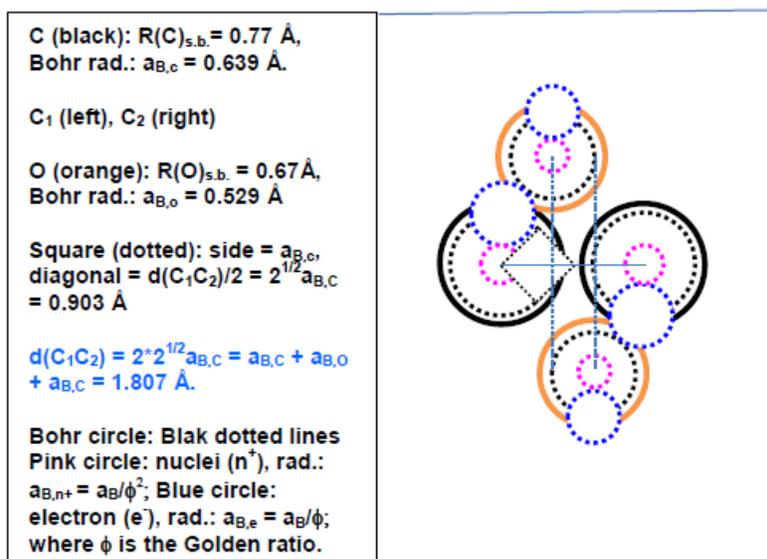


Figure 1. The long C_1-C_2 distance as the sum of the Bohr radii of C and O.

It can be seen that $d(C_1C_2)$ is exactly equal to the sum,

$$d(C_1C_2) = a_{B,C} + a_{B,O} + a_{B,C} = 0.639 + 0.529 + 0.639 = 2 \cdot 2^{1/2} a_{B,C} = 1.807 \text{ Å} \dots (1)$$

which is also exactly equal to twice the diagonal of a square with Bohr radius of carbon as a side.

References

1. Y. Ishigaki, T. Shimajiri, T. Takeda, R. Katoono, T. Suzuki, Longest C–C Single Bond among Neutral Hydrocarbons with a Bond Length beyond 1.8 Å. *Chem* **2018**, *in press*. [DOI: [10.1016/j.chempr.2018.01.011](https://doi.org/10.1016/j.chempr.2018.01.011)]
2. T. Nguyen, Chemists break record for longest C–C bond. *C&EN*, Vol. 96 Issue 11 | p. 11 | Issue Date: March 12, 2018 | Web Date: March 8, 2018.
3. R. Heyrovska, The long O-O bond in HOON, <http://comments.sciencemag.org/content/10.1126/science.1244180> and slide 16 in: <https://www.researchgate.net/publication/281270357>
4. R. Heyrovska, Direct dependence 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. <http://arxiv.org/ftp/arxiv/papers/0708/0708.1108.pdf>
5. R. Heyrovska, Atomic and Ionic Radi of Elements and Bohr Radii from Ionization Potentials are Linked Through the Golden Ratio, *International J. Sciences* 03(2013):82-92 , <http://www.ijsciences.com/pub/article/155>
6. R. Heyrovska, Bond Lengths, Bond Angles and Bohr Radii from Ionization Potentials Related via the Golden Ratio for H₂⁺, O₂, O₃, H₂O, SO₂, NO₂ and CO₂. *International J. Sci.*, Vol 2, 1-4, Issue: Apr-2013. <http://www.ijsciences.com/pub/pdf/V2-201304-08.pdf>
7. R. Heyrovska, 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>
8. 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. Sci.*, Vol 2, 30-32, Issue: Dec-2013. <http://www.ijsciences.com/pub/pdf/V220131214.pdf>
9. 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 . Full text of Keynote talk in: 2014 - Sustainable Industrial processing summit/Shechtman International Symposium; Volume 5: Composite, Ceramic, Quasicrystals, Nanomaterials, High temperature Protection Coatings. Edited by Florian Kongoli, Flogen 2014, pp 395 - 402. <https://www.researchgate.net/publication/321292841>