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Benzene C-C Bond Mirroring P-Energy on Double-Surface

(Proto-Science Paper)

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Abstract: *With the help of carbon p-energy the benzene C-C bond length of 139.72 pm is calculated. And further, the double-surface characteristics of pi electron pathway are found.*

Keywords: *benzene C-C bond length, carbon p-energy, effective nuclear charge, heat of benzene hydrogenation, double surface geometry*

1. PREFACE

The subject of interest of this paper is with the help of released heat at benzene hydrogenation [1]to relate the effective nuclear charge of carbon valence electrons [2]to the benzene C-C bond length [3]. And further, with the help of double-surface geometry [4] see the characteristics of pi electron pathway.

2. THE CARBON P-ENERGY

Neglecting the energetic influence of orbital hybridization the carbon p-orbital energy (p-energy) in cyclohexane molecule $E_p^{cyclo\ hexane}$ should equal that one in carbon atom $E_p^{carbon\ \ atom}$:

$$E_p^{cyclo\ hexane} \approx E_p^{carbon\ \ atom}. \quad (1)$$

But the p-energy $E_p$is significantly elevated in benzene molecule for the energy of dehydrogen-ation $E_{dehydrogenation}$ becoming:

$$E_p^{benzene} = E_p^{cyclo\ hexane} + E_{dehydrogenation}. \quad (2)$$

3. THE CARBON P-ENERGY MIRRORING THE EFFECTIVE NUCLEAR CHARGE

The carbon p-energy in the carbon atom $E_p^{carbon\ \ atom}$ mirrors the effective nuclear charge seen by electrons in the carbon atom 2p orbital [2]. Thus:

$$E_p^{carbon\ \ atom} = -\frac{Z_{effective}}{n^2}\ x\ \frac{m_e c^2}{2\alpha^{-2}}. \quad (3)$$

Where:

$Z_{effective} = effective\ nuclear\ charge\ of\ carbon\ 2p\ electrons = 3.1358,$

$n = excited\ state\ of\ carbon\ p\ electrons = 2,$

$$\frac{m_e c^2}{2\alpha^{-2}} = Ry = Rydberg\ unit\ of\ energy = 13.605693009\ eV. \quad (4)$$

So applying $(1), (3), (4)$ the carbon p-energy in the cyclohexane molecule yields:

$$E_p^{cyclo\ hexane} = -10.6661830344\ eV. \quad (5)$$

4. THE CARBON DEHYDROGENATION ENERGY

Respecting conservation laws the dehydrogenation energy $E_{dehydrogenation}$ is the opposite of the hydrogenation energy $E_{hydrogenation}$:

$$E_{dehydrogenation} = -E_{hydrogenation}. \quad (6)$$

The experimental value of released heat at benzene hydrogenation is known from chemistry books [1].Its value calculated per benzene carbon atom is the next:

$$E_{hydrogenation} = \frac{\Delta H}{6\ x\ N_{Avogadro}}. \quad (7)$$

Where:

$\Delta H = heat\ of\ benzene\ hydrogenation = -208.5\ kJmol^{-1} = -1.301354653\ x\ 10^{24}\ eVmol^{-1}$,

$6 = number\ of\ carbon\ atoms\ in\ benzene$,

$N_{Avogadro} = Avogadro\ number = 0.602214086\ x\ 10^{24} mol^{-1}$. (8)

So applying(6),(7) the carbon dehydrogenation energy yields:

$$E_{de\,hydrogenation} = 0.360158368\ eV. \quad (9)$$

5. THE CARBON P-ENERGY IN THE BENZENE MOLECULE

Applying(2), (5) , (9) the carbon p-energy value in the benzene molecule is given:

$$E_p^{benzene} = -10.666183034\ eV + 0.360158368\ eV = -10.306024667\ eV. \quad (10)$$

6. THE CARBON P-ORBIT AND C-C BOND LENGTH

The p-energy as an orbital energy is at the same time the electron energy on the original orbit of that orbital [5]. Since the orbit length and energy are in inverse proportion [6] the original carbon p-orbit length $s_{original}$ can be calculated as:

$$s_{original} = \frac{-Ry}{E_p^{benzene}}\ x\ \alpha^{-1} = 180.910670459\ \lambda_e. \quad (11)$$

The C-C bond length, denotedl_{C-C}, enabling the circular bridge between carbonatoms for pi electrons (electrons originated from the concerned p orbitals) should be $\pi - times$ smaller:

$$l_{C-C} = \frac{s_{original}}{\pi} = 57.585654921\ \lambda_e = 139.72\ pm. \quad (12)$$

The above value is in accordance with the experimental value $l_{c-c}^{experimental}$ known from chemistry books [3]:

$$l_{c-c}^{experimental} - l_{c-c}^{calculated} = 139.7\ pm - 139.7\ pm = 0.0\ pm. \quad (13)$$

7. THE BENZENE RING PATHWAYS

The geometric characteristics of benzene are represented in Figure 1.

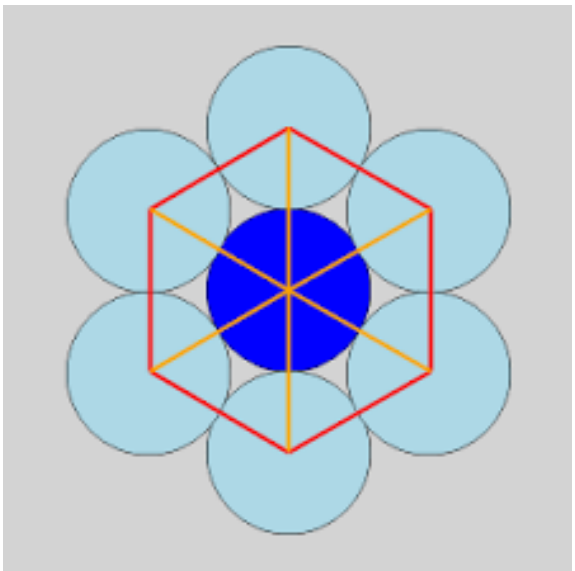

Figure1. *The benzene geometry*

The bright blue circles represent benzene carbon atoms and dark blue circle the empty space inside the benzene ring. The yellow segments are the distances between non-adjacent carbon atoms. The circumferences of bright blue circles show the circular and the orange circumference of hexagon the diametrical pathway of pi electrons. The circular pathway enables the passage between both – upper and lower – ring sides but the diametrical pathway offers travel above and below the ring. Interesting are the double-surface[4] characteristics of the diametrical pathway. The pi electron average elliptic-hyperbolic path on the whole benzene ring s_{ring} equals the circumference of benzene hexagon:

$$s_{ring} = 6\,x\,l_{C-C} = 6\,x\,57.58565\,\lambda_e = 345.5139\,\lambda_e. \quad (14)$$

The corresponding elliptic path n[4] seems to possess the half-integer value of Compton wave lengths of the electron. Indeed for $n = 345.5$ holds:

$$s(n) = n\left(2 - \frac{1}{\sqrt{1+\frac{\pi^2}{n^2}}}\right) = 345.5143\ldots \quad (15)$$

The above number (15) differs from the proposed diametrical ring route(14) on the fourth decimal place:

$$s(345.5) - s_{ring} = 0.0004. \quad (16)$$

This means that the pi electron wave should rotate once around its path axis or on the other hand the pathway should be the Möbius strip to escape the electron ouroboros destiny (vanishing point) after one diametrical ring route. As illustrated by Haltopub [7]:

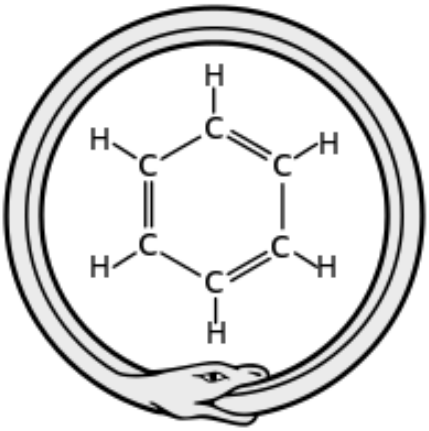

Figure2. *The ouroboros, Kekulė's inspiration for the structure of benzene*

8. CONCLUSIONS

The benzene C-C bond length is explained by the carbon p-energy as well as benzene pi electron pathway viewed in the light of double surface geometry.

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DEDICATION

This fragment is dedicated to – according to the folk tradition miraculous – Ivanov izvir (Ivan's water spring) to inspire recently revitalized unit of Pharmacy Špringer located in Razkrižje, Slovenia.

AUTHOR'S BIOGRAPHY

Janez Špringer, is an independent scientist and pharmacist.