

Double-Surface Characteristics of Trihydrogen Cation Common Orbit

Janez Špringer

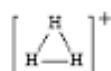
Cankarjeva cesta 2, 9250 Gornja Radgona, Slovenia, EU

Abstract: With the help of trihydrogen cation enthalpy of formation the common orbit length of $[H_3]^+$ yielding 161.03 Compton wave lengths of the electron is calculated what implies the stable double-surface characteristics of delocalized electron pathway.

Keywords: trihydrogen cation enthalpy of formation, trihydrogen cation s-energy, double-surface characteristics of trihydrogen cation common orbit

1. PREFACE

The subject of interest of this paper is with the help of hydrogen s-energy –mirroring Rydberg unit of energy $Ry[1]$ as well as trihydrogen cation enthalpy of formation [2] –to calculate the length of the common trihydrogen cation orbit [1]. And further, check the double-surface characteristics of delocalized electron pathway [1] of trihydrogen cation:



2. THE S-ENERGY

The s-energy E_s is the orbital energy of electron originated from the atomic s-orbital. For instance, in the ground state of Hydrogen atom that energy equals the negative value of Rydberg unit of energy Ry [1]:

$$E_s^{\text{Hydrogen atom}} = -Ry = -13.605693009 \text{ eV}. \quad (1)$$

But s-energy in the trihydrogen cation $E_s^{[H_3]^+}$ is significantly elevated for the enthalpy of cation formation calculated per one hydrogen atom $E_{\text{formation}}^{[H_3]^+}$ becoming:

$$E_s^{[H_3]^+} = E_s^{\text{Hydrogen atom}} + E_{\text{formation}}^{[H_3]^+}. \quad (2)$$

3. THE TRIHYDROGEN CATION ENTHALPY OF FORMATION

The trihydrogen cation formation is the opposite of its degradation:



The experimental value of trihydrogen cation enthalpy of formation ΔH is known from the thermochemical references [2]. Its value calculated per hydrogen atom of trihydrogen cation can be then given as:

$$E_{\text{formation}}^{[H_3]^+} = \frac{1}{3} \times \frac{2}{3} \times \frac{\Delta H}{N_{\text{Avogadro}}}. \quad (4)$$

Where:

$$\Delta H = \text{trihydrogen cation enthalpy of formation} = 1106.697 \text{ kJmol}^{-1} = 6.907459425 \times 10^{24} \text{ eVmol}^{-1},$$

$$N_{\text{Avogadro}} = \text{Avogadro number} = 0.602214086 \times 10^{24} \text{ mol}^{-1},$$

$$\frac{2}{3} = \text{electron share} = \frac{2 \text{ delocalized } e^- \text{ of the compound } [H_3]^+ e^-(g)}{\text{total } 3 e^- \text{ of the compound } [H_3]^+ e^-(g)},$$

$$\frac{1}{3} = \text{Hydrogen atom share} = \frac{1 \text{ H} - \text{atom of the cation } [H_3]^+}{\text{total } 3 \text{ H} - \text{atoms of the cation } [H_3]^+} \quad (5)$$

So applying (4), (5) the trihydrogen cation enthalpy of formation calculated per one hydrogen atom yields:

$$E_{\text{formation}}^{[H_3]^+} = 2.548912455 \text{ eV}. \quad (6)$$

4. THE S-ENERGY IN THE TRIHYDROGEN CATION

Applying(1), (2) , (6) the s-energy value in the trihydrogen cation is given:

$$E_s^{[H_3]^+} = -13.605693009 \text{ eV} + 2.548912454 \text{ eV} = -11.056780554 \text{ eV}. \quad (7)$$

5. THE HYDROGEN ORBIT AND H-H BOND LENGTH

The s-energy as an orbital energy is at the same time the electron energy on the original orbit of that orbital [1]. Since the orbit length and energy are in inverse proportion [1] the original hydrogen orbit lengths s_{original} in the trihydrogen cation can be calculated as:

$$s_{\text{original}} = \frac{-Ry \times \alpha^{-1}}{E_p^{[H_3]^+}} = 168.626827948 \lambda_e. \quad (8)$$

The H-H bond length, denoted l_{H-H} , enabling the circular bridge for the electrons located on the original orbits of H-atoms should be $\pi - \text{times}$ smaller:

$$l_{H-H} = \frac{s_{\text{original}}}{\pi} = 57.585654921 \lambda_e = 130.2 \text{ pm}. \quad (9)$$

Unfortunately the above value differs from the experimental values $l_{H-H}^{\text{experimental}}$ known from chemistry references [3]:

$$\frac{l_{H-H}^{\text{calculated}}}{l_{H-H}^{\text{experimental}}} = \frac{130.2 \text{ pm}}{\text{from } 87 \text{ to } 90 \text{ pm}} \approx 1.5. \quad (10)$$

The approximately 1.5 – times smaller mentioned experimental value means that the $H - H$ bond length of trihydrogen cation cannot be explained on classical way having in mind only the original orbits. The problem can be over passed on one hand with the help of distributive orbits[4]and on the other hand with the common orbit[1]derived from the three single original orbits.

6. THE DISTRIBUTIVE ORBIT EXPLANATION

Keeping the total orbital energy W_{total} untouched the original orbit s_{original} can be transformed to the discrete number of distributed orbits $s_{\text{distributed}}$ [4]. With other words, the electron is able to circulate on them with the same total but different kinetic energy. Thus [4]:

$$W_k^{\text{distributed}} = W_k^{\text{original}} \left(2 \times \frac{s_{\text{original}}}{s_{\text{distributed}}} - 1 \right). \quad (11)$$

And since the original kinetic and total energy are of the opposite values $W_k^{\text{original}} = -W_{\text{total}}$ [4] holds:

$$W_k^{\text{distributed}} = -W_{\text{total}} \times \left(2 \times \frac{s_{\text{original}}}{s_{\text{distributed}}} - 1 \right). \quad (12)$$

In the case of trihydrogen cation we have $W_{\text{total}} = E_s^{[H_3]^+} = 11.06 \text{ eV}$ (7) and $\frac{s_{\text{original}}}{s_{\text{distributed}}} \approx 1.5$ (10). So:

$$W_k^{\text{distributed}} \approx -2 \times E_s^{[H_3]^+} = 22,1 \text{ eV}. \quad (13)$$

Following the non-classical explanation the electron circulating in the trihydrogen cation should possess twice as much kinetic energy as would be expected from the classical approach.

7. THE COMMON ORBIT EXPLANATION

Interesting are the double-surface [5] characteristics of the diametrical pathway performed on the common orbit derived from the three single original orbits of trihydrogen cation. The average elliptic-

hyperbolic path [5] used by the two delocalized electrons circulating on the trihydrogen cation ring s_{ring} equals the circumference of the equilateral triangle:

$$s_{ring} = 3 \times l_{H-H}^{calculated} = 3 \times 53.675586412 \lambda_e = 161.0268 \lambda_e. \quad (14)$$

The corresponding elliptic path n [5] seems to measure the integer value of Compton wavelengths of the electron. Indeed for $n = 161$ holds:

$$s(n) = n \left(2 - \frac{1}{\sqrt{1 + \frac{\pi^2}{n^2}}} \right) = 161.0306 \dots \quad (15)$$

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

$$s(161) - s_{ring} = 0.004. \quad (16)$$

This means that the electron wave provided on the common orbit of trihydrogen cation experiences favourable double-surface characteristics of the given elliptic-hyperbolic pathway.

8. CONCLUSIONS

The trihydrogen cation H-H bond length is explained by the s-energy taking into account the non-classical distributive orbits. Besides the common electron pathway is viewed in the light of double surface geometry.

DEDICATION AND ACKNOWLEDGEMENT

This fragment is dedicated to the ten fruitful years of Lekarna Špringer (Špringer Pharmacy) being present in the Pannon region of Slovenia since 2007. Special thanks to the hospitality of the city of Gornja Radgona located inside the triangle “Apače, Razkrižje and Rogašovci”.

REFERENCES

- [1] Špringer J. Benzene C-C Bond Mirroring P-Energy on Double-Surface(Proto-Science Paper). International Journal of Advanced Research in Physical Science (IJARPS), Volume 4, Issue 4, May 2017, 12-15.
- [2] Ruscic B. and Bross D. H. Active Thermochemical Tables (AtcT) values based on ver. 1.122 of the Thermochemical Network (2016) available at AtcT anl. Gov
- [3] Wang Z., Wang H., Tse J.S., Itaka T. and Ma Y. Stabilization of H_3^+ in the high pressure crystalline structure of H_nCl ($n = 2 - 7$). Chem. Sci. 2015 Jan 1; 6(1): 522-526
- [4] Špringer J. Upper Limit in Mendeleev's Periodic Table Uhq Unhexquadium. International Journal of Advanced Research in Physical Science (IJARPS), Volume 4, Issue 3, March 2017, 14-18.
- [5] Špringer J. Double Surface and Fine Structure. Progress in Physics, 2013, v. 2, 105-106.

AUTHOR'S BIOGRAPHY



Janez Špringer, is an independent scientist and pharmacist from Slovenia.