Double-Surface Characteristics of Protonated Guanidine

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Abstract: *The double-surface characteristics of the carbocation and nitrogen orbit in the protonated guanidine yielding 190.03 and 301.02 Compton wavelengths of the electron, respectively, are proposed.*

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1. PREFACE

In this paper we shall try with the help of carbon and nitrogen p-energy to reveal the double-surface characteristics [1] of the carbocation and nitrogen orbit in the protonated guanidine (briefly Gu^+)[2]:
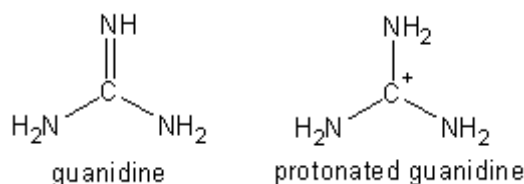
2. THE TRIANGLE GEOMETRY

Let us propose that 6 electrons of Gu^+[2] are delocalized between the nitrogen atoms. The distance between the planar nitrogen atoms l_{N-N} located at the edges of an Isosceles triangle (having angles $30^o, 30^o \ and \ 120^o$ [3]) is $\sqrt{3} - times$ longer than the bond length between the carbon and nitrogen atom l_{C-N}:

$$l_{NN} = \sqrt{3} \ x \ l_{C-N}. \tag{1}$$

For $l_{C-N} = 134.24 \ pm$ [3] we have:

$$l_{NN} = 232,511 \ pm. \tag{2}$$

3. THE NITROGEN ORBIT

The distance between nitrogen atoms l_{NN} is at the same time the diameter of the orbit spread around each of the three nitrogen atoms. The concerned three equal nitrogen orbits are in the point touch with each other. For such a subtle touch the zero kinetic energy of the electron on the nitrogen orbit of the circumference $s_N = \pi \ x \ l_{NN}$ is plausible. Then we have deal with the nitrogen longest distributed orbit [4]:

$$s_{N-distributed}^{max} = \pi \ x \ l_{NN} = 730.453 \ pm. \tag{3}$$

4. THE DOUBLE-SURFACE CHARACTERISTICS OF NITROGEN ORBIT

Interesting are favourable double-surface characteristics [1] of the nitrogen orbit implied from the length given in the units of Compton wave length of the electron:

$$s_{N-distributed}^{max} = 730.453 \ pm \ = 301.055. \tag{4}$$

Indeed, the average elliptic-hyperbolic path s corresponding to the elliptic path $n = 301$ lies very close to the above value [1]:

$$s(n = 301) = n \left(2 - \frac{1}{\sqrt{1 + \frac{\pi^2}{n^2}}} \right) = 301.016 \ \dots \approx 301.055. \tag{5}$$

5. THE NITROGEN ORIGINAL ORBIT

The longest distributed orbit around nitrogen atom is twice longer than the corresponding original orbit and vice versa – the original orbit is twice shorter [4]:

$$s_{N-original} = \frac{s_{N-distributed}^{max}}{2} = 150.528. \tag{6}$$

6. THE NITROGEN P-ENERGY IN Gu^+

The energy of the electron on the original orbit around nitrogen atom in Gu^+ is at the same time the nitrogen p-orbital energy (nitrogen p-energy, denoted E_{N-p}) in that cation given by the relation [5]:

$$E_{N-p}^{Gu^+} = \frac{Ry \, x \, \alpha^{-1}}{s_{N-original}} = -\frac{13.606 \, eV \, x \, 137.036}{150.528} = -12.386 \, eV. \tag{7}$$

7. THE FUNDAMENTAL NITROGEN P-ENERGY

The nitrogen p-energy in Gu^+ is greater than the fundamental one in the nitrogen atom $E_{N-p}^{Nitrogen \ atom}$. [5]The latter reflects the effective nuclear charge seen by 2p electrons [6]:

$$E_{N-p}^{Nitrogen \ atom} = -\frac{Z_{effective}}{n^2} \, x \, Ry. \tag{8}$$

For [7] $Z_{effective} = 3.8340$ and $n = 2$ we have:

$$E_{N-p}^{Nitrogen \ atom} = -13,041 \, eV. \tag{9}$$

8. THE NITROGEN P-ENERGY INCREMENT IN Gu^+

The nitrogen p-energy increment E_{N-p} ↑per one electron is the next [4]:

$$E_{N-p} \uparrow = E_{N-p}^{Gu^+e^-} - E_{N-p}^{Nitrogen \ atom} = -12.3863 \, eV - (-13,041 \, eV) = 0.655 \, eV. \tag{10}$$

The energy increment per all six delocalized electrons in three nitrogen orbits is six times greater:

$$6 \, x \, E_{N-p} \uparrow = 3.929 \, eV. \tag{11}$$

9. THE WHOLE NITROGEN P-ENERGY INCREMENT IN Gu^+ VERSUS THE ENTHALPY OF ONE MOLECULE Gu^+e^- FORMATION

The whole nitrogen p-energy increment in Gu^+(11) is less than the whole energy increment needed for one molecule of Gu^+e^- formation [2]:

$$Gu^+e^-(g) \rightarrow Gu(g) + H^+(g) + e^- + E_{Formation}^{Gu^+e^-} \ . \tag{12}$$

Where [2]:

$$E_{Formation}^{Gu^+e^-} = \frac{(462 \mp 3)kJmol^{-1}}{N_{Avogadro}} = (4.788 \mp 0.031) \, eV. \tag{13}$$

Since(11), (13):

$$6 \, x \, E_{N-p} \uparrow = 3.929 \, eV < E_{Formation}^{Gu^+e^-} = (4.788 \mp 0.031) \, eV. \tag{14}$$

10. THE POSSIBLE EXPLANATION OF THE ENERGY INCREMENT DISCREPANCY

Let us propose that the difference between the enthalpy of one molecule Gu^+e^- formation [2], denoted $E_{Formation}^{Gu^+e^-}$ (13), on one side and the whole nitrogen p-energy increment in Gu^+, denoted $6 \, x \, E_{N-p}$ ↑ (11), on the other side is due to the carbon p-energy increment, denoted E_{C-p} ↑ (15), belonging to the electron generated from the guanidine anion A^- but being localized on the carbocation orbit of Gu^+:

$$E_{C-p} \uparrow = E_{Formation}^{Gu^+e^-} - 6 \, x \, E_{N-p} \uparrow = (0.859 \mp 0.031) \, eV. \tag{15}$$

11. THE CARBON P-ENERGY IN Gu^+

Knowing the carbon p-energy in the carbon atom $E_{C-p}^{Carbon \ atom} = -10.666 \, eV$ [5] the whole carbon p-energy in the Gu^+e^- molecule, denoted $E_{C-p}^{Gu^+e^-}$, can be calculated [5]:

$$E_{C-p}^{Gu^+e^-} = E_{C-p}^{Carbon \ atom} + E_{C-p} \uparrow = -10.666 \, eV + (0.859 \mp 0.031) \, eV) = (-9.807 \mp 0.031) \, eV. \tag{16}$$

12. THE CARBOCATION ORIGINAL ORBIT

The carbocation original orbit $s_{C-original}$ related to the carbon p-energy is given as follows (7):

$$s_{C-original} = \frac{Ry \; x \; \alpha^{-1}}{E_{p-C}^{Gu^+e^-}} = -\frac{13.606 \; eV \; x \; 137.036}{(9.807 \mp 0.031) \; eV} = 190.12 \mp 0.60 \,. \tag{17}$$

13. THE DOUBLE-SURFACE CHARACTERISTICS OF THE CARBOCATION ORIGINAL ORBIT

Interesting are favourable double-surface characteristics [1] of the carbocation original orbit. Indeed, the average elliptic-hyperbolic path s corresponding to the elliptic path $n = 190$ lies inside the interval of the above values (17):

$$189.52 \; < s(n = 190) = n \left(2 - \frac{1}{\sqrt{1 + \frac{\pi^2}{n^2}}} \right) = 190.03 < 190.72 \,. \tag{18}$$

14. CONCLUSIONS

Following the p-energy concept the carbocation and nitrogen orbit in the protonated guanidine shows favourable double-surface characteristics as the original 190th and longest distributed 301th orbit, respectively.

DEDICATION AND ACKNOWLEDGEMENT

This fragment is dedicated to the Štajerski most-Steirerbrücke (Styrian Bridge) enabling the subtle touch over the Mura River for Pannon pleasure.

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