International Journal of Advanced Research in Physical Science (IJARPS)
Volume 5, Issue 5, 2018, PP 13-16
ISSN No. (Online) 2349-7882
www.arcjournals.org

Extreme Water Molecule Extension

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Abstract: *Respecting zero water molecule enthalpy of transformation and double-surface geometry the maximal water molecule extension to HOH angle of 162.5° is expected.*

Keywords: *Original and subtle electron orbit, covalent and subtle bond, double-surface geometry, deactivation of non-bound and activation of bound electrons, maximal HOH angle*

1. PREFACE

Previously one respecting zero water molecule enthalpy of transformation calculated the extreme water molecule contraction expressed in HOH angle of 39.5°.[1]. In the present paper the concept proposes the reverse process where the extension of gaseous water molecule is enabled by the deactivation of non-bound Oxygen electrons and balanced by the activation of bound Hydrogen electrons in the water molecule.

2. THE OUTER WATER MOLECULE ELECTRONS

Let us recall the outer electron structure of water molecule from the reference [1]. It consists of four non-bound Oxygen electrons creating the negative pole as well as two bound Hydrogen electrons and two bound Oxygen electrons enabling the positive pole of molecule as presented in figure(1):

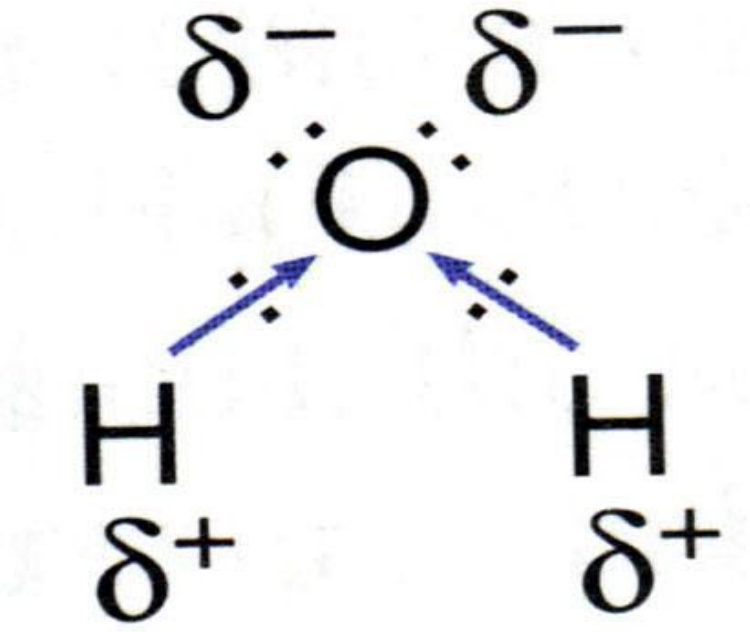

Figure1. *Outer water molecule electrons*

3. THE WATER MOLECULE EXTENSION

At zero water molecule enthalpy of transformation [1] the deactivation energy of four non-bound Oxygen electrons can be balanced by the activation energy of two bound Hydrogen and two bound Oxygen electrons [1]:

$$4\Delta E_{O\ non-bound} = 2\Delta E_{OH\ bound} = 2\Delta E_{O\ bound} + 2\Delta E_{H\ bound}\,. \quad (1)$$

The deactivation of non-bound electrons and activation of bound electrons in the water molecule is accompanied by stretching the covalent OH and subtle HH bond length as well as increasing or decreasing the HOH angle. The subject of interest of this paper is to find the maximal extension of both chemical bond lengths and angle between covalent bonds. Starting with the water molecule in the gas state where the non-bound Oxygen electrons are proposed to be in the ground atomic state (initial state) and finishing with the maximal deactivated state where the deactivated non-bound Oxygen electrons are balanced by the optimal activated bound Oxygen electrons and Hydrogen electrons (final state). The energy equation (1) then takes the next form:

$$2(E^{initial}_{O\ non-bound} - E^{final}_{O\ non-bound}) = (E^{final}_{O\ bound} - E^{initial}_{O\ bound}) + (E^{final}_{H\ bound} - E^{initial}_{H\ bound}). \quad (2)$$

4. THE ORBITAL ENERGIES

The maximal orbital energy of bound Oxygen electron in the final state, denoted $E^{final}_{O\ bound}$, and maximal orbital energy of bound Hydrogen electron in the final state, denoted $E^{final}_{H\ bound}$, is zero by definition:

$$E^{final}_{O\ bound} = E^{final}_{H\ bound} = 0. \quad (3)$$

The initial orbital energies in the equation (2) are given respecting zero water molecule enthalpy of transformation from the solid to gas state [1].

The orbital energy of non-bound Oxygen electron in the initial state of gaseous water molecule yields:

$$E^{initial}_{O\ non-bound} = -15{,}147\ 218\ eV. \quad (4)$$

The orbital energy of bound Oxygen electron in the initial state of gaseous water molecule yields:

$$E^{initial}_{O\ bound} = -24.881\ 679\ eV\ . \quad (5)$$

The orbital energy of bound Hydrogen electron in the initial state of gaseous water molecule yields:

$$E^{initial}_{H\ bound} = -19.023\ 237\ eV. \quad (6)$$

5. THE EXTREME HOH ANGLE EXTENSION

It can be examined that the greatest extension in HOH angle is achieved when only the bound Hydrogen electrons are activated. The activation of bound Oxygen electrons contributes only to the OH bond length extension and is neutral to the HH subtle bond length enhancement what consequently causes the opposite effect, i.e. the HOH angle contraction.

Taking into account the deactivation of non-bound Oxygen electrons and only the activation of bound Hydrogen electrons the energy equation (2) takes the next form:

$$2(E^{initial}_{O\ non-bound} - E^{final}_{O\ non-bound}) = (E^{final}_{H\ bound} - E^{initial}_{H\ bound}). \quad (7)$$

Inserting data (3), (4), (6) in the above equation (7) the orbital energy of non-bound Oxygen electron in the final state is given:

$$E^{final}_{O\ non-bound} = E^{initial}_{O\ non-bound} - \frac{E^{final}_{H\ bound} - E^{initial}_{H\ bound}}{2} = -15{,}147\ 218\ eV - \frac{0-(-19.023\ 237\ eV)}{2}$$
$$= -24.658\ 837\ eV. \quad (8)$$

Since the orbital energy and the orbit length are in inverse proportion the corresponding orbit length of non-bound Oxygen electron in the final state is the next:

$$s^{final}_{o\ non-bound} = -\frac{Ry\ x\ \alpha^{-1}}{E^{final}_{O\ non-bound}} = -\frac{13.605\ 693\ 009\ \text{eV}\ x\ 137.035\ 999\ 139\lambda_e}{-24.658\ 837\ eV} = 75.610\ 611\ \lambda_e. \quad (9)$$

The given value is not conceptual [1]. The nearest conceptual orbit length enabling a stable circulation of the electron on the double-surface is a little longer[1]:

$$s^{final\ conceptual}_{o\ non-bound} = s(n) = n\left(2 - \frac{1}{\sqrt{1+\frac{\pi^2}{n^2}}}\right) = 76.064\ 849\ \ldots\ for\ n = 76. \quad (10)$$

Applying again the inverse proportion between the orbital energy and orbit length the corresponding conceptual orbital energy of non-bound Oxygen electron in the final state is the next [1]:

$$E_{O\ non-bound}^{final\ conceptual} = -\frac{Ry\ x\ \alpha^{-1}}{s_{o\ non-bound}^{final\ conceptual}} = -\frac{13.605\ 693\ 009\ \text{eV}\ x\ 137.035\ 999\ 139\ \lambda_e}{76.064\ 849\ \lambda_e}$$
$$= -24.511\ 582\ eV. \quad (11)$$

The conceptual orbital energy of bound Hydrogen electron in the final state $\boldsymbol{E_{H\ bound}^{final\ conceptual}}$ is then according to the equation (7) and inserted data (4), (6),(11) of non-zero value:

$$2(E_{O\ non-bound}^{initial} - E_{O\ non-bound}^{final\ conceptual}) = \boldsymbol{E_{H\ bound}^{final\ conceptual}} - E_{H\ bound}^{initial}. \quad (12a)$$

And

$$2(-15{,}147\ 218\ eV - (-24.511\ 582\ eV)) = \boldsymbol{E_{H\ bound}^{final\ conceptual}} - (-19.023\ 237\ eV). \quad (12b)$$

Yielding

$$\boldsymbol{E_{H\ bound}^{final\ conceptual}} = -0.294\ 510\ eV. \quad (12c)$$

Let us also calculate the corresponding conceptual orbit length of bound Hydrogen electron in the conceptual final state since we need it for the maximal HOH angle calculation:

$$s_{H\ bound}^{final\ conceptual} = -\frac{Ry\ x\ \alpha^{-1}}{E_{H\ bound}^{final\ conceptual}} = -\frac{13.605\ 693\ 009\ \text{eV}\ x\ 137.035\ 999\ 139\ \lambda_e}{-0.294\ 510\ eV}$$
$$= 6330.7519\ \lambda_e. \quad (13)$$

For the same reason is welcome also the known value of the unchanged orbit length of bound Oxygen electron in the final state:

$$s_{O\ bound}^{unchanged} = -\frac{Ry\ x\ \alpha^{-1}}{E_{O\ bound}^{unchanged}} = -\frac{13.605\ 693\ 009\ \text{eV}\ x\ 137.035\ 999\ 139\ \lambda_e}{-24.881\ 679\ eV} = 74.933\ 438\ \lambda_e. \quad (14)$$

6. The Maximal HOH Angle Calculation

The maximal HOH angle can be given applying cosine rule [1]:

$$HH_{subtle} = OH\sqrt{2(1-cos\varphi)}. \quad (15a)$$

$$\frac{2\ x\ s_{H\ bound}^{final\ conceptual}}{\pi} = \frac{(s_{O\ bound}^{unchanged} + s_{H\ bound}^{final\ conceptual})}{\pi}\ x\ \sqrt{2(1-cos\ \varphi)}. \quad (15b)$$

Inserting the data (13), (14) in the above equation (15b) we have:

$$2\ x\ 6330.7519\lambda_e = (74.933\ 438\ \lambda_e + 6330.7519\lambda_e)x\ \sqrt{2(1-cos\varphi_{max})}. \quad (15c)$$

Thus

$$\varphi_{max} = 162.455°. \quad (15d)$$

Of course, at zero orbital energy of bound Hydrogen electron in the final state, $E_{H\ bound}^{final} = 0$, the corresponding final orbit length would be infinite, $s_{H\ bound}^{final} = \infty$, and consequently the maximal HOH angle would be the straight one, $\varphi_{max} = 180°$.

7. Conclusions

Respecting zero water molecule enthalpy of transformation and double-surface geometry the maximal HOH angle of about 162.5° is expected due to the deactivation of non-bound Oxygen electrons and activation of bound Hydrogen electrons in the gaseous water molecule. Further extension of HOH angle could be achieved only by the deactivation of bound Oxygen electrons on the account of activation of some other energy inside or outside the water molecule.

Acknowledgement

Gratitude to the cold water in the hot summer of 2018

DEDICATION

This fragment is dedicated to my residence – the spa town Radenci, Slovenia, EU

REFERENCE

[1] J. Špringer, "Extreme Water Molecule Contraction", International Journal of Advanced Research in Physical Science (IJARPS), vol. 5, no. 5, pp. 1-4, 2018.

Citation: *J. Springer, "Extreme Water Molecule Extension", International Journal of Advanced Research in Physical Science (IJARPS), vol. 5, no. 5, pp. 13-16, 2018.*