Extreme Water Molecule Contraction

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Abstract: *Respecting zero water molecule enthalpy of transformation the maximal water molecule contraction to HOH angle of 39.2° is calculated. Respecting double surface geometry, too, a little larger minimal HOH angle of 39.7°is given.*

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

1. PREFACE

Previously one proposed zero water molecule enthalpy of transformation from solid to gas state [1]. In the present paper the concept proposes further contraction of gaseous water molecule enabled by the extreme activation of non-bound Oxygen electrons and balanced by the deactivation of bound Oxygen and Hydrogen electrons in water molecule.

2. OUTER WATER MOLECULE ELECTRONS

In figure1 [2]outer water molecule electrons are presented:

a)Four non-bound Oxygen electrons creating the negative pole.

b)As well as two bound Hydrogen and two bound Oxygen electrons enabling the positive pole of molecule.
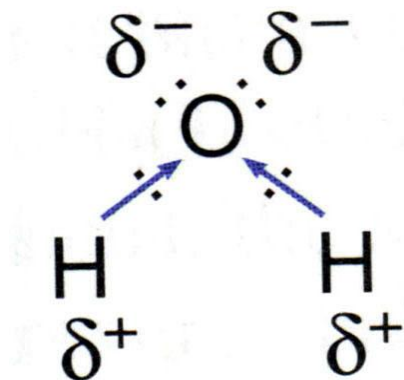

Figure1. *Outer water molecule electrons*

3. ZERO WATER MOLECULE ENTHALPY OF TRANSFORMATION

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

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

The activation of non-bound and deactivation of bound electrons in water molecule is accompanied by shortening the covalent OH and subtle HH bond length as well as shrinking the HOH angle. The subject of interest of this paper is to find the maximal reduction of both chemical bond lengths and angle between covalent bonds. Starting with 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 activated state where the non-bound Oxygen electrons are almost out of the Oxygen atom (final state). The energy equation (1) then takes the next form:

$$2(E_{O\ non-bound}^{final} - E_{O\ non-bound}^{initial}) = (E_{O\ bound}^{initial} - \boldsymbol{E_{O\ bound}^{final}}) + (E_{H\ bound}^{initial} - \boldsymbol{E_{H\ bound}^{final}}). \tag{2}$$

The maximal orbital energy of non-bound Oxygen electron, denoted $E_{O\ non-bound}^{final}$ (2), is zero by definition:

$$E_{O\ non-bound}^{final} = 0. \tag{3}$$

Other orbital energies written in non-bold print of the equations (1) and (2) are given respecting zero water molecule enthalpy of transformation from solid to gas state[1].

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

$$E_{O\ non-bound}^{initial} = -15{,}147\ 218\ eV. \tag{4}$$

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

$$E_{O\ bound}^{initial} = -24.881\ 679\ eV. \tag{5}$$

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

$$E_{H\ bound}^{initial} = -19.023\ 237\ eV. \tag{6}$$

The maximal activation energy of non-bound Oxygen electron $\Delta E_{O\ non-bound}$ according to (3) equals the opposite value of non-bound Oxygen electron orbital energy $E_{O\ non-bound}^{initial}$ as follows:

$$\Delta E_{O\ non-bound} = 0 - E_{O\ non-bound}^{initial} = -E_{O\ non-bound}^{initial} = 15{,}147\ 218\ eV. \tag{7}$$

It can be examined that the greatest reduction in bond lengths and angle is achieved when only the bound Hydrogen electrons are deactivated since they possess greater initial orbital energy than the bound Oxygen electrons (5), (6):

$$E_{H\ bound}^{initial} = -19.023\ 237\ eV > E_{O\ bound}^{initial} = -24.881\ 679\ eV. \tag{8}$$

4. ZERO DEACTIVATION ENERGY OF BOUND OXYGEN ELECTRONS

At zero deactivation energy of bound Oxygen electrons we have (1):

$$\Delta E_{H\ bound} = 2\Delta E_{O\ non-bound} - \Delta E_{O\ bound} = 2\ x\ 15{,}147\ 218\ eV - 0 = 30.294\ 436\ eV. \tag{9}$$

And (2)

$$E_{H\ bound}^{final} = E_{H\ bound}^{initial} - \Delta E_{H\ bound} = -19.023\ 237\ eV - 30.294\ 436\ eV = -49.317\ 673\ eV. \tag{10}$$

Corresponding original and subtle orbit lengths of bound Hydrogen electron in the final state are the next [1]:

$$s_{H-original}^{final} = -\frac{Ry\ x\ \alpha^{-1}}{E_{H\ bound}^{final}} = -\frac{13.605\ 693\ 009\ eV\ x\ 137.035\ 999\ 139\lambda_e}{-49.317\ 673\ eV} = 37.805\ 306\ \lambda_e. \tag{11}$$

And

$$s_{H-subtle}^{final} = 2\ x\ s_{H-original}^{final} = 2\ x\ 37.805\ 306 = 75.610\ 613\ \lambda_e. \tag{12}$$

The above subtle orbit length (12) is not in accordance with the double-surface geometry[1] to provide a stable electron circulation on the orbit since for all natural numbers $n \in \mathbb{N}$ holds the non-equality:

$$s(n) = n\left(2 - \frac{1}{\sqrt{1 + \frac{\pi^2}{n^2}}}\right) \neq s_{H-subtle}^{final} = 75.610\ 613\ \lambda_e,\ if\ n \in \mathbb{N}. \tag{13}$$

The nearest conceptual orbit length expressed in Compton wavelengths of electron is a little longer:

$$s_{H-subtle}^{conceptual} = s(76) = 76.064\ 849\dots \tag{14}$$

Consequently it means that some excitation energy of non-bound Oxygen electrons could not origin from the deactivation of bound Hydrogen electrons. Some deactivation energy of bound Oxygen electrons may fulfil the task. Let us also keep in mind for further calculations that the original orbit length of bound Oxygen electron in the initial state is the next (5):

$$s_{O-original}^{initial} = -\frac{Ry \; x \; \alpha^{-1}}{E_{O \; bound}^{initial}} = -\frac{13.605\,693\,009 \; eV \; x \; 137.035\,999\,139\lambda_e}{-24.881\,679 \; eV} = 74.933\,437 \; \lambda_{e.}. \tag{15}$$

5. NON-ZERO DEACTIVATION ENERGY OF BOUND OXYGEN ELECTRONS

The conceptual final original orbit length of bound Hydrogen electron is twice shorter than the conceptual final subtle orbit length of that electron (14):

$$s_{H-original}^{conceptual} = \frac{s_{H-subtle}^{conceptual}}{2} = 38.032\,424 \; \lambda_{e.} \tag{16}$$

The conceptual final original orbit length of bound Hydrogen electron is in inverse proportion with the conceptual final orbital energy of bound Hydrogen electron (11):

$$E_{H \; bound}^{final} = -\frac{Ry \; x \; \alpha^{-1}}{s_{H-original}^{final}} = -\frac{13.605\,693\,009 \; eV \; x \; 137.035\,999\,139 \; \lambda_{e.}}{38.032\,424 \; \lambda_{e.}} = -49.023\,163 \; eV. \tag{17}$$

The conceptual final orbital energy of bound Hydrogen electron is related to the conceptual deactivation energy of bound Hydrogen electron (10):

$$\Delta E_{H \; bound} = E_{H \; bound}^{initial} - E_{H \; bound}^{final} = -19.023\,237 \; eV - (-49.023\,163 \; eV) = -29.999\,926 \; eV. \tag{18}$$

The conceptual deactivation energy of bound Hydrogen electron is related to the conceptual deactivation energy of bound Oxygen electron (9):

$$\Delta E_{O \; bound} = 2\Delta E_{O \; non-bound} - \Delta E_{H \; bound} = 2 \; x \; 15{,}147\,218 \; eV - 29.999\,926 \; eV = 0.294\,510 \; eV. \tag{19}$$

The conceptual deactivation energy of bound Oxygen electron is related to the conceptual final orbital energy of bound Oxygen electron (1), (2):

$$E_{O \; bound}^{final} = E_{O \; bound}^{initial} - \Delta E_{O \; bound} = -24.881\,679 \; eV - 0.294\,510 \; eV = -25.176\,789 \; eV \tag{20}$$

The conceptual final orbital energy of bound Oxygen electron is in inverse proportion with the conceptual original orbit length (11):

$$s_{O-original}^{final} = -\frac{Ry \; x \; \alpha^{-1}}{E_{O \; bound}^{final}} = -\frac{13.605\,693\,009 \; eV \; x \; 137.035\,999\,139}{-25.176\,189 \; eV.} = 74.056\,869 \; \lambda_e. \tag{21}$$

Indeed, the given value is approximately conceptual (13):

$$s_{O-original}^{final} = 74.056\,869 \; \lambda_e \approx s(74) = 74.066\,597 \ldots \lambda_e. \tag{22}$$

6. MINIMAL HOH ANGLE

Minimal HOH angle is given applying cosine rule [1]:

$$HH_{subtle} = OH\sqrt{2(1 - cos\varphi)}. \tag{23a}$$

$$\frac{s_{H-subtle}^{final}}{\pi} = \frac{(s_{O-original}^{final} + s_{H-original}^{final})}{\pi} \; x \; \sqrt{2(1 - cos\,\varphi)}. \tag{23b}$$

Inserting data in the case of zero deactivation energy of bound Oxygen electrons from section 4 we have:

$$75.610\,613 \; \lambda_e = \left(74.933\,437 \; \lambda_e + \frac{75.610\,613 \; \lambda_{e.}}{2}\right) x \; \sqrt{2(1 - cos\,\varphi)}. \tag{24a}$$

And

$$\varphi = 39.186°. \tag{24b}$$

Inserting data in the case of non-zero deactivation energy of bound Oxygen electrons from section 5 we have:

$$76.064\,849\,\lambda_e = \left(74.056\,869\,\lambda_e + \frac{76.064\,849\,\lambda_e}{2}\right) x \sqrt{2(1 - cos\,\varphi)}. \tag{25a}$$

And

$$\varphi = 39.669°. \tag{25b}$$

7. CONCLUSIONS

Respecting zero water molecule enthalpy of transformation approximately the same minimal HOH angle of about 39.5° is expected in the case of zero as well as non-zero deactivation energy of bound Oxygen electrons in water molecule.

ACKNOWLEDGEMENT

Thanks God for Life and Water

DEDICATION

This fragment is dedicated to my dear daughter Alenka

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