

Zero Water Molecule Enthalpy of Transformation

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Abstract: Respecting the subtle touch of Hydrogen atoms in water molecule during the transformation from bend to tetrahedral shape and vice versa the balance between de-excitation energy of bound and non-bound valence electrons is introduced and zero water molecule enthalpy of transformation proposed.

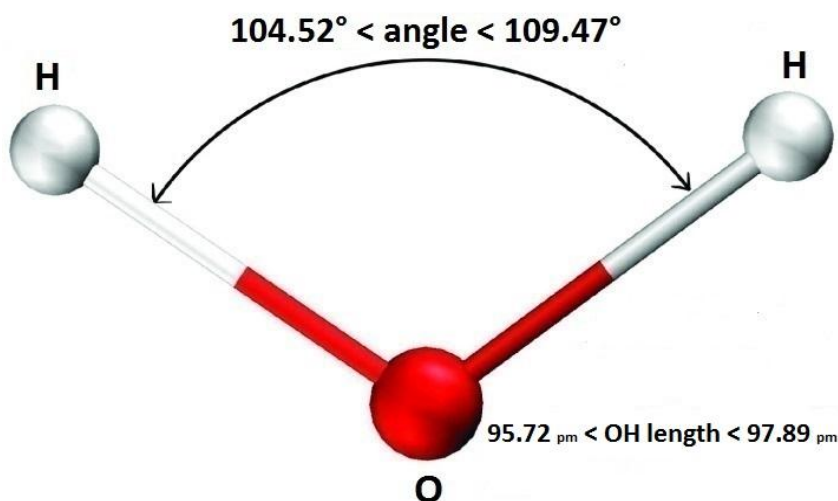
Keywords: Water molecule geometry, subtle and original orbit, double-surface orbit length, Hydrogen s-energy and Oxygen p-energy increment, Oxygen p-energy decrement, zero water molecule enthalpy of transformation

1. PREFACE

Our task in this paper is with the help of subtle touch of Hydrogen atoms [1] in water molecule to introduce zero water molecule enthalpy of transformation.

2. THE GEOMETRY OF WATER MOLECULE

The geometry of water molecule H_2O depends on the belonging physical state as presented below [2]:



Geometry of water molecule from gas to solid state

In the above image the interval of bond lengths l_{O-H} as well as bond angles $\angle HOH$ is given. The concerned lower values belong to the gas state and are based on the experimental OH bond length and angle in the gas phase from spectroscopic data [3]. The parameters of the isolated water molecule are altered significantly in liquid water and even more in hexagonal ice crystals. [3] The concerned upper values belong to the solid state since the hydrogen bonding in the liquid state alters the OH bond length around 97 pm [3] as well as in hexagonal ice crystals the bond angle $\angle HOH$ approaches tetrahedral angle, 109.47° [3]. All the values inside the given interval are expected to be allowed in the liquid phase. Both extreme states are collected in Table 1.

Table 1. The bond length and angle of water molecule in the solid and gas state

Solid state	Gas state
$l_{O-H}^{solid} = 97.89 \text{ pm}$	$l_{O-H}^{gas} = 95.72 \text{ pm}$
$\angle HOH^{solid} = 109.47^\circ$	$\angle HOH^{gas} = 104.52^\circ$

The distance between Hydrogen atoms $l_{H...H}$ in water molecule can be calculated using the cosine rule $l_{H...H} = l_{OH} \times \sqrt{2(1 - \cos \varphi)}$ for each physical state. For the solid state holds:

$$l_{H...H}^{solid} = 97.89 \sqrt{2(1 - \cos(109.47))} = 159.853\ 700\ pm = 65.833\ 455\ \lambda_e \tag{1}$$

And for gas state we have:

$$l_{H...H}^{gas} = 95.72 \sqrt{2(1 - \cos(104.52))} = 151.390\ 065\ pm = 62.395\ 181\ \lambda_e \tag{2}$$

The distance between hydrogen atoms in both physical states of water molecule are shown in table2:

Table2. The distance between Hydrogen atoms of water molecule in the solid and gas state, denoted $l_{H...H}^{solid}$ and $l_{H...H}^{gas}$, respectively

Solid State	Gas state
$l_{H...H}^{solid} = 65.833\ 455\ \lambda_e$	$l_{H...H}^{gas} = 62.395\ 181\ \lambda_e$

3. THE HYDROGEN SUBTLE ORBIT LENGTH

The distance between Hydrogen atoms in solid state, denoted $l_{H...H}^{solid}$, and gas state, denoted $l_{H...H}^{gas}$, equals the diameter of Hydrogen subtle orbit in the concerned physical state [1]. The Hydrogen subtle orbit length in the solid state of water molecule, denoted $s_{H-subtle}^{solid}$, and gas state, denoted $s_{H-subtle}^{gas}$, expressed in Compton wavelengths of the electron λ_e then applying data from Table 2 yields:

$$s_{H-subtle}^{solid} = \pi \times l_{H...H}^{gas} = 206.978\ 977\ \lambda_e \tag{3a}$$

$$s_{H-subtle}^{gas} = \pi \times l_{H...H}^{gas} = 196.020\ 241\ \lambda_e \tag{3b}$$

4. THE DOUBLE-SURFACE CHARACTERISTICS OF SUBTLE-ORBITS

The given subtle-orbit lengths (3a), (3b) are close to the double-surface orbit length $s(n) =$

$$n \left(2 - \frac{1}{\sqrt{1 + \frac{\pi^2}{n^2}}} \right) \text{ enabling a stable electron circulation on the orbit [1]:}$$

$$s_{H-subtle}^{solid\ H_2O} = 206.978\ 977 \approx s(207) = 207.024 \dots \tag{4a}$$

$$s_{H-subtle}^{gas\ H_2O} = 196.020\ 241 \approx s(196) = 196.025 \dots \tag{4b}$$

5. THE HYDROGEN ORIGINAL ORBIT LENGTH AND CORRESPONDING ORBITAL S-ENERGY

The original orbit length $s_{H-original}$ is twice shorter than the subtle orbit length $s_{H-subtle}$ [1]. The corresponding Hydrogen orbital energy (s-energy) in water molecule $E_{H-s}^{H_2O}$ is related to the former [1] as follows:

$$E_{H-s}^{H_2O} = - \frac{Ry \times \alpha^{-1}}{s_{H-original}} \tag{5}$$

Here Ry is Rydberg constant expressed in energy units and α^{-1} is the inverse fine structure constant.

Both extreme Hydrogen original orbit lengths and corresponding orbital s-energies in water molecule are collected in table3:

Table3. The Hydrogen original orbit lengths and corresponding orbital energies (s-energies) in the solid and gas state of water, denoted $s_{H-original}^{solid\ H_2O}$ and $s_{H-original}^{gas\ H_2O}$, respectively

Solid state	Gas state
$s_{H-original}^{solid\ H_2O} = 103.489\ 490\ \lambda_e$	$s_{H-original}^{gas\ H_2O} = 98.010\ 121\ \lambda_e$
$E_{H-s}^{solid\ H_2O} = -18.016\ 030\ eV$	$E_{H-s}^{gas\ H_2O} = -19.023\ 237\ eV$

According to the data in Table 3 the Hydrogen electron in water molecule is in the de-excited state. The de-excitation energy is lower in the gas than solid state as follows:

$$E_{H-s}^{gas\ H_2O} = -19.023\ 237\ eV < E_{H-s}^{solid\ H_2O} = -18.016\ 030\ eV < -Ry = -13.605\ 693\ eV \tag{6}$$

6. THE OXYGEN ORIGINAL ORBIT LENGTH AND CORRESPONDING ORBITAL P-ENERGY

The Oxygen original orbit radius $r_{O-original}$ is the difference between the OH bond length l_{OH} and hydrogen original orbit radius $r_{H-original}$:

$$r_{O-original} = l_{OH} - r_{H-original} \tag{7}$$

And Oxygen original orbit length is 2π – times longer:

$$s_{O-original} = 2\pi \times (l_{OH} - r_{H-original}) = 2\pi \times l_{OH} - s_{H-original} \tag{8}$$

The Oxygen orbital energy (p-energy) in OH bond of water molecule $E_{O-p}^{H_2O}$ is related to the former(5) as follows:

$$E_{O-p}^{H_2O} = -\frac{Ry \times \alpha^{-1}}{s_{O-original}} \tag{9}$$

Both extreme Oxygen original orbit lengths and corresponding orbital p-energies in the OH bond of water molecule are collected in table4:

Table4. The Oxygen original orbit lengths and corresponding orbital energies (p-energies) in the OH bond of water molecule in solid and gas state, denoted $s_{O-original}^{solid H_2O}$ and $s_{O-original}^{gas H_2O}$, respectively

Solid state	Gas state
$s_{O-original}^{solid H_2O} = 75.003\ 476\ \lambda_e$	$s_{O-original}^{gas H_2O} = 74.933\ 439\ \lambda_e$
$E_{O-p}^{solid H_2O} = -24.858\ 444\ eV$	$E_{O-p}^{gas H_2O} = -24.881\ 679\ eV$

According to the data in Table 4 the Oxygen electron in water molecule is in the de-excited state. The de-excitation energy is again lower in the gas than solid state as follows:

$$E_{O-p}^{gas H_2O} = -24.881\ 679\ eV < E_{O-p}^{solid H_2O} = -24.858\ 444\ eV < E_{O-p}^{Oxygen\ atom} \tag{19}$$

$$= -15,147\ 218\ eV. \tag{10}$$

7. THE S-ENERGY INCREMENT

For calculating the Hydrogen s-energy increment E_{H-s} in water during the transformation from the bent gas to tetrahedral solid state the following equation is applicable[1]:

$$E_{H-s} \uparrow = Ry \times \alpha^{-1} \left(\frac{1}{s_{H-original}^{solid}} - \frac{1}{s_{H-original}^{gas}} \right) \tag{11}$$

Applying the data from Table 3 the next s-energy increment per one bound Hydrogen electron is given:

$$E_{H-s} \uparrow = 1.007\ 207\ eV. \tag{12}$$

For the amount of above energy the Hydrogen electron in OH bond of water molecule is more excited in the solid than gas state of water.

8. THE P-ENERGY INCREMENT

For calculating the Oxygen p-energy increment $E_{O-p} \uparrow$ in water during the transformation from the bent gas to tetrahedral solid state the following equation is applicable (11):

$$E_{O-p} \uparrow = Ry \times \alpha^{-1} \left(\frac{1}{s_{O-original}^{solid}} - \frac{1}{s_{O-original}^{gas}} \right) \tag{13}$$

Applying the data from Table 4 the next p-energy increment per one bound Oxygen electron is given:

$$E_{O-p} \uparrow = 0.023\ 234\ eV. \tag{14}$$

For the amount of above energy the Oxygen electron in OH bond of water molecule is more excited in the solid than gas state of water.

9. THE WHOLE S-ENERGY AND P-ENERGY INCREMENT

The whole energy increment in two OH bonds of water molecule is the sum of the energy increments of four valence electrons forming the two bonds (12), (14):

$$E_{OH} \uparrow = 2 \times (E_{H-s} \uparrow + E_{O-p} \uparrow) = 1.030\ 441\ eV. \tag{15}$$

For the amount of above energy the electrons in OH bonds of water molecule are more excited in the solid than gas state of water.

10. THE ORIGIN OF WHOLE ENERGY INCREMENT

The OH bonds in the tetrahedral water molecule have higher energy than OH bonds in bent molecule. But contrarily the whole tetrahedral molecule being present in solid state possesses lower energy than bent molecule being present in gas state. So no energy from outside the water molecule can carry out the energy increment of OH bonds inside water molecule during the transformation from the energetic higher gas state to energetic lower solid state. Only the inner energy of Oxygen non-bound valence electrons can do it. And to do it the energy decrement of Oxygen non-bound electrons $E_O \downarrow$ should happen.

11. THE WHOLE P-ENERGY DECREMENT

The whole orbital energy increment in two OH bonds of water molecule should happen at the zero net energy change in the whole water molecule:

$$E_{OH} \uparrow - E_O \downarrow = 0. \quad (16a)$$

Said explicitly: the energy increment of Oxygen bound valence electrons in OH bonds $E_{OH} \uparrow$ should equal the energy decrement of Oxygen non-bound valence electrons $E_O \downarrow$:

$$E_O \downarrow = E_{OH} \uparrow = 1.030\,441\,eV. \quad (16b)$$

The p-energy decrement of four Oxygen non-bound valence electrons $E_O \downarrow$ thus equals the s-energy and p-energy increment of four bound valence electrons in OH bonds $E_{OH} \uparrow$.

12. THE P-ENERGY DECREMENT PER OXYGEN NON-BOUND VALENCE ELECTRON

The p-energy decrement per one Oxygen non-bound valence electron is a quarter of the whole p-energy decrement:

$$\frac{E_O \downarrow}{4} = 0.257\,610\,eV. \quad (17)$$

For the amount of above energy the Oxygen non-bound valence electron is less excited in the solid than gas state of water.

13. THE P-ENERGY OF OXYGEN NON-BOUND VALENCE ELECTRON IN THE GAS STATE OF WATER MOLECULE

Let us propose that the p-energy of Oxygen non-bound valence electron in gas state of water molecule, denoted $E_{non-bound}^{gas\ H_2O}$, equals that one in the oxygen atom $E_{O-p}^{Oxygen\ atom}$. The latter reflects the effective nuclear charge seen by 2p electrons [4]:

$$E_{O-p}^{Oxygen\ atom} = -\frac{Z_{effective}}{n^2} \times Ry. \quad (18)$$

For $Z_{effective} = 4.4532$ and $n = 2$ [5] we have:

$$E_{O-p}^{Oxygen\ atom} = -15,147\,218\,eV. \quad (19)$$

The p-energy of Oxygen non-bound valence electron in gas state of water molecule yields the above value:

$$E_{non-bound}^{gas\ H_2O} = E_{O-p}^{Oxygen\ atom} = -15,147\,218\,eV. \quad (20)$$

14. THE P-ENERGY OF OXYGEN NON-BOUND VALENCE ELECTRON IN THE SOLID STATE OF WATER MOLECULE

The p-energy per one Oxygen non-bound valence electron of water molecule in the gas state, denoted $E_{non-bound}^{gas\ H_2O}$, is for the p-energy decrement $\frac{E_O \downarrow}{4} = 0.257\,610\,eV$ higher than in solid state, denoted $E_{non-bound}^{solid\ H_2O}$. Then the p-energy per one Oxygen non-bound valence electron of water molecule in solid state possesses the following value:

$$E_{non-bound}^{solid\ H_2O} = E_{non-bound}^{gas\ H_2O} - \frac{E_O \downarrow}{4} = -15,147\,218\,eV - 0.257\,610\,eV = -15.404\,828\,eV. \quad (21)$$

15. THE ORIGINAL ORBIT LENGTH OF OXYGEN NON-BOUND VALENCE ELECTRON

Applying the equation (9) the original orbit lengths of Oxygen non-bound valence electron in both extreme physical states is given. Together with the corresponding p-energies the values are collected in Table 5.

Table 5. The original orbit lengths of Oxygen non-bound valence electrons and corresponding p-energies in the solid and gas state of water molecule

Solid state	Gas state
$s_{non-bound}^{solid H_2O} = 121.031\ 518\ \lambda_e$	$s_{non-bound}^{gas H_2O} = 123.089\ 913\ \lambda_e$
$E_{non-bound}^{solid H_2O} = -15.404\ 828\ eV$	$E_{non-bound}^{gas H_2O} = -15.147\ 218\ eV$

According to the data in Table 5 the Oxygen non-bound valence electrons in water molecule are non-excited in the gas state and de-excited in solid state. The de-excitation energy is – on the contrary as in the case of bound electrons – higher in the gas than solid state:

$$E_{O-p}^{Oxygen\ atom} = -E_{non-bound}^{gas H_2O} = -15.147\ 218\ eV > E_{non-bound}^{solid H_2O} = -15.404\ 828\ eV. \quad (22)$$

16. THE DOUBLE-SURFACE CHARACTERISTICS OF ORIGINAL ORBITS OF OXYGEN NON-BOUND VALENCE ELECTRONS

The given original orbit lengths of Oxygen non-bound valence electrons in gas and solid state of

water molecule are close to the double-surface orbit length $s(n) = n \left(2 - \frac{1}{\sqrt{1 + \frac{\pi^2}{n^2}}} \right)$ enabling a stable

electron circulation on the orbit [2]:

$$s_{non-bound}^{solid H_2O} = 121.031\ 518 \approx s(121) = 121.041 \dots \quad (23)$$

$$s_{non-bound}^{gas H_2O} = 123.089\ 913 \approx s(123) = 123.040 \dots \quad (24)$$

17. CONCLUSIONS

During the transformation of water molecule from the bend shape in the gas state to tetrahedral shape in solid state no energy change in water molecule is expected. From macro point of view we have deal with zero water molecule enthalpy of transformation.

DEDICATION

This fragment is dedicated to all the hidden talents in us who eagerly want to be revealed

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