Double Surface Characteristics of Confined Water Molecule

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Abstract: *The double surface characteristics of shrunk water molecule can help to explain the path of electrons trough the energy barriers in the confined water molecule.*

Keywords: *atom tunnelling, confined and shrunk water molecule, double-surface characteristics*

1. INTRODUCTION

A confined water molecule should accommodate in new circumstances. In a beryl channel, for instance, as shown in Figure1[1]:
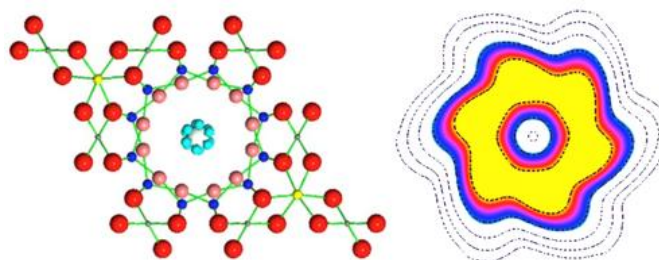

Fig1. *Water ring in beryl channel* [1]

A single water molecule can be confined inside a hexagonally shaped channel of the gemstone beryl (left). The light-blue spheres show the positions of one hydrogen atom in a water molecule as it takes on six different rotational orientations in the water ring [1].

The crystal structure of beryl ($Be_3Al_2Si_6O_{18}$) contains channels with hexagonal cross-sections that can trap water molecules.[1] The channels periodically narrow into "cages" roughly 500 pm wide by 900 pm long and only big enough for one water molecule.[1] Water molecule can occupy six symmetrical orientations in a beryl channel, in agreement with the known crystal structure.[1] A single orientation has the oxygen atom roughly in the center of the channel, with the two hydrogens pointing to the same side (like a "<" symbol) toward one of the channel's six hexagonal faces. [1] Other orientations point to other faces, but are separated from each other by energy barriers of around 0.05eV.[1] However, these barriers don't stop the hydrogens from tunneling among the six orientations and thereby splitting the ground-state energy into multiple levels.[1] Thus the water molecules confined in nanochannels exhibit tunneling behavior that smears out the positions of the hydrogen atoms into a pair of corrugated rings. [1] The subject of interest of this article is to examine the double surface characteristics of such water molecule.

2. THE GEOMETRY OF WATER MOLECULE IN GAS STATE

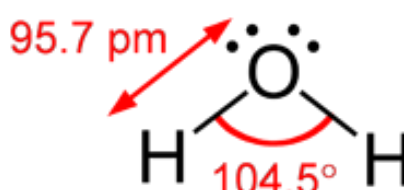The geometry of free water molecule in gas state is shown in Figure2:

Fig2. *Geometry of water molecule in gas state*

The octet of valence electrons consisting of two bound hydrogen electrons and two bound oxygen electrons as well as four non-bound oxygen electrons provides a bent molecule with OH bond length of 95.7 pm and HOH angle of 104.5° in the gas state.[2]

3. THE GEOMETRY OF THE SHRUNK WATER MOLECULE

Respecting the zero enthalpy of water molecule contraction as a consequence of the deactivation of two bound hydrogen electrons and the activation of four non-bound oxygen electrons [3] one can propose that the ratio of HH distance (as well as $\pi - times\ longer\ subtle\ orbit$) and HOH angle in the water molecule is approximately constant:

$$\frac{s_{HH}^{subtle}}{\varphi_{HOH}} = constant. \tag{1}$$

Then applying the data known for the gas state [2] the next constant is given:

$$constant = \frac{s_{HH}^{subtle} = s_{196} = 196.025\ 173\ ...\lambda_e}{\varphi_{HOH} = 104.5°} = 1.875\ 584\ ... \frac{\lambda_e}{°}. \tag{2}$$

4. THE GEOMETRY OF THE CONFINED WATER MOLECULE

To occupy six symmetrical orientations[1] the HOH angle of the confined water molecule should be shrunk from 104.5° to 60°. Then the next subtle orbit length between Hydrogen atoms is expected (2):

$$s_{HH}^{60°} = constant\ x\ 60° = 112.5\mathbf{5}\ ...\lambda_e \approx s_{112.5} = 112.5\mathbf{4}\ ...\lambda_e. \tag{3}$$

Such result (3) does not meet the double surface criteria for a stable orbit which should otherwise obey the next equation[2]:

$$s_n = n\left(2 - \frac{1}{\sqrt{1 + \frac{\pi^2}{n^2}}}\right), n \in \mathbb{N}. \tag{4}$$

On the contrary, with $n = 112.5$ the concerned orbit is completely self-destructive to the fourth number after one circular path. But fortunately just this is exactly what is needed for the beginning of the new life of the electron wave on the next hydrogen orientation. To make this transition feasible all six electrons must perform the electron transition between hydrogen orientations on the pair of corrugated rings simultaneously.

5. THE ENERGY OF THE TEMPORALLY STABLE HH BOND OF THE CONFINED WATER MOLECULE

Taking into account $Ry = 13.606\ \text{eV}$ and $\alpha^{-1} = 137.036$ the energy released at forming the intramolecular subtle HH bond in the confined water molecule contracted to the HOH angle of 60° is given by[4]:

$$\Delta E = Ry\ x\ \alpha^{-1}\left(\frac{1}{\frac{s(112.5)}{2}} - \frac{1}{s(\frac{112.5}{2})}\right) \approx 0.04\ eV. \tag{8}$$

The above energy is close to the energy of 0.05 eV needed for splitting the energy barrier between water molecule orientations in the gemstone beryl [1] seen in Fig3:
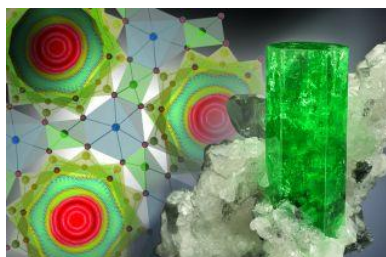

Fig3. *New state of water molecule seen in gemstone beryl (Image: © Jeff Scovil)*

6. CONCLUSION

It looks like a confined water molecule accommodates in new circumstances as a shrunk molecule which uses its double surface characteristics to come through energy barriers.

DEDICATION

This fragment is dedicated to bravery

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