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Subtle Touch of Hydrogen Atoms in Hydrogen Peroxide Molecule

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Abstract: *Respecting the subtle touch of Hydrogen atoms in Hydrogen peroxide molecule the Hydrogen peroxide enthalpy of formation yielding* $\Delta H = 193.177\ kJ/mol$ *is given what is inside the range of the value* $\Delta H(0\ K) = 193.158 \mp \frac{0.080\ kj}{mol}$ *known from Chemistry and Physics references.*

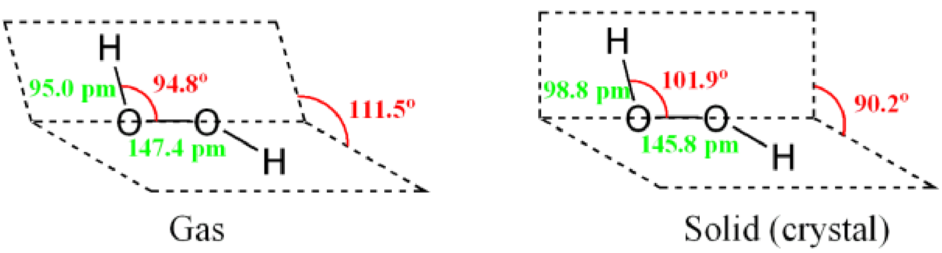
Keywords: *Hydrogen peroxide geometry in solid and gas state, subtle and original orbit, double-surface orbit length, Hydrogen s-energy increment, Hydrogen peroxide enthalpy of formation*

1. Preface

Our task in this paper is to explain the Hydrogen peroxide enthalpy of formation [1] with the help of subtle touch of Hydrogen atoms [2] in Hydrogen peroxide molecule.

2. The Geometry of Hydrogen Peroxide Molecule

The geometry of Hydrogen peroxide molecule H_2O_2 depends on the belonging physical state as presented below [3]:



In the above images the bond length l_{O-H} and l_{O-O} as well as bond angles $\angle HOO$ and $\angle HOH$ are given. For the sake of transparency they are also collected in Table 1:

Table1. *The bond length and angle of Hydrogen peroxide in the solid and gas state*

Solid state	Gas State
$l_{O-H}^{solid} = 98.8\ pm$	$l_{O-H}^{gas} = 95.0\ pm$
$l_{O-O}^{solid} = 145.8\ pm$	$l_{O-O}^{gas} = 147.4\ pm$
$\angle HOO^{solid} = 101.9^o$	$\angle HOO^{gas} = 94.8^o$
$\angle HOH^{solid} = 90.2^o$	$\angle HOO^{gas} = 111.5^o$

The distance between Hydrogen atoms $l_{H...H}$ in H_2O_2 can be calculated using the cosine rule twice for each physical state. For the solid state holds:

$$l_{O...H}^{solid} = \sqrt{98{,}8^2 + 145{,}8^2 - 2\ x\ 98{,}8\ x\ 145{,}8\ x\ cos\ (101{,}9)} = 192.24942\ pm,$$

$$l_{H...H}^{solid} = \sqrt{98{,}8^2 + 192.24942^2 - 2\ x\ 98{,}8\ x\ 192{,}24942\ x\ cos(90{,}2} = 216{,}45758\ pm. \quad (1)$$

And for gas state we have:

$$l_{O...H}^{gas} = \sqrt{95^2 + 147{,}4^2 - 2\ x\ 95\ x\ 147{,}4\ x\ cos\ (94{,}8)} = 181{,}92098\ pm,$$

$$l_{H...H}^{gas} = \sqrt{95^2 + 181{,}9210 - 2\ x\ 95\ x\ 181{,}92098\ x\ \cos(111{,}5))} = 234{,}06914\ pm. \quad (2)$$

The distances between hydrogen atoms in the both physical states of Hydrogen peroxide, denoted $l_{H...H}^{solid}$ and $l_{H...H}^{gas}$, are shown in Table2:

Table2. *The distance between Hydrogen atoms of Hydrogen peroxide in the solid* $l_{H...H}^{solid}$ *and gas state* $l_{H...H}^{gas}$

Solid State	Gas state
$l_{H...H}^{solid} = 216{,}45758\, pm$	$l_{H...H}^{gas} = 234{,}06914\, pm$

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[2]. The Hydrogen subtle orbit length in the solid state of Hydrogen molecule, denoted $s_{H-subtle}^{solid}$, and gas state, denoted $s_{H-subtle}^{gas}$, expressed in Compton wavelengths of the electron λ_e then yields[2]:

$$s_{H-subtle}^{solid} = \pi\ x\ l_{H...H}^{gas} = 280.26985\ \lambda_e. \qquad (3a)$$

$$s_{H-subtle}^{gas} = \pi\ x\ l_{H...H}^{gas} = 303.07332\ \lambda_e. \qquad (3b)$$

4. The Double-Surface Characteristics

The given orbit lengths 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]:

$$s_{H-subtle}^{solid} = 280.26985 \approx s(280) = 280.018\ ... \qquad (4a)$$

$$s_{H-subtle}^{gas} = 303.07332 \approx s(303) = 303{,}016\ ... \qquad (4b)$$

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 $s_{\ H-subtle}$ [2]. The orbital energy (s- energy) of Hydrogen electron in Hydrogen peroxide $E_{H-s}^{Hydrogen\ \ peroxide}$ is related to the former [2] as follows:

$$E_{H-s}^{Hydrogen\ \ peroxide} = -\frac{Ry\ x\ \alpha^{-1}}{s_{H-original}}. \qquad (5)$$

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

Both Hydrogen original orbit lengths and s-energies in the Hydrogen peroxide are collected in Table3:

Table3. *Hydrogen original orbit length and orbital energy (s-energy) in the solid and gas state of Hydrogen peroxide*

Solid state	Gas state
$s_{H-original}^{solid\ Hydrogen\ \ peroxide} = 140.13493\ \lambda_e$	$s_{H-original}^{gas\ Hydrogen\ \ peroxide} = 151.53666\lambda_e$
$E_{H-s}^{solid\ Hydrogen\ \ peroxide} = -13.30482\ eV$	$E_{H-s}^{gas\ Hydrogen\ \ peroxide} = -12{,}30375$ eV

According to the data in Table 3 the electron generated from the Hydrogen atom in Hydrogen peroxide is in the excited state. The excitation energy is higher in gas than solid state:

$$E_{H-s}^{gas\ H_2O_2} = -12{,}30375\ eV > E_{H-s}^{solid\ \ H_2O_2} = -13.30482\ eV > -Ry = -13.60569\ eV. \qquad (6)$$

6. The S-Energy Increment

For calculating the Hydrogen s-energy increment $E_{H-s}\uparrow$ in Hydrogen peroxide during the transformation from the solid to gas state the following equation is applicable:

$$E_{H-s}\uparrow = 2\ x\ Ry\ x\ \alpha^{-1}\left(\frac{1}{s_{H-subtle}^{solid}} - \frac{1}{s_{H-subtle}^{gas}}\right). \qquad (7)$$

Applying the data $(4a), (4b)$ the next s-energy increment per one Hydrogen atom is given:

$$E_{H-s}\uparrow = 1.00107\ eV. \qquad (8)$$

7. The Enthalpy of Formation

Taking into account the s-energy increment $E_{H-s}\uparrow$ of both Hydrogen atoms consisting Hydrogen peroxide the Hydrogen peroxide enthalpy of formation ΔH should be given:

$$\Delta H = 2\ x\ E_{H-s}\uparrow\ x\ N_{Avogadro} = 12.05717\ x\frac{10^{23} eV}{mol} = 193.177\ kJ/mol. \qquad (9)$$

Indeed the above result is inside the range of the value known from Chemistry and Physics references $\Delta H(0\ K) = 193.158 \mp \frac{0.080\, kj}{mol}$ [1]. Since:

$$H_{H_2O_2} - H(0\ K) = 193.177\frac{kJ}{mol} - 193.158\frac{kJ}{mol} = 0.02\frac{kJ}{mol} < 0.08\ \frac{kJ}{mol}. \qquad (10)$$

8. Conclusion

In the present paper calculated Hydrogen peroxide enthalpy of formation yielding 193.2 kJ/mol is in accordance with the known values from Chemistry and Physics references what encourages one to extend the concept of subtle touch electron orbits – previously examined for some planar molecules – to the non-planar molecules, too.

Dedication

This fragment is dedicated to Peace and Beauty

References

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