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 $\Delta H = 193.177 \text{kJ/mol}$ is given what is inside the range of the value $\Delta H(0 \text{ K}) = 193.158 \pm 0.080 \text{kJ/mol}$ 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:

Table 1. The bond length and angle of Hydrogen peroxide in the solid and gas state

<table>
<thead>
<tr>
<th>Solid state</th>
<th>Gas State</th>
</tr>
</thead>
<tbody>
<tr>
<td>$l_{O-H}^{\text{solid}} = 98.8 \text{ pm}$</td>
<td>$l_{O-H}^{\text{gas}} = 95.0 \text{ pm}$</td>
</tr>
<tr>
<td>$l_{O-O}^{\text{solid}} = 145.8 \text{ pm}$</td>
<td>$l_{O-O}^{\text{gas}} = 147.4 \text{ pm}$</td>
</tr>
<tr>
<td>$\angle{HOO}^{\text{solid}} = 101.9^\circ$</td>
<td>$\angle{HOO}^{\text{gas}} = 94.8^\circ$</td>
</tr>
<tr>
<td>$\angle{HOH}^{\text{solid}} = 90.2^\circ$</td>
<td>$\angle{HOH}^{\text{gas}} = 111.5^\circ$</td>
</tr>
</tbody>
</table>

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:

$$
l_{H-H}^{\text{solid}} = \sqrt{98.8^2 + 145.8^2 - 2 \times 98.8 \times 145.8 \times \cos(101.9^\circ)} = 192.24942 \text{ pm},
$$

$$
l_{H-H}^{\text{solid}} = \sqrt{98.8^2 + 192.24942^2 - 2 \times 98.8 \times 192.24942 \times \cos(90.2^\circ)} = 216.45758 \text{ pm}.
$$

(1)

And for gas state we have:

$$
l_{H-H}^{\text{gas}} = \sqrt{95.2^2 + 147.4^2 - 2 \times 95 \times 147.4 \times \cos(94.8^\circ)} = 181.92098 \text{ pm},
$$

$$
l_{H-H}^{\text{gas}} = \sqrt{95.2^2 + 181.92098^2 - 2 \times 95 \times 181.92098 \times \cos(111.5^\circ)} = 234.06914 \text{ pm}.
$$

(2)
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The distances between hydrogen atoms in the both physical states of Hydrogen peroxide, denoted \( l_{\text{H-H}}^{\text{solid}} \) and \( l_{\text{H-H}}^{\text{gas}} \), are shown in Table2:

<table>
<thead>
<tr>
<th>Solid State</th>
<th>Gas state</th>
</tr>
</thead>
<tbody>
<tr>
<td>( l_{\text{H-H}}^{\text{solid}} = 216.45758 \text{ pm} )</td>
<td>( l_{\text{H-H}}^{\text{gas}} = 234.06914 \text{ pm} )</td>
</tr>
</tbody>
</table>

3. THE HYDROGEN SUBTLE ORBIT LENGTH

The distance between Hydrogen atoms in solid state, denoted \( l_{\text{H-H}}^{\text{solid}} \), and gas state, denoted \( l_{\text{H-H}}^{\text{gas}} \), 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 \( s_{\text{H-subtle}}^{\text{solid}} \), and gas state, denoted \( s_{\text{H-subtle}}^{\text{gas}} \), expressed in Compton wavelengths of the electron \( \lambda_e \) then yields[2]:

\[
\begin{align*}
  s_{\text{H-subtle}}^{\text{solid}} &= \pi x l_{\text{H-H}}^{\text{gas}} = 280.26985 \lambda_e. \\
  s_{\text{H-subtle}}^{\text{gas}} &= \pi x l_{\text{H-H}}^{\text{gas}} = 303.07332 \lambda_e.
\end{align*}
\]

4. THE DOUBLE-SURFACE CHARACTERISTICS

The given orbit lengths are close to the double-surface orbit length \( s(n) = n \left( 2 - \frac{1}{\sqrt{1+n^2}} \right) \) enabling a stable electron circulation on the orbit [2]:

\[
\begin{align*}
  s_{\text{H-subtle}}^{\text{solid}} &= 280.26985 \approx s(280) = 280.018 ... \\
  s_{\text{H-subtle}}^{\text{gas}} &= 303.07332 \approx s(303) = 303,016 ...
\end{align*}
\]

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

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

\[
E_{\text{H-peroxide}}^{\text{H}} = -\frac{\text{Ry} x \alpha^{-1}}{s_{\text{H-original}}}.
\]

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

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

<table>
<thead>
<tr>
<th>Solid state</th>
<th>Gas state</th>
</tr>
</thead>
<tbody>
<tr>
<td>( s_{\text{H-original}}^{\text{H}} = 140.13493 \lambda_e )</td>
<td>( s_{\text{H-original}}^{\text{gas}} = 151.53666 \lambda_e )</td>
</tr>
<tr>
<td>( E_{\text{H-peroxide}}^{\text{H}} = -13.30482 \text{ eV} )</td>
<td>( E_{\text{gas}}^{\text{H-peroxide}} = -12.30375 \text{ eV} )</td>
</tr>
</tbody>
</table>

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:

\[
E_{\text{H-peroxide}}^{\text{H}}^{\text{gas}} = -12.30375 \text{ eV} > E_{\text{H-peroxide}}^{\text{H}}^{\text{solid}} = -13.30482 \text{ eV} > -\text{Ry} = -13.60569 \text{ eV}.
\]

6. THE S-ENERGY INCREMENT

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

\[
E_{\text{H-peroxide}}^{\text{H}} \uparrow = 2 x \text{Ry} x \alpha^{-1} \left( \frac{1}{s_{\text{H-subtle}}^{\text{solid}}} - \frac{1}{s_{\text{H-subtle}}^{\text{gas}}} \right).
\]

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

\[
E_{\text{H-peroxide}}^{\text{H}} \uparrow = 1.00107 \text{ eV}.
\]
7. THE ENTHALPY OF FORMATION

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

$$\Delta H = 2 \times E_{H−s} \uparrow \times N_{\text{Avogadro}} = 12.05717 \times 10^{23} \text{eV} \frac{\text{mol}}{\text{mol}} = 193.177 \text{kJ/mol}. \quad (9)$$

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

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

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

