Water Molecule Thermal Stability (Second Side of Fragment)

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Abstract: *Respecting the temperature dependent lengths of the initial bound Hydrogen and initial non-bound Oxygen orbits in the water molecule as well as the double surface geometry the endothermic water molecule thermolysis can be expected to begin at about 1900°C reaching zero Gibbs free energy and the unit equilibrium constant at about 4200°C and being completed at about 6400°C.*

Keywords: *temperature dependent initial orbit lengths, double-surface geometry, Gibbs free energy, water molecule decomposition, equilibrium constant*

1. Preface

Previously[1] the water molecule thermolysis above 1850°C was proposed due to limitations in the zero enthalpy electron energy exchange between Hydrogen and Oxygen orbitals. The aim of the present paper is to extend the validity of the theory to the equilibrium reaction of the water molecule decomposition occurred after this temperature, too.

2. The Temperature Dependent Length of the Initial Orbits

The next temperature dependence expressed in Celsius degrees is expected for the initial bound Hydrogen electron orbit length[1]:

$$s_H = s(103.5) - \frac{s(103.5) - s(98)}{100°C} \, x \, T = 103.547\,646 - 0.054\,973 \, x \, \frac{T}{°C}. \tag{1}$$

And for the initial non-bound Oxygen electron orbit length we have [1]:

$$s_0 = s(121) + \frac{s(123) - s(121)}{100°C} \, x \, T = 121.040\,763 + 0.019\,993 \, x \, \frac{T}{°C}. \tag{2}$$

Where n and $s_x(n)$ is the orbit number and orbit length, respectively, related as follows [1]:

$$s_x(n) = n \left(2 - \frac{1}{\sqrt{1 + \frac{\pi^2}{n^2}}} \right) \; for \; x = O \; or \; H. \tag{3}$$

3. The Role of the Initial Hydrogen and Oxygen Orbit Lengths

At given set of the initial bound Hydrogen and the initial non-bound Oxygen orbit lengths in the water molecule the zero enthalpy of the electron energy exchange can be provided by two mechanisms.[2] The first mechanism is the contraction of the initial bound Hydrogen orbit lengths as the source of the electron energy exchange. It is temperature limited because at some enough high temperature the existence of the initial Hydrogen orbit length with its negative value becomes doubtful in the water molecule(1).The second mechanism is the contraction of the initial non-bound Oxygen orbit lengths as the source of the electron energy exchange. It is temperature limitless (2). When both mechanisms are possible they are in principle equally probable.[2] When only the second mechanism with Oxygen source of the electron energy exchange is available the water molecule decomposition becomes possible. The task of this paper is to answer the question: "How much possible?"

4. The Allowed Temperature for the Electron Energy Exchange in the Water Molecule

The highest temperature for the electron energy exchange in the water molecule can be achieved at the shortest initial bound Hydrogen electron orbit length (1):

$$s_H(1) = 1.6967 = 103.547\ 646 - 0.054\ 973\ x\ \frac{T}{°C}. \tag{4}$$

Yielding:

$$T_1 = 1852.75°C. \tag{5}$$

Taking into account the possibility of forming the subtle-touch orbit a little higher temperature for the electron energy exchange in the water molecule can be achieved (1):

$$s_H(0.5) = 0.9214 = 103.547\ 646 - 0.054\ 973\ x\ \frac{T}{°C}. \tag{6}$$

Yielding:

$$T_{0.5} = 1866.85°C. \tag{7}$$

The electron cannot fall into the nucleus so the initial zero-orbit is impossible and consequently the water molecule cannot be decomposed neither at the corresponding temperature (1):

$$s_H(0) = 0 = 103.547\ 646 - 0.054\ 973\ x\ \frac{T}{°C}. \tag{8}$$

Yielding:

$$T_0 = 1883.61°C. \tag{9}$$

5. THE LOWEST TEMPERATURE OF THE WATER MOLECULE DECOMPOSITION

Obliged to be discrete the first initial bound Hydrogen orbit enabling the water molecule decomposition is the -0.5th orbit because of its negative orbit length (3):

$$s_H(-0.5) = -0.0058 = 103.547\ 646 - 0.054\ 973\ x\ \frac{T}{°C}. \tag{10}$$

Occurring at the next temperature:

$$T_{-0.5} = 1900.37°C. \tag{11}$$

The next initial non-bound Oxygen orbit length corresponds to the initial bound Hydrogen orbit length at given temperature $1900.37°C$ (11) accompanying the water molecule decomposition:

$$s_O(1900.37°C) = 121.040\ 763 + 0.019\ 993\ x\ \frac{T}{°C} = 159.0349 \approx s_O(159) = 159.0310. \tag{12}$$

6. THE MEASURE OF THE WATER MOLECULE DECOMPOSITION

The initial negative bound Hydrogen orbit length value is a measure of the water molecule decomposition. Higher is the temperature more negative is the initial bound Hydrogen orbit length and more water molecules are decomposed. More applicable is the positive value of the ratio of initial negative bound Hydrogen orbit length and initial positive non-bound Oxygen orbit length representing the share of decomposed water molecules:

$$x = -\frac{s_H}{s_O}. \tag{13}$$

Let us see how trustful is above measure.

7. THE LOWEST SHARE OF THE WATER MOLECULE DECOMPOSITION

The lowest share of the water molecule decomposition is the next:

$$x_{min} = -\frac{s_H(T_{min})}{s_O(T_{min})} = -\frac{s_H(1900.37°C)}{s_O(1900.37°C)} = -\frac{s_H(-0.5)}{s_O(159)} = -\frac{-0.9214}{159,0310} = 0,0058. \tag{14}$$

8. THE HIGHEST TEMPERATURE OF THE WATER MOLECULE DECOMPOSITION

The highest temperature of the water molecule decomposition can be achieved at the unit share of decomposition(13):

$$1 = -\frac{s_H}{s_O} = -\frac{s_H(-249)}{s_O(249)}. \tag{15}$$

Since for the initial -249th bound Hydrogen orbit holds $(1), (3)$:

$$s_H(-249) = -249.019\,816 = 103.547\,646 - 0.054\,973\,x\,\frac{T}{°C}. \tag{16}$$

Yielding the highest temperature of the water molecule decomposition:

$$T_{-249} = 6413.47°C. \tag{17}$$

And for the initial 249th non-bound Oxygen orbit we have $(2), (3)$:

$$s_0(249) = 121.040\,763 + 0.019\,993\,x\,\frac{T}{°C}. \tag{18}$$

Yielding to the $6413.47°C$ the nearest possible discrete temperature:

$$T_{249} = 6401.19°C \approx 6413.47°C. \tag{19}$$

9. THE DECOMPOSITION OF THE WATER MOLECULE

The decomposition of the water molecule proceeds in two steps[3]:

$$H_2O \rightarrow HO + H. \tag{20}$$

$$HO \rightarrow H + O. \tag{21}$$

The recombination of H and O atoms produces molecules of H_2 and O_2 and OH as follows[3]:

$$2H \rightarrow H_2. \tag{22}$$

$$2O \rightarrow O_2. \tag{23}$$

$$O + H \rightarrow OH. \tag{24}$$

10. THE FIRST STEP OF THE WATER MOLECULE DECOMPOSITION

We are focused in the first step of the water molecule decomposition (20):

$$H_2O \rightleftharpoons HO + H. \tag{25}$$

In the endothermic reaction the equilibrium constant increases with temperature:

$$k_1 = \frac{x.x}{1-x}. \tag{26}$$

Becoming of unit value at some share of the water molecule decomposition as follows:

$$1 = \frac{x.x}{1-x}. \tag{27a}$$

$$x^2 + x - 1 = 0. \tag{27b}$$

Solving the quadratic equation the next share of the water molecule decomposition is given:

$$x = \frac{-1 + \sqrt{1+4}}{2} = \frac{-1 + \sqrt{5}}{2} = 0.6180. \tag{27c}$$

At this share the Gibbs free energy should be zero. It happens at $4176.35°C$ $(1), (2), (3)$ when the non-bound Oxygen electrons occupy the initial 204th orbit and the bound Hydrogen electrons are dislocated at the initial -126th orbit. After the above temperature the first step of the water molecule decomposition could be spontaneous. The given result of $4449.50\,K$ is in accordance with that one of $4500K$ known from the thermodynamics references [3].

11. THE ONE STEP WATER MOLECULE DECOMPOSITION

If the decomposition possesses only one step we would have:

$$H_2O \rightleftharpoons 2H + O. \tag{28}$$

In the endothermic reaction the equilibrium constant increases with temperature:

$$k_2 = \frac{x^2x}{1-x}. \tag{29}$$

Becoming of unit value at some share of the water molecule decomposition as follows:

$$1 = \frac{x^3}{1-x}. \tag{30a}$$

$$x^3 = -x + 1. \tag{30b}$$

Solving the reduced cubic equation $x^3 = mx + n$ for $m = -1$ and $n = 1$ the next decomposition share is given:

$$x = \sqrt[3]{\frac{n}{2} + \sqrt{\frac{n^2}{4} - \frac{m^3}{27}}} + \sqrt[3]{\frac{n}{2} - \sqrt{\frac{n^2}{4} - \frac{m^3}{27}}} = 0.6823. \tag{30c}$$

At this share Gibbs free energy should be zero. It would happen at $4503.70°C$ $(1), (2), (3)$ when the non-bound Oxygen electrons occupy the initial 211th orbit and the bound Hydrogen electrons are dislocated at the initial -144th orbit. After the above temperature the one step water molecule decomposition could be spontaneous. The given result of $4776.85\ K$ is in poorer accordance with that one of $4500 K$ known from the thermodynamics references [3].

12. CONCLUSION

From the thermodynamic point of view the present theory supports the water molecule decomposition proceeding in two steps as well as the spontaneous decomposition reaction at the turning temperature of about $4500\ K$.

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