Quantized Gibbs Energy of Water Molecule Decomposition

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Abstract: *Respecting the restrictions of the zero enthalpy Hydrogen and Oxygen orbital energy exchange in the water molecule the temperature dependent Gibbs energy of water molecule decomposition is quantized and temperature limited.*

Keywords: *Gibbs energy, water molecule decomposition, equilibrium constant*

1. PREFACE

The subject of interest of this paper is to introduce the temperature dependent Gibbs energy of water molecule decomposition $H_2O \rightarrow H_2 + \frac{1}{2}O_2$ in the light of restrictions of the zero enthalpy Hydrogen and Oxygen orbital energy exchange.[1]

2. TEMPERATURE DEPENDENT GIBBS ENERGY OF WATER MOLECULE DECOMPOSITION

Respecting thermodynamics references [2] Gibbs energy of the water molecule decomposition ΔG is linearly related to the temperature T:

$$\Delta G = aT + b. \tag{1}$$

The constants $a \; and \; b$ can be found solving two equations with two unknowns [2]:

$$228.71 \frac{kJ}{mol} = a \; x \; 373.15 + b. \tag{2a}$$

$$0 = a \; x \; 4500K + b. \tag{2b}$$

Yielding a linear function:

$$\Delta G = -55.42 \; Jmol^{-1}K^{-1} \; x \; T + 249\,389.\,97 \; Jmol^{-1}. \tag{3}$$

The relation should be valid for the water in gas phase at total pressure of 1 atm in principle for all temperatures equal or higher than 373.15 K.

3. RESTRICTIONS OF THE ZERO ENTHALPY ORBITAL ENERGY EXCHANGE

Applying the data from the theory of Hydrogen and Oxygen orbital energy exchange [1] a very similar linear function for Gibbs energy of water molecule decomposition is given. But since here Gibbs energy is quantized as a consequence of quantized orbital energies the relation is valid only as a trend in which all 500 possible Gibbs energies should be found [1]. Unfortunately the unit equilibrium constant and the belonging zero Gibbs energy is not available [1].The smallest positive Gibbs energy belonging to the highest sub-unit equilibrium constant $k = 0.998\,431$ emerges at $T = 4449.5 \; K$ [1]. Taking into account the given data the fictitious zero Gibbs energy can be attributed to the temperature of $T = 4456.5 \; K$. However Gibbs energy remains of the smallest positive value at this temperature and up to the temperature $T = 4458.6 \; K$, too, where it turns to become negative. With the help of the just mentioned temperature of the fictitious zero Gibbs energy instead of the previously applied 4500 K (2b) the next relation is given:

$$\Delta G = -56.01 \; Jmol^{-1}K^{-1} \; x \; T + 249\,610.\,27 \; Jmol^{-1}. \tag{4}$$

The above modified relation (4) of temperature dependent Gibbs energy is valid for water in gas phase at total pressure of 1 atm inside the temperature interval (2156.8 K ; 6686.6 K). Outside this interval Gibbs energy is not defined due to lack of decomposition equilibrium. [1]

4. CONCLUSION

The zero enthalpy Hydrogen and Oxygen orbital energy exchange does not support the presence of decomposed water molecules below 2156.8 K neither water molecules above 6686.6 K. But the quantized Gibbs energy implies the existence of quantized equilibrium of decomposed water molecules inside the concerned interval.

REFERENCES

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