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Determination of the Band Gap of Water

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Abstract **Short Communication**

The study determined the band gap of water. The obtained value is among the band gaps of known semiconductors. The hypothesis that water and ice are semiconductors was confirmed. The law of electrolytic ionization was formulated.

Keywords: electrolyte, semiconductor, band gap, ionization, dissociation.

INTRODUCTION

The identity of the mathematical models of electrolyte solutions and doped semiconductors, which was shown in our previous works (Yefimov, S. 2023), (Yefimov, S. 2023), (Yefimov, S. 2024), (Yefimov, S. 2024), indicates the direction of the search for semiconductor properties of water. Such a property has been discovered and claimed to be an invention called: "Diode made of ice" (Yefimov, S. 2025). In this invention, the analogue of a crystalline semiconductor doped with an n-type impurity is ice doped with an acid, and the analogue of a semiconductor doped with a p-type impurity is ice doped with a base. The obtained experimental data and their interpretation allowed us to draw a conclusion about the mechanism of ionization of electrolytes in water (Yefimov, S. 2025). The proposed mechanism complements and expands the Arrhenius hypothesis of electrolytic dissociation (Arrenius, S. 1903). In this paper, we determined the band gap for water. The resulting value ranks among the band gaps of known semiconductors.

MATERIALS AND METHODS

The calculation of the band gap (Electrons and Holes in Semiconductors. 2009) for water was carried out using reference data on the dependence of the ionic product of water (Kw) on temperature (Рабинович, В. А. Хавин, З. Я. 1977). The data was processed in a Microsoft Excel spreadsheet. Using reference data, the pKw dependence on the reciprocal absolute temperature (1/T) was plotted. Using the Least Squares Method, the experimental points were approximated by a straight line. The band gap (Eg) was extracted from the slope of the line.

RESULTS AND DISCUSSION

The Theory of Electrolytic Ionization considers water as a semiconductor, which means that the expression for the product of charge carrier concentrations in semiconductors (Yefimov, S. 2025) is applicable to it, and this product is the ionic product of water ($Kw = n_e \times n_h$). Let's write down the equation for Kw:

$$Kw = C^2 \times e^{\frac{-Eg}{kT}} (M^2) \text{ (1)},$$

where C- constant, k=1.38E-23 (J/K)-Boltzmann constant, Eg - the energy band gap, T-absolute temperature, $Kw = n_e \times n_h$, n_e and n_h - the molar concentration of mobile charge carriers, electrons (n_e) and holes (n_h) (Electrons and Holes in Semiconductors. 2009). Taking the logarithm of expression (1), we obtain the pKw.

$$pKw = -2 \times lgC + (\frac{E_g \times lge}{k}) \times \frac{1}{T} \text{ (2)}$$

Using reference data (Рабинович, В. А. Хавин, З. Я. 1977), we construct the dependence of pKw on 1/T (Fig. 1). The experimental points are approximated by a straight line (Fig. 1, dotted line) using the least squares method. As a result, we obtain the slope and the intercept with the ordinate axis.

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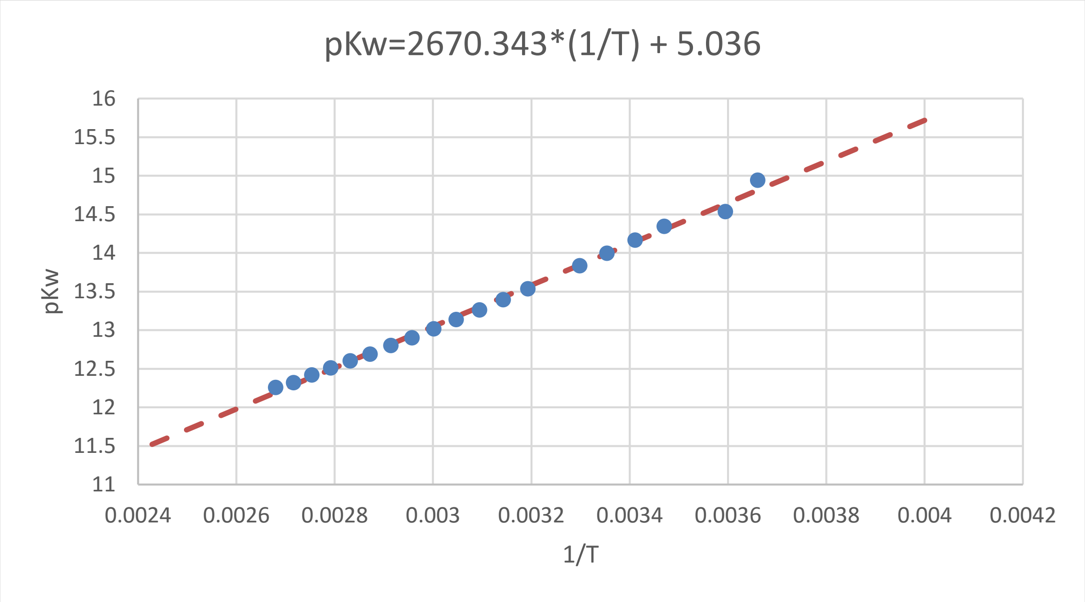

Figure 1: Dependence of pKw on 1/T. Circles – reference data (Рабинович, В. А. Хавин, З. Я. 1977), dotted line – linear regression

Having performed simple calculations, we obtained the energy of the water band gap $Eg = 8.49 \times 10^{-20}$J (0.53 eV**)**, and the constant C=0.003033. To check the correctness of the calculations, we substituted the obtained energy Eg, the constant, and the temperature T=298.15ºK into equation (2) and obtained the expected result: pKw=14.0. The band gap energy of water, 0.53 eV. In the series of semiconductors, water is located between InSb (Eg=0.18eV) and Ge (Eg=0.67eV) (Electrons and Holes in Semiconductors. 2009). The Eg of water proves that water is a semiconductor.

The similarity of theoretical models and semiconductor properties of crystalline semiconductors and aqueous solutions indicates the need to unify them. Such unification would be convenient. As a general model, one should choose a model suitable for crystalline semiconductors, and it is the only possible option. **Law of electrolytic ionization**: *"Water is a semiconductor. In water, acids ionize by donating an electron to the conduction band, while bases ionize by accepting an electron from the hole conduction band, forming a hole. Salt solutions are the product of the interaction of an ionized acid and an ionized base"*.

From this point of view the dissociation schemes should be replaced by corresponding ionization schemes. So, for tri-basic acids, these schemes look like this:

$H_3A = H_3A^+ + e^-$ first stage of ionization
$H_3A^+ = H_3A^{2+} + e^-$ second stage of ionization
$H_3A^{2+} = H_3A^{3+} + e^-$ third stage of ionization
For the bases, these schemes look like this:
$B(OH)_2 = B(OH)_2^- + e^+$ first stage of ionization
$B(OH)_2^- = B(OH)_2^{2-} + e^+$ second stage of ionization
The acid and base ionization constants (K_a, K_b) look like this:

$$K_a{}^1 = \frac{[H_3A^+]\times[e^-]}{[H_3A]}$$

$$K_b{}^1 = \frac{[B(OH)_2{}^-]\times[e^+]}{[B(OH)_2]}$$

These constants' numerical values are equal to those of the known constants of acid and base dissociation.

Now let's compare two competing models:

1. Arrhenius's theory of electrolytic dissociation, and
2. The law of electrolytic ionization.

Common. Both the electrolytic ionization law and the theory of electrolytic dissociation state that during the dissolution of an electrolyte, the number of particles in the solution increases by a factor "**I**" – the number of particles formed when a compound dissolves. Moreover, this factor is numerically equal for both models. It follows that the Colligative properties (Freezing Point Depression and Boiling Point Elevation) such as a boiling point elevation $\Delta T = k \times m \times i$, (where k is constant, m is molality of the solution) a freezing point depression $\Delta T = k \times m \times i$, and an increase in the osmotic pressure of electrolyte solutions (Osmosis and Osmotic Pressure) indirectly confirm both models equally. Oswald's dilution law (Theory of Electrolytic Conductance) also indirectly supports both models equally, in its expression $K = \frac{C\times\alpha^2}{1-\alpha}$, K is the dissociation or ionization constant, and alpha is the degree of dissociation or ionization.

Different. 1. The law of electrolytic ionization predicts semiconducting properties of an aqueous solution of electrolytes, but the Arrhenius theory does not.

2. As we know, the specific electrical conductivity of an electrolyte increases with increasing temperature (Does Temperature Affect Conductivity?).

The law of electrolytic ionization treats water as a semiconductor with all the properties inherent to semiconductors, specifically, it predicts that the specific conductivity of electrolyte solutions should increase with increasing temperature, however, this does not follow from Arrhenius's theory. 3. Ionic product of water within the framework of the theory of electrolytic dissociation: $Kw = [H^+] \times [OH^-] = 10^{-14} (M^2)$ does not contain any information about the dependence of the Kw on temperature. In contrast, the law of electrolytic ionization considers water as a semiconductor, which means that the expression for the product of charge carrier concentrations in semiconductors is applicable to it, and this product is the ionic product of water (1).

CONCLUSION

The determined band gap of water (0.53 eV) is a good confirmation of the law of electrolytic ionization. Among semiconductors, water occupies a position between Indium antimonide (Eg=0.18 eV) and Germanium (Eg=0.67 eV). The law of electrolytic ionization does not replace the Arrhenius dissociation model but rather complements and expands the methods for describing the behavior of electrolyte solutions. Where it is convenient to consider the dissociation of molecules into ions, the Arrhenius's model can be used, but where it is necessary to consider the semiconductor properties of aqueous solutions, the electrolytic ionization model should be used.

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