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Inter-molecular interactions between water and ethanol

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Abstract. The structure and properties of alcohol-water mixtures are of great significance in the study of mass transfer theory and industrial applications. When dissolving in water, alcohols form hydrogen bonds with water, further complicating the properties of the binary mixture. The properties of the mixture they form are quite different from those of the corresponding pure substance. However, although ethanol-aqueous solutions have been widely used, the physical and chemical properties of ethanol-aqueous solutions have not been thoroughly explained. In this paper, various physical changes of ethanol and water after dissolution were observed by experiments, and the possible causes of these changes were analyzed from the perspective of molecular dynamics. It is of positive significance to further understand the molecular interaction between ethanol and water in mixtures and the properties of ethanol aqueous solution.

Keywords: List the; keywords covered; in your paper.

1. Introduction

The ethanol-water binary system has always been a research hotspot. It also has important real-world applications. Ethanol is an bisexual molecule composed of hydrophilic hydroxyl and hydrophobic ethyl. Ethanol molecules dissolved in water combine with water molecules to form hydration molecules and release heat in a process called hydration.

The hydration of ethanol with water molecules can be divided into hydrophobic and hydrophilic types. Marczak and Spurek(2004) believed that in low-concentration ethanol-aqueous solution, hydrophobic coordination played a dominant role, and Franks and Ives(1966) found that water molecules were wrapped in hydrophobic groups of ethanol molecules to form a cage structure. Research by Sikorska et al.(2010) proposed that when the concentration of ethanol increased to 3 mol%, the number of water molecules was not enough to form a cage structure, and the hydrogen bond between ethanol molecules and the hydrophilic groups of water molecules began to dominate, and the hydrogen bond force was very strong, which was also the main reason for the solubility of ethanol in water.

Through experiments and data analysis, combined with the theoretical basis provided by predecessors, this paper tries to explain various phenomena caused by the mixing of ethanol and water from a deeper level, studies the molecular interaction between water and ethanol, and further understands the hydration process of ethanol-aqueous solution and the hydration kinetics of amphoteric ethanol.

2. Results

In the experiment, a certain amount of ethanol was slowly poured into a glass jar filled with water, so that the amount of ethanol in the mixture gradually increased while the temperature of the mixture was recorded periodically. Density changes in ethanol and water mixtures were calculated by measuring changes in volume and weight. In order to ensure the accuracy of the experimental results, five parallel experiments were conducted simultaneously.

3. Density Changes

First, when a small amount of ethanol was added to the water, the volume and weight of the mixture were measured using a cylinder and an electronic balance, and the weight data was divided by the volume data to calculate the density of the mixture. In the course of the experiment, we

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observed that when a very small amount of ethanol has been added to water, the total volume of the solution decreased instead of increasing, resulting in the density of the mixture being greater than that of water. This abnormal phenomenon can be attributed to the hydrophobic cooperation between ethanol molecules and water molecules. Then more ethanol was added to the water, the volume and weight of the mixture were also measured, and the density was calculated. It was then observed that the density of the mixture gradually decreased and became less than that of water as the ethanol was poured continuously. When ethanol of the same volume as water was poured into water, the density of the mixture was greater than 0.9g/cm3 but less than 1g/com3. (Alcohol has a density of 0.8g/cm3 and water has a density of 1g/cm3.)

When the mixture was stored in the air for a period of time, the volume and weight of the mixture were measured again, and it was found that the density of the mixture increased.

4. Temperature Changes

When water and ethanol were mixed, the temperature continued to increase with the slow addition of ethanol. When the ethanol was fully poured in, the temperature reached its maximum and then gradually dropped closer to the room temperature.

In each of the five parallel experiments, the temperature rose rapidly and then gradually dropped to the room temperature. Maximum temperatures for each run were 27, 28, 26.5, 25.4 and 28.2 degrees Celsius.

5. Analysis of Experimental results

5.1 Experimental analysis of temperature changes

The results show that when ethanol was mixed with water molecules, the temperature rose rapidly and then dropped to near the room temperature.

Firstly, the reason for the temperature changes of ethanol after it dissolved in water was analyzed. The substance dissolves in water, usually through two processes: One is the diffusion process of solute molecules, which is a physical process and needs to absorb heat. The other is the process of solute molecules interacting with solvent molecules to form hydration ions or hydration molecules. This process is a chemical process, in which chemical bonds are formed between solvent and solute molecules and heat is released.

Thus, when the solute ethanol molecules enter the solution, they first undergo a process of molecular diffusion, which is endothermic, followed by hydration to form hydrating ions or hydrating molecules, which give off energy. Specifically, hydrogen bonds are formed between ethanol molecules and water molecules through hydration, and the reason why ethanol and water can be miscible in any proportion is also because of the easy formation of hydrogen bonds between them.

By analyzing the experimental phenomenon, we know that in the five parallel experiments in which ethanol dissolved in water, the temperature of the mixtures were increased. It is proved that the heat absorbed by the diffusion endothermic process is less than the heat released by the hydration exothermic process in the physical and chemical process of ethanol dissolving in water. Therefore, the temperature rose when ethanol dissolved in water.

5.2 Experimental analysis of density changes

The experimental results show that when a very small amount of ethanol was mixed with aqueous solution, the volume of the mixed solution decreased slightly at first, resulting in a slight increase in the density of the mixed solution. Then, with the continuous increase of the ethanol solution, the volume of the mixed solution increased gradually, but the total volume is always less than the sum of the volume of added ethanol and the volume of water in the cylinder. When ethanol of the same volume as water was poured into water, the density of the mixture was greater than

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0.9g/cm3 but less than 1g/com3. (Alcohol has a density of 0.8g/cm3 and water has a density of 1g/cm3).Later, when the ethanol completely dissolved in water for a period of time, the volume and weight of the mixture were measured, and it was found that the volume and weight of the mixture decreased slightly, while the density gradually increased.

First of all, the strange phenomenon that the volume of the mixture decreased and the overall density increased slightly after a very small amount of ethanol was added to the water solution is analyzed. This may be caused by the hydrophobic cooperation between ethanol molecules and water molecules, specifically: When a small amount of ethanol is added to water, the alcohol hydroxyl group and water molecules form hydrogen bonds, and the hydrophobic carbon chain of ethanol promotes the water molecules to be closely arranged around it. The interaction between ethanol and water molecules leads to the decrease of the molecular distance between them. From the macro level, it is shown that after a small amount of ethanol is added to the aqueous solution, the volume of the mixture decreases slightly instead of increasing.

Then, it was analyzed why: although the volume of ethanol-water mixture increased with the continuous addition of ethanol, the volume after mixing was always less than the sum of the volume of added ethanol and the volume of water in the measuring cylinder.

There are two reasons why the total volume decreases when ethanol and water are mixed. One is because any molecule is in constant motion, and the other is because there are Spaces between the molecules of the substance. Specifically, the ethanol molecules entering the aqueous solution rapidly diffused into the space of water molecules through motion, and formed hydrogen bonds with water molecules. The gravitational action of chemical bonds reduced the distance between ethanol molecules and water molecules. As a result, the volume of the mixture is less than the sum of the two.

Then, the reasons for density changes of the mixed system during the whole process of ethanol dissolved in water were analyzed. The first is why the mixture becomed slightly denser when a very small amount of ethanol was added to the water. According to the previous analysis, after a very small amount of ethanol is added to water, the hydrophobic cooperation between ethanol molecules and water molecules is dominant. Specifically, When a small amount of ethanol is added to water, the alcohol hydroxyl group and water molecules form hydrogen bonds, and the hydrophobic carbon chain of ethanol promotes the water molecules to be closely arranged around it. The interaction between ethanol and water molecules leads to the decrease of the molecular distance between them. From the macro level, it is shown that after a small amount of ethanol is added to the aqueous solution, the volume of the mixture decreases slightly instead of increasing.

Therefore, through the density formula $\rho=m/v$, it can be known that the density of the mixed system also increases slightly, greater than the density of water (1g/cm3).

Subsequently, we analyzed the reason why the density of the mixed system began to decrease gradually after the continuous addition of ethanol to the water, but was always higher than that of ethanol. The density of ethanol used in the experiment is 0.8g/cm3, and the density of distilled water is 1g/cm3, through comparison we know that the density of ethanol is less than the density of water, according to the density formula $\rho=m/v$, we can quickly know that the density of the mixture of the two should always be greater than the density of ethanol (0.8g/cm3), Less than the density of water (1g/cm3). When ethanol with the same volume as water is added into water, assuming that after mixing, the volume of ethanol and water remains unchanged, the theoretical density of the mixture should be 0.9g/cm3. However, due to the continuous movement between molecules and the space between water molecules and ethanol molecules, hydrogen bonds are formed between ethanol molecules and water molecules. Thus, the volume of the mixture is less than the sum of the two volumes, and the density of the mixture is finally greater than the theoretical 0.9g/cm3.

Finally, the reason why the density of the mixture gradually increased to close to that of water after ethanol completely dissolved in water for a period of time is analyzed. This may be caused by the volatile nature of ethanol. The water-soluble ethanol continued to escape from the mixture

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through the molecular diffusion movement, resulting in the reduction of the weight and volume of ethanol-aqueous solution, while the density gradually approached that of distilled water.

6. Conclusions

Through the experiment of ethanol dissolved in water and the analysis of the experimental results, we have a deeper understanding of the interaction between ethanol molecules and water molecules and the hydration kinetics of ethanol molecules.Specifically, the following conclusions are drawn.

When ethanol dissolved in water, ethanol molecules and water molecules will form hydrogen bonds, and the formation of chemical bonds is an exothermic reaction, which eventually leads to a rise in the temperature of the mixed system.

As ethanol dissolves in water, ethanol molecules continue to spread into the space of water molecules, and form hydrogen bonds with them, resulting in the volume of the mixture is less than the sum of the two volumes.

When a very small amount of ethanol is added to water, the alcohol hydroxyl group and water molecules form hydrogen bonds, and the hydrophobic carbon chain of ethanol promotes the water molecules to be closely arranged around it. The interaction between ethanol and water molecules leads to the decrease of the molecular distance between them. Therefore,after a small amount of ethanol was added to the aqueous solution, the volume of the mixture decreased slightly instead of increasing.

7. Experiments Section

In the experiment, a glass cylinder with a scale of 0.1 mm was used and the ethanol concentration was 99.5%. In addition, distilled water, glass rods, electronic balances and thermometers were used.

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