A Study of the Liquid Structure of 1, 4-Dioxane Aqueous Solution Using the Chemical Shift of ^{17}O-NMR

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Abstract

In the process of investigating the physical and chemical properties of 1, 4-dioxane aqueous solution, the authors discovered an unprecedented phenomenon in which the water-solubility of various types of salt increases. From partial knowledge about the state of both components of the solution, it is thought that the breaking of hydrogen bonds by 1, 4-dioxane generates smaller water-clusters that have high physical or chemical activities. In other words, controlling the liquid structure of water through the addition of 1, 4-dioxane may be possible. The present study investigated the state of both components of the solution and control of the liquid structure of water by 1, 4-dioxane and used ^{17}O-NMR chemical shift to perform a quantitative evaluation of the process by which hydrogen bonds are broken. The following conclusions were obtained:

1) The addition of 1, 4-dioxane, which is capable of breaking hydrogen bonds, can be used to effectively control the liquid structure of water.
2) The process by which hydrogen bonds are broken can be evaluated quantitatively using ^{17}O-NMR chemical shift.

Keywords: ^{17}O-NMR, chemical shift, 1, 4-Dioxane, hydrogen bonds

1. Introduction

In the process of investigating the physical and chemical properties of 1, 4-dioxane aqueous solution, the authors discovered an unprecedented phenomenon in which the water-solubility of various types of salt increases. A state of 1, 4-dioxane existing in 1, 4-dioxane aqueous solution had been examined using low-frequency Raman scattering and water and monomeric 1, 4-dioxane were found to be independently and uniformly mixed. Therefore, we believe that smaller water-clusters having high physical or chemical activities are generated through the breaking of hydrogen bonds by 1, 4-dioxane. In other words, we believe that the liquid structure of water can be controlled by the addition of 1, 4-dioxane.

Although many studies have been performed concerning the liquid structure of water, specifically, clarification of the tetra-coordinated structure, and the existence of clusters that are formed from pentamers, no research has been performed with respect to controlling the liquid structure of water. Although various agents reported to be capable of controlling the

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