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Structural Change of the Mixtures of Ionic Liquid and Water Studied by Infrared Absorption Spectroscopy DOSEOK KIM, YOONNAM JEON, JAEHO SUNG, Department of Physics and Interdisciplinary Program of Integrated Biotechnology, Sogang University, Seoul 121-742 Korea, YUKIO OUCHI, Department of Chemistry, Nagoya University, Chikusa-ku, Nagoya 464-8602 Japan — Infrared absorption spectra of the mixtures of ionic liquid and water (1-butyl-3-methylimidazolium tetrafluoroborate, [BMIM]BF₄) with varying concentrations were obtained by Attenuated Total Reflection (ATR) method. Investigation of the spectra in the OH-stretch vibration range indicated the structural change of the water with the change in the concentration. At very low concentration of water, two peaks around 3600cm⁻¹ were assigned to the monomeric form of water molecules weakly hydrogen bonded to the BF₄⁻ anions. With the increase in the water concentration, the broad feature at ~3460cm⁻¹ corresponding to the bulk water took over the above monomeric peaks, which gradually redshifted with the increased water concentration. In the range from 2800 to 3200cm⁻¹ for the various CH-stretch vibration modes in the cation, the peaks in this ranged blueshifted with the increase in the water concentration. This blueshift was as much as ~7cm⁻¹ for the CH₃ vibration modes of butyl chain while it hardly changed for the modes for the CH attached to the imidazolium core, suggesting varying degree of interactions between the carbon-bonded hydrogen and the water molecules.

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