Changes of H-bond network on cooling in 2-propanol-water liquid mixtures over the entire concentration range

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Due to the fact that 2-propanol molecules show both hydrophobic and hydrophilic characters, its aqueous mixtures provide a good opportunity for studying effects of temperature and composition on the variations of the hydrogen-bonded (H-bonded) network. Understanding these changes at a microscopic level can be a substantial step toward a better understanding the behaviour of aqueous solutions of more complex amphiphilic molecules.

A series of Molecular Dynamics (MD) simulations were performed for 2-propanol—water mixtures over the entire concentration range, between room temperature and the freezing points of the liquids. All-Atom Optimized Potential for Liquid Simulations (OPLS-AA) [1] was used for isopropanol molecules. For water molecules the improved Transferable Intermolecular Potential with four Particles (TIP4P-2005) [2] was applied. The goodness of our models was assessed by the goodness of agreement between total scattering structure factors from the MD models and measured X-ray diffraction data [3,4].

Percolation was monitored by comparing the calculated cluster size distribution functions for the present systems with that obtained for random percolation on a 3D cubic lattice. In percolating systems the cluster size distribution exceeds this predicted function at large cluster size values. It was found that the size of the percolated clusters is decreasing with the increasing ratio of 2-propanol molecules in the mixtures.

Observable trends on varying the temperature and the composition were revealed in terms of the average H-bond number, the fraction of 2-propanol molecules as H-acceptors and as H-donors in the H-bonds, as well as in terms of size distributions of cyclic entities [6].

[1] W. L. Jorgensen; D. Maxwell, S. Tirado-Rives, J. Am. Chem. Soc., 118, 11225−11236 (1996).
[2] J. L. F. Abascal, C. Vega, J. Chem. Phys., 123, 234505/1−12 (2005).
[3] T. Takamuku, K. Saisho, S. Nozawa, T. Yamaguchi, J. Mol. Liq., 119, 133– 146 (2005).
[4] I. Pethes, L. Temleitner, L. Pusztai, unpublished results
[5] I. Bakó, J. Oláh, A. Lábas, Sz. Bálint, L. Pusztai, M.C. Bellissent Funel, J. Mol. Liq., 228, 25-31 (2017).
[6] Sz. Pothoczki, L. Pusztai, I. Bakó, J. Phys. Chem. B 122, 6790−6800 (2018).