

Study of the self-diffusion coefficient in the water-methanol binary mixture from the hydrogen bonding viewpoint using DOSY NMR

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Self-diffusion coefficient in the water-methanol binary mixture was measured by NMR diffusion-order spectroscopy (DOSY) experiment [1] at different concentrations. The self-diffusion coefficient of both water and methanol decreases exponentially as methanol mole fraction increases. This behavior is similar to the concentration dependence of the diffusivity in the water-glycerol binary mixture but the rate of exponential decay is different for two solutions. This trend gives information about the intermolecular interactions specially the hydrogen bonds. The effect of the temperature on the self-diffusion coefficient was also analyzed. An Arrhenius temperature behavior was observed for the self-diffusion coefficient of both water and alcohol. The self-diffusion activation energy of water was measured 24.8 and 23.2 kJ mol⁻¹ in methanol and glycerol solutions, respectively. Likewise, this value was obtained 13.6 for methanol and 28.5 kJ mol⁻¹ for glycerol. The results help to reveal some aspects of the molecular structure of the alcohol solutions with the focus on the hydrogen bonds.

References

- [1] C. S. Johnson Jr.: *Diffusion ordered nuclear magnetic resonance spectroscopy: principles and applications*. Progress in Nuclear Magnetic Resonance Spectroscopy. **34**, 203–256 (1999)

