

# Large-Angle X-ray Scattering Investigation of the Structure of 2-Propanol–Water Mixtures

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The structure of 2-propanol and its aqueous mixtures has been investigated at 25°C, using a large-angle X-ray scattering (LAXS) technique. The total radial distribution function of neat 2-propanol has shown that hydrogen-bonded chains of 2-propanol molecules are formed. In the 2-propanol-water mixtures, 2-propanol chains predominate at mole fractions  $x_{\text{pr}} > \sim 0.1$ . When  $x_{2\text{pr}}$  decreases from  $x_{2\text{pr}} = 1$ , the number of hydrogen bonds reaches a plateau of  $3.4 \pm 0.1$  at  $x_{\text{pr}} \leq \sim 0.1$ , suggesting that the tetrahedral-like structure of water is mainly formed. On the basis of the present findings, together with previous results on methanol-water and ethanol-water mixtures, effects of hydrophobic groups on the structure of the alcohol-water mixtures are discussed. The heat of mixing at 25°C as a function of  $x_{2\text{pr}}$  has been interpreted in terms of the structural transition of solvent clusters.

*Key words:* 2-Propanol–water Mixtures; Structure; LAXS; Hydrogen Bonds; Hydrophobic Group.