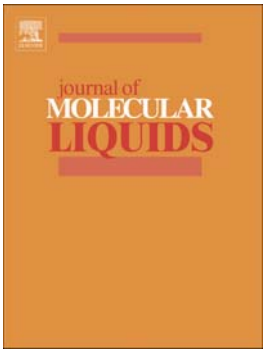

On the micro-heterogeneous structure of neat and aqueous propylamine mixtures: a computer simulation study

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On the micro-heterogeneous structure of neat and aqueous propylamine mixtures: a computer simulation study

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Abstract

The micro-heterogeneous structure of neat and aqueous propylamine is examined through computer simulations. Neat propylamine is found to have a pre-peak in the nitrogen-nitrogen structure factor, due to the presence of branched chain-like aminogen clusters. Aqueous propylamine mixtures are found to be micro-segregated at all amine concentrations. Both the water-water and the amine nitrogen-nitrogen structure factors show the characteristic domain pre-peaks in their respective moderate to high contents. The amine cluster pre-peak, still visible at high amine content, disappears into the domain pre-peak at lower amine contents. Interestingly, water domains forms linears clusters for water concentrations below equimolar. We discuss the specificity the amine brings to the nature of the water clustering as compared with other type of solutes. In particular, we find that the Kirkwood-Buff integrals are quasi-ideal in the amine mole fraction range $0.3 < x < 1$, which we interpret as being consistent with the linear water clusters observed in this range, and which act as individual supra-molecular entities. We conjecture that such cluster shapes are consistent with the existence of a lower critical solution temperature for this system as well as other aqueous amines.

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