

What Quantum Chemists Owe to Molecular Physicists: Aqueous Mixtures of Alcohols

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Accurate pure fluid intermolecular potential models are used to study aqueous mixtures of methanol over the entire composition range. It is shown that when these potentials are used for mixtures, only rough qualitative agreement is obtained for excess properties and that the potentials fail to reproduce, at least qualitatively, the partial molar volume of methanol.

This failure is associated with the cross water-alcohol interaction for which no theoretically-based combination rules have been developed yet.

In addition, the same mixtures are also studied using primitive models and the same results are obtained. Agreement with experimental findings is found only when the cross interaction is empirically adjusted.