Dimerization of Carboxylic Acids: An Equation of State Approach

The association term of the nonrandom hydrogen bonding theory, which is an equation of state model, is extended to describe the dimerization of carboxylic acids in binary mixtures with inert solvents and in systems of two different acids. Subsequently, the model is applied to describe the excess enthalpies and the vapor-liquid equilibrium of relevant binary mixtures containing low molecular weight organic acids. The model sheds light on the interplay of intermolecular interactions through the calculation of the various contributions to the mixing enthalpies, namely from hydrogen bonding and non-hydrogen bonding (dipolar, induced polar or dispersive) interactions. According to model predictions, the acid molecules are so strongly associated that the addition of inert solvents to carboxylic acids with small carbon numbers at ambient temperature does not dramatically alter their degree of association. Consequently, the observed endothermic dissolution process is mainly attributed to the hindering of polar interactions. Furthermore, upon mixing of two carboxylic acids, the rearrangement of hydrogen bonds due to the formation of cross associating species results in an insignificant contribution to the heats of mixing due to the rather constant dimerization enthalpy that is revealed by the available experimental data for low molecular weight compounds.

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