A Group-Contribution Lattice Fluid Equation of State with Hydrogen Bonding Involving COSMO-RS

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Group contribution based models are widely used in industrial applications for its convenience and flexibility. Although a number of group contribution models have been proposed, there were certain limitations inherent to those models. Models based on group contribution excess Gibbs free energy are only limited to low pressures and models based on equation of state (EOS) cannot properly describe highly nonideal mixtures including acids without introducing additional modification such as chemical theory. In the present study new a new appoach derived from quantum chemistry have been used to calculate necessary group interaction parameters. The COSMO-RS method, based on quantum mechanic, provides an reliable tool for fluid phase thermodynamics. Benefits of the group contribution EOS are the consistent extension to hydrogen-bonded mixtures and the capability to predict polymersolvent equilibria up to high pressures. The authors are confident that with a sufficient parameter matrix the performance of the lattice EOS can be improved significantly.