167d Thermodynamic Modeling of the Phase Behavior of Binary Systems of Ionic Liquids and Carbon Dioxide with the Gc-Eos

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Over the past decade, ionic liquids have attracted a great deal of attention as possible replacements for conventional solvents in a number of synthetic processes. Ionic liquids have a couple of features that make them attractive as solvents, including their negligible vapor pressure, their good solubility characteristics, their wide liquid temperature range and the fact that their physical and chemical properties can be changed through appropriate modifications of the cation, the anion, or the alkyl chains. Numerous chemical reactions have been performed successfully in ionic liquids. However, separation of the products from the reaction medium sometimes exhibits some problems. A promising separation technique for ionic liquids is the extraction of solutes with supercritical carbon dioxide (CO2). By employing CO2 for product recovery, it is not only possible to quantitatively extract the organic solute from the ionic liquid, but also to eliminate the problem of cross-contamination; CO2 can easily be removed by simple depressurization. In the case of extraction with supercritical CO2, knowledge of the phase behavior of binary systems of ionic liquids and CO2 is essential for evaluating the viability of the separation process. Considering the large variety of ionic liquids that may be formed, methods for the prediction of phase equilibria involving ionic liquids are needed. In this work, an equation of state approach is used for the modeling of the phase behavior of binary systems of ionic liquids and CO2. The Group Contribution Equation of State (GC-EOS) developed by Skjold-Jørgensen is used to predict the phase behavior of binary systems consisting of CO2 and ionic liquids of the homologous family 1-alkyl-3-methylimidazolium hexafluorophosphate. The agreements between experimental and predicted bubble point data for the ionic liquids [emim][PF6], [bmim][PF6] and [hmim][PF6] are excellent for pressures up to 10 MPa and even for pressures up to about 100 MPa the agreements are good. These results show the capability of the GC-EOS model to describe the phase behavior of binary systems of ionic liquids and CO2 and its potential for modeling supercritical processes involving ionic liquids.