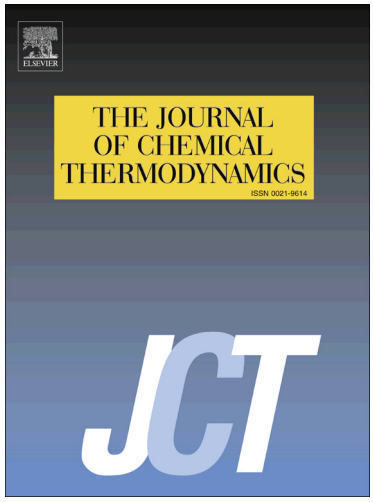

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PII: S0021-9614(16)30310-X
DOI: http://dx.doi.org/10.1016/j.jct.2016.10.011
Reference: YJCHT 4841

To appear in: *J. Chem. Thermodynamics*

Received Date: 23 January 2016
Revised Date: 26 September 2016
Accepted Date: 5 October 2016

Please cite this article as: B. Long, Y. Xia, Z. Deng, Y. Ding, Understanding the enhanced solubility of 1,3-benzenedicarboxylic acid in polar binary solvents of (acetone + water) at various temperatures, *J. Chem. Thermodynamics* (2016), doi: http://dx.doi.org/10.1016/j.jct.2016.10.011

Understanding the enhanced solubility of 1,3-benzenedicarboxylic acid in polar binary solvents of (acetone + water) at various temperatures

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Abstract: Understanding solid dissolution in polar binary solvents showing maximum or minimum solubility phenomenon is essential for the design and operation of anti-solvent crystallization process. Solubilities of 1,3-benzenedicarboxylic acid in binary solvents of acetone with water are measured from 278.15 to 323.15 K using the static equilibrium method, covering the entire range of solvent composition. The solubility always increases with increasing temperature, while, at fixed temperature, a maximum solubility is observed in mixed solvents of certain composition. The experimental temperature-dependent solubility data of 1,3-benzenedicarboxylic acid in coslovents of different compositions are correlated using the Apelblat model with an average relative deviation (ARD) of 0.18%. Calculations of the derived thermodynamic functions show that the dissolution of 1,3-benzenedicarboxylic acid in the solvent mixtures is endothermic and mainly driven by the enthalpy change. The simplified Modified Wilson (SMW) model is adopted to reproduce the isothermal solubility data over the entire acetone composition with an overall ARD of 1.41%, with which the maximum mole fraction solubility and the corresponding solvent composition at different temperatures are determined, and are subsequently used to estimate the solubility parameter of 1,3-benzenedicarboxylic acid.

Keywords: Solubility, Mixed solvents, 1,3-Benzenedicarboxylic acid, Synergistic effect, Modeling

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