

Solubilities, Henry's Law Constants and Direct Correlation Function Integrals of Gases in Ionic Liquids

Jens Abildskov^{C, S} and Martin D. Ellegaard

Department of Chemical and Biochemical Engineering, Technical University of Denmark, Kgs. Lyngby, Denmark

John P. O'Connell

Department of Chemical Engineering, University of Virginia, School of Applied Science and Engineering, Charlottesville, VA, U.S.A.

We describe a combination of experimental gas (hydrogen, carbon monoxide, oxygen, methane etc.) solubilities in ionic liquids with a two-parameter, corresponding-states form for direct correlation function integrals in liquids. Previously [Campanella E.A. et al., 1987, AIChE J., 33(12): 2057] this method was applied to many types of systems with one substance being supercritical. That gave a quantitative correlation for volumetric behavior of pure and mixed systems, pure and mixed solvent Henry's law constants, and Henry's Law deviations over wide ranges of conditions using only pure component information and (possibly) a single binary parameter. Details of the method and results obtained for hydrogen, carbon monoxide, oxygen and methane in the ionic liquids 1-butyl-3-methyl-imidazolium hexafluorophosphate ([bmim][PF₆]) and 1-hexyl-3-methyl-imidazolium bis(trifluoromethylsulfonyl)imide ([hmim][Tf₂N]) are presented. In addition, a procedure is explored for predicting Henry's law constants without using experimental gas solubility data at isothermal conditions.

[1] E.A. Campanella, P.M. Mathias, and J.P. O'Connell, 1987. "Equilibrium Properties of Liquids Containing Supercritical Substances", AIChE J., 33(12): 2057-2066.