Solubility of Halogenated Benzene Isomers in Room-Temperature Ionic Liquid: 1-Ethyl-3-Methylimidazolium Bis(Trifluoromethylsulfonyl)Imide

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Binary liquid-liquid equilibria (LLE) in mixtures of halogenated benzenes and room-temperature ionic liquid, 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ([emim][Tf_2N]), have been measured using the volumetric method over a temperature range from about (283 to 373) K. The observed solubility data for the binary systems of benzene + [emim][Tf_2N] and hexafluorobenzene + [emim][Tf_2N] have been used to develop our equation-of-state (EOS) model. Ternary phase diagrams for the present three component system (benzene + hexalfluorobenzene + [emim][Tf_2N]) have been constructed and extractive separations of the benzene/hexafluorobenzene azeotropes are discussed. The measured LLE for other fluorinated benzene isomers + [emim][Tf_2N] were well correlated by use of the nonrandom two liquid (NRTL) solution model. A general trend between the magnitude of the dipole moment (polarity) and the immiscibility gap was found, although other intermolecular interactions (higher-order moments, p-electron effects, and hydrogen bonding) may also be involved. The fluorinated benzenes having the largest dipole moments (1,2-difluorobenzene, 1,2,3-trifluorobenzene, and 1,2,3,4-tetrafluorobenzene) were completely miscible in the [emim][Tf_2N]. The binary systems (1,4-difluorobenzene, 1,3,5-trifluorobenzene, and 1,2,4,5-tetrafluorobenzene) with zero dipole moments, and the binary systems (fluorobenzene, 1,3-difluorobenzene, 1,2,4-trifluorobenzene, 1,2,3,5-tetraflurobenzene, and pentafluorobenzene) with dipole moments of about 1.4 D were only partially miscible in [emim][Tf_2N]. LLE behavior for mono-substituted chlorobenzene, bromobenzene, and iodobenzene have been measured and compared with fluorobenzene indicate that molecular size may also play a role in determining the miscibility behavior.