A Lattice Group Contribution Equation of State Involving COSMO-RS Applied to Systems Containing Ionic Liquids

알렉산더, 윤지은, 강정원[1], 임종성, 유기풍[*]
서강대학교; [1]고려대학교
(kpyoo@sogang.ac.kr[*])

Group contribution based models are widely used in industrial applications for its convenience and flexibility. In previous studies we introduced the COSMO-RS, based on quantum mechanic, to obtain energy parameters for the lattice group contribution equation of state. Since our previous results have been promising the new method of obtaining parameters has been evaluated for binary systems containing ionic liquids and carbon dioxide. The current approach showed a satisfying agreement with the experimental data sets. The authors are confident that with the new method the performance of the lattice EOS can be improved significantly and new apply able areas such as solvent screening can be opened.