Abstract

Dispersion of asphaltene in crude oil using ionic liquids (ILs) is being considered as a viable solution, in extraction and transportation processes. In this work, the interplay between asphaltene and ILs has been studied systematically to understand the effect of structural variation of ILs on asphaltene solubility. The activity coefficient of the total of 1517 ILs with different combinations of cation and anion of ILs for representative asphaltene molecule (asphaltene) was estimated via COSMO-RS (Conductor-like Screening Model for Real Solvents). COSMO\_RS predictions were validated using experimental data on asphaltene solubility. Among the studied ILs, asphaltene showed high solubility in imidazolium-based ILs with hydrophobic anions. The present approach paved a way forward to rationally understand the impact of structural variation of ILs on their interaction with asphaltene molecule and to design new ILs for the dispersion and stabilization of asphaltene.