Abstract

Significance of Ionic Liquids (ILs), designer solvents, on inhibiting the asphaltene deposition provided the alternative solution to the problem. In this work, 34 anions and 3 cations comprising of 102 combinations of ILs were investigated for a model asphaltene molecule via quantum solvation software tool COSMO-RS (Conductor like Screening for Real Solvents). Validation is done by comparing literature values of activity coefficient at infinite dilution (IDAC) of alkanes, cycloalkanes and aromatic in 3 ILs with 111 data points at 3 sets of different temperatures. Percent relative absolute average deviation (%RAAD) was found to be 10%. Thereafter IDAC values were predicted for model asphaltene compound in the cations and anions combinations for performance analysis. It is found that smaller cation with sterically shielded large anion gave the large performance for removal of upgrading the asphaltenic crude oil.