

Density functional theory on ionic liquid as carbonate scale dissolver in petroleum pipelines

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ABSTRACT

The carbonate scale is the common oilfield scale found in the petroleum pipeline, which will cause flow assurance problems. In the purpose to conquer this problem, the alternative approach is to use ionic liquids (ILs) particularly in dissolving carbonate scale. The main objective of this study is to determine the effective ILs to dissolve carbonate scale in petroleum pipelines, and to evaluate the effect of intermolecular interaction in ILs toward their properties such as dissolution capabilities. The density functional theory (DFT) calculation is used to investigate the intermolecular interaction of a series of different ion pair, namely cations and anions-based of ILs with carbonate ion. All the calculations are completed by Gaussian software at the hybrid Becke 3-Lee-Yang-Parr (B3LYP) level using the 6-311++G(d, p) basis set. The optimized structure of carbonate ion and ion pairs of ILs have been obtained from the calculation which was further complemented by harmonic vibrational frequency, binding energies, bond type, bond order, and natural bond orbital (NBO). The binding energy for the cation and anion-based ILs are obtained where the ammonium ion is -302.2627 kJ/mol and tetrafluoroborate ion is -562.9194 kJ/mol which depict to have the highest value compare to others. Both of them are made up of the single bond and are characterized as the polar covalent bond. The NBO analysis pointed out the higher second-order perturbation energy, $E(2)$ for ammonium ion is at a lone pair, LP (1) N 9 to antibonding sigma, $BD^*(1)$ O 3H 6 while BF_4 ion is at lone pair LP (3) F 2 to antibonding lone pair, $LP^*(1)$ Ca 6. The selective ILs, ammonium tetrafluoroborate shown the higher negative binding energy which is -371.93 kJ/mol having the same nature of bond type and bond order from the findings in cation and anion-based ILs.

KEYWORDS

Binding energy; Bond type and bond order; Density functional theory (DFT); Gaussian software; Natural bond orbital (NBO); Optimized structure

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