Theoretical probing of anion-cation interaction in 1-butylpyridinium based ionic liquids

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ABSTRACT

The 1-butylpyridinium based-ionic liquids composed of 1-butylpyridinium cation in combination with three different anions: Cl^-, Br^- and BF_4^- was optimized by DFT method using 6311++G (d, p)/B3LYP basis set in G09 software. The results have been analysed using multiwfn software [1] to study the differences arising in the electron localization function (ELF), reduced density gradient (RDG) and molecular electrostatic potential (ESP) of the three ionic liquid molecules due to the difference in the accompanying anions. The plot of total density of states (TDOS), partial density of states (PDOS) and overlap density of states (OPDOS) for the three ILs have been compared.

Observation of OPDOS curves in these plots confirms that a strong chemical bond formation between the anion and cation in these ILs is not possible. This observation was further confirmed by observing isosurfaces of corresponding molecular orbitals. The nature of interaction between the anion and cation in these ILs have been probed by analysing the critical points (CP) of bonding paths between the anion and cation which satisfied the Poincare-Hopf relationship [2] and also from the RDG plots. The RDG isosurface representing the weak interaction region between the anion and cation was clearly observed.

Key words: ionic liquids, ELF plot, RDG, ESP, critical points, bond order analysis, radial distribution function

References

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