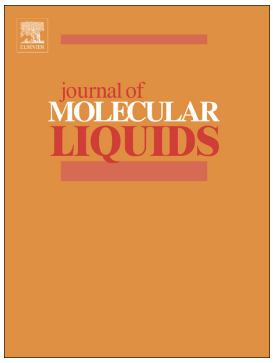

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Tuning the structural, electronic and electrochemical properties of the 4-methyl-1-phenyl triazolium based [PhMeTAZ][Y_{1-8}] ionic liquids through changing anions: A quantum chemical study

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Abstract

The many ionic liquids properties can be tuned for specific applications by changing their constituent ions. In the present work, the effect of anion variations on the structural, electronic and thermodynamic characteristics of the tunable phenyl methyl triazolium based ionic liquids [PhMeTAZ][Y_{1-8}] (Y = CH_3COO^-, NO_3^-, CF_3COO^-, BF_4^-, ClO_4^-, $N(CN)_2^-$, Tf_2N^- and $C(CN)_3^-$ were explored at M06–2X/6-311++G(d,p) level of theory. Thermodynamic binding energy of ion pairs were assessed using M06-2X and dispersion corrected M06-2X-D3, B2PLYP-D and mPW2PLYP-D functionals. Based on the Grimme's dispersion corrected binding ΔG values, strength of the inter-ionic interactions in the ILs decreases in the following order: [PhMeTAZ][CH_3COO] > [PhMeTAZ][CF_3COO] > [PhMeTAZ][NO_3] > [PhMeTAZ][BF_4] > [PhMeTAZ][ClO_4] > [PhMeTAZ][$N(CN)_2$] > [PhMeTAZ] [Tf_2N] > [PhMeTAZ] [$C(CN)_3$]. In addition, thermodynamic functions of formation and combustion of ionic liquids ($\Delta H_f^{\circ},_{298}$, $\Delta G_f^{\circ},_{298}$ and $\Delta H^{\circ}_{c,298}$ using CBS-QB3 composite method), electrochemical stability of the caions and anions, electrochemical window (ECW), crystal lattice energy and volumetric based properties were assessed. The $\Delta H_f^{\circ},_{298}$ and $\Delta G_f^{\circ},_{298}$ of all ILs are positive and those of Y_3, Y_5 and Y_6 based ILs are greater than others, indicating that formation of these ionic liquids is high energetic. The molar enthalpy of combustion for Y1, Y4 and Y6 based ILs is greater than 1500.0 kcal mol^{-1}. Our results also show that

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