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Tuning the structural, electronic and electrochemical properties of the 4-methyl-1-phenyl triazolium based [PhMeTAZ][Y₁₋₈] 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][Y₁₋₈] (Y = CH₃COO⁻, NO₃⁻, CF₃COO⁻, BF₄⁻, ClO₄⁻, N(CN)₂⁻, Tf₂N⁻ 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][CH₃COO] > [PhMeTAZ][CF₃COO] > [PhMeTAZ][NO₃] > [PhMeTAZ][BF₄] > [PhMeTAZ][ClO₄] > [PhMeTAZ][N(CN)₂] > [PhMeTAZ][Tf₂N] > [PhMeTAZ][C(CN)₃]. In addition, thermodynamic functions of formation and combustion of ionic liquids ($\Delta H_{f,298}^{\circ}$, $\Delta G_{f,298}^{\circ}$ and $\Delta H_{c,298}^{\circ}$ using CBS-QB3 composite method), electrochemical stability of the cations and anions, electrochemical window (ECW), crystal lattice energy and volumetric based properties were assessed. The $\Delta H_{f,298}^{\circ}$ and $\Delta G_{f,298}^{\circ}$ of all ILs are positive and those of Y₃, Y₅ and Y₆ 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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