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Ali Ounissi, Yacine Benguerba, Nadia Ouddai

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## Theoretical investigation on structural and physicochemical properties of some ionic liquids

Ali OUNISSI<sup>A,b</sup>, Yacine BENGUERBA<sup>a</sup>, Nadia OUDDAI<sup>b</sup>

<sup>a</sup> Laboratoire de Génie des procédés chimiques, Université Setif-1.

<sup>b</sup> Laboratoire de Chimie des Matériaux et des Vivants : Activité & Réactivité (LCMVAR), Université Batna1.

### Abstract

Theoretical studies were carried out using density functional theory (DFT) method, including the explicit dispersion (functional B97D), on a group of five Ionic liquids (**ILs**), selected based on their hardness. The results of all the theoretical approaches show that there is no covalent bond between anion and cation of the **ILs**. The quantum theory of atoms in molecules (AIM) allowed us to confirm the existence of weak hydrogen bonds. The physicochemical properties were determined using the program Cosmotherm. A correlation between viscosity and energy of **ILs** Van der Waals energy was obtained. The distribution of the electron density displayed by "molecular electrostatic potential" (MEP) cards shows the effect of introducing the oxygen atom in MoEMIM.

### Keywords

Density functional; theoretical chemistry; ionic liquids; physicochemical properties; geometry optimization; cations/anions

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