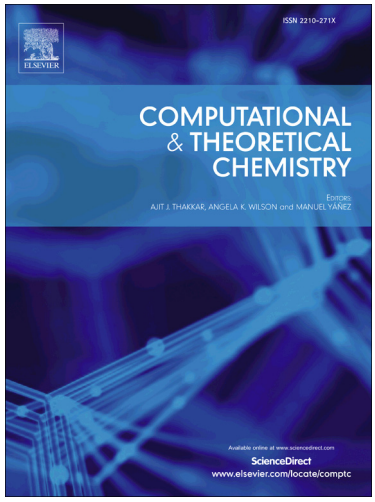

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PII: S2210-271X(16)30298-5
DOI: http://dx.doi.org/10.1016/j.comptc.2016.08.007
Reference: COMPTC 2217

To appear in: *Computational & Theoretical Chemistry*

Received Date: 24 July 2016
Accepted Date: 3 August 2016

Please cite this article as: A. Ounissi, Y. Benguerba, N. Ouddai, Theoretical investigation on structural and physicochemical properties of some ionic liquids, *Computational & Theoretical Chemistry* (2016), doi: http://dx.doi.org/10.1016/j.comptc.2016.08.007

Theoretical investigation on structural and physicochemical properties of some ionic liquids

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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