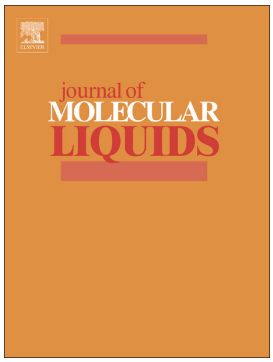

para'Xylyl bis'1'methylimidazolium bis(trifluoromethanesulfonyl)imide: Synthesis, crystal structure, thermal stability, vibrational studies

Boumediene Haddad, Annalisa Paolone, Didier Villemin, Jean-François Lohier, Mokhtar Drai, Serge Bresson, Ouissam Abbas, El-habib Belarbi

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Para-xylyl bis-1-methylimidazolium bis(trifluoromethanesulfonyl)imide: synthesis, crystal structure, thermal stability, vibrational studies.

Boumediene Haddad [1,2,3], Annalisa Paolone [4], Didier Villemin [3], Jean-François Lohier [3], Mokhtar Drai [2,5], Serge Bresson [6], Ouissam Abbas [7], El-habib Belarbi [2]

[1] Department of Chemistry, Dr Moulay Tahar University of Saida, Saida, Algeria
[2] Synthesis and Catalysis Laboratory LSCT, Tiaret University, Tiaret, Algeria
[3] LCMT, ENSICAEN, UMR 6507 CNRS, University of Caen, 6 bd Ml Juin, 14050 Caen, France
[4] CNR-ISC, U.O.S. La Sapienza, Piazzale A. Moro 5, 00185 Roma, Italy
[5] Université Djillali Liabes, BP 89, 22000 Sidi-Bel-Abbes, Algeria
[6] Laboratoire de Physique des Systèmes Complexes, Université Picardie Jules Verne, 33 rue St Leu, 80039 Amiens cedex, France.
[7] Centre Wallon de Recherche Agronomique, CRA-W, Bâtiment Maurice Henseval, Chaussée de Namur, 24, 50030 Gembloux, Belgium.

ABSTRACT

In this study, a new para-xylyl linked di-imidazolium [p-$C_6H_4(CH_2ImMe)_2^+$] ionic liquid (DIL) containing the bis(trifluoromethanesulfonyl)imide [$(CF_3SO_2)_2N^-$] anion is synthesized. The method is based on the alkylation reaction of 1-methyl imidazole, followed by anion exchange. The obtained DIL is characterized by ^{1}H-NMR, ^{13}C-NMR, ^{19}F-NMR and FT-IR spectroscopy. The melting point and the subsequent decomposition of [p-$C_6H_4(CH_2ImMe)_2^+$][$(CF_3SO_2)_2N^-$]$_2$ are measured by using differential scanning calorimetry (DSC) and thermogravimetric (TGA) analyses in the temperature range from 25 to 700 °C. Thermal analysis indicated that this DIL melted below 100 °C and can, therefore, be classified as an ionic liquid. Vibrational spectroscopy studies were conducted by infrared (IR), Raman (FT-Raman) spectroscopy and DFT calculations. Moreover, the crystal structure is investigated by single crystal X-ray diffraction (XRD) method. The X-ray studies on [p-$C_6H_4(CH_2ImMe)_2^+$][$(CF_3SO_2)_2N^-$]$_2$ show that it crystallizes in the monoclinic system with space group P21/c. The theoretical structural parameters such as bond lengths, bond angles and dihedral angles determined by DFT methods are in good agreement with the XRD results.

KEYWORDS: di-imidazolium; bis(trifluoromethanesulfonyl)imide; para-xylyl; crystal structure; vibrational spectra; thermal stability; Raman measurements; DFT.