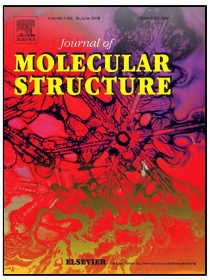
Accepted Manuscript



Synthesis, X-Ray Structural, Hirshfeld surface analysis, FTIR, MEP and NBO analysis using DFT study of a 4-chlorobenzylammonium nitrate $(C_7ClH_9N)^+(NO_3)^-$

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PII:	S0022-2860(18)30357-0
DOI:	10.1016/j.molstruc.2018.03.068
Reference:	MOLSTR 25007
To appear in:	*Journal of Molecular Structure*
Received Date:	27 December 2017
Revised Date:	16 March 2018
Accepted Date:	18 March 2018

Please cite this article as: R. Hakiri, I. Ameur, S. Abid, N. Derbel, Synthesis, X-Ray Structural, Hirshfeld surface analysis, FTIR, MEP and NBO analysis using DFT study of a 4-chlorobenzylammonium nitrate $(C_7ClH_9N)^+(NO_3)^-$, *Journal of Molecular Structure* (2018), doi: 10.1016/j.molstruc.2018.03.068

Synthesis, X-Ray Structural, Hirshfeld surface analysis, FTIR, MEP and NBO analysis using DFT study of a 4-chlorobenzylammonium nitrate $(C_7ClH_9N)^+(NO_3)^-$

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ABSTRACT

A new compound, 4-chlorobenzylammonium nitrate, was obtained by a reaction between 4-chlorobenzylamine and nitric acid, and characterized by X-ray diffraction and FT-IR spectroscopy. The phenyl ring and the nitro group were essentially coplanar in the obtained crystal. The aminomethyl substituent $-CH_2-NH_3^+$ lies out the plane of the aromatic ring as evidenced by the torsion angle $N_1-C_7-C_1-C_6$ of 88.2°. The crystal packing was formed by an infinite bi-dimensional layers with graph-set motif $R_4^8(16)$, and stabilized by N-H···O hydrogen bond-type intermolecular interactions. In addition, molecular geometry in the electronic ground state, Hirshfeld surface, vibrational wavenumbers, molecular electronic plane (MEP), and Natural bond orbital (NBO) analysis were performed using the density functional theory (DFT/B3LYP) with 6-31+G* basis set. Theoretical and experimental results are in good agreement. The NBO analysis confirms that the N–H...O intermolecular interactions notably affect crystal packing in this molecule.

Keywords: Crystal structure; Hirshfeld surface analysis; DFT; FT-IR; MEP; NBO.