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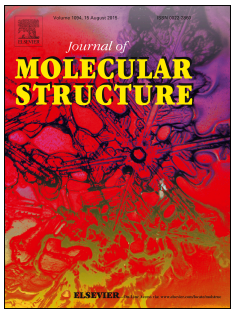

Single crystal, vibrational and computational studies of Theophylline (a bronchodilator drug) and its chloride salt

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Single crystal, vibrational and computational studies of Theophylline (a bronchodilator drug) and its chloride salt

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Abstract:

The crystal structure of Theophyilline (TH) and Theophyillinium chloride monohydrate (THC) and its complete molecular structure analysis on theoretical and experimental methods is reported here. The hydrogen bonding studies were carried out as a special note of the present work. The electron density analyses of the compounds were also analyzed in view of the intermolecular interactions. Moreover, it is an ever first quantum chemical report of this drug (TH) and its chloride salt. In TH crystal, the water molecule connects the Theophylline molecules through O–H···N hydrogen bond forming chain $C_2^2(7)$ motif and dimer $R_2^2(10)$ motif through N–H···O hydrogen bond. In THC, the two classical (N-H···O, N–H···Cl) and one non-classical (C–H···O) hydrogen bonds produce two pentameric chain motifs C_5^5 (16) and $C_5^5(17)$. These two chain motifs are interconnected by O–H···O hydrogen bond and cross linked by N–H···Cl and O–H···Cl hydrogen bonds to produce octametric ring motifs $R_8^8(27)$ and $R_8^8(28)$. The solubility test is carried out to enhance the drug solubility and the therapeutic effectiveness of the drug. Experimentally obtained vibrational wavenumbers are compared with the spectra obtained theoretically for both the compound. The strong intensity bands and the shifting of bands due to intermolecular hydrogen bonds are also investigated. The Mulliken atomic charges, HOMO-LUMO and thermodynamic properties are calculated using Density Functional Theory (DFT) and Hartree-Fock Theory (HF) using 6-311++G(d,p) basis set.

Keywords: Theophylline, hydrogen bond, Mulliken charge, HOMO-LUMO, DFT/HF.