Poster Sessions

Experimental and DFT studies of (E)-1-((3-iodophenylimino)met hylnaphthalene 2-ol
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The experimental geometry of (2-Hydroxyethyl)trihenylphosphoniumchloride
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Triphenylphosphonium compounds and their various derivatives are key reagents in the Wittig reactions and are used to convert aldehydes and ketones into alkynes [1], specifically in applications ranging from the synthesis of simple alkynes to the construction of complex biologically active molecules in the pharma-ceutical research [2]. They are also an important class of isoaromatic compounds and have widespread applications for their antimicrobial and anticancer activities [3].

In the crystal structure of the title compound, C20H16OPCl, the cations and anions are linked by intermolecular C—Cl hydrogen bonds forming zig-zag chains running parallel to the b axis.

The experimental geometry of (2-Hydroxyethyl)trihenylphosphoniumchloride was calculated using a density functional theory (DFT) method with the B3LYP functional and 6-31G basis set. The parameters of unit cell are a=6.9404, b=8.7757, c=8.7200 α=68.564, β=78.640, γ=81.260 and Z=1. The crystal structure of the title compound, [Mg(H2O)6]·(CH3NO3)2, was determined at 296 K. The complex crystallizes in centrosymmetric triclinic space group P1 and Mg2+ atom is coordinated by six O atoms from six water molecules. The ligands in the Hexaaquamagnesium(II) Acesulfamate are linked with three dimension via O—H—O and O—H—N interactions.

In this paper, the geometric parameters which are obtained from X-ray determination and theoretical parameters which are calculated by using density functional theory (B3LYP) with the 6-31G basis sets were compared. Experimental IR study, theoretical IR calculations, molecular electrostatic potential and frontier molecular orbital calculations were also put in this paper.

Keywords: acesulfame, X-ray, DFT

Experimental and DFT computational study on hexaquaamagnesium(II) acesulfamate
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Keywords: density functional theory(DFT), crystal and molecular structure studies, tautomerism