THE EFFECT OF THE SOLVENT ON THE GEOMETRIC STRUCTURE OF THE CRYSTAL DERIVED FROM CHALCONE

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In this work we study the effect of the solvent on the geometry structure of the compound (2E)-3-(3-methylphenyl)-1-(4-nitrophenyl) prop-2-en-1-one (3MPNP), with molecular formula C16H13NO3, have been synthesized and crystallized by Shobha R. Prabhu et al. We use the Polarizable Continuum Model (PCM) that treat the solvent by means of dielectric constants (\(\epsilon\)). This method has found very good results in different applications. The static and dynamic electric properties of a (3MPNP) isolated molecule when embedded in solvent medium present important changes, to study the solvent effects on the averages dipole moment, linear polarizability, first and second hyperpolarizability we have considered the solvents media: gas-phase (\(\epsilon\) =1.00), chloroform (\(\epsilon\)=4.71), dichloromethane (\(\epsilon\)=8.93), acetone (\(\epsilon\)=20.49), ethanol (\(\epsilon\) = 24.85), methanol (\(\epsilon\)=32.61), dimethyl sulfoxide (\(\epsilon\) =46.70), water (\(\epsilon\) =78.36) and where \(\epsilon\) is the dielectric constant of the medium. We also studied in gas phase. The computations were performed numerically based on finite field method and using the B3LYP/6-311+G(d) level of theory.

Key-words: Electrical Properties, Electrostatic iteration, Supermolecule approach.

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