

Poster Presentations

[MS25-P09] Analysis on Hydrogen-Bond Patterns of a New Coumarin Ester

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It has been discovered a wide range of biological activities for the derivatives of cinnamic acid. There are reports that the derivatives *trans*-cinnamic acid possess hepatoprotective activity, antimalarial, antimicrobial, antioxidant and α -glucosidase. The cinnamic esters are also important intermediates in chemical reactions, such as hydroarylation in the presence of strong acid and Phenol forming the dihydrocoumarins^[3]. The single crystals of the Ethyl-(2E)-3-(4-hydroxy-3,5-dimethoxyphenyl)-prop-2enoate (C₁₃H₁₆O₅) were obtained by slow evaporation technique using ethyl ether as solvent. The structure was solved by Direct Methods and refined by full matrix Least Square methods on F^2 , using WINGX package. Non H atoms were refined anisotropically and all H atoms were placed geometrically, except those of the water molecule and hydroxyl, that were placed by D.W. Smith method. The compound crystallizes in the C2/c monoclinic space group with 23018 measured reflections and 4279 unique and 2587 observed [$I > 2\sigma(I)$]. The final residual factor RI is 0.0607 for 181 refined parameters using 25 restraints. In the asymmetric unit there is a disordered water molecule that causes a partial disorder on the ester molecule. The water molecule of this compound does five intramolecular hydrogen bonds and three of them are significantly smaller than the sum of their van der Waals radii^[4], indicating one strong intra molecular interaction between the oxygen charge centers, and another one of this bonds is directed to a hydroxyl of the ester molecule.

Throughout the electron density map we observed two peaks of residual electron density instead of one around the oxygen atom of this hydroxyl, suggesting that the hydrogen of this hydroxyl was also occupying two site positions. The observed disorder may be caused by a repulsive interaction between the hydrogen of the water molecule and the hydroxyl of the coumarin ester. The importance of it is due its harmonic characteristic that the atoms involved in the disorder show all the components in the disorder have the same site occupancy factor (about 48% through 52%) for each group, that may be indicating a resonance along the structure. Finally, the water-coumarin calculations using the DFT method have strengthened this structural finding, since our theoretical approaches also suggest two well-defined conformations of similar energies which resemble the molecular geometries determined by X-ray diffraction.

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