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X-Ray and DFT Electrostatics Parameters Determination of a Coumarin Derivative Compound C17H13NO3

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Abstract : The crystal structure of 4-Methyl-7-(salicylideneamino)coumarin C17H13NO3has been determined using X-ray diffraction to establish the configuration and stereochemistry of the molecule. This crystal is characterized by its nolinear activity. The molecular electron charge density distribution of the title compound is described accurately using the multipolar model of Hansen and Coppens. The net atomic charge and the molecular dipole moment in-crystal have been determined in order to understand the nature of inter-and intramolecular charge transfer. The study present the thermal motion and the structural analysis obtained from the least-square refinement on F2,this study has also allowed us to determine the electrostatic potential and therefore locate the electropositive part and the electronegative part in molecular scale of the title compound.

Keywords : electron charge density, net atomic charge, molecular dipole moment, X-ray diffraction
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