Poster Presentation

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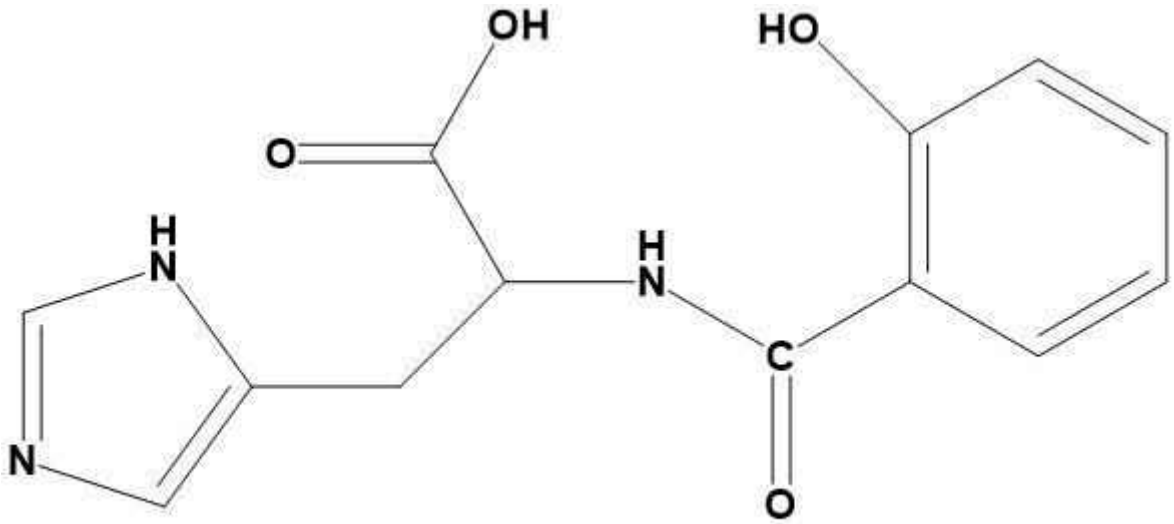
Ab initio and DFT study on Cu (II) complex salicylate derivative

K. Natarajan[1], S. Duraisamy[1], S. Kandasamy[1]
[1]*Anna University, Department of Physics, Chennai, India*

X -ray diffraction becomes a routine process these decades for determining crystal structure of the materials. Most of the crystal structures solved nowadays is based on single crystal X-ray diffraction because it solves the crystal and molecular structures from small molecules to macro molecules without much human intervention. However it is difficult to grow single crystals of sufficient size and quality for conventional single-crystal X-ray diffraction studies. In such cases it becomes essential that structural information can be determined from powder diffraction data. With the recent developments in the direct-space approaches for structure solution, ab initio crystal structure analysis of molecular solids can be accomplished from X-ray powder diffraction data. It should be recalled that crystal structure determination from laboratory X-ray powder diffraction data is a far more difficult task than that of its single-crystal counterpart, particularly when the molecule possesses considerable flexibility or there are multiple molecules in the asymmetric unit. Salicylic acid and its derivatives used as an anti-inflammatory drug are known for its numerous medicinal applications. In our study, we synthesized mononuclear copper (II) complex of salicylate derivative. The structural characterization of the prepared compound was carried out using powder X-ray diffraction studies. Crystal structure of the compound has been solved by direct-space approach and refined by a combination of Rietveld method using TOPAS Academic V4.1. Density Functional Theory (DFT) calculations have to be carried in the solid state for the compound using GaussianW9.0 in the frame work of a generalized-gradient approximation (GGA). The geometry optimization was to be performed using B3LYP density functional theory. The atomic coordinates were taken from the final X-ray refinement cycle.

[1] *Crystal Structure Determination from Powder Diffraction Data, Chem. Mater. 1996, 8, 2554-2570,* ***[2]*** *Ab-initio Crystal Structure Determination FromX-ray Powder Diffraction Dta, Alok K. Mukherjee, Journal of the Indian Institute of Science VOL 87:2 Apr–Jun 2007,* ***[3]*** *Synthesis, X-ray powder structure analysis and biological properties of a mononuclear Cu(II) complex of N-2-hydroxyhippuric acid, Soumya Basu, Basab Chattopadhyay, A. Ganguly, P. Chakraborty, P. Roy Chowdhury, S. Samanta, M. Mukherjee, A. K. Mukherjee and*



Derivative of Salicylic acid

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