Poster Presentation

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Investigation of topological and electrostatic properties of anti-inflammatory drug Aceclofenac.

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In the present work, the crystallization of the potent anti-inflammatory drug Aceclofenac has been done using slow evaporation technique and the structure has been re-determined at 105.01(10)K. An experimental electron density distribution of Aceclofenac has been accomplished along with the periodic theoretical calculations which were performed at the B3LYP/6-31G** level of theory. In order to visualize and quantify the intermolecular interactions, the Hirshfeld surface analysis and enrichment ratio calculations have been carried out and further the finger print provides the details of various contributions of the contacts for the crystal packing. The experimental and theoretical multipole electron density distribution analysis has been carried out to examine the bonding details, concentration/depletion of charges and the topological properties of the Aceclofenac molecule. Global Reactivity descriptors calculation has been executed to understand the molecule's nature of reactivity and site selectivity. Comparison of experimental as well as theoretical charges yields better information of the charge distribution in the molecule. The K and L sub-shells of Cl atoms and the lone pairs of the N atoms can be visualized through the electron localization function. The sigma hole of Cl atom has been traced out. The electrostatic potential helps to identify the sites of electrophilic and nucleophilic regions where the molecular interactions likely to happen. On the whole this study provides a clear description of the structural, topological and electrostatic and reactivity properties of the drug Aceclofenac in a detailed manner which further will be useful in the design of new potential drugs with improved efficiency and reduced side effects.

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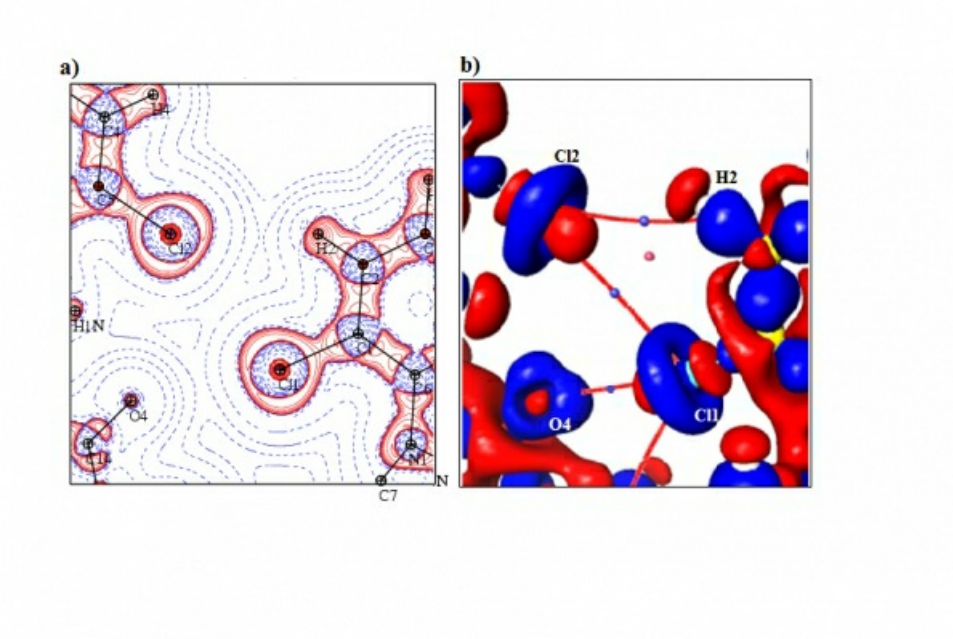

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