

*Charge density and Electrostatic properties of curcumin: An experimental study*Saravanan Kandasamy¹¹Department Of Physics, Periyar University, Salem, India

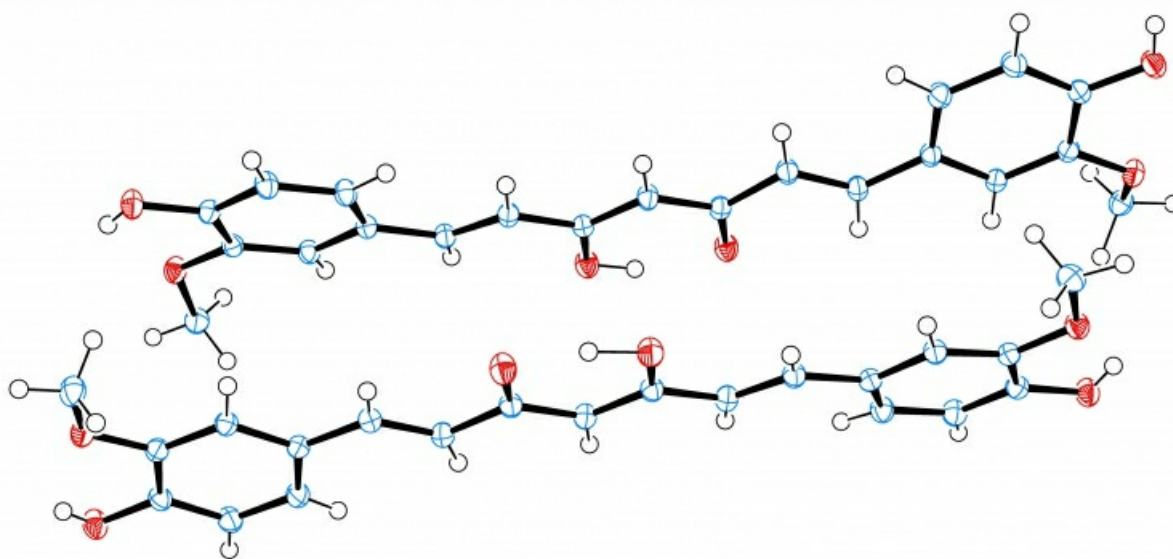
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Curcumin is one of the tautomeric compound, naturally occurs in turmeric (*curcuma longa*). It exhibits wide medicinal application; recent years, extensive studies have been performed to understand its structural properties and to relate with the physical and chemical properties [1]. In the present study, we have grown curcumin crystals from ethanol to determine its structure, bond topological and electrostatic properties from high resolution X-ray diffraction and charge density analysis. The X-ray diffraction intensity data has been collected up to the resolution 1.1 Å⁻¹ at the low temperature 100K. The structure was solved by direct methods and refined by least-squares methods. The structural analysis reveals that curcumin crystallizes two molecules in the asymmetric unit and are found to be conformationally different, this was confirmed from their torsion angles. The molecular packing is stabilized by strong O–H...O and C–H...O type of hydrogen bonding. The keto-enol group of both molecules forms strong O–H...O intra-molecular hydrogen bonding interactions. The Hirshfeld surface analysis [2] and fingerprint plot shows that the crystal packing environment around the surface and the contribution of intermolecular interactions. Further, multipole model refinement was carried out using Hansen-Coppens multipole formalism using XD2006 [3]. The topological analysis of the electron density of two molecules in the asymmetric unit reveals that they differ in their charge density distribution. The electrostatic properties of the molecule have been determined; notably, the electrostatic potential (ESP) surface of both molecules displays high electronegative and electropositive ESP regions. The topological properties of intermolecular interactions also carried out, which gives the strength of intermolecular interactions. The complete results of charge density analysis will be presented.

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Keywords: [Crystal structure of Curcumin](#); [Hirshfeld surface analysis](#); [Topological electron density analysis](#)