Poster Presentation

MS19.P01

Charge-density analysis and electrostatic properties of a new hybrid compound

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2-carboxy-4-methylaniline is a biologically active molecule serving as a pharmaceutical intermediate [1]. We've synthesized, studied and refined the crystal structure of its derivative 2-carboxy-4-methylanilinium chloride monohydrate using three different electron-density models. In the first model, the ELMAM2 multipolar electron-density database [2] was transferred to the molecule. Theoretical structure factors were also computed from periodic density functional theory calculations [3] and yielded, after multipolar-atoms refinement, the second charge-density model. An alternative electron-density modelling, based on spherical atoms and additional charges on the covalent bonds and electron lone-pair sites, was used in the third model in the refinement versus the theoretical data. The crystallographic refinements, structural properties, electron-density distributions and molecular electrostatic potentials obtained from the different charge-density models were compared.

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Keywords: atomic charges, bonding electron density, lone pairs