Electron-density Properties of the Functionally-substituted Hydropyrimidines

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This work reports the results of the study of electron density and electronic energy density in the new functionally substituted hydropyrimidines. We performed the accurate X-ray diffraction measurements at 110 K and reconstructed the electron density and electronic energy density for three compounds of this series. *Ab initio* calculations were performed for different molecular conformations as well. In this work, we shall focus on the study of ethyl 4,6-dimethyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate. The topological analysis of the experimental and theoretical electron densities was fulfilled for all the conformations and the bonding network was quantitative described in terms of the electron density and energy density topological features. In addition, the analysis of critical points of molecular orbitals (i.e. HOMO, LUMO) has been performed. Similar considerations were done for the other functionally substituted hydropyrimidines. New electron-localization/delocalization indices like the exchange energy density and correlation energy density and its Laplacians are introduced. The electron-density-based similarity of the pharmacophoric parts of the conformers of the hydropyrimidines studied has been estimated using new original algorithm.

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