MS41.P19

Charge density studies on N-n-butyltetrachlorophthalimide
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The charge density distribution in N-n-butyltetrachloro-phthalimide has been determined by means of high-resolution X-ray diffraction at 100K. The supramolecular structure of the title compound is stabilized by intermolecular halogen bonds C-Cl∙∙∙O and intermolecular Cl∙∙∙Cl interactions [1]. In the current presentation the deformation density distribution of electron density and topological analysis of electron interactions [1] are reported. The comparison of molecular electrostatic potentials has important implications on their function as anti-infective agents. Molecular electrostatic potentials for the same protonation states show a striking degree of similarity for the whole class of compounds. The relevance of this similarity for rational drug design and optimization of lead structures is discussed. The rapid calculation of electrostatic potentials directly from the invariom database makes the procedure suitable for high-throughput screening.

This research was supported by a grant of the Polish Ministry of Education and Science (Grant No. N N204 028138).

Keywords: halogen bonding, electron density, deformation density topology

MS41.P20

Electrostatics of fluoroquinolone antibiotics derived from crystal structures
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A comparison of nine fluoroquinolone antibiotics [1] with respect to their solid-state electrostatic properties is reported. Molecular electrostatic potentials and dipole moments were derived from the electron density distribution after crystal structure refinement with Invarions. The comparison of molecular electrostatic potentials has important implications on their function as anti-infective agents. Molecular electrostatic potentials for the same protonation states show a striking degree of similarity for the whole class of compounds. The relevance of this similarity for rational drug design and optimization of lead structures is discussed. The rapid calculation of electrostatic potentials directly from the invariom database makes the procedure suitable for high-throughput screening.

Deposited, newly determined and re-measured single-crystal diffraction data of varying quality were evaluated in this manner. The structure of lomefloxacin hydrochloride tetrahydrate is reported for the first time and the structural model of enoxacin methanol solvate as reported by Yoon et al. [2] needed revision: it turns out to be a water solvate. An in silico validation procedure for invariom database entries [3] is presented.


Keywords: Z-DNA, sub-atomic resolution, deformation density

MS41.P21

Dipole moment determination in push-pull chromophores from charge density data
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Push-pull chromophores find use in organic optical materials and for many applications their ground state dipole moment and polarizability are important properties. [1] In the condensed phase intermolecular interactions influence these properties and may lead to an enhancement of the dipole moment. The crystalline state provides a rigid surrounding for the intermolecular interactions, thus maximizing the effects. Experimental charge density studies facilitate the determination of molecular “in-crystal” dipole moments. However, the dipole moment values determined in this way have to be examined critically and are prone to systematic errors. [2] In this study dipole moments obtained from multipole refinements of structure factor amplitudes determined experimentally by diffraction and theoretically by ab-initio calculations are compared. The applicability of the invariom model [3]