

[1] K. Brzezinski, A. Brzuszkiewicz, M. Dauter, M. Kubicki, M. Jaskolski, Z. Dauter *Nucleic Acids Research* **2011**, in press. [2] C. Jelsch, B. Guillot, A. Lagoutte, C. Lecomte *J. Applied Cryst.* **2005**, *38*, 38-54, [3] S. Domagala, C. Jelsch *J. Appl. Cryst.* **2008**, *41*, 1140-1149.

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

MS41.P19

Acta Cryst. (2011) A67, C514

Charge density studies on N-n-butyltetrachlorophthalimide

Teresa Borowiak,^a Grzegorz Dutkiewicz,^a Agnieszka Paul,^a Maciej Kubicki,^a Bogusław Misterkiewicz,^b ^aDepartment of Crystallography, Faculty of Chemistry, Adam Mickiewicz University. ^bLaboratory of Organic Chemistry, Technical University of Radom (Poland). E-mail: borowiak@amu.edu.pl

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 density for the title compound crystal are shown. The deformation density clearly indicates a significantly anisotropic distribution of electrons in the halogen atom with less of them in the direction of C-Cl bond and more in the other two directions (see Figure 1 below). The topological analysis confirms conclusions derived from the deformation density distribution.

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

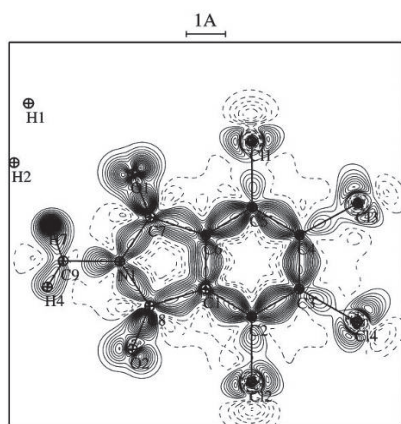


Fig. 1. Deformation density distribution for N-n-butyltetrachlorophthalimide

[1] T. Borowiak, I. Wolska, B. Brycki, A. Zieliński, I. Kowalczyk, *J. Mol. Struct.* **2007**, *833*, 197-202.

Keywords: halogen bonding, electron density, electron density topology

MS41.P20

Acta Cryst. (2011) A67, C514

Electrostatics of fluoroquinolone antibiotics derived from crystal structures

Julian J. Holstein, Christian B. Huebschle, Birger Dittrich *fuor Anorganische Chemie, Georg-August-Universität Goettingen, Tammannstr. 4, D-37077 (Germany)*. E-mail: jholste@gwdg.de

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 *Invarioms*. 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.

[1] L.A. Mitscher, *Chem. Rev.* **2005**, *105*, 559-592. [2] I. Yoon, K. Bark, M.S. Yang, S.S. Lee, *Anal. Sci.* **2003**, *19*, x11-x12 [3] B. Dittrich, C.B. Huebschle, P. Luger, M.A. Spackman, *Acta Cryst.* **2006**, *D62*, 1325-1335.

Keywords: ntibacterial, electrostatics, charge density

MS41.P21

Acta Cryst. (2011) A67, C514-C515

Dipole moment determination in push-pull chromophores from charge density data

Christian W. Lehmann, Thomas Dols, *Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr (Germany)*. E-mail: lehmann@kofo.mpg.de

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]