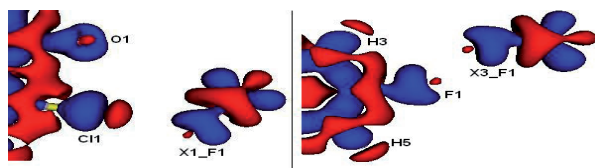


nature of F...F interactions in 4-fluorobenzamide show indication of a minor decrease in repulsion (type I interaction), though the extent of polarization on the fluorine atom is limited [4].



[1] (a) T.T.T. Bui, S. Dahaoui, C. Lecomte, G.R. Desiraju, E. Espinosa, *Angew. Chem. Int. Ed.* **2009**, *48*, 3838-3841. (b) V.R. Hathwar, T.N.G. Row, *J. Phys. Chem. A* **2010**, *114*, 13434-13441. [2] (a) K. Reichenbacher, H.I. Süss, J. Hulliger, *Chem. Soc. Rev.* **2005**, *34*, 22-30. (b) D. Chopra, T.N.G. Row, *CrystEngComm* **2011**, *13*, 2175-2186. [3] R.F.W. Bader, *Atoms in Molecules-A Quantum Theory*, Oxford: Clarendon, **1990**. [4] V.R. Hathwar, T.N.G. Row, *Cryst. Growth Des.* **2011**, DOI: 10.1021/cg1015862.

Keywords: charge density, halogen interaction, organic fluorine

MS34.P12

Acta Cryst. (2011) **A67**, C448

Experimental and theoretical charge density studies and topological analysis of 2-methyl-4-nitro-1-phenyl-1H-imidazole-5-carbonitrile: case of antiparallel cyano-cyano interaction

Agnieszka Paul,^{a,b} Adam Kubas,^c Christian Jelsch,^b Maciej Kubicki,^a Claude Lecomte,^b ^aDepartment of Crystallography, Adam Mickiewicz University in Poznań (Poland). ^bCRM2 UMR7036 CNRS, Henri Poincaré University Nancy 1 (France). ^cKarlsruhe Institute of Technology (Germany). E-mail: agapaul@amu.edu.pl

High resolution diffraction data were collected on laboratories diffractometers for 2-methyl-4-nitro-1-phenyl-1H-imidazole-5-carbonitrile, as part of our studies on intermolecular interactions in 4-nitro-1H-imidazole derivatives series.

The standard data processing within the Independent Atom Model (IAM) approximation, where the atoms are treated as 'spherical balls' in their ground state ie free, neutral and non interacting with neighbors does not take into account the density moved to the bonding regions and the charge transfer related to intermolecular interactions.

More realistic picture of the charge density distribution in crystals, which allows for inter- and intramolecular analysis can be derived from the Hansen-Coppens formalism [1] and Atoms-In-Molecule approach topological analysis [2]. The multipole model implemented in MoPro program suite [3] allows electrostatic and topological calculations either for small molecules or biological molecules at subatomic resolution.

The communication presents the experimental charge density analysis of the title compound, supported with the theoretical calculations. The standard resolution crystal structure was published some time ago [4], however no detailed analysis of the substituent's effect on the imidazole ring was performed. 2-methyl-4-nitro-1-phenyl-1H-imidazole-5-carbonitrile consists of two strongly electronegative and withdrawing groups, and the main interactions in its crystal structure are four weak hydrogen bonds (C-H...N; C-H...O) and interesting antiparallel cyano-cyano interactions. This dipole dipole interaction is found to be the most common type of C≡N...C≡N contacts (which in fact are similar to C=O...C=O interaction), and will be analyzed in details by means of experimental data and theoretical calculations.

[1] P. Coppens, T.S. Koritsanszky, *Chem. Rev.* **2001**, *101*, 1583-1627. [2] R.F.W. Bader **1990**. *Atoms in Molecules: A Quantum Theory*. Oxford University Press. [3] C. Jelsch, B. Guillot, A. Lagoutte, C. Lecomte *J. Applied Crystallography* **2005**, *38*, 38-54. [4] M. Kubicki *Acta Cryst.* **2004**. *C60*, o255-o257.

Keywords: 4-nitro-1H-imidazole derivatives, multipole, refinement, antiparallel cyano interactions

MS34.P13

Acta Cryst. (2011) **A67**, C448

Observation of a conserved "selenium bond synthon" involving Se...O interaction

Sajesh P.Thomas, Tayur N. Guru Row, *Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore 560012 (India)*. E-mail: sajesh@sscu.iisc.ernet.in

Organoselenium compounds have gained extreme importance in recent years due to their diverse biological, medicinal and catalytic activities which essentially stem from the presence of a seemingly divalent selenium atom. An in depth understanding of the non bonded Se...X interactions (X=heteroatom like N, O etc) becomes essential as they play crucial role in enzyme-mimetic reactions and protein engineering [1,2]. Three polymorphs of the organoselenium antioxidant drug *m-Ebselenol*, 2-(3-hydroxyphenyl)-1,2-benzisoxazol-3(2H)-one [3] have been generated by tuning the solvent polarity and their crystal structures have been analyzed. Polymorph I, which crystallizes in a noncentrosymmetric space group *Pna2₁* has O-H...O hydrogen bond chains propagating in a catemeric fashion whereas polymorphs II and III which crystallize in centrosymmetric space groups, *Pbcn* and *P2₁/c* respectively form centrosymmetric O-H...O hydrogen bond dimers. In all polymorphic forms as well as in the original drug *Ebselen* [4] and its derivatives we have identified a new conserved "selenium bond synthon". This is formed by strong Se...O and a surrogate C-H...O interaction which is conserved in all the structures as shown in Figure 1. The intricate nature of the Se...O interactions analyzed by both experimental and theoretical charge density analysis will be presented[5].

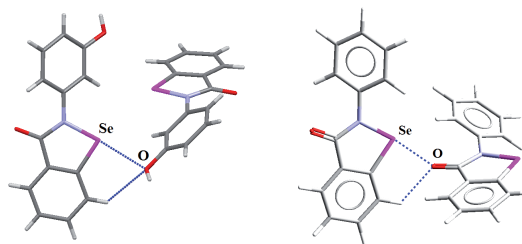


Figure1. Conserved "selenium bond" interactions in m-Ebselenol and Ebselen

[1] A.J. Mukherjee, S.S. Zade, H.B. Singh, R.B. Sunoj, *Chemical Reviews* **2010**, *110*, 4357-4416.[2] B.K. Sarma, G. Mugesh, *ChemPhysChem* **2009**, *10*, 3013-3020.[3] K.P. Bhabak, G. Mugesh, *Chemistry: A European Journal* **2007**, *13*, 4594-4601.[4] P.L. Dupont, O.Dideberg, *Acta Cryst.* **1990**, *C46*, 484-486. [5] R.F.W. Bader, *Atoms in Molecules-A Quantum Theory*, Oxford: Clarendon, **1990**.

Keywords: Se...O interaction, Selenium bond synthon, crystal engineering

MS34.P14

Acta Cryst. (2011) **A67**, C448-C449

Non-Covalent Interactions descriptor using experimental electron densities

Gabriele Saleh,^{a,c} Carlo Gatti,^{b,c} Leonardo Lo Presti,^a Julia Contreras-Garcia,^d ^aDept. of Physical Chemistry and Electrochemistry,