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

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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-benziselenazon-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 noncentrosymmetry space group Pna2, has O-H···O hydrogen bond chains propagating in a catemetic 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].

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

MS34.P13

Observation of a conserved “selenium bond synthon” involving Se···O interaction
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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 ic 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: case of antiparallel cyano-cyano interaction

Keywords: charge density, halogen interaction, organic fluorine

MS34.P12

Experimetal 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
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MS34.P14

Non–Covalent Interactions descriptor using experimental electron densities
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Non covalent interactions (NCI) play a crucial role in biology (protein-drug recognition) and in the design of new materials (self-assembly). A novel electron density (ED) based descriptor of non covalent interaction was proposed in 2010 by Johnson et al.[1]. It exploits a key quantity in DFT, the reduced density gradient $\nabla^2 \rho/\rho^{4/3}$, and reveals NCI in terms of low $s$-value isosurfaces, defined in low-ED regions and on which the ED is mapped with a colour related to the sign of the local density curvature along the second largest variation direction and to the magnitude of the ED itself. Though directly obtainable from experimental EDs, up to now such descriptor has been applied only to theoretical EDs or to independent atom model (IAM) densities.

In this work, we explore the application of this new descriptor to NCI in the bulk, using X-ray derived EDs. In particular, molecular crystals represent ideal supramolecular entities for studying non covalent interactions and the global effect that the crystal field has on them. Austidiol [2], benzene [3] and the two polymorphs of the anti-ulcer drug famotidine [4] were chosen as representative case studies. Atom-centred multipole expansions (XD2006 package [5]) were adopted in the refinement against the experimental structure factors and the grid files for implementing the NCI descriptor were obtained with an ad-hoc code. The NCI isosurfaces obtained from experiment have been also compared with those calculated using ab-initio periodic wavefunctions and the IAM densities.

On the basis of the experience gained on the investigated systems, it turns out that when applied to experimental EDs the NCI descriptor gives essentially similar information to that found for theoretical EDs. For instance, as shown in the figure below for benzene crystal, we find that interactions having a presumably delocalized nature, such as $\pi-\pi$ stackings or C-H-$\pi$ contacts, are indeed seen as extended surfaces, at variance with the localized and discontinuous picture unavoidably provided by the bond path analysis. Moreover, we confirm that mapping the ED on the $s$ isosurface highlights the strength of the various interactions, while the sign of the curvature helps to distinguish true stabilizing interactions from simple steric repulsions. The visible difference between the NCI isosurfaces portrait found in benzene crystal on passing from the multipolar to the IAM density corroborates the stabilizing and not simply steric nature of the $\pi-\pi$ stacking and C-H-$\pi$ interactions.

NCl isosurfaces [1] ($s=0.3$) in the molecular crystal of benzene. Left: multipolar ED. Right: IAM-ED


Keywords: non covalent interactions, electron density