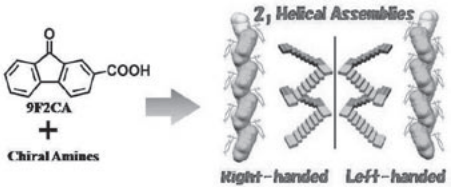
of the method proposed from our laboratory. Furthermore, solid-state fluorescence spectral analysis and circular dichroic analysis were performed on the crystals. We also discuss these optical properties of those enantiomorphic two crystals.



Keywords: 21 helical assembly, single crystal X-ray diffraction analysis, optical property

P08.08.65

Acta Cryst. (2008). A**64**, C438

Energy of interactions in polymorphs as calculated within the molecular pairs approach

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Our crystal structure prediction studies of nitrobenzene derivatives [1] resulted in the properly predicted crystal structures of the polymorphs stable at ambient. The crystal structures of the metastable polymorphs have not been found among the lowest energy predicted structures. This encouraged us to perform *ab initio* calculations aiming at the evaluation of the individual atom-atom force field in the case of polymorphic *p*-nitrophenol. The calculation at the second-order MP2 level have been applied to different molecular dimers modeling the crystal structures. The experimental atomic coordinates have been assumed in the calculations. The proton positions have been adjusted. The energy decomposition scheme has been applied to the energy of interactions that has been partitioned into the first-order electrostatic, exchange (corresponding to the repulsion energy) and delocalisation (corresponding to the charge transfer energy) terms. Additionally the electron correlation corresponding to the dispersion contribution to the interaction energy has been calculated. The details of the theoretical method used are given in [2]. The results give an insight into the intermolecular interactions in the polymorphs and enable to determine relevant interactions leading to the polymorphic structures. The results also indicate that the close values of the lattice energy of polymorphic structures originate from rather different values of the energetic contributions. The individual force-field determined for *p*-nitrophenol crystals may be validated by comparison of the simulated and experimental crystal properties, e.g. thermal expansion.

[1] Mossakowska I. ; Wojcik G., in preparation.
[2] Wojcik, G.; Holband, J.; Szymczak, J; Roszak, S.; Leszczynski, J., Cryst. Growth Des., 2006, 6, 274.

Keywords: intermolecular potentials, quantum chemical calculations, polymorphic structures

P08.08.66

Acta Cryst. (2008). A**64**, C438

Cocrystals of monoguanidinobenzene with benzoic acid derivatives

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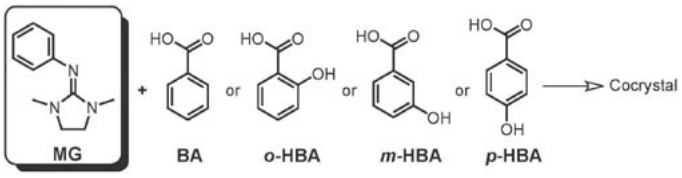
We have developed guanidine chemistry forcusing on the potential abilities of the guanidino groups to act as chiral auxiliaries, for example. We have previously reported interesting cocrystal properties based on the cluster formation of bisguanidinobenzene and benzoic acid (BA). As a part of our investigation in guanidine chemistry, we present cocrystals of newly prepared monoguanidinobenzene (MG) and BA, *o*-hydroxybenzoic acid (*o*-HBA), *m*-hydroxybenzoic acid (*m*-HBA), or *p*-hydroxybenzoic acid (*p*-HBA).



Keywords: cocrystallization and complexation of small molecu, intermolecular interactions, organic molecules

P08.08.67

Acta Cryst. (2008). A**64**, C438-439

Electrostatic interaction energy computation: The human aldose reductase - Fidarestat complex case

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Aldose reductase hAR is a 36-kDa enzyme member of the aldo-keto reductase superfamily, involved in the reduction of glucose into sorbitol. The accumulation of sorbitol in cells leads to diabetes complications. Thus, inhibition of hAR is a potential therapeutic way to treat the pathologies related to chronic hyperglycemia like retinopathy, nephropathy and neuropathy. Many aldose reductase inhibitors (ARIs) have been identified and studied for several years [1]. Most of them have unacceptable side effects or lack of efficacy. Fidarestat is a cyclic imide group inhibitor which shows higher activity and selectivity than the others. Taking into account the pharmaceutical stake, hAR in complex with Fidarestat has been subject to many studies [2,3]. The main purpose of these studies is the understanding of Fidarestat affinity and selectivity with hAR which leads to characterize the interactions between the inhibitor and the hAR active site. We will present the advancement of the crystallographic software suite MoPro & VMoPro [4] for the estimation of protein-ligand interaction energy. These calculations are performed from the subatomic charge distribution modelling according to the multipolar formalism of Hansen & Coppens [5] and take into account atomic valence electron cloud deformation due to the chemical environment. These new developments allow the precise estimations of electrostatic interaction energies which are useful to understand affinity and specificity of Fidarestat with hAR compared to other ARIs.

[1]El-Kabbani et al., Proteins, 2004, 55, 805
[2]El-Kabbani et al., Proteins, 2003, 50, 230
[3]Oka et al., J. Med. Chem., 2000, 43, 2479