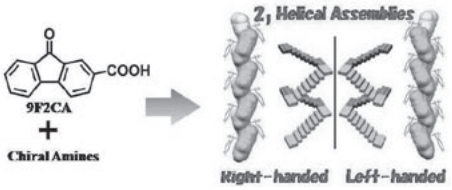
of the method proposed from our laboratory. Furthermore, solid-state fluorescence spectral analysis and circular dichroic analysis were performed on the crystals. We also discuss these optical properties of those enantiomorphic two crystals.



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

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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

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Cocrystals of monoguanidinobenzene with benzoic acid derivatives

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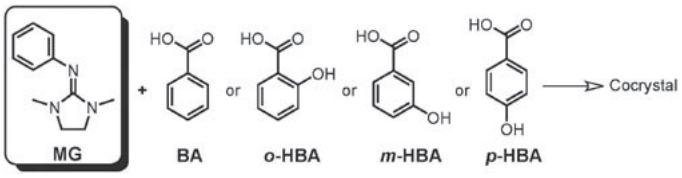
We have developed guanidine chemistry forcusing on the potential abilities of the guanidino groups to act as chiral auxiliaries, for example. We have previously reported interesting cocrystal properties based on the cluster formation of bisguanidinobenzene and benzoic acid (BA). As a part of our investigation 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

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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

[4]Jelsch et al., J. Appl. Cryst., 2005, 38, 38
[5]Hansen & Coppens, Acta. Cryst., 1978, A34, 909

Keywords: human aldose reductase, protein-ligand complex, interaction energies

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X-ray visualization of protein biotinylation

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Biotin-dependent carboxylases play essential roles in the metabolism of all organisms. Their activation by biotinylation is catalysed by biotin protein ligase (BPL). The crystal structures of the archaeal BPL (PhBPL), the biotinyl domain of archaeal biotin carboxyl carrier protein (PhBCCP) and the PhBPL:PhBCCP complex have been determined by X-ray diffraction. The structural feature of the intermediate (biotinyl-5'-AMP) formation was studied using the PhBPL structures liganded with biotin, ATP and biotinyl-5'-AMP [1]. The BPL:BCCP complex was obtained using two BPL mutants R48A and R48A&K111A [2]. The mutants retain functionality as an enzyme but likely with lower activity, thereby providing the complex crystals. Structural funding of the transient BPL:BCCP complexes at formation (BPL:apo-BCCP) and product (BPL:holo-BCCP) stages allow us to visualize the biotinylation process. The catalytic N- and C-terminal domains of BPL and the biotinyl domain of BCCP act as three rigid-body parts of the complex. The C-terminal domain of BPL shows large conformational motions to accommodate BCCP, suggesting its functional importance. Additionally, the C-domain has a flexible loop that must open every time when BCCP attaches to BPL, and it allows the specific lysine of BCCP to enter the active site of BPL with the intermediate biotinyl-5'-AMP. These structural details are useful to understand the protein biotinylation which is widely used in purification, quantum dots targeting as well as in the design of anti-obesity drugs.
[1] Bagautdinov B., Kuroishi C., Sugahara M., Kunishima N. (2005). JMB, 353, 322.
[2] Bagautdinov, B., Matsuura, Y., Bagautdinova, S., Kunishima, N. (2008). (JBC in press, M709116200)

Keywords: biotinylation, protein-protein complex, X-ray diffraction

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Optical and electric properties depending on molecular arrangement of dehydro[12]annulene derivative

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To develop a novel π-conjugated molecule-based supramolecular assembly, we designed and synthesized trisdehydrotribenzo[12]-annulene ([12]DBA) derivative **1** which has three carboxyl groups at the periphery. Recrystallization of **1** from DMSO gave a crystal of the solvate **1**/DMSO. Crystallographic analysis revealed that a face-to-face π-stacked one-dimensional (1D) assembly of **1** was achieved and that the DMSO molecule played a significant role as a "structure-dominant element" in the crystal. This is the first example of [12]DBA to stack completely orthogonal to the columnar axis. To reveal its superstructure-dependent optical and electrical properties, **1** and its parent molecule **2**, which crystallizes in a herringbone fashion, were subjected to fluorescence spectroscopic analysis and charge-carrier mobility measurements in crystalline states. The 1D stacked structure of **1** provides a red-shifted, structureless, weakened fluorescence profile compared to **2**, due to strong interactions between the π-orbitals of the stacked molecules. The charge-carrier mobility of the single crystal of **1**/DMSO, as well as **2**, was determined by flash photolysis time-resolved microwave conductivity measurements. The single crystal of **1**/DMSO revealed significantly-anisotropic charge mobility along the columnar axis. This value is 12 times larger than that along the orthogonal axis.

Keywords: one dimensional structure, pi interactions, charge carrier mobility

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X-ray crystal structure analyses of methionine γ-lyase 1 and 2 from *Entamoeba histolytica*

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Methionine γ-lyase (MGL) is a member of the γ-family of pyridoxal 5-phosphate (PLP)-dependent enzymes and catalyzes α, γ or α, β - elimination of sulfur-containing amino acids such as methionine, homocysteine and cysteine to produce ammonia, α-keto acid and volatile thiol (hydrogen sulfide or methanethiol). There are two isoenzymes (MGL1 and MGL2; amino acid sequence identity of 70%) in *E. histolytica* showing somewhat different substrate specificities. Since MGL is not present in mammalian hosts, MGL1 and 2 are promising targets for structure-based drug design of amebicides. In this study, we succeeded in crystallizing MGL1 and 2, and carried out X-ray structure analyses for the enzymes. MGL1 and 2 were crystallized using ammonium sulfate and polyethylene glycol 400 as a precipitant, respectively. The structures of MGL1 and 2 were solved by the molecular replacement method using MGL from *P. putida* (PDB code 1gc2) as a search model and refined to R=17.2% (1.93 Å resolution) and R=18.2% (1.80 Å resolution), respectively, based on diffraction data collected at BL5A of Photon Factory or BL44XU at SPring-8. The refined structures of MGL1 and 2 as well as those complexed with methionine reveal that both enzymes exist as homotetramers consisting of two catalytic dimers, and that the PLPs are covalently bound to the ε-amino group of lysine residues (205/208) in the active sites of the enzymes. Furthermore, it is also indicated that tyrosine residues (108/111) play a crucial role as a general acid catalyst in γ- elimination of methionine. Currently, we are trying to prepare crystals of MGL1 and 2 complexed with compounds such as trifluoromethionine, a suicide substrate of MGL, to develop potential pro-drugs.

Keywords: methionine gamma-lyase, X-ray structure analyses, gamma-elimination