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Chloride Intracellular Channel (CLIC) proteins are recently discovered members of the chloride ion channels family that have the unusual property of existing as both soluble proteins and integral membrane channels. There are 6 members in the human CLIC family (CLIC1-6). Most of CLICs exist in cells as both soluble and integral membrane proteins. Although the specific cellular function of these CLIC proteins remains unclear, CLICs have been associated with some cellular functions such as cell cycle regulation and maintenance of intracellular membranes. The mechanism of CLIC insertion into the membrane remains unclear, however previous studies suggest that this process may involve structural changes and/or protein-protein interactions. CLIC proteins are believed to form a complex with the N-terminus FERM domain (band Four-point-one, Ezrin, Radixin, Moesin domain) of the ERM (Ezrin-Radixin-Moesin) proteins. ERM is a member of protein 4.1 superfamily which is characterised by the ~300kDa FERM domain. This superfamily mediates the cross-linking between the cytoskeleton and the plasma membrane. Current studies using both blue native polyacrylamide gel electrophoresis and Western Blots indicate that CLIC1 forms a complex with the FERM domain of Ezrin. Further crystallographic studies of these complexes are necessary to reveal the nature of the complex.

Keywords: CLIC, FERM domain, macromolecular complexes

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Interaction of sols on a dispersion containing only the couterions dissociated from the surface

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The electrical potential for the case of two identical, planar parallel sols immersed in a salt-free medium, where the ionic species is the counterions come solely from that dissociated from the surfaces, is evaluated. We show that in a salt-free dispersion if the separation distance between two sols is sufficiently far, the electrical repulsive force dominates, that is, the total energy is positive and does not have a secondary minimum, which is not the case for a dispersion where both coions and counterions are present. Also, the conditions used to calculate the critical coagulation concentration in the classic DLVO (Derjaguin, Landau, Verwey, and Overbeek) theory become inappropriate and Derjaguin approximation is inapplicable. We show that if the surface charge density exceeds ca. 0.04 C/m^2, the stability of a salt-free dispersion remains essentially the same. If the surface charge density is sufficiently high, the maximum separation distance between two particles below which coagulation occurs is in the range [0,1 nm] and [1,7 nm] for the case where Hamaker constant are 10^-20 J and 10^-19 J, respectively.

Keywords: salt-free dipersion, Posisson-Boltzmann equation, stability

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The origin of polar ordering in high pressure phases of chloroform and bromoform

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The majority of materials crystallize in centrosymmetric or nonpolar space groups. One of the examples are chloroform ($CHCl_3$, CF) and bromoform ($CHBr_3$, BF). Despite their pyramidal molecular structure all their low-temperature (LT) crystalline phases are centrosymmetric. This contrasts with most of crystals built of pyramidal molecules or ions, like a prototypical pyroelectric α-$LiIO_3$. Therefore we undertook to perform an X-ray diffraction study of pressure-frozen CF and BF. Only one LT phase of CF of was reported (space group *Pnma*) [1], while BF is known to exist in 3 phases: a disordered one ($P6_3/m$), formed just below melting point, which transforms on cooling further to ordered *P*-1 or *P*-3 polymorphs [2]. Due to the less attractive character of Cl...Cl interactions the structure of CF is distinct from the BF phases, in which the molecules are arranged in bipolar sheets interacting by a cooperative triangular motif of Br...Br bridges. We revealed that CF crystallizes at 0.62 GPa yielding a LT phase, which transforms between 0.62 and 0.75 GPa to a polar $P6_3$ phase. Isochorically frozen BF forms isostructural polar crystals already at the freezing pressure of ca. 0.1 GPa. It can be shown that X...X and H...X interactions in the structures of CF and BF can be rationalized in terms of electrostatic forces and molecular electrostatic potential mapped onto molecular surfaces. The polar crystals of CF and BF contribute to a better understanding of the structural mechanism responsible for polar symmetries of materials, required for technological applications [3].

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Keywords: polarity, halogens, high-pressure polymorphism

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Construction of 2_1 helical assemblies of fluorescent molecules and the study on their properties

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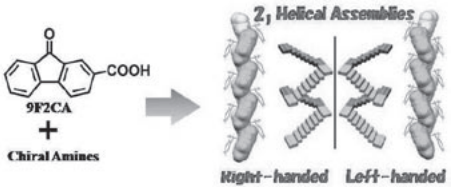
2_1 helical assemblies are often found and general in crystals. Conventionally, it has been assumed that right- or left- handedness of 2_1 helical assemblies cannot be determined on the basis of mathematical viewpoint, because the two-fold screw axis operation includes just 180 degrees rotation and translation. We had, however, been aware of that those can be chiral when the objects consisting of themselves are not spherically-symmetric. Recently, we have suggested that it is possible to define the handedness of 2_1 helical aggregates observed in crystals on the basis of the molecular tilt against the 2_1 axis. In this study, we prepared the crystals in which fluorescent molecules form 2_1 helical assemblies. Namely, crystallization of 9-fluorenone-2-carboxylic acid (9F2CA) and chiral amines yielded homo-chiral 2_1 helical structures (Figure). We determined the handedness of the 2_1 helical assemblies on the basis

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.

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Keywords: intermolecular potentials, quantum chemical calculations, polymorphic structures

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Cocrystals of monoguanidinobenzene with benzoic acid derivatives

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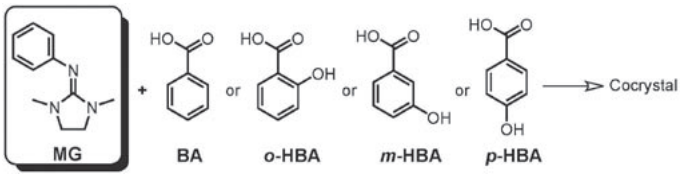
We have developed guanidine chemistry forcusing on the potential abilities of the guanidino groups to act as chiral auxiliaries, for example. We have previously reported interesting cocrystal properties based on the cluster formation of bisguanidinobenzene and benzoic acid (BA). As a part of our investigation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

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