signalling networks. Identification of disordered regions in protein sequences can help identify such proteins and to reduce bias in sequence similarity analysis. A practical spin-off for structural biology work is to delineate boundaries of protein domains to guide structural and functional studies (Ferron, et al., 2006). Several state-of-the-art approaches have been proposed for prediction of ordered and disordered residues, such as neural networks, NNs, and Support Vector Machines, SVMs. We introduce Conditional Random Fields, CRFs (Lafferty, et al., 2001), as a new method for accurately predicting the transition between structured and highly flexible or disordered regions in proteins. Our Order and Disorder predictor, OnD-CRF, relies only on features which are generated from the amino acids sequence and from the predicted secondary structure. Benchmarking results rank the OnD-CRF model highest among the fully automatic server group (Wang and Sauer, 2008). Availability: http://babel.ucmp.umu.se/ond-crf/

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Keywords: protein disorder, flexibility, domain boundary

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The remarkable “polymorphism” of aspirin

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The crystal structure of aspirin, *ortho*-acetylsalicylic acid, has been established since 1964. A second polymorph was reported in 2005. The new crystal structure (“form II”) is closely related to the long-established structure (“form I”). Both structures contain identical layers of centrosymmetric dimers, linked by O-H···O hydrogen bonds between their carboxyl groups. In the form I structure, adjacent layers are arranged so that their acetyl groups meet to form a centrosymmetric arrangement of C-H···O contacts. In the form II structure, adjacent layers are translated relative to each other so that C-H···O contacts link the acetyl groups into catemeric motifs. The two arrangements have been calculated to be approximately isoenergetic. Diffraction patterns reveal that aspirin crystals can exhibit one-dimensional stacking disorder, incorporating both interlayer arrangements. Two sets of Bragg reflections demonstrate extended domains with the form I and form II structures, while diffuse features reveal less ordered regions. The relative proportions of the two interlayer arrangements are variable. Pure form I crystals are commonplace but pure form II crystals have not so far been realised. This disordered system raises interesting questions with regard to the definition of polymorphism in molecular crystals: is aspirin polymorphic, and if so, how many polymorphs exist? The question is especially relevant given the pharmaceutical prominence of aspirin, and may prove to be significant in the context of the patentability of crystalline forms.

Keywords: pharmaceuticals, polymorphism, disordered solids

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Polymorphism and structural mechanism of the phase transformation of phenyl carbamate (PC)

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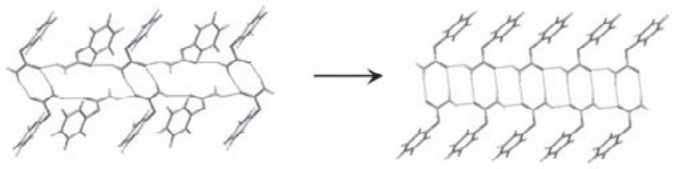
Co-crystallization experiments with phenyl carbamate (PC) as a hydrogen bond donor with crown ethers have led to the serendipitous discovery of three crystal forms of PC. These newly discovered polymorphs have been characterized by a variety of methods including variable temperature powder X-ray diffraction (PXRD), vibrational spectroscopy (Infrared and Raman), calorimetry (DSC) and optical hot stage microscopy (HSM). Forms I and II have been obtained from a number of solvents while Form III was obtained only by heating Form II and was observed only transiently in the DSC, HSM and PXRD. Form I transformed to Form II both through solution-mediated phase transformation and solid state transformation. A comparison of the two structures of Form I and Form II provides a qualitative model for the structural mechanism of the transformation. The relatively small changes in IR and Raman peak positions imply that the major differences between the two structures are associated with changes in the environment of the phenyl ring as revealed in the single crystal structure analysis.



Keywords: polymorphism, hydrogen bonds, structurally dependent related phase transformatio

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Polymorphic study of the model system hexamidine diisethionate

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Polymorphism in drug substances may cause severe problems during manufacturing processes. Hexamidine diisethionate (HDI) is an aromatic diamidine linked by a flexible eight-membered chain and resembles the type of molecules which form liquid crystals. Since HDI is used as a preservative mainly in solution, no polymorphism has been described to date. The drug is closely related to the polymorphic pentamidine diisethionate [1], which has a seven-membered connecting chain, so that the existence of multiple crystal forms of HDI was anticipated. By applying multiple analytical techniques, ten anhydrous crystal forms were discovered. In particular, thermal-analytical techniques and temperature controlled X-ray diffraction turned out to be superior analytical tools to identify and characterize the various polymorphic transitions. Additionally, two enantiotropically related triclinic dihydrates were

characterized. Single crystal structure determination revealed only slight conformational differences of the hexamidine molecule, which causes a doubling of the primitive unit cell volume of the low temperature form. However, the overall packing of both forms is maintained. Based on the thermo-chemical data a semi-schematic energy-temperature diagram [2] was constructed, which permits the visualization of the relationships and relative thermodynamic stability of the polymorphic forms in this complex system. This knowledge allows us to derive valuable information that is relevant for the design and control of the production and formulation strategy of a particular polymorph.

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Keywords: polymorphs, pharmaceuticals, thermal analysis

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Order and disorder in the $Sr_2VO(XO_4)_2$ (X=V,P) phases

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The $M_2VO(XO_4)_2$ compounds (M = Sr, Ba, Pb; X = V^{+5}, P) ("239 phases") have been actively studied during the last decade as low-dimensional magnetic systems. Among these oxides the Sr239 phases are especially interesting since they have similar crystal structures for X = V and P. The crystal structures of these phases contain infinite chains of the corner shared $V^{+4}O_6$ octahedra linked into layers by XO_4 tetrahedra. The vanadium cation is slightly shifted by about 0.2 Å towards one of the O-ion. This results in a formation of one short V-O vanadyl bond, elongated opposite V-O bond. In the Sr239 phases the vanadyl bond, pointing toward the oxygen atom connecting the octahedra along the chain, but it is not clear in which sense it is directed since the reported refinement of the X-ray diffraction data led to a splitting of the V-position towards both directions with statistical occupancy of 50%. Order-disorder in the crystal structures of the S239 phases were investigated by means of single crystal and powder X-ray diffraction, electron diffraction (ED) and high-resolution electron microscopy (HREM). We succeeded in obtaining of $Sr_2VO(VO_4)_2$ and $Sr_2VO(PO_4)_2$ single crystals having ordered structures where the short vanadyl bonds have same direction inside the layers and are directed oppositely in the adjacent layers. Such ordering results in a decrease of the symmetry from the body-centered unit cell to primitive one. Electron microscopy study revealed a presence of both primitive and body-centered crystallites in the samples as well as a new type of superstructure. Additionally, the different types of defects were observed on the HREM images. Magnetic properties of the compounds are briefly described.

Keywords: order-disorder transitions, low-dimensional materials, vanadium compounds

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Powder X-ray diffraction study of polymorphic drugs: fluconazole and mebendazole

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Polymorphism and pseudopolymorphism in pharmaceutical compounds can affect bioavailability and therapeutic efficiency of drugs. Therefore, this characteristic that might affect the stability or availability of the drug substance in a solid dosage form must be monitored and controlled [1]. The aim of this work is to characterize the solid state crystalline forms presents in raw material and drug product tablets of the pharmaceutical active compounds fluconazole (FCZ) and mebendazole (MBZ). The samples were studied by powder X-ray diffraction (XRD) using synchrotron radiation and thermal analysis (TGA and DSC), respectively. The raw material of FCZ employed to manufacture drug product usually is identified as a mixture of a monohydrate and anhydrate form I. In the case of MBZ, for which up to now is known three polymorphic forms (A, B e C), is well established that the form C is the only one therapeutically efficient. The XRD, TGA, and DSC results obtained for FCZ showed significant polymorphic differences comparing the five samples manufactured by different makers. Of the eleven raw materials of MBZ studied here, four were identified as form A, which is considered therapeutically inactive. The more alarming result is that the drug tablets analyzed here do not show the presence of the active form. It is important to emphasize that the XRD data collected using synchrotron facilities was mandatory to characterize the pharmaceutics solids studied here. The high resolution was important to identify the mixture of polymorphic forms, especially to FCZ and MBZ for which as of yet the crystal structures of some polymorphic forms was not determined.

Aknowlegments: FAPEMIG and FUNED.

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Keywords: pharmaceutical crystallography, polymorphism, powder crystallography

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Low temperature and ambient phases of decane-1,10-diammonium dichloride monohydrate

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Investigations into structure-property relationships and applications of *n*-alkyl-ammonium and *n*-alkyl-diammonium salts are of continued interest and form the basis of our continuing investigations of these materials. In particular, we have focused on the structural characteristics of the *n*-alkyl-diammonium salts as they are precursors to layered inorganic-organic perovskite-type hybrids(1); they are bidentate ligands in transition metal complexes that have applications in propellants, explosives and pyrotechnic compositions(2); they have structure directing properties in the synthesis of a number of