bioactivities, antifungal bioactivities and inhibitor activities against viruses. In the past few years, we have pursued investigations on the new thiourea derivatives. As a continuation of these studies, *N*-(2,2-diphenylacetyl)-*N'*-(naphthalen-1yl)-thiourea (PANT) has been synthesized and characterized by elemental analysis, IR spectroscopy and ^{1}H-NMR spectroscopy. The crystal and molecular structure of the title compound has been determined from single crystal X-ray diffraction data. It crystallizes in the triclinic space group *P*-1, *Z* = 2 with *a* = 10.284(2) Å, *b* = 10.790(2) Å, *c* = 11.305(2) Å, α= 64.92(3) °, β= 89.88(3) °, γ= 62.99(3) °, *V* = 983.7(3) Å^3 and *Dcalc* = 1.339 Mg/m^3. The molecular structure, vibrational frequencies and infrared intensities of PANT were calculated by the Hartree-Fock and Density Functional Theory methods (BLYP and B3LYP) using 6-31G(d) basis set. The calculated geometric parameters were compared to the corresponding X-ray structure of the title compound. We obtained 22 stable conformers for the title compound; however the Conformer 1 is approximately 9.53 kcal/mol more stable than the Conformer 22. The comparison of the theoretical and experimental geometry of the title compound shows that the X-ray parameters fairly well reproduce the geometry of the Conformer 17. The harmonic vibrations computed of this compound by the B3LYP/6-31G(d) method are in a good agreement with the observed IR spectral data. Theoretical vibrational spectra of the title compound were interpreted by means of PEDs using VEDA 4 program. A general better performance of the investigated methods was calculated by PAVF 1.0 program.

Keywords: crystal structure, *ab-initio* calculations, thiourea derivatives

P08.01.91

Acta Cryst. (2008). A**64**, C446

Molecular complex formation of medicinal cationic surfactants with aromatic compounds

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Some aromatic drugs (4-chlro-m-cresol of germicide, flopropione of antispasmodic agent, etc) make molecular complexes with quaternary ammonium halides such as hexadecyltrimethylammonium bromide (abbreviated as CTAB). The structures of the complex crystals have been analyzed by X-rays.[1] They were shown to be very similar to each other. Moreover, we confirmed that these surfactant complexes had new characteristics. If an aromatic drug is a water insoluble drug, the dissolution rate is increase. If it easily takes oxygen damage, it is kept out to oxygenate. The complexes can control of the vaporization of drugs by heat treatment, too.[2, 3] We recently studied molecular complex formation between surfactant of different type in cationic surfactants, medicinal surfactants such as 1-hexadecylpyridinium bromide (abbreviated as CPB), benzyl(hexadecyl) dimethylammonium chloride (abbreviated as BCDAC), and aromatic compounds containing drugs (hydroquinone of treatment of skin pigmentation, etc). After many trials, we obtained complexes above fifteen, three of which were suitable for X-ray analysis. The three complexes, CPB/guaiacol, CPB/9-anthracenecarboxylic acid, and BCDAC/hydroquinone were obtained from alcohol or aqueous solutions. Their crystal structures were similar to that observed in the quaternary ammonium surfactant complexes. Therefore, these complexes will show the similar characteristics to those of the quaternary ammonium complexes.

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Keywords: molecular complex, surfactant, stabilization of drug

P08.01.92

Acta Cryst. (2008). A**64**, C446

Chiral recognition in cholamide crystals: Four-location model for hydrogen and stereogenic carbon

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A four-location model for enantioselective inclusion of secondary aliphatic and aromatic alcohols with steroidal acids and their derivatives is presented. In principle, two kinds of disordered structures of guest components may be observed in a concave cavity at least. The one is that a stereogenic carbon of the guest is disordered with a substituent, such as a hydrogen. The other is that the stereogenic carbon is almost fixed while two neighboring substituents, such as a hydrogen and a methyl group, are disordered. For example, cholamide accommodates 2-methyl-3-hexanol (**1**) and 2,2-dimethyl-3-hexanol (**2**) into its channels. (*S*)-isomer of **1** is separated in less than 20% ee, while that of **2** in more than 98% ee. Crystallographic studies brought us a profound insight for such one methyl group effect in chiral recognition. It was confirmed that the inclusion crystal of **1** exhibits a disordered structure of hydrogen around a stereogenic carbon, while that of **2** a definite structure. Such a difference requires a chirality recognition model which explains selective locations of the forth substituent, hydrogen, together with chiral carbon. Employment of a four-location model resulted in a successful interpretation for the chirality recognition. Moreover, cholamide includes various 1-phenylethanol derivatives. Among them, (*S*)-isomers of ortho-substituted 1-phenylethanols showed higher enantioselectivity than those of para-substituted ones. X-ray crystallographic analysis clarified that the former has a definite structure in the channels, while the latter has a disordered structure between hydrogen and methyl group. The four-location model enabled us to explain these experimental results for enantioresolution.

Keywords: chiral recognition, inclusion compounds, alcohols

P08.01.93

Acta Cryst. (2008). A**64**, C446–447

Protein intrinsic disorder predicted with conditional random fields

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A large fraction of eukaryotic proteins harbour significant intervals of disordered residues which allow the protein to adopt multiple, alternate conformations (Dunker, et al., 2002). Frequently, such proteins have important biological functions in the cell, such as in

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

P08.10.94

Acta Cryst. (2008). A**64**, C447

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

P08.10.95

Acta Cryst. (2008). A**64**, C447

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

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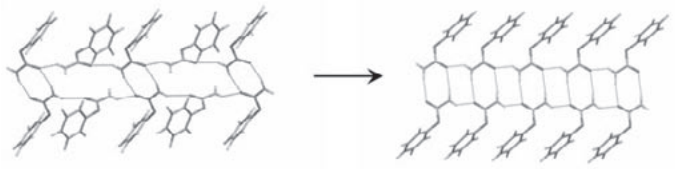
Co-crystallization experiments with phenyl carbamate (PC) as a hydrogen bond donor with crown ethers have led to the serendipitous discovery of three crystal forms of PC. These newly discovered polymorphs have been characterized by a variety of methods including variable temperature powder X-ray diffraction (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

P08.10.96

Acta Cryst. (2008). A**64**, C447-448

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