

this compound is crystallized from solutions in acetophenone as a host-guest complex with a ratio 2:3. In the crystal structure DEDA molecules form infinite chains in a direction [01-1] through a pair of centrosymmetric hydrogen bonds. The acetophenone molecules are situated inside different channels formed at stacking of these chains and running along [100] and [0-11] directions.

At decreasing of crystallization temperature until 5°C from the same solution DEDA crystallizes as new complex - hydrate with 1:3 host-guest ratio. In the crystal structure one carboxylic group of DEDA molecules is connected via centrosymmetric H-bonding with the carboxylic group of the other host molecule, while other carboxylic group is deprotonated giving rise to a network of intermolecular H-bonds associating with one ion of hydroxonium ( $\text{H}_3\text{O}^+$ ) and two molecules of water. The structure may be described as intercalate type complex with strict separation of the hydrophobic and hydrophilic areas.

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[1] Weber E., Csöregi I., Ahrendt J., Finge S., Czugler M., *J. Org. Chem.*, 1988, **53**, 5831-5839.

**Keywords:** versatile host, host-guest complex, intercalate

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#### Different Building Modes of $\alpha$ -Cyclodextrin/Monoalkyl Amphiphile Complexes

Delphine Gallois-Montbrun<sup>a</sup>, Sylviane Lesieur<sup>a</sup>, Thierry Prangé<sup>b</sup>, Dominique Durand<sup>b</sup>, Michel Ollivon<sup>a</sup>, Geneviève Le Bas<sup>a</sup>, <sup>a</sup>UMR CNRS 8612, Faculté de Pharmacie, Université Paris Sud, Châtenay-Malabry, France. <sup>b</sup>LURE, Université Paris Sud, Orsay, France. E-mail: delphine.gallois@cep.u-psud.fr

In this study, the impact of the length of the guest molecule alkyl chain and the crystallization conditions on the structural parameters of  $\alpha$ -cyclodextrin ( $\alpha$ -CD)/monoalkyl complexes was determined. Several procedures to crystallize those complexes were developed for different alkylalcohols as model guest molecules, as a function of temperature. Three different crystalline structures were identified depending on the alkyl chain length, using synchrotron X-ray diffraction (LURE, Orsay, France). In all cases, complexes crystallize in channel-type structures, where  $\alpha$ -CD molecules are stacked like coins in a roll and the alkyl chain of the guest compound is embedded in the tubular cavity of the  $\alpha$ -CDs. However, depending on the length of the chains and the crystallization conditions, the channels are organized differently.  $\text{C}_6$ - $\text{C}_8$  chains give rise to a pseudo-hexagonal lattice, a packing mode already observed for polyiodide complexes [1].  $\text{C}_{10}$ - $\text{C}_{12}$  chains crystallize in a triclinic pseudo-monoclinic C2 lattice, while longer chains up to  $\text{C}_{18}$  form hexagonal crystals with R3 symmetry. These two novel crystal structures are described. Understanding these structures opens new routes to nanotube formation through amphiphile-driven crystallization of cyclodextrin templates.

[1] Noltemeyer M., Saenger W., *J. Am. Chem. Soc.*, 1980, **102**, 8, 2710.

**Keywords:** cyclodextrin, nanotubes, supramolecular assembly

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#### Inclusion Compounds of Isomeric Xanthenol Hosts with Aniline

Ayesha Jacobs<sup>a</sup>, Luigi R. Nassimbeni<sup>a</sup>, Benjamin Taljaard<sup>b</sup>, <sup>a</sup>Faculty of Applied Sciences, Cape Town Campus, Cape Peninsula University of Technology, Cape Town. <sup>b</sup>Nelson Mandela Metropolitan University, South Campus, Port Elizabeth, South Africa. E-mail: jacobsa@cput.ac.za

Two isomeric xanthenol host compounds have been found to form inclusion compounds with aniline. These hosts are H1 = 9-(4-methoxyphenyl)-9H-xanthen-9-ol and H2 = 9-(3-methoxyphenyl)-9H-xanthen-9-ol. We have elucidated the structures of the inclusion compounds and determined their kinetics of desolvation. H1•½aniline crystallises in the triclinic space group  $P\bar{1}$  with the host in general positions and the aniline guest on a centre of symmetry. H2•aniline

was solved successfully in the monoclinic space group  $P2_1/c$  with both the host and guest molecules in general positions. For H1•½aniline there is (Host)—OH•••O—(Host) hydrogen bonding whereas in H2•aniline (Host)—OH•••N—(Guest) hydrogen bonding occurs. We have correlated the structures with the thermal stabilities of the compounds.

**Keywords:** isomeric hosts, aniline, desolvation

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#### Structural Features of Some Schiff Base Disulfide Compounds

Ömer Celik<sup>a</sup>, Nilgün Ancin<sup>b</sup>, Selma Gül Öztaş<sup>b</sup>, Semra İde<sup>a</sup>, <sup>a</sup>Hacettepe University, Department of Physics Engineering, 06800 Beytepe-Ankara, Turkey. <sup>b</sup>Ankara University, Department of Chemistry, 06100 Besevler-Ankara, Turkey. E-mail: ocelik@hacettepe.edu.tr

Schiff bases bearing imine N and anionic S atoms constitute an important class of polydentate ligands and their metal complexes have previously been used as models for biological systems. The molecule and crystal structure of a new synthesized disulfide compound [ $\text{C}_{30}\text{H}_{22}\text{F}_6\text{N}_2\text{O}_2\text{S}_2$ ] has been undertaken with a view to obtaining accurate structural parameters of interest in disulfide compounds. Crystal data:  $M=620.62$ , Triclinic,  $a=7.639(2)\text{Å}$ ,  $b=8.526(8)\text{Å}$ ,  $c=23.349(5)\text{Å}$ ,  $\alpha=89.04(4)^\circ$ ,  $\beta=89.99(2)^\circ$ ,  $\gamma=63.41(4)^\circ$ ,  $V=1359.6(9)\text{Å}^3$ ,  $P\bar{1}$ ,  $R=0.0538$ ,  $R_w=0.0944$ . The structure was solved by direct methods and refined by least squares on  $F_{\text{obs}}^2$  by using SHELX-97.

In the second phase of the study, structural results have been compared with the values found in our previous studies related at least four Schiff base disulfides [1-4]. The molecular conformation around central S-S bond has been affected by trifluoromethyl groups in the molecule. High electronegativity in the  $\text{CF}_3$  groups has been cause to conformational changes in the torsion angle of C-S-S-C [ $77.8(4)^\circ$ ]. Two strong intramolecular hydrogen bonds [O-H•••N, O•••N: 2.612(9) and 2.612(8)Å] have been observed and cause to increasing of the planarity in the main parts of the molecule.

[1] İde S., Öztaş G., Ancin N., Tüzün M., *Acta Cryst.*, 1997, **C53**, 376-378. [2] Özbey S., Temel A., Ancin N., Öztaş S.G., Tüzün M., *Z. Kristallogr.*, 1998, **213**, 207-208. [3] Candan M.M., İde S., Kendi E., Öztaş G., Ancin N., *Spectroscopy Letters*, 1998, **31(4)**, 891-900. [4] İde S., Ancin N., Öztaş S.G., Tüzün M., *Pharm. Acta. Helv.*, 1998, **72**, 291-294.

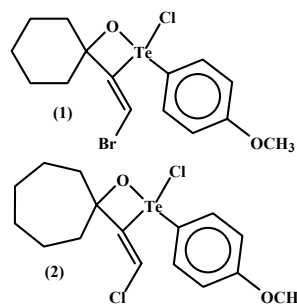
**Keywords:** Schiff base, disulfides, crystal structure

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#### Structural Studies of Human Cathepsin B Inhibitors: Telluroxetanes

Julio Zukerman-Schpector<sup>a</sup>, Ignez Caracelli<sup>b</sup>, Rodrigo L.O.R. Cunha<sup>c</sup>, João V. Comasseto<sup>c</sup>, Miriam E. Urano<sup>d</sup>, Ivarne L.S. Tersariol<sup>d</sup>, <sup>a</sup>Chemistry Department, UFSCar-São Carlos. <sup>b</sup>Department of Physics, UNESP-Bauru. <sup>c</sup>IQ-USP, São Paulo, <sup>d</sup>CIIB-UMC, Mogi das Cruzes, Brazil. E-mail: julio@power.ufscar.br



The inhibition of cathepsin B has been postulated to be directly responsible for the abrogation of the invasion process in several tumor cells lines [1], and, as it was shown that AS-101 [2], a  $\text{Te}^{\text{IV}}$  compound, was a cathepsin B inhibitor, compounds (1) and (2) were synthesized and studied.

In both compounds, if intra and two intermolecular secondary bonds and the electron lone pair are considered, then the  $\text{Te}^{\text{IV}}$  is coordinated in a  $\psi$ -pentagonal bipyramidal fashion. The secondary interactions join the molecules in chains of centrosymmetric dimers. These compounds, have higher second-order rate constants for the inactivation of cathepsin B, than that of AS-101. Moreover, the compound with a cyclohexane ring is 20-fold more active than (2) and 4-fold than (1), so that it can be