this compound is crystallized from solutions in acethophenone 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 acethophenone 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 (H_3O^+) 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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Keywords: versatile host, host-guest complex, intercalate

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Different Building Modes of α-Cyclodextrin/Monoalkyl Amphiphile Complexes

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In this study, the impact of the length of the guest molecule alkyl chain and the crystallization conditions on the structural parameters of α-cyclodextrin (α-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 α-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 α-CDs. However, depending on the length of the chains and the crystallization conditions, the channels are organized differently. C_6-C_8 chains give rise to a pseudo-hexagonal lattice, a packing mode already observed for polyiodide complexes [1]. C_{10}-C_{12} chains crystallize in a triclinic pseudo-monoclinic C2 lattice, while longer chains up to 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

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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

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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 [$C_{30}H_{22}F_6N_2O_2S_2$] 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)Å, b=8.526(8)Å, c=23.349(5)Å, α=89.04(4)°, β=89.99(2)°, γ=63.41(4)°, V=1359.6(9)Å^3, Pī, R=0.0538, Rw=0.0944. The structure was solved by direct methods and refined by least squares on F_{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 trifloromethyl groups in the molecule. High electronegativity in the CF_3 groups has been cause to conformational changes in the torsion angle of C-S-S-C [77.8(4)º]. 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., Ancın N., Tüzün M., Acta Cryst., 1997, **C53**, 376-378. [2] Özbey S., Temel A., Ancın N., Öztaş S.G., Tüzün M., *Z. Kristallogr*., 1998, **213**, 207-208. [3]Candan M.M., İde S., Kendi E., Öztaş G., Ancın N., *Spectroscopy Letters*, 1998, **31(4)**, 891-900. [4] İde S., Ancın 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: Tellurooxetanes

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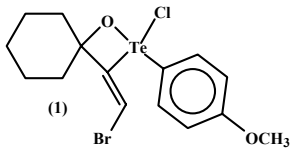

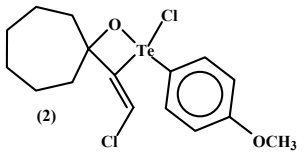

The inhibition of cathepsin B has been postulated to be directly responsible for the abrogation of the invasion process in several tumor cells lines [1], and, as it was shown that AS-101 [2], a Te^{IV} compound, was a cathepsin B inhibitor, compounds (1) and (2) were synthesized and studied.

In both compounds, if intra and two intermolecular secondary bonds and the electron lone pair are considered, then the Te^{IV} is coordinated in a ψ-pentagonal bipyramidal fashion. The secondary interactions join the molecules in chains of centrosymmetric dimmers. 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