

MS18 P01

A Comparison of the Inclusion Ability of Two Related Hosts Ayesha Jacobs^a, Kanyisa L. Nohako^a, Luigi R. Nassimbeni^a, Jana H. Taljaard^b, *Department of Chemistry, Cape Peninsula University of Technology, Cape Town, South Africa*, ^b*Nelson Mandela Metropolitan University, Port Elizabeth, South Africa*. E-mail: jacobsa@cput.ac.za

Keywords: inclusion compounds, kinetics, organic compounds

The inclusion ability of two host compounds H1, 9-(1-naphthyl)-9H-xanthen-9-ol, and H2, 9-(1-naphthyl)-9H-thioxanthen-9-ol was studied. We have previously shown that H1 successfully forms inclusion compounds with 1,4-dioxane[1] and acetone[2]. Here we report on the structures of **H1•DMF** and **H1•DMA** where DMF = N,N-dimethylformamide and DMA = N,N-dimethylacetamide. Numerous attempts at forming inclusion compounds between H2 and selected small organic guests including DMF and DMA were unsuccessful and yielded powders of the host alone. Both **H1•DMF** and **H1•DMA** successfully solved in P(-1), the host: guest ratios were 1:1 and their structures were stabilized by hydrogen bonding of the type (Host)-OH•••O-Guest.

Sulphur is less electronegative than oxygen and is less likely to be involved in hydrogen bonding. Interestingly even though the hydrogen bonding in the inclusion compounds of H1 does not involve the ether oxygen of the host, still no inclusion is found for H2.

The kinetics of desolvation for **H1•DMF** and **H1•DMA** were analysed as well as competition experiments.

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MS18 P02

Clathrates with Mixed Guests Tanya le roex^a, Luigi R. Nassimbeni,^b Edwin Weber^c ^a*Department of Chemistry & Polymer Science, University of Stellenbosch, South Africa*. ^b*Department of Chemistry, University of Cape Town, South Africa*. ^c*Institut für Organische Chemie, Technische Universität Bergakademie Freiberg, Germany*. E-mail: tlr@sun.ac.za

Keywords: clathrates, molecular recognition, crystal structures

Investigation of the selectivities of two diol organic hosts for pairs of small organic guests gave very interesting results which could be correlated with the crystal structures of the inclusion compounds containing mixtures of the two guests. This study comprises two separate investigations and in the first investigation the selectivity of the host 9,9'-(biphenyl-4,4'-diyl)difluoren-9-ol (**H1**) for a pair of guests with very similar chemical compositions but significantly different boiling points was examined. The second investigation involved a pair of guests with very similar boiling points and which form inclusion compounds with a particular host which have different host:guest ratios when crystallised at different temperatures. We thus investigated the selectivity of the host 9,9'-(ethyne-1,2-diyl)difluoren-9-ol (**H2**) for these guests and carried out the competition experiments at two different temperatures in order to see whether the selectivity would change with changing temperature.

Clathrate compounds are an important aspect of supramolecular chemistry and this study displays some novel results showing interesting selectivity profiles, and more importantly giving new insight into clathrates with mixed guests through crystal structure analysis, which in each case could be correlated with the selectivity profiles.

MS18 P03

Inclusion Complexes of β -Cyclodextrin with N-acetyl-L-Tryptophan and N-acetyl-D-Tryptophan I. M. Mavridis, S. D. Chatziefthimiou, *Institute of Physical Chemistry, National Center for Scientific Research "Demokritos", P. O. Box 60228, Aghia Paraskevi 15310, Athens, Greece*. Email: mavridi@chem.demokritos.gr

Keywords: beta-cyclodextrin; N-acetyl-tryptophan; crystal structure

Natural cyclodextrins (CDs), cyclic oligosaccharides consisting mainly of six (α CD), seven (β CD) or eight (γ CD) α -(1,4)-linked D-glucopyranosyl residues have a hydrophobic, relatively rigid cavity able to host a plethora of molecules. Being chiral compounds, CDs can, in principle, discriminate between enantiomers (guests) forming preferentially with one of the two a more stable inclusion complex [1,2]. X-ray crystallography can provide details of the factors that lead to chiral recognition. Structures of CD inclusion complexes with each enantiomer separately suggest that not only the cavity, which undergoes "induced fit" by the presence of the guest, but the guest's H-bonding potential, solvent interactions and packing forces also play a role in chiral discrimination [3].

The crystal structures of the complexes of β CD with N-acetyl-L-Tryptophan (triclinic P1, a=17.760 Å, b=15.158 Å, c=15.237 Å, α =102.774°, β =99.346°, γ =112.997°) and N-acetyl-D-Tryptophan. (Orthorhombic C222₁, a=19.162 Å, b=23.965 Å, c=32.597), with data collected by synchrotron radiation at 100K, are reported presently. In both complexes the β CD forms dimers accommodating two molecules of the guest. The differences in the arrangement of the two enantiomers with respect to the host, as well as the impact of the different packing modes are discussed with respect to chiral discrimination.

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MS18 P04

Polymorphism, selectivity and reactivity of inclusion Compounds Luigi Nassimbeni^a, Hong Su^a, Edwin Weber^b, ^a*Department of Chemistry, University of Cape Town, South Africa*, ^b*Institut für Organische Chemie, Technische Universität Bergakademie Freiberg, D-09596 Freiberg, Germany*. E-mail: luigi.nassimbeni@uct.ac.za

Keywords: inclusion, selectivity, reactivity

Host molecules which are exposed to a mixture of guests form inclusion compounds whose Guest:Host (G/H) ratio depends on the conditions of the crystallisation experiment. Thus the G/H ratio tends to decrease with rising crystallisation temperature [1] while the