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Keywords: silver coordination complexes; fluorescence; antibacterial properties

FA4-MS04-P04

From X-ray Structure to Gel – Can We Predict Gelation Abilities of Small Molecules? Roman Luboradzki[a,b], Monika Pyzalska[b], Zbigniew Pakulski[c]. [a]*Institute of Physical Chemistry, Polish Academy of Sciences, Poland.* [b]*Cardinal Stefan Wyszynski University, Warsaw, Poland.* [c]*Institute of Organic Chemistry, Polish Academy of Sciences, Poland.*
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In recent years, gels derived from low-molecular-mass compounds have attracted special interest on account of their unique features, potential applications and relative simplicity of the gelator molecules [1], [2]. These gels fall within the physical gels (in contradistinction to chemical gels) since, only non-covalent interactions between the gelator molecules are involved. The formation of the gel based on spontaneous self-assembly of gelator molecules under non-equilibrium conditions such as the cooling of oversaturated solutions which is used as the typical preparation method. Despite gels are, in general, amorphous an x-ray crystallography may be used as a tool for predicting the presence (or absence) of gelation abilities since the basic feature of the gelator molecules is their ability to stack into one-dimensional chains (e.g. by using intermolecular hydrogen bonds). Moreover, crystallographic data can be an inspiration for design more complicated systems, as two component gels [3]. The authors acknowledge the financial support from the Polish Ministry of Science and Higher Education (Grant No. N204 058 32/1514)

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Keywords: gels; saccharides; self-assembly

FA4-MS04-P05

β-Cyclodextrin Inclusion Complexes of L- and D-tryptophan. Chiral Discrimination. Irene M. Mavridis[a], Spyros D. Chatziefthymiou[a], Anastasia Paulidou[a]. [a]*National Center for Scientific Research "Demokritos", Athens, Greece.*
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Cyclodextrins (CDs) are well known cyclic oligosaccharides, consisting mainly of six (*α*CD), seven (*β*CD) or eight (*γ*CD) glucopyranose residues, which are water soluble and they are used for micro encapsulation of organic molecules inside their relatively apolar cavity. CDs are chiral hosts forming diastereomeric inclusion complexes with chiral substrates, a feature that makes them potential agents for enantiomeric discrimination, which is the basis of enantiomeric resolution of racemic mixtures by chiral gas and liquid chromatography. Enantiomeric discrimination by CDs is achieved by weak intermolecular interactions that may or may not include H-bonding, established by the embrace of the guest by the CD host, in order to obtain maximum contact. Resolution of racemates by natural *α*-, *β*-, and *γ*-CDs is generally poor, because the secondary hydroxyl groups of adjacent glucose units form strong intramolecular H-bonds that keep the cavity rigid and symmetrical. As a consequence, strict shape complementarity with a particular chiral guest, of the type "lock and key", is required for complete enantioselective complexation. On the other hand, in per-derivatized CDs the above strong H-bonding network has been destroyed and the macrocycles can be distorted readily, thus they can perform enantiomeric discrimination via "induced fit", leading even to complete resolution of racemates [1-2]. Presently, we report the crystal and molecular structures of the inclusion complexes of N-acetyl-L- tryptophan and N-acetyl-D-tryptophan with βCD, which are isomorphous, triclinic P1, a=17.760, b=15.158, c=15.237, α=102.774, β=99.346, γ=112.997. The host forms dimers that include two guest molecules (host:guest ratio 1:1), their aromatic moieties being in parallel arrangement (π...π interactions). The host-guest interactions involve H-bonding of the carboxylic terminal group and the indole part. Chiral discrimination of βCD is discussed based on similarities and differences of the inclusion complexes of the two enantiomeric guests and the corresponding complexes of the N-acetyl-L- and D- phenylalanine.

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Keywords: cyclodextrin; tryptophan; chiral discrimination

FA4-MS04-P06

Conformational Adaptations of Podands as a Base for Selective Binding of Stereoisomers. Krunoslav Užarević[a], Ivica Đilović[a], Marina Cindrić[a], Dubravka Matković-Čalogović[a]. [a]*Laboratory of General and Inorganic Chemistry, Chemistry Department, Faculty of Science and Mathematics, University of Zagreb, Zagreb, Croatia.*
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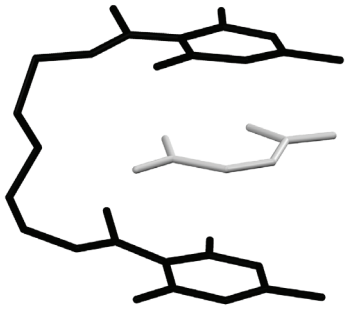
Flexible anion receptors draw significant scientific attention in the last few decades.[1] Although they usually display lower binding constants than rigid hosts, many interesting features are connected with this class of compounds. Binding

to anion often includes extreme spatial rearrangements of the flexible host. Such movement provides valuable information about the nature of host-guest binding and can further serve in developing of more efficient receptors in the field of anion sensing and signal transduction.
N,N'-3-azapentane-1,5-bis[3-(1-aminoethylidene)-6-methyl-3*H*-pyran-2,4-dione], **L**, is a podand known to be selective for nitrate and sulfate by self-assembling to pseudomacrocyclic host.[2] No similar pseudomacrocycle appears in the binding of HL^+ with maleinate or fumarate, well known *cis-trans* isomers. L displays new kind of conformes for each anion. In the case of maleinate, HL^+ take a "tweezers" conformation and the complex is additionally stabilized by π-π interactions between the pyrone rings and the π-system of the maleinate (A). Main motif in the binding of fumarate is the "letter Z" conformation of HL^+ with no π-π interactions between the host and named anion (B).
Competitive crystallization experiments in solutions containing both maleinate and fumarate provided only maleinate complex in high yield, thus suggesting higher affinity of **L** for this anion.



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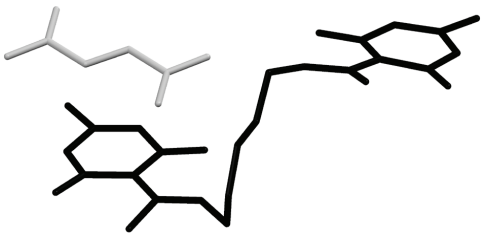

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Keywords: anion receptors; molecular tweezers; selectivity

FA4-MS04-P07

Crystal Structure of Cyclodextrin Complexes with Antioxidant Substances. Elias Christoforides[a], Fransceska Tsorteki[a], Areti Kokkinou[a], Pavlos Tzamalis[a], Athanassios Hountas[a], Kostas Bethanis[a], Christos Pappas[b], Dimitrios Mentzafos[a]. [a]*Department of Science, Physics Laboratory.* [b]*Laboratory of Chemistry, Agricultural University of Athens, Iera Odos 75, Athens,Greece.*
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Cyclodextrins (CDs) are a family of cyclic oligosaccharides that are composed of α-(1,4)-linked glucopyranose subunits. As a result of their molecular structure and shape, the cyclodextrins possess a unique ability to act as molecular containers (molecular capsules) by entrapping guest molecules in their apolar, hydrophophic, internal cavity. The use of natural cyclodextrins, frequently reported as "native", has been well established in cosmetic, pharmaceutical and industrial formulations, including food industry, as it provides a number of benefits: bioavailability enhancement; active stabilization; odor or taste masking; compatibility improvement; material handling benefits; and irritation reduction [1].
As part of a systematic study of the inclusion compounds of antioxidant substances extracted from Mediterranean plants in CDs, we report here the crystal structure of thymol, carvacrol (antifungal compounds found in thyme and origanum oils) and eugenol complexes with β-CD. Despite the similarities in the chemical structure of the above substances their inclusion compounds in β-CD exhibit differences in space group and host:guest stoichiometry. The thymol/β-CD complex crystallizes as a head-to-head dimmer in a triclinic unit cell (host:guest stoichiometry 1:1). Both carvacrol and eugenol/ β-CD (Figure 1) complexes crystallize in the space group *C2*, but the former exhibits host:guest stoichiometry 1:1, while the latter exhibits host:guest stoichiometry 2:3. All of them crystallize in a channel packing mode.
The stability of the above inclusion compounds has been confirmed by FT-IR spectra studies.

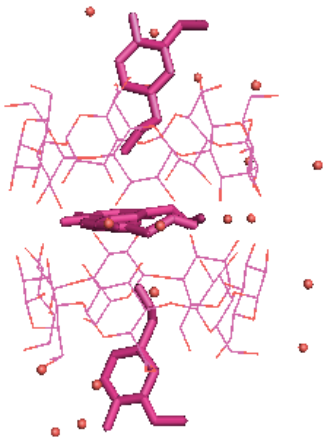

Figure 1: Eugenol inclusion compound with β- cyclodextrin.

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Keywords: cyclodextrins; antioxidants; inclusion compounds