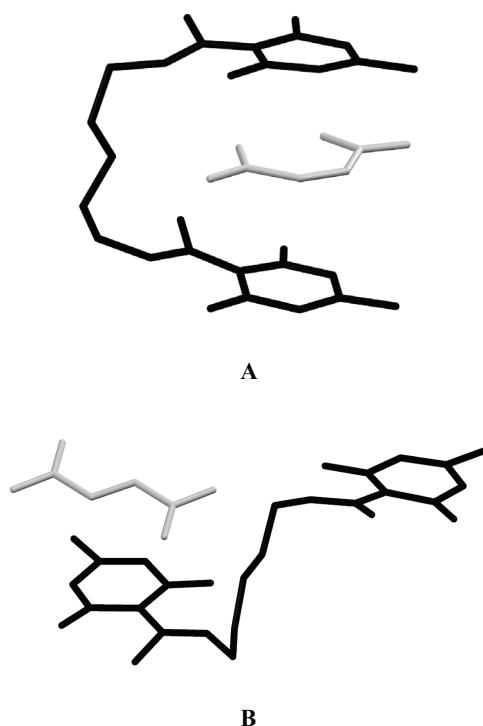


to anion often includes extreme spatial rearrangements of the flexible host. Such movement provides valuable information about the nature of host-guest binding and can further serve in developing of more efficient receptors in the field of anion sensing and signal transduction.

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.



[1] Steed, J. W., *Chem. Commun.* **2006**, 2637. [2] Užarević, K.; Đilović, I.; Matković-Čalogović, D.; Šišak, D.; Cindrić, M., *Angew. Chem. Int. Ed.*, **47**, **2008**, 7022.

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Crystal Structure of Cyclodextrin Complexes with Antioxidant Substances. Elias Christoforides^a, Fransceska Tsorteki^a, Areti Kokkinou^a, Pavlos Tzamalīs^a, Athanassios Hountas^a, Kostas Bethanis^a,

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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, hydrophobic, 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 dimer 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.

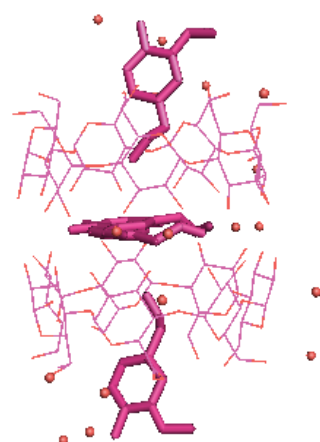


Figure 1: Eugenol inclusion compound with β - cyclodextrin.

[1] J. Szejtli, “Cyclodextrin Technology”, Kluwer Academic Publishers, **1988**.

Keywords: cyclodextrins; antioxidants; inclusion compounds