

representative points.

The crystals of (MDABCO<sup>+</sup>)-(C<sub>60</sub><sup>-</sup>)-TPC show metallic conductivity which is realized in the ordered layer of the C<sub>60</sub><sup>-</sup> radical anions due to effective overlapping of the C<sub>60</sub> LUMO orbitals. Ordering in the second layer below 200K is accompanied with the essential increase of the conductivity. Other physical properties affected by these ordering processes are also considered.

**Keywords:** fullerene; order-disorder phenomena; phase transition

#### FA4-MS03-P06

**Structural Effects of Lateral Substitution and Solvation on a Calixarene.** Petra Bombicz<sup>a</sup>, Tobias Gruber<sup>b</sup>, Margit Gruner<sup>c</sup>, Conrad Fischer<sup>b</sup>, Wilhelm Seichter<sup>b</sup>, Edwin Weber<sup>b</sup>. <sup>a</sup>*Institute of Structural Chemistry, Chemical Research Center, Hungarian Academy of Sciences, Hungary.* <sup>b</sup>*Institut für Organische Chemie, Technische Universität Bergakademie Freiberg, Germany.* <sup>c</sup>*Institut für Organische Chemie, Technische Universität Dresden, Germany.*  
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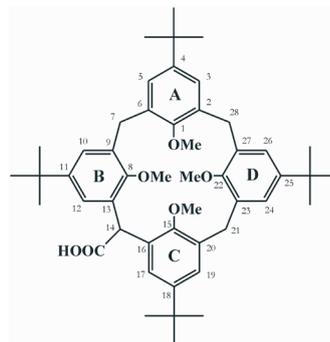
Modification of the upper and the lower rim of calixarenes using a vast number of different substituents has already been performed and widely investigated, including their conformational behaviour, inclusion property etc. Derivatives of calixarene with modified methylene unit attached to the backbone of the central ring are far less studied [1]. The monolateral substitution may open prospects for the design of new host structures, functional units and supramolecular aggregates.

Solvent-free calyx[4]arene **1** (Scheme) was subjected to single crystal X-ray structure determination: space group  $P2_1/n$ ,  $Z=1$ . Crystallization of **1** from aqueous ethanol/ethylacetate or an ethanol/tetrahydrofuran mixture yields the ternary inclusion compounds **1a** [1 EtOH H<sub>2</sub>O (1:1:1)] and **1b** [1 EtOH THF (1:1:1)], respectively, with identical space group ( $Pca2_1$ ,  $Z=1$ ) and close cell parameters. The structures are compared with the parent calixarene without carboxylic acid substituent on the methylene bridge (KEVXUE,  $P2_1/a$ ,  $Z=2$ ). The calix[4]arene molecules in all structures adopt distorted *partial cone* conformation but they show marked differences. Cell similarity ( $\pi$ ), isostructurality [ $I(s)$ ] and molecular isometricity indices [ $I(m)$ ] were calculated allowing detailed comparison of the investigated structures.

Both in the unsolvated compound **1** and the solvent inclusions **1a** and **1b** the methoxy group of the down oriented aromatic ring pointing into the cavity of the calixarene molecule. The solvents are thus not accommodated in the calixarene cavity but are located in the voids between the host molecules. The presence of a water molecule instead of THF neither affects the semirigid calixarene molecular structure nor influences the packing behaviour of the calixarene and alcohol molecules. In the non-carboxylic parent compound the methoxy groups of the down oriented aromatic rings point outwards the cavity.

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[1] Gruber T., Gruner M., Fischer C., Seichter W., Bombicz P., Weber E., *New J. of Chemistry*, submitted 2009.

**Keywords:** inclusion compounds; isostructurality; conformational flexibility

#### FA4-MS03-P07

**Cyclodextrin Inclusion of Agrochemicals: Complexes of the Herbicides Metobromuron and Monolinuron.** Vincent J Smith<sup>a</sup>, Mino R Cairn<sup>a</sup>, Susan A Bourne<sup>a</sup>. <sup>a</sup>*Department of Chemistry, University of Cape Town, Rondebosch 7701, RSA.*  
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Agrochemicals are often poorly soluble, light sensitive and some have high contact toxicity. These reasons serve as the motivation for attempts at cyclodextrin inclusion of these herbicides. Successful cyclodextrin inclusion may result in enhanced solubility, photo stability, a reduction in the contact toxicity and may simultaneously reduce the environmental pollution resulting from overdosing [1]. Cyclodextrin inclusion studies with metobromuron (3-(*p*-bromophenyl)-1-methoxy-1-methylurea) and monolinuron (3-(*p*-chlorophenyl)-1-methoxy-1-methylurea), yielded cyclodextrin inclusion complexes with TRIMEB (heptakis(2,3,6-tri-O-methyl)- $\beta$ -cyclodextrin). These complexes were subjected to characterization by single crystal X-ray diffraction, powder X-ray diffraction and thermal analysis. Single crystal X-ray diffraction showed that the complexes between TRIMEB and the guests (metobromuron and monolinuron) are isostructural crystallising in the orthorhombic space group  $P2_12_12_1$ . It also revealed the rotational disorder of the guest metobromuron in the complex. Furthermore, the structures also showed the diverse modes of guest inclusion of these isostructural complexes.

[1] Dodziuk, H. In *Cyclodextrins and Their Complexes*, (Ed. H. Dodziuk), Wiley-VCH Verlag GmbH & Co. KGaA, 2006, 1-26.

**Keywords:** cyclodextrin inclusion; isostructural; herbicides