

SHELXL97 program. Samples had significantly different colors, depending on the growth atmosphere (Ar+O₂: yellow or orange) and post-grown treatment (Ar and vacuum: almost colorless; air: bright orange). The analysis of the color and crystal composition of La₃(Ga_xTa_{1-x})Ga₅O_y allowed to divide them into four groups: colorless (y~14), orange (y~13.95-13.97), yellow (y~13.92-13.93), and colorless (y~13.90). These results are agreed with transmission spectroscopy («Specord-M40», wave range 11000-50000 cm⁻¹): the yellow crystals with the oxygen vacancies (□) have the band 28500 cm⁻¹. The low-grade band 20800 cm⁻¹ is present at colored crystals and absent at colorless ones (the like result has been wrote in [1]). At that the study of their chromaticity diagrams showed the different shade for the samples of the like visual color. The orange and colorless (the last group) Y54°-crystals, Y54° cut and the orange, yellow and colorless (the first group) Z-crystals, Z cut have the microhardness value ~13.8, ~12.2 GPa and ~12.6, ~10.4 and ~9.7Gpa, respectively. It was found that the temperature maximum of the yellow plate (Z-crystal, Z-cut) dielectric loss tangent has an effusive relaxation maximum in the temperature range 300-550°C. The topography by Shultz method (reflection 50.0) of the yellow plate (Z-crystal, Z-cut) with the refined composition La₃(Ga_{0.58}Ta_{0.42})Ga₅(O_{13.92}□_{0.08}) shown absence of blocks. According to the rocking curves (the scheme of a double-crystal X-ray diffractometer: Si (400) monochromator, (n, -n)) of the same sample, the half-width of the Bragg 50.0 and 40.0 peaks (value β_{exp}) are ~22" in contrast to the Z-crystal LGT, Y cut [2], in which β_{exp} ~6". So, a series of properties of LGT can be associated with the atmosphere of growth and post-grown treatment (the composition of crystals and their color), the growth and cut directions (the microhardness and structural perfection). Moreover langatate crystals are more appropriate for the high temperature applications compared with langasite ones.

[1] O.A.Buzanov et al., Crystallography Reports, 52(4) 2007,691-696. [2] D.V.Roshchupkin et al. Bulletin of the Russian Academy of Science: Physics. 72 (2) 2008, 184-187

Keywords: piezoelectrics; single crystal X-ray diffraction; microstructure characterization

FA4-MS03-P04

Simple Decoration of Inclusion Cavities within Isostructural Two-Component Organic Salts. Judit Galcera^a, Tomislav Friščić^b, Elies Molins^a, William Jones^b. ^aInstitut de Ciència de Materials de Barcelona Campus UAB, 08193 Bellaterra, Spain. ^bDepartment of Chemistry, University of Cambridge Lensfield Road, CB21EW Cambridge, UK. E-mail: jgalcera@icmab.es, wj10@cam.ac.uk

The rational design of multi-component crystalline organic solids is an important developing area in chemistry, especially for its applications in pharmaceutical and material sciences. The synthesis and screening for such multi-component solids (e.g. cocrystals) is significantly facilitated by using liquid-assisted grinding (LAG)¹. In this contribution, we

describe how LAG revealed an unprecedented number of 30 isostructural three-component molecular solids, based on the pharmaceutical compound lamotrigine. The solids are based on a two-component ionic inclusion host, composed of lamotrigine cations and a variable anion, along with an included solvent.² The ability to modify the anion components of the host provides a unique opportunity to manipulate the size and shape of the inclusion cavity, whilst maintaining the isostructurality of the material.

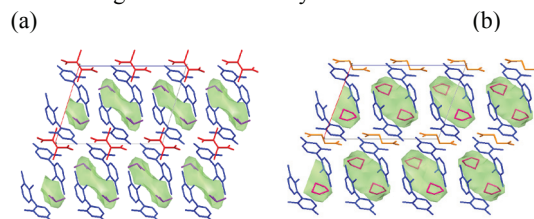


Figure 1. Different shapes of the inclusion cavities in lamotrigine D,L-chlorosuccinate (a) and lamotrigine succinate (b).

Consequently, the materials that will be described in this presentation illustrate a novel methodology to functionalise inclusion cavities and achieve control over molecular inclusion in organic solids, without resorting to rigid structures, such as metal-organic frameworks.

[1] T. Friščić, A.V. Trask, W. Jones and W. D. S. Motherwell *Angew. Chem. Int Ed.* 2006, 45, 7546. [2] J.Galcera and E.Molins *Cryst. Growth Des.* 2009, 9, 327.

Keywords: isostructurality; organic inclusion compounds; supramolecular host-guest chemistry

FA4-MS03-P05

Orientation ordering of the fullerene molecules in the ionic multicomponent complex (MDABCO⁺)(C₆₀⁻)·TPC. Salavat Khasanov^a, Dmitry Konarev^b, Gunzi Saito^c. ^aInstitute of Solid State Physics, Chernogolovka, Russia. ^bInstitute of Problems of Chemical Physics, Chernogolovka, Russia, ^cMeijo University, Nagoya, Japan. E-mail: khasanov@issp.ac.ru

The crystal structure of the ionic multicomponent complex (MDABCO⁺)(C₆₀⁻)·TPC incorporates two crystallographically independent close packed fullerene layers. At room temperature one of them completely ordered while in the other one the molecules are almost freely rotating. There are three stages of fullerene ordering in the disordered layer. Firstly it takes place a dynamical ordering down to 200K, when the fullerene motion can be approximated well by jumping only between three orientations with equal occupancies (33%). Occupational ordering in the temperature range 200-180K lowers the crystal structure symmetry from the trigonal to the monoclinic one. Complete ordering is resulted in the lattice distortion to the triclinic symmetry, which is accompanied by twinning of crystal sample. Full crystal structure analysis has been carried out for the all temperature ranges with

representative points.

The crystals of (MDABCO⁺)-(C₆₀^{•-})-TPC show metallic conductivity which is realized in the ordered layer of the C₆₀^{•-} radical anions due to effective overlapping of the C₆₀ 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^a, Tobias Gruber^b, Margit Gruner^c, Conrad Fischer^b, Wilhelm Seichter^b, Edwin Weber^b. ^a*Institute of Structural Chemistry, Chemical Research Center, Hungarian Academy of Sciences, Hungary.* ^b*Institut für Organische Chemie, Technische Universität Bergakademie Freiberg, Germany.* ^c*Institut für Organische Chemie, Technische Universität Dresden, Germany.*
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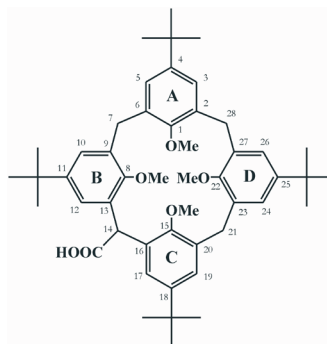
Modification of the upper and the lower rim of calixarenes using a vast number of different substituents has already been performed and widely investigated, including their conformational behaviour, inclusion property etc. Derivatives of calixarene with modified methylene unit attached to the backbone 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 H₂O (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 (π), 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^a, Mino R Cairra^a, Susan A Bourne^a. ^a*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)- β -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