

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

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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.

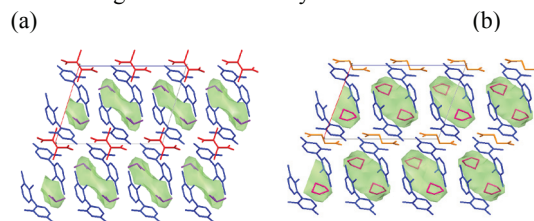


Figure 1. Different shapes of the inclusion cavities in lamotrigine D,L-chlorosuccinate (a) and lamotrigine succinate (b).

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.

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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