

waves devices. Single crystals of various properties have been grown by the Czochralski method from different melt compositions ($\text{La}_3\text{Ga}_4(\text{GaSi})\text{O}_{14}$ and $\text{La}_3\text{Ga}_4(\text{Ga}_{1.14}\text{Si}_{0.86})\text{O}_{14}$) using different conditions: the growth direction ($\langle 0001 \rangle$ -Z-crystals, $\langle 01-11 \rangle$ - $Y54^\circ$ -crystals), the growth atmosphere (Ar - colorless crystals, $99 \pm 98\% \text{Ar} + 1 \pm 2\% \text{O}_2$ -colored crystals), and post-grown treatment (vacuum or air at the 1000° ; ultraviolet or γ -irradiations). The other technology parameters ("Kristall-3M", the pulling and rotation rates - 1.2 mm/h and 1-15 rpm, respectively) did not vary. The aim of this work is to find a relationship between composition, color, microhardness, optical properties, and specific conductivity of LGS.

The peculiarities of the crystal structure and the refined composition of all samples have been determined by the diffraction methods: X-ray (the single crystals - CAD-4 diffractometer, MoK_α ; ground in powder crystals - HZG-4 diffractometer: Ni - filter, CuK_α , 2θ $10-115^\circ$), neutron (the single crystals - TriCS diffractometer: $\lambda=1.18\text{\AA}$; diffractometer located at the channel 5C2, $\lambda=0.830\text{\AA}$).

It is supposed, that color of $\text{La}_3\text{Ga}_4(\text{GaSi})\text{O}_y$ is caused by the oxygen contain: $y \sim 14$ (I-colorless), $y \sim 13.7$ (II-orange), $y \sim 13.6$ (III-yellow), $y \sim 13.4$ (IV-colorless). The colorless crystals can have both the stoichiometric composition (I) and to contain a plenty of oxygen vacancies- $\text{V}_\text{O}^\bullet$ (IV). These results agree with the optical properties (spectrophotometer "Specord-M40"): the bands 28500, 26000, 25000 cm^{-1} are connected with $\text{V}_\text{O}^\bullet$ and the band 20800 cm^{-1} -with color centres. At that the crystals of like visual coloration can have a different shade of color according to the chromaticity diagrams: for example, with the increase a ratio Ga/Si in $\text{La}_3\text{Ga}_4(\text{GaSi})\text{O}_{14}$ orange crystals changes the shade of color from yellow to pale blue over pale green. It has been concluded that the increase in the concentration of oxygen vacancies is of particular value for color crystals, the microhardness, the tangent of dielectric losses and specific conductivity. The frequency and elastic coefficients depend on common crystal composition. The $Y54^\circ$ -crystals, $Y54^\circ$ -cut possess the greater value of microhardness ($MH=14.6$ GPa) and the more structural perfection (the half-width of the Bragg $02\bar{2}2$ peak is $\beta_{\text{exp}}=36.22^\circ$) in comparison with Z-crystals, Z-cut ($MH=14.3$ GPa; $\beta_{\text{exp}}=94.54^\circ$ for 0002 peak). $Y54^\circ$ -crystals, $Y54^\circ$ -cut have the greater value of activation energy ($E_a=1.01$ eV) than Z-crystals, X and Y cuts ($E_a=0.92$ eV). Obtaining of homogeneous on compositions LGS crystals is possible at partial replacement Si on Ge or at contents of Ga excesses in initial composition.

Keywords: piezoelectric; point defect; physical properties

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Magnetic Structure of the Molecular Compound $[\text{Co}_2(\text{bta})]_n$ (H_4bta : Pyromellitic acid). Oscar Fabelo^a, Laura Cañadillas-Delgado^a, Jorge Pasán^a, Fernando S. Delgado^a, Ines Puente-Orench^{b,c}, Javier Campo^{b,c}, Juan Rodriguez-Carvajal^c, Catalina Ruiz-Pérez^a. ^aLaboratorio de Rayos X y Materiales Moleculares,

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The design and construction of new polymeric compounds of tuneable dimensionality, through adapted synthetic routes, is of strong interest in molecular materials [1]. In particular, the hydrothermal synthesis is currently being developed in solid-state and coordination chemistry for the design of new architectures. The magnetic behaviour of $[\text{Co}_2(\text{bta})]_n$ is complex and controversial. DC magnetic measurements without applied magnetic field in the range of temperature 2-300K show different features, a maximum at 16 K which has been explained as a long-range antiferromagnetic order confirmed by a lambda-shaped maximum in the specific-heat plot. At 13 K, another maximum appears together with a maximum in the out-of-phase signal (no frequency dependent). Some authors suggest that this is a field-dependent spin-canting region. [2-4]. Along this line, we have the possibility to shed light on the magnetic properties of a cobalt(II) complex of formula $[\text{Co}_2(\text{bta})]_n$. We have performed a neutron experiment in D1B diffractometer at ILL intending to clarify this situation. We are able to discard the presence of structural phase transitions at low temperatures and to obtain, preliminarily, the antiferromagnetic structure of $[\text{Co}_2(\text{bta})]_n$ below 16K without applied field, but no traces of spin canting has been observed, including that the SC is incompatible with the magnetic space group of the AF phase.

[1] Yaghi O., Li H., Davis C., Richardson D., Groy T.L., *Acc. Chem. Res.*, **1998**, 31, 474. [2] Sneško N., Gutierrez-Puebla E., Martínez J.L., Monge M.A., Ruiz-Valero C., *Chem.Mater.*, **2002**, 14, 1879. [3] Kumagai H., Kepert C.J., Kurmoo M., *Inorg. Chem.*, **2002**, 41, 3410. [4] Kumagai H., Chapman K.W., Kepert C.J., Kurmoo M., *Polyhedron*, **2003**, 22, 1921.

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Crystal Structures and Magnetic Properties of a Series of Copper(II)-Methylmalonate Complexes with 4,4'-Bipyridine. Jorge Pasán^a, Pau Diaz-Gallifa^a, Mariadel Déniz^a, Laura Cañadillas-Delgado^a, Oscar Fabelo^a, Joaquín Sanchiz^b, Francesc Lloret^c, Miguel Julve^c, Catalina Ruiz-Pérez^a. ^aDepartamento de Física Fundamental II, Facultad de Física, Universidad de La Laguna. La Laguna, Tenerife. Spain. ^bDepartamento de Química Inorgánica, Universidad de La Laguna, Tenerife, Spain. ^cICMol, Departament de Química Inorgánica, Universitat de València, Valencia, Spain. E-mail: jpasang@ull.es

The construction of one-, two-, or three-dimensional (1-D, 2-D, or 3-D) coordination polymers with various architectures is based upon the directionality and control