crystal diffraction, dilatometry, specific heat, calorimetry and impedance spectroscopy together with an attempt to present our view on the nature and origin of anomalies in $Li_2B_4O_7$.

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Keywords: neutron diffraction; noncentrosymmetric oxides; boron compounds

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Spectroscopic Study and Third-order Nonlinear Optical Behavior of N-(2-Hydroxy-4-methoxybenzylidene)-3-nitroaniline.

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N-(2-hydroxy-4-methoxybenzylidene)-3-nitroaniline (1) has been synthesized and characterized by X-ray diffraction analysis, FTIR and 1H NMR spectroscopy. The maximum one-photon absorption (OPA) wavelengths recorded by quantum mechanical computations using a configuration interaction (CI) method are estimated in the UV region to be shorter than 450 nm, showing good optical transparency to the visible light. We have computed both dispersion-free (static) and also frequency-dependent (dynamic) linear polarizabilities and second hyperpolarizabilities by using the time-dependent Hartree-Fock (TDHF) method to provide an insight into the microscopic third-order nonlinear optical (NLO) behavior of the title compound. The ab initio calculation results with non-zero values on (hyper) polarizabilities indicate that the synthesized molecule might possess microscopic third order NLO phenomena.

Keywords: hyperpolarizability; nonlinear optical behavior; spectroscopy

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The Peculiarities of Angular Width of Diffracted X-Rays at The Presence of Temperature Gradient.

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As it is known ref. [1] under the external influences (temperature gradient, ultrasound excitations) in the result of X-ray reflection from (10-11) plain sets of SiO2 single crystal in Laue geometry at certain values of influences it is observed the full pumping from the transmitting direction into the reflection direction.

To study the noted phenomena and to discover the peculiarities numerous theoretical and experimental works by different authors have been done. The angular width and energetic dispersions of full pumped X-rays have been studied. Particularly in ref. [2] it is shown that the angular width of the beam reflected from the transmitting direction into the reflected direction is strongly depends on the width of the pumping single crystal.

The submitted investigation is linked to the study of the dependence of the full pumped monochromatic X-ray angular width from the transmitting direction depending on the distance between source-pumping single crystal (sample).

To carry out the noted investigations it has been used MoK monochromatic radiation obtained of the Brag reflection from SiO_2 single crystal (10-11) plain sets. As a sample it has been selected the parallel samples of SiO_2 single crystal of different width in order to obtain to observe reflections from plain sets in Laue geometry.

To study the influence of X-ray full pumping angular width from the transmitting beam from the source-sample distance the sample was placed on distances of L_1=27cm and L_2=110cm and the section topograms of the transmitting beam have been obtained in the full pumping mode.

The investigations of the section topograms of the transmitting beam from the samples of L_1 and L_2 distances show that the X-ray angular width full pumped from the transmitting beam is decreased with increasing of the source-sample distance.

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Keywords: X-ray diffraction; topography X-ray; X-ray optics

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Effect of Cobalt Doping on the Gahnite Structure.

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Zinc aluminate ($ZnAl_2O_4$) is known by mineral name gahnite. It is a semiconductor with a wide energy band gap of ~3.8 eV, transparent for wavelengths greater than 320 nm which makes it useful in ultraviolet photoelectronic devices [1,2]. When doped with Co^{2+}, Mn^{3+} or rare-earth cations, it exhibits luminescence and can be used as a cathodoluminescent material [3]. Gahnite is cubic with the normal spinel structure, space group *Fd*-3*m*. Powder

gahnite samples doped with 0-100 at% Co were prepared by a sol-gel technique. XRD patterns of the prepared samples indicated that all gahnite samples had a characteristic cubic spinel structure. The unit-cell parameter *a* increased with Co-doping level, the increase being nonuniform. However, with Co doping the decrease of unit-cell parameter should be expected considering that ionic radius of 4-coordinated Co^{2+} is smaller than that of 4-coordinated Zn^{2+}. The observed lattice expansion is an indication of a considerable level of structure inversion: a part of Co^{2+} substitutes for Zn^{2+} on tetrahedral cation sites, and remaining Co^{2+} substitutes for Al^{3+} on octahedral cation sites in the $ZnAl_2O_4$ lattice. The location of Co^{2+} in the structure was determined by EPR spectroscopy. The structure of Co-doped gahnite samples was refined by the Rietveld method, which confirmed that Co doping induced the inverse spinel structure. It was found that metal-oxide distances in the $(Al,Co)O_6$ octahedra dominantly influenced the unit-cell parameter of Co-doped gahnite.

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