

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 $\text{Li}_2\text{B}_4\text{O}_7$.

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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.

Hüseyin Ünver^a, Aslı Karakaş^b, Ayhan Elmali^a, Tahsin Nuri Durlu^a. ^aAnkara University, Ankara, Turkey. ^bSelçuk University, Konya, Turkey.

E-mail: unver@science.ankara.edu.tr

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.

Vardan V. Margaryan^a, Karlen T. Hayrapetyan^a, Serob N. Noreyan^a. ^aX-Ray Pungs Laboratory, Yerevan, Republic of Armenia.

Email: x-ray@web.am

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 SiO_2 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 α monochromatic radiation obtained of the Bragg 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 $L_1=27\text{cm}$ and $L_2=110\text{cm}$ 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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Effect of Cobalt Doping on the Gahnite Structure.

Biserka Grzeta^a, Jasminka Popovic^a, Emilija Tkalcic^b, Stanislav Kurajica^b, Boris Rakvin^c. ^aDivision of Materials Physics, Rudjer Boskovic Institute, Bijenicka cesta 54, HR-10000 Zagreb, Croatia. ^bFaculty of Chemical Engineering and Technology, University of Zagreb, Marulicev trg 19, HR-10000 Zagreb, Croatia. ^cDivision of Physical Chemistry, Rudjer Boskovic Institute, Bijenicka cesta 54, HR-10000 Zagreb, Croatia.

E-mail: grzeta@irb.hr

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 $Fd\bar{3}m$. Powder