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**Phase equilibria and β-BaB₄O₆ crystal growth in the Ba, Na, B // O, F system**

Tatyana Bekker, Alexander Kokh, Pavel Fedorov, Institute of Geology and Mineralogy, Siberian Branch of Russian Academy of Science, Novosibirsk, General Physics Institute, Russian Academy of Science, Moscow. E-mail: tatyana_bekker@mail.ru

Due to the phase transition at 925°C, nonlinear optical crystals of low temperature modification of β-BaB₄O₆ (BBO) are commonly grown from high-temperature solution by top-seeded solution growth technique. Main solvents are some compositions in the BaO-B₂O₃-NaO ternary system, the BaB₂O₄–NaF system, the BaB₂O₄–BaF₂ system and also some mixed sodium oxide-fluoride compositions. The information in the available literature has been often contradictory and segmental. We believe that it’s more appropriate to consider mentioned solvents as one four-component mutual system Ba, Na, B // O, F. It represents a trigonal prism with the corresponding oxide (BaO-B₂O₃-NaO) and fluoride (BaF₂-BF₃-NaF) concentration triangles at the bases.

Our investigation of the BaB₂O₄–NaF system has shown that it includes a primary crystallization area of the new compound Ba₄Na₂[B₂O₄]₅F (hexagonal system, P6₃/m, a=7.346(1) Å, c=12.637(2) Å) [1,2]. Faceted bulk crystals of the new compound have been grown. Thus, BaB₂O₄–NaF section belongs to the Ba, Na // BO₂, F (BaB₂O₄–NaB₂O₄)–(NaF)–(BaF₂) ternary mutual system, which is the prism section. Comprehensive investigation of the phase equilibria and crystal growth has been carried out. It has been shown that the BaB₂O₄–Ba₄Na₂[B₂O₄]₅F system is suitable for BBO crystal growth. The fast pyrohydrolysis of BaF₂ in air causes gradual transformation of the BaB₂O₄–BaF₂ system into the BaB₂O₄–BaO system and results in the co-cristallization of BaB₂O₄ and BaB₂O₃ phases, making the growth of large high-quality β-BaB₂O₄ crystals in air impossible [3]. The BaB₂O₃ phase (PDF 00-058-0115) was earlier found in the BaO-B₂O₃-Na₂O system [4].

High-quality crystals of about 400 g in weight with the convex form of the crystallization front, which has a sufficient area of the crystallization process, are reproducibly obtained. Currently the maximum aperture of NLO element cut from the crystals is 30 x 30 x 6 mm³ [5].

3. T.B. Bekker, A.E. Kokh, P.P. Fedorov, CrystEngComm 2011, D01-01039 C1CE05071K.

**Keywords:** phase, equilibrium, NLO

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**Transition metal sheet-like systems based on dicarboxylic ligands**

Antonio Diego Lozano-Gorrín, Pau Diaz-Gallifa, Óscar Fabelo, Jorge Pasán, Catalina Ruiz-Pérez, Laboratorio de Rayos X y Materiales Moleculares, Departament de Fundamental Physics II, Facultat de Física, Universitat de La Laguna, Tenerife (Spain). E-mail: adlozano@ull.es

The preparation, the structure determination by means of X-ray diffraction and the study of magnetic properties of different transition metals sheet-like systems based on dicarboxylic ligands have been done.

1. 1-Cyclohexanediacidic and 1,1-cyclopentanediacidic acids, dicarboxylic acid-substituted C-6 and C-5 alicyclic hydrocarbons, can exhibit typical carboxyl group chemistry in variety of industrial applications. There are almost infinite esters obtained from thousands of potential starting materials. Esters are formed by removal of water from an acid and an alcohol, e.g., carboxylic acid esters, phosphoric acid esters, and sulfonic acid esters. Carboxylic acid esters are used as in a variety of direct and indirect applications. Lower chain esters are used as flavouring base materials, plasticizers, solvent carriers and coupling agents. Higher chain compounds are used as components in metalworking fluids, surfactants, lubricants, detergents, oiling agents, emulsifiers, wetting agents textile treatments and emollients.

Both acids are metal chelators. Chelation is applied in metal complex chemistry, organic and inorganic chemistry, biochemistry, and environment protection. It is used in chemotherapy treatments for metal poisoning. An example of end product derived from 1,1-cyclohexanediacidic acid is gabapentin, an anti-epileptic agent, chemically described as 1-(aminomethyl)cyclohexane acetic acid.

Polynuclear compounds of high-spin cobalt(II) ions bridged by carboxylic acid groups exhibit different magnetic behaviors depending on the bridging mode of the carboxylic acid and on its coordination number [1-3]. Concerning the magnetic properties, a relationship between the nature of the magnetic coupling and the type of bridge that links the metal center has been proposed.

**Keywords:** crystal engineering, X-ray diffraction, magnetic properties

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**Peculiarities of crystal growth and morphology of carbonate-synthetic diamonds**

Natalia Solopova, Anna Spivak, Yuriy Litvin, Institute of Experimental mineralogy RAS, 142432, (Russia), Chernogolovka, str. Akademika Osipyanu 4. Moscow State University. E-mail: solopenok@yandex.ru

Diamond formation in multicomponent K-Na-Ca-Mg-melts oversaturated with dissolved carbon in respect to diamond is studied at 7.0 – 8.5 GPa. Experiments on diamond spontaneous crystallization and seeded growth were carried out in the “anvil-with-hole” high-pressure apparatus. Diamond-forming processes are high-effective [1] and characterized by estimated density of nucleation of no less than 3 – 510¹⁰ nuclei in cm³ for individual crystal of up to 200 μm size, spinel-law and polycrystalline twins, polycrystalline aggregates of