A NEW FAMILY OF INDIUM RARE EARTH COMPOUNDS HAVING THE THORTVEITITE STRUCTURE

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In the last twenty years, a great deal of research has been carried out to identify new compounds having potential applications in different fields as scintillators, dosimeters or lasers. Some of these compounds show the characteristic laminar structure presented by the thortveitite mineral $Sc_2Si_2O_7$, as $InFeGe_2O_7$ and $InYGe_2O_7$. The monoclinic space group $C2/m$ (No. 12) describes the crystal symmetry exhibited by them in which only one octahedral site is disposed of for all the non-germanium cations. Recently, our work has been focused to obtain new laminar structures with potential applications as scintillators. Among these compounds we have synthesized and characterized the crystal structure data of $InGdGe_2O_7$ and $InTbGe_2O_7$ pyrogermanates, which have a thortveitite-like structure. For these two compounds we have employed a model in which the mirror plane symmetry present in the thortveitite structure is broken. That is to say, the space group $C2$ (No. 5) was used to perform a Rietveld refinement of the powder diffraction data. The cell parameters obtained for $InGdGe_2O_7$ and $InTbGe_2O_7$ were a = 6.8714(5) Å, b = 8.8799(6) Å, c = 4.8978(4) Å, β = 101.522(2)° and a = 6.8816(3) Å, b = 8.8770(3) Å, c = 4.8943(2) Å, β = 101.402(2)° respectively. In this point is important to rebound that only one laminar compound with symmetry $C2$ was found in the literature. A remarkable photo-luminescence effect was observed when the sample was irradiated with alpha-particles beam and during the incidence of X-rays. Finally we can say that these compounds should be interesting in possible optical applications.

Keywords: THORTVEITITE, PYROGERMANATE, LAYERED STRUCTURES

GRAPHITE SINGLE CRYSTAL INCLUSIONS IN DIAMOND

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Graphite in natural diamond usually occurs as oriented sheet-like masses on octahedral planes.   Here we present the results of an investigation of graphite in colourless, clear, single crystal diamond octahedra with rounded edges of 2–3 mm in length from the Panda kimberlite in the Ekati Mine district of Canada [1].   The diamond-graphite assemblage is unusual because: - Each diamond contains a single central graphite inclusion of up to 300 micrometer in linear dimension. - X-ray diffraction reveals all but one of these inclusions to be single crystals exhibiting sharp reflections. No deviation from hexagonal symmetry is observed. - The graphite occurs in two euhedral forms: tabular hexagonal prisms (the vast majority), and hexagonal dipyramids with pinacoids. - Distinct, yet not perfect, mutual crystallographic orientations between graphite and diamond are observed. - One very thin inclusion shows possibly dissolution or imperfect growth near one of its corners. - Another graphite consists of countless thin patches inside a sharp hexagonal borderline, again of about 300 micrometer edge length.   These observations give strong evidence for a heterotactic (topotactic) formation of the diamonds.

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Keywords: **GRAPHITE INCLUSION DIAMOND**

SYNTHESIS AND CHARACTERIZATION OF AN OPEN-FRAMEWORK AMMONIUM-IRON-GALLOPHOSPHATE

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The intense search for new materials with enhanced catalytic activities, like zeolites with heteroatoms in their framework, has led to the discovery of several new open framework structures. Particularly, new microporous metalphosphates have been synthesized. Here we report on synthesis and structural characterization of a new iron-gallophosphate.

Solvothermal synthesis experiments at 463K, using imidazole, Ga_2O_3, $FeCl_2$ and H_3PO_4 yield a brown-violet crystalline product with the chemical composition $NH_4(FeGa_2P_3O_{12}(H_2O)_2)$. Phase analysis from powder diffraction measurements revealed that the material is isotype to a former described cobaltphosphate (Chippindale, 1996). An X-ray data set was collected with MoKα radiation and a CCD detector at 152K from a single crystal, and a structure refinement was performed.   The product crystallizes in the monoclinic space group C2/c with cell constants of 13.445(3) Å, 10.184(2) Å, 8.894(2) Å and 108.36(2)°. The microporous 3-dimensional framework is built up of PO_4-tetrahedra, pseudo-trigonal GaO_5-bipyramids and distorted $FeO_4(H_2O)_2$-octahedra. Bands of cornersharing Ga-polyhedra and PO_4-units are running parallel to the c-direction. They are connected by Fe-octahedra which are edgeshared with further PO_4-terahedra. By this way, 2 intersecting channel systems are formed, which are filled by NH_4-groups and water molecules. Removing the NH_4-groups by thermal treatment up to 473K cause the decomposition of the compound.

The formation of new microporous metalphosphates with open framework structures are supported by solvo-thermal synthesis conditions. The low thermal stability and the small channel openings of the irongallophosphate are limiting factors for an industrial application of this compound.

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Keywords: **OPEN FRAMEWORK GALLOPHOSPHATE STRUCTURE ANALYSIS**

SOME α'-LOW TEMP. STRUCTURES IN Ca_2SiO_4-Sr_2SiO_4 SOLID SOLUTIONS

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Alkaline-earth orthosilicates have been extensively studied from the view points of crystal chemistry as well as earth sciences. Among them, Ca_2SiO_4-Sr_2SiO_4 solid solutions characteristic of having five polymorphic modifications (α, α' -prime-high temp., α'-low temp., β, γ) were studied by a number of researchers. They found that the basic structures of those five modifications were almost the same. Saalfeld (1975) carried out high temperature experiments on β-Ca_2SiO_4 and succeeded in transforming it into alpha-prime-low temp. above 1070K. In addition, he found a three-layers superstructure (a = 5.53 Å, b = 6.81 Å, c = 9.4 Å) . Udagawa and Urabe (1978) obtained details of the structure for the $Ca_{1.7}Sr_{0.3}SiO_4$. They found that their crystals had the same superstructure as that of Saalfeld (1975). Il'inets and Bikbau (1990) studied $Ca_{0.8}Sr_{1.2}SiO_4$ and they found a superstructure of the same kind which was obtained by Saalfeld (1975) and Udagawa & Urabe (1978).

On the contrary, any structure in Ca_2SiO_4-Sr_2SiO_4 solid solutions did not show superstructures (Catti, Gazzoni, Ivaldi and Zanini, 1983; Catti, Gazzoni and Ivaldi, 1984).   We tried synthesizing some crystals having chemical components of Ca_2SiO_4-Sr_2SiO_4 solid solutions and we obtained four different alpha-prime-low temp. crystals. They are $Ca_{1.5}Sr_{0.5}SiO_4$, $CaSrSiO_4$, $Ca_{0.5}Sr_{1.5}SiO_4$ and Sr_2SiO_4. Among four, $Ca_{1.5}Sr_{0.5}SiO_4$ and $Ca_{0.5}Sr_{1.5}SiO_4$ show the same superstructure as that of Saalfeld (1975), Udagawa & Urabe (1978) and Il'inets & Bikbau (1990). $CaSrSiO_4$ and Sr_2SiO_4 do not show any superstructure.

Keywords: **CRYSTAL STRUCTURE, SILICATE, SUPERSTRUCTURE**