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been reported. Among examples, can be named the following ones: anilinium nitrate [7], anilinium hydrogenophosphate and anilinium hydrogenoxalate [8]. This structure may be described as formed by alternating sheets of cations and anions which are held together with four five centered N-H...O bonds to form C₄(10) C₂(10) infinite chains running through the c direction. Moreover, strong O-H...O hydrogen bonds observed between bisulfate anions generate C₃(8) chains in the a axis direction. The infinite chains resulting from anion-anion and anion-cation interactions can be described as zigzag layers parallel (ac) plans. The crossing of these chains builds up different rings with R₃(10) and R₃(16) graph set motifs [9].

Keywords: graph theory, hybrid compounds, hydrogen bonds.

MS53.P33


Thiodiazolo[2,3-a][py] as an oxidative cyclization of (py)carbamothioyl by Cu²⁺

Forogh Adhami, Farzaneh Simyari, Maryam Ehsani, Department of Chemistry, Shahr-ray Branch, IAU, Tehran (Iran). E-mail: fadhami@gmail.com

Some compounds are worth from different aspects. The existences of specific functional groups cause unique properties for them. Reaction of benzoyl chloride, potassium thiocyanate with 2-aminopyridine and 2-amino-picoline in one pot produces carbamothioyl benzamide derivatives. These compounds possess various sites to react with numerous reactants.

When 2-aminopyridine was used in above reaction, N-(pyridine-2-ylcarbamothioyl) benzamide was formed. This compound and the other synthesized derivatives were characterized by CHN, IR-, ¹H NMR- and ¹³C NMR spectroscopies. Also their crystal structures were determined.

The reaction of 2-aminopyridine and 2-amino-picoline with Cu(II) salts resulted in oxidative cyclization. There are two possibilities of oxidative cyclization and two different structures (a & b) for these compounds. The products were characterized CHN, IR-, ¹H NMR- and ¹³C NMR spectroscopies.

The obtained crystals and x-ray single crystal diffraction confirmed the structure b is correct. The structure b of different derivatives is able to act as anti cancers.

Increasing of the anti cancer property of these products will be increased by changes and replacement of various groups and functions in both of aromatic rings.

Table 1. Characteristic of growing tourmalines.

<table>
<thead>
<tr>
<th>Snmp</th>
<th>Color</th>
<th>3d-elements cont., wt.%</th>
<th>Unit cell parameters, A</th>
<th>Rc</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>green</td>
<td>NiO-7.4 CrO-5.3</td>
<td>15.897(5) 7.145(2)</td>
<td>0.038</td>
</tr>
<tr>
<td>2</td>
<td>green</td>
<td>NiO-13.4 CrO₂-10.2 FeO-0.3</td>
<td>15.945(5) 7.208(2)</td>
<td>0.051</td>
</tr>
<tr>
<td>3</td>
<td>pink</td>
<td>CoO-14.4</td>
<td>15.753(8) 7.053(3)</td>
<td>0.057</td>
</tr>
<tr>
<td>4</td>
<td>blue</td>
<td>CuO-8.4</td>
<td>15.840(4) 7.093(1)</td>
<td>0.041</td>
</tr>
</tbody>
</table>

MS54.P01


Ion substitution in tourmaline with chromophore elements growing in hydrothermal conditions

O.S. Vereshchagin, IV. Rozhdestvenskaya, O.V. Frank-Kamenetskaya, T.V. Sergeyeva, Yu.B. Shapovalov, Institute of Experimental Mineralogy, Saint-Petersburg, (Russia). Institute of Experimental Mineralogy, Saint-Petersburg State University, Saint-Petersburg, (Russia). E-mail: oleg-vereschagin@yandex.ru

Unique physical properties of tourmaline crystals (pyroelectric, piezoelectric) and possibility of their use in jewelry makes the growing of synthetic tourmalines a topic of the most immediate interest. Our work is devoted to the crystal chemistry of synthetic tourmalines doped by transition metal (3d) elements (Ni, Cr, Co, Fe, Cu) which are identified as coloring agents (table 1).
Single crystals of samples 1-3 have been grown from complex boron-containing hydrothermal solutions at range of temperatures of 400-750°C and pressures of up to 150 MPa in the IEM RAS [1]. Cu- bearing tourmaline (sample 4) has been synthesised in the Institute of Mineralogy and Petrography SB RAS [2]. X-ray experiment was carried out on four-circle single-crystal diffractometer Nicolet R3.

The content of 3d-elements in multicolor synthetic tourmalines can rise up to 24 wt. % (in oxide form) and in the case of Ni, Co, Cu-tourmalines it is significantly higher than that found in natural specimens. The total content of 3d-elements and the ratio of its’ ionic radii are the reason for the unit cell parameters and octahedral dimensions variations. In all cases chromophore elements occupied Y (mainly) and Z octahedra (table 2).

Table 2. Characteristic of Y and Z octahedral.

<table>
<thead>
<tr>
<th>Smp</th>
<th>Y octahedron</th>
<th>Z-octahedron</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Occupation, apfu</td>
<td>&lt;Y-O&gt;, A</td>
</tr>
<tr>
<td>1</td>
<td>Al_{1,06}Ni_{0,04}Fe_{0,55}</td>
<td>1.991</td>
</tr>
<tr>
<td>2</td>
<td>Ni_{0,35}Fe_{0,65}Al_{0,35}</td>
<td>2.008</td>
</tr>
<tr>
<td>3</td>
<td>Al_{1,06}Co_{0,10}</td>
<td>1.949</td>
</tr>
<tr>
<td>4</td>
<td>Al_{1,06}Cu_{0,14}</td>
<td>1.978</td>
</tr>
</tbody>
</table>

In the structure of samples 1, 3, 4 the main element in Y and Z sites is aluminium. The samples 3 and 4 (sodium in X site) are analogues of sample 2 in nature. This work was supported by the RFBR (grant no. 09-05-00769-a).


Keywords: crystallochemistry, silicate, X-ray.

MS54.P02

First Silicate Mineral with Triple Tetrahedral Layer

Sergey M. Aksenov,* Ramiza K. Rastsvetaeva,* Nikita V. Chukanov,* Shubnikov Institute of Crystallography, RAS, Moscow (Russia). Institute of Problems of Chemical Physics, RAS, Chernogolovka (Russia). E-mail: rasti@ns.crys.ras.ru

The crystal structure of a new silicate mineral from the Eifel paleovolcanic area, Rhineland-Palatinate, Germany was studied by X-ray single crystal diffraction (diffractometer Xceliber Oxford Diffraction, CCD-detector). The orthorhombic unit-cell parameters are: a=6.528(1) Å, b=6.970(1) Å, c=37.216(5) Å, V=1693.33(4) Å³, space group Pnm2. The structure was solved by direct methods and refined to R=4.9%, 2706 /F > 3σ(F). Idealized crystal-chemical formula is: (K,Ca,Na)[Fe, Ca, Mg, Na]((Si,Al))_{2}O_{5}·(OH)·7H_{2}O.

The mineral is representative of a new structure type. The most important specific feature of its structure is a block [Si_{6}O_{18}] consisting of three connected single layers formed by four- and eight-membered rings of tetrahedra (T) centered by Si and Al. Two outer layers [Si_{3}O_{9}]

MS54.P03

New members in sodium cadmium bisulfate: structure, property and thermal studies

Dipankar Sah,* Giridhar Madras,* Tayur N. Guru Row,* Solid State and Structural Chemistry Unit. *Department of Chemical Engineering, Indian Institute of Science, Bangalore 560 012 (India). E-mail: s.dipankar@iisc.ernet.in

Bimetallic sulfates form an important constituent of the earth’s crust and are recognized to provide essential link to mineral evolution. Depending on the level of hydration they form different class of minerals. The omnipresent water plays a decisive role in the formation of hydrates of complex inorganic materials generating complicated structural frameworks. These compounds exhibit properties like ionic conductivity, phase transitions in the context of electric, magnetic and elastic properties [1, 2] and believed to have played an important role in the formation of earth’s atmosphere oxygen [3]. We have synthesized polymorphs of sodium cadmium bisulfate which differ in the extent of hydration and have studied their thermal properties and phase transition. Na_{2}Cd(SO_{4})_{3}·3H_{2}O, Na_{2}Cd(SO_{4})_{3}·2H_{2}O, Na_{2}Cd(SO_{4})_{3}·4H_{2}O, were crystallized by slow evaporation method form water. Na_{2}Cd(SO_{4})_{3}·3H_{2}O crystallizes in a trigonal system with the space group P3c. It loses water completely after 250 °C and transforms to a dehydrated phase whose structure has been established using abinitio powder diffraction. The dehydrated form crystallizes in the space group I 43d. The phase transitions have been investigated using DSC, TGA and ionic conductivity studies. β-Na_{2}Cd(SO_{4})_{3}, a polymorphic form of α-Na_{2}Cd(SO_{4})_{3}, has been isolated by quenching the parent compound α-Na_{2}Cd(SO_{4})_{3} and characterised to belong to a monoclinic system, space group P2_1/c. β-Na_{2}Cd(SO_{4})_{3} takes up water from the atmosphere and gets converted to a Krekhinite type mineral Na_{2}Cd(SO_{4})_{3}·2H_{2}O. Upon heating, mineral loses water and gets converted to α-Na_{2}Cd(SO_{4})_{3}.

The phase transition analysis provides inputs for exploring the origin of Krekhinite mineral. Na_{2}Cd(SO_{4})_{3}·4H_{2}O crystallizes in a monoclinic system with a space group P2_1/c. It is isosstructural with the mineral Astrakhanite which is also known as Blodite [4]. This work describes a structure based analysis of phase transitions involved in these complexes, thus providing insights into their evolutionary aspects.

Keywords: X-ray analysis, mineral, silicate.

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