Phosphate(II)-tetrahedra, NaO$_2$- and SeO$_{3.5}$- octahedra together form a (3, 6)-connected net. Thermochemical property studies show that during heating hydrogen and water are released while part of the phosphate(III) groups are oxidized to phosphate(V). Se[PO$_4$]$_2$ is formed as the main crystalline decomposition product. NaSe$_2$[HPO$_2$]$_2$[HPO$_2$(OH)]$_2$ represents the first example containing scandium within the family of $MM'$ metal phosphates(III). The replacement of phosphate(V) tetrahedra by phosphate(III) groups leads to a reduction of $M'$–O–P connections, resulting in more open frameworks.


**Keywords:** scandium, phosphate(III), thermal analysis

**MS81.P63**


Effect of magnesium on the thermal stability of the hydroxyfluorapatite

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The biological apatite contains minor substituents such as F, Cl, CO$_2$, SiO$_2$, Na, K$^+$, Sr$^{2+}$ and Mg$^{2+}$. Therefore, the incorporation of such ions into the synthetic hydroxyapatite would enhance its biocompatibility and bioactivity. Magnesium and fluoride co-substituted hydroxyapatites with the general formula Ca$_x$Mg$_y$(PO$_{4-y}$)(OH)$_y$F$_z$ (y = 0, 0.5, 1, 1.5 and 2) have been synthesized through a hydrothermal method. The obtained powders have been characterized using different analyses. The results showed that the substitution of F by OH was continuous between the limiting compositions Ca$_x$Mg$_y$(PO$_{4-y}$)(OH)$_y$ and Ca$_x$Mg$_y$(PO$_{1.5}$)F$_{0.5}$. Indeed, no secondary phases were formed. Furthermore, the incorporation of Mg into the hydroxyfluorapatite lattice influenced considerably its thermal behavior by lowering its decomposition temperature with respect to the nonsubstituted HFA. Also, the nature of the decomposition products tightly depended on the fluorine content. The Fullprof program was used to determine the phase distribution for the powders calcined at different temperatures. The obtained results showed that the amounts of the decomposition products increased with the increase of the calcination temperature. According to the nature of the decomposition products, it seems that the MHF$_A$ samples exhibit a thermal behavior similar to that of MHA rather than that of MFA.

**Keywords:** apatite, magnesium

**MS81.P64**


Role of supramolecular interactions on electronic absorption spectra of metal dithiolen complexes

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Metal-maleonitrileditholate (mnt) complexes have received considerable attention in the areas of conducting and magnetic materials, dyes, non-linear optics, and catalysis [1]. Typically, the geometry around the transition metal ions (Cu, Ni) possesses square-planar arrangement, and in case of Mn, Fe, Co-mnt complexes, the geometry is noticeably distorted square-planar [2]. We describe here a series of highly distorted square-planar ion-pair complexes in which $M$(mnt)$_2$ ($M$= Cu, Ni) anions are associated with alkyl imidazolium cations of varied alkyl chain lengths. In the present study, a systematic study of variation of square planar geometries (in terms of distortion) around the metal ion in customary square planar metal-dithiolen complexes has been discussed. This distortion in the geometry around the metal ion can be ascribed due to un-balanced supramolecular interactions, that include S–H, N–H and M–S type of weak contacts. The title complexes show a moderate absorption band in the NIR region at 1210 nm and 800 nm, in their solid states for the copper and nickel dithiolene complexes.


**Keywords:** supramolecular interactions, diffuse reflectance spectra.

**MS81.P65**

Crystal structure and phase transition of Rb$_{(x+y)}$(NH$_{3}$)$_{1.6}$IO$_3$ mixed crystal

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Ammonium iodate, NH$_4$IO$_3$, is a well known electro-optic material [1] and exhibits a strong piezoelectric effect [2]. Ferroelectricity was reported at 1975 with a transition temperature to paraelectric phase near 85°C [3]. In RbN$_2$I$_4$ iodate, RBIO$_3$, there is no report of the existence of ferroelectricity and phase transition. On the other hand, Potassium iodate, KIO$_3$, is known as successive phase transition within ferroelectricity [4]. Therefore, it is strange that RbIO$_3$ does not undergo the phase transition, like as KIO$_3$, or NH$_4$IO$_3$. In order to clarify this question, we carried out the measurement of differential scanning calorimetry and the experiment of powder X-ray diffraction of Rb$_{x}$(NH$_{3}$)$_{1.6}$IO$_3$ with $x$=$0.0$, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0. According to the results, the following things have become clear now. In all compositions of $x$, Rb$_{(x+y)}$(NH$_{3}$)$_{1.6}$IO$_3$, mixed crystals were the single crystalline solid solution. The crystal structure of $x$=$0.1$, 0.2 and 0.3 is approximately-same crystal structure of RBIO$_3$, and one
of x=0.7, 0.8 and 0.9 was almost same one of NH₄IO₃. Meanwhile, the crystal structure of the middle compositions (x=0.4, 0.5 and 0.6) was different from both of Rb₂O, and NH₄IO₃.

The measurement of DSC in temperature range from room temperature to 135°C, Rb₂(NH₄)₂IO₃ with x=0.0 to 0.6 indicate no anomaly. However, single anomaly in DSC was observed in the each sample of x=0.7 to 1.0. From a reported temperature of ferroelectric phase transition in NH₄IO₃ [3], it was considered that these DSC anomalous temperatures were equivalent to temperature of the ferroelectric phase transition. These temperatures of ferroelectric phase transition were decreased with decreasing the value of composition x from x=1.0 to x=0.7. The values of the entropy change at the ferroelectric phase transition of x=0.8, 0.9 and 1.0 were obtained from the value of these heat anomaly in DSC measurement of each samples. As a result, it was considered these ferroelectric phase transition was an order-disorder type.

Now, we are carrying out the low temperature DCS measurement and the identification of the crystal structure of middle composition region (x=0.4, 0.5 and 0.6). In congress, we will show the crystal structures and DSC measurements, and will discuss the phase diagram and the mechanism of phase transition in Rb₂(NH₄)₂IO₃ mixed crystals.

Some peroxy-nicotinic acid complexes of Mo, have been investigated by Djordjevic et al., [4], their samples were not investigated by X-ray methods, but with the use of chem. analysis, spectroscopic, ¹H and ⁱ³C NMR studies they proposed structures which differ from ours.

Acknowledgement: The research has been partly supported by the EU Human Capital Operation Program, Polish Project No. POKL.04.0101-00-434/08-00.

Keywords: catalyst, molybdate

**Indiallade and cordierite in glass ceramics for millimeterwave dielectrics**


Dielectrics for millimeterwave communications are expected to have low dielectric constant and high quality factor (high Q). Cordierite ceramics is a candidate for millimeterwave dielectrics, because of low dielectric constant 4.7, and high Q of more than 200,000 GHz. Cordierite has two polymorphs: disordered phase indiallite (hexagonal, P6/mcc (No. 192)) and ordered phase cordierite (orthorhombic, Cccm (No.66)). As Ni-doped cordierite ceramics with good dielectric properties tend to disordered, indiallite was expected to have high Q. As indiallite

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**Table 1. Crystal data of new peroxy-molybdates with nicotinic acid.**

<table>
<thead>
<tr>
<th>Chemical formula</th>
<th>C₅H₇Mo₅N₅O₁₈</th>
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</tr>
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<tbody>
<tr>
<td>SG</td>
<td>P-1 (2)</td>
<td>P₂₁/c (14)</td>
<td>Pc (7)</td>
</tr>
<tr>
<td>Cell parameters</td>
<td>a=6.687(4) b=6.965(4) c=12.012(7) α=76.421(4) β=7.777(2) γ=69.478(4)</td>
<td>a=7.504(2) b=28.473(7) c=111.425(1)</td>
<td>a=5.416(3) b=5.350(2) c=16.976(7)</td>
</tr>
<tr>
<td>V (Å³)</td>
<td>503.66(2), 1</td>
<td>1546.82(3), 2</td>
<td>472.29(4), 2</td>
</tr>
<tr>
<td>R₁, R₂</td>
<td>0.0422; 0.0902</td>
<td>0.0282; 0.0622</td>
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**Keywords: catalyst, molybdate**

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**Figure 1, a) Anion coordination polyhedron and b) asymmetric unit of compound I (Mo-green, O-blue, N-red, C-grey).**

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MS81.P67


**Indiallade and cordierite in glass ceramics for millimeterwave dielectrics**


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**Keywords: catalyst, molybdate**

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