Phosphate(III)-tetrahedra, NaO_2- and SeO_6- octahedra together form a (3, 6)-connected net. Thermochromic property studies show that during heating hydrogen and water are released while the phosphate(III) groups are oxidized to phosphate(V). Sc[PO_4]_2 is formed as the main crystalline decomposition product. NaSe[PO_4]_2[PO_4(OH)] represents the first example containing scandium within the family of MPO_4 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.[2]


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

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**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_3^2-, 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)_{z}(OH)_w have been synthesized through a hydrothermal method. The obtained powders have been characterized using different analyses. The results showed that the substitution of F for OH was continuous between the limiting compositions Ca_{x}Mg_{y}(PO_4)_{z}(OH)_w and Ca_{x}Mg_{y}(PO_4)_{z}F_w. 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**

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**MS81.P64**


**Role of supramolecular interactions on electronic absorption spectra of metal dithiole 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 [Mmnt]_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-dithiole 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 solution states for the copper and nickel dithiolene ion-pair complexes respectively. The absorption maxima in the solid-state diffuse reflectance spectra is mainly depends on the geometry around the copper metal, e.g., the square planar copper-dithiole complexes exhibit broad band at 1150 nm whereas distorted square planar (λ = 38.31°) copper-dithiole complexes show an broad band at 1260 nm, indicating a bathochromic for the more distorted square planar copper complexes. All the compounds are unambiguously characterized by single crystal X-ray crystallography, and further characterized by IR, ^1^H NMR, LCMS, EPR spectral- and electrochemical-studies.

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**MS81.P65**


**Crystal structure and phase transition of Rb_3(NH_4)_3IO_3 mixed crystal**

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Ammonium iodate, NH_4IO_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 Rubidium 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_4IO_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_3(NH_4)_3IO_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. Accordingly the results, the following things have become clear now. In all compositions of x, Rb_3(NH_4)_3IO_3 mixed crystals were the single crystalline solid solution. The crystal structure of x=0.1, 0.2 and 0.3 was approximately-same crystal structure of RbIO_3, and one