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**Synthesis and structural study of photoluminescent lanthanide-organic frameworks.**

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**Keywords:** ruthenium, carboxylate, amidate

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**Synthesis, crystal structure and thermal decomposition of NaSc[HP2O7][HP2O7(OH)]8.**

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NaSc[HP2O7][HP2O7(OH)]8 was prepared by use of a phosphorous acid flux route (H2PO3, mp: 73.6 °C).[1] The crystal structure was determined from single-crystal X-ray diffraction data: triclinic, space group P1 (No. 2), a = 7.4507(1) Å, b = 9.6253(17) Å, c = 9.6141(16) Å, α = 115.798(4)°, β = 101.395(4)°, γ = 101.136(3)°, V = 777.29(16) Å3 and Z = 1. The crystal structure of NaSc[HP2O7][HP2O7(OH)]8 contains two kinds of phosphate(III) groups: H2PO3 and HPO32−.

**Keywords:** lanthanide-organic frameworks, phosphonates, photoluminescence

C726
Phosphate(III)-tetrahedra, NaO₆- and ScO₆- octahedra together form a (3, 6)-connected net. Thermochromic property studies show that during heating hydrogen and water are released while part of the phosphate(III) groups are oxidized to phosphate(V). Sc[PO₄]₂⁻ is formed as the main crystalline decomposition product. NaSc[HP0₄]₂[HPO₄(OH)] represents the first example containing scandium within the family of M[MP] 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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Effect of magnesium on the thermal stability of the hydroxyfluorapatite

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The biological apatite contains minor substituents such as F, Cl, CO₂⁻, SiO₂⁻, Na⁺, K⁺, Sr²⁻ and Mg²⁻. Therefore, the incorporation of such ions into the synthetic hydroxyapatite would enhance its biocompatibility and bioactivity. Magnesium and fluoride co-substituted hydroxypatites with the general formula Ca₃Mg[PO₄]₂(OH)₁₋₂Fₓ 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 Ca₃Mg[PO₄]₂(OH)₁₋₂Fₓ and Ca₃Mg[PO₄]₂F₂. 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 depends 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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Role of supramolecular interactions on electronic absorption spectra of metal dithiolene 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-dithiolene 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-dithiolene complexes exhibit broad band at 1150 nm whereas distorted square planar (κ = 38.31°) copper-dithiolene complexes show a 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, 1H NMR, LCMS, EPR spectral- and electrochemical-studies.


Keywords: supramolecular interactions, diffuse reflectance spectra.

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Crystal structure and phase transition of RB₆(NH₄)₂IO₃ mixed crystal

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Ammonium iodate, NH₄IO₃, 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, Rb(IO₃), there is no report of the existence of ferroelectricity and phase transition. On the other hand, Potassium iodate, K(IO₃), is known as successive phase transition within ferroelectricity [4]. Therefore, it is strange that Rb(IO₃) does not undergo the phase transition, like as K(IO₃) or NH₄IO₃. In order to clarify this question, we carried out the measurement of differential scanning calorimetry and the experiment of powder X-ray diffraction of RB₆(NH₄)₂IO₃ 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, RB₆(NH₄)₂IO₃, 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 Rb(IO₃), and one