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Keywords: MD simulation, hydrates, nucleic acid

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A Novel Spin Transition Curve in [tris(2-picolylamine)Fe(II)]Cl_2 Allyl Solvate
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The title compound exhibits a temperature dependent spin crossover with an intermediate plateau in the spin transition curve (STC) around 111K at an unusual high-spin concentration of about 30%. This is well below the plateau with a 50% concentration observed for the isomorphous ethanol solvate [1].

We report here single crystal diffraction data collected at 200, 132, 111 and 94K. The systematic absences are consistent with $B2_1/c$ space group symmetry at 200 and 132K. At 111K, *i.e.* in the range of the plateau, a superstructure is observed. The consequential reflections violate the original *B*-centering and lead to $P2_1/c$ space group symmetry with a doubled unit cell volume. At 94K the original $B2_1/c$ symmetry is recovered, thus indicating a reentrant sequence of phase transformations [2].

This observation shows that, as in the cases of the ethanol and 2-propanol solvates [1,3], a plateau in the STC reflects the appearance of a new ordered structure. The plateau region is likely a result of the coupling of the spin conversion with the concurrent conformational ordering of the crystal architecture.

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Keywords: spin crossover, phase transition, order-disorder

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Solid State Synthesis and Characterization of Some Novel Sodium Rare Earth Phosphates
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Recently, much attention has been paid to the rare earth phosphates because of their potential applications for optical materials, including laser, phosphors, and more recently, anti-UV materials [1]. $MOPO_4$ type materials possess properties that make them potentially useful for catalytic, electronic and ion exchange applications[2].

In this work, Ln_2O_3 (where Ln= La, Nd, Sm, Eu, Gd, Dy, Ho, Er, Yb) were used as a rare earth source, $NH_4H_2PO_4$ was used as a phosphate source and Na_2CO_3 was used as a sodium source to obtain sodium rare earth oxyphosphates. Reactants were heated at 1100 ^{0}C for 20 hours. X-ray difraction patterns, IR and Raman analysis, SEM pictures and EDX analysis were taken for characterization. According to these results, structures of these products were compared with previous ones[2-3].

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Keywords: rare-earths, oxyphosphates, solid-state

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The Systems Li-Ho-P-O and K-Ho-P-O: A Study in Inert Atmosphere
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The phosphates with open frameworks are materials that are composed by (PO_4) tetrahedral and by others polyhedral as octahedral (XO_6) and dodecahedral (XO_8) units. So, this structural conformation prove several applications of such materials as ionic conductors, ion exchangers, scintillating materials for gamma ray detection [1], catalysts [2], anticorrosive [3], etc. As part of our phosphates with open frameworks research, we study the phases present in the systems Li-Ho-P-O and K-Ho-P-O using different temperatures reaction and atmospheres. In this work, different phosphates compound like rare earth phosphate (Xenotime-type $HoPO_4$), alkali metaphosphate (APO_3, A= Li, K) and an alkali-rare earth pyrophosphate ($LiHoP_2O_7$) [4] were synthesized. These phases were characterized by X ray powder diffraction, differential thermal analysis and microscopy methods. A crystallochemistry study relating the crystal structures was performed.

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Keywords: phosphates, phase identification, X-ray diffraction

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Studies of Spin Crossover Complexes via Solvo-thermal Syntheses and their Thermal Relaxation of Light Excited Kinetic Phenomena
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The unique spin crossover 1D ladder complex $[Fe_2(bpt)_2(NCS)_2(bpy)_2]\cdot MeOH$ (**1**) have been synthesized successfully by one-step solvo-thermal syntheses or directly transformed from *trans*-$[Fe(abpt)_2(NCS)_2]$ complex by hydrothermal process.

The magnetic measurement reveals that the 1D spin-crossover complex **1** has an abrupt spin transition at 130 K and possesses an unusual magnetic behavior. The π-π interactions of **1** do vary slightly with spin transition. The distances along the (110) and (101) planes are 3.65(1) Å and 3.52(5) Å at 295 K but 3.53(3) Å and 3.45(2) Å at 100 K.

The novel dinuclear Double bridging complex $[Fe_2(\mu\text{-}bpt)_2(NCS)_2(CH_3OH)_2]$(**2**) and $[Fe_2(\mu\text{-}bpt)_2(NCS)_2(py)_2]$ (**3**) have also been synthesized and characterized by x-ray diffraction. The bond lengths of Fe-N are 2.292(3) Å, 2.094(3) Å for complex **2** and 2.110(2) Å, 2.321(2) Å for complex **3** at HS state.

The variable-temperature magnetic susceptibility measurement reveals that **2** and **3** are in high-spin state during 60-400 K. Interestingly, the complex **3** has a spin transition from HS to LS at low temperature under 808 nm radiation and the thermal relaxation behavior of such induced LS state will be disscussed.
Keywords: LIESST, spin crossover, thermal relaxation

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Study of the Mechanism of Cu-Zn Mechanical Alloying by X-ray Powder Diffraction
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