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Nickel ferrite is an important high frequency magnetic material due to its ultrahigh resistivity. Nanocrystals of NiFe<sub>2</sub>O<sub>4</sub> ferrite have been synthesized by the chemical co-precipitation of the amorphous metal hydroxides (under controlled pH values). The prepared powders have been sintered at 800 C. Room temperature X-ray measurements of the prepared samples of NiFe<sub>2</sub>O<sub>4</sub> reveal the production of single cubic phase with average crystallites size of about 30 nm, Results confirmed by transmission electron microscope (TEM) investigations. The lattice parameters, the oxygen position and the cation distribution have been determined by using Rietveld analysis. The study shows clearly surprising departure of the cation distribution from the known inverse distribution and reduce concentration of iron ions on tetrahedral sites, the degree of inversion is determined. The results of Mossbauer Effect spectroscopy (ME) and the Vibrating Sample Magnetometer (VSM) indicate the correlation between the magnetic properties and the nanocrystallinity of the investigated nickel ferrite.

Keywords: nanomagnetism, ferrites, magnetic - structure properties

**P08.14.172**

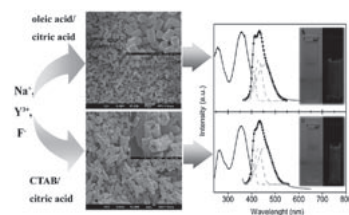
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**Synthesis and intense blue luminescence of sodium yttrium fluoride microcrystals**

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NaYF<sub>4</sub>:Eu<sup>2+</sup> microcrystals with an intense blue luminescence were fabricated. Oleic acid and cetyltrimethylammonium bromide were used as the surfactants to tune the morphology, while citric acid was taken as a ligand to stabilize the beta phase NaYF<sub>4</sub> and to reduce Eu<sup>3+</sup> to Eu<sup>2+</sup> for activation of blue luminescence. All as-prepared samples were found to crystallize in hexagonal rods or tubes. Both rods and tubes were capped with surfactants which enabled their stable dispersion in glycol to form transparent solutions. This observation seems to be the first example of the successful preparation of stable dispersion of micron luminescence solids. These transparent solutions showed an intense blue luminescent emission of Eu<sup>2+</sup> with a quantum yield of about 14 percent. Finally, the mechanism for the fabrication of the rods and tubes as well as the reduction of Eu<sup>3+</sup> ions was discussed.



Keywords: hydrothermal synthesis, inorganic luminescence, surfactants

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**Solid-state optical properties of CT complexes with ammonium anthracene-2,6-disulfonate and TCNB**

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The tuning of electronic properties by controlling the molecular arrangements in organic solid is an effective approach for both fundamental and practical research of the organic material. We have proposed that tunable solid-state optical properties of organic salts of anthracenedisulfonic(ADS) acid with aliphatic amines ascribed to arrangements of anthracene moieties. Recently we applied the tuning method to charge transfer (CT) complexes and founded that ammonium anthracene-2,6-disulfonate included 1,2,4,5-tetracyanobenzene(TCNB) to form CT complexes. Here we report several crystal structures and solid-state optical properties of the CT complexes composed of diisopropylamine, anthracene-2,6-disulfonate and TCNB. From crystallization under different conditions, we obtained three CT complex crystals, 1-3. X-ray structure analysis revealed that complex 2 and 3 have alternating stacks of 2,6ADS and TCNB molecules in which ratio are 1:1 and 1:2, respectively. On the other hand, Complex 1 has 1:1 segregated stacks. They showed very different solid-state optical properties depending on their different manners of molecular packing.

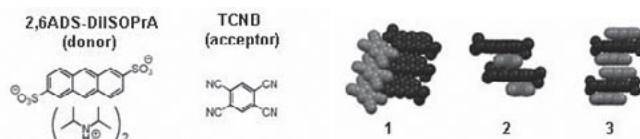


Fig.1 Molecular structure of donor and acceptor. Fig.2 crystal structure of complex 1,2 and 3.

Keywords: charge-transfer complexes, solid-state spectroscopy, single-crystal X-ray analysis

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**Crystal and magnetic structure of quantum spin-trimer compounds Ca<sub>3</sub>Cu<sub>3-x</sub>Ni<sub>x</sub>(PO<sub>4</sub>)<sub>4</sub>**

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Ca<sub>3</sub>Cu<sub>3</sub>(PO<sub>4</sub>)<sub>4</sub> is a novel quantum spin trimer system in which the three Cu<sup>2+</sup> (S=1/2) spins are antiferromagnetically coupled giving rise to a doublet ground state (TN<1 K). By substituting a Cu<sup>2+</sup> spin in the trimer by Ni<sup>2+</sup> (S=1) a singlet ground state can eventually be realized offering for the first time the observation of the Bose-Einstein condensation (BEC) in a quantum spin trimer system. Neutron diffraction experiments with the powder samples of Ca<sub>3</sub>Cu<sub>3-x</sub>Ni<sub>x</sub>(PO<sub>4</sub>)<sub>4</sub> (x=1,2) have been carried out on HRPT and DMC instruments at SINQ to determine the arrangement of the Cu and Ni atoms in the trimers and to study possible magnetic ordering. The composition with one Ni per trimer (x=1) crystallizes in a monoclinic structure (sp. gr. P21/a, N14) with the cell parameters a=17.714 Å, b=4.885 Å, c=8.846 Å and β=123.845° at T=290K. Each trimer is formed by two crystallographic positions (2a) in the middle and (4e) at the ends of the trimer. We found that the middle position is occupied by the Cu<sup>2+</sup>, whereas the end positions are statistically equally populated with the Cu<sup>2+</sup> and Ni<sup>2+</sup>. Thus, the three different types of trimers are present: Cu-Cu-Cu, Ni-Cu-Ni and Ni-Cu-Cu.

The  $x=2$  composition crystallizes in the  $C2/c$  space group (N15) with the doubled unit cell along  $c$ -axis. The trimers were found to be of only one type Ni-Cu-Ni. Below  $T_N=20$  K a magnetic ordering with the propagation vector  $k=[1/2,1/2,0]$  has been found. The magnetic diffraction patterns are well described by the antiferromagnetic structure given by the irreducible representation 2 for both Ni (8f) and Cu (4b) sites. The exchange interactions within the trimers are dominated by Heisenberg-type nearest-neighbor interactions  $J_{Cu-Cu}=-4.92(6)$  meV,  $J_{Cu-Ni}=-0.85(10)$  meV and  $D_{Ni}=-0.7(1)$  for  $x=2$ .

Keywords: magnetic structure, symmetry analysis, quantum system

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**Temperature-dependent disordered structure of (BEDT-TTF)<sub>3</sub>Cl<sub>2</sub>.5H<sub>2</sub>O**

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Chlorine complexes of BEDT-TTF (bis(ethylenedithio) tetrathiafulvalene) crystallize as hydrates. Among them, (BEDT-TTF)<sub>3</sub>Cl<sub>2</sub>.5H<sub>2</sub>O was obtained by electro-crystallization in the presence of a small amount of water. It showed a rectifying effect of resistivity. Temperature dependence of the resistivity showed hysteresis around 250K. The dynamic behaviour of chlorine ions and water molecules would correlate with the physical property. X-ray diffractions indicated significant disorder. The averaged structure had space group  $C2/c$  with four BEDT-TTF molecules per asymmetric unit. Organic layers of BEDT-TTF and inorganic layers of hydrated chlorine ions exist alternatively along the  $c$  axis. The observed characteristics of the X-ray diffractions were: For even values of  $h$  and  $k$ , the diffractions of  $h+k=4n+2$ , which were scarcely observed at 300K and weakly observed at 100K, were almost continuous along  $c^*$ . For odd values of  $h$  and  $k$ , the diffractions of  $h \pm k=8n$  were strong and broadened along  $c^*$  at both 300K and 100K. The characteristics are explained by the stacking fault. The model of the disordered structure and its temperature dependence will be discussed.

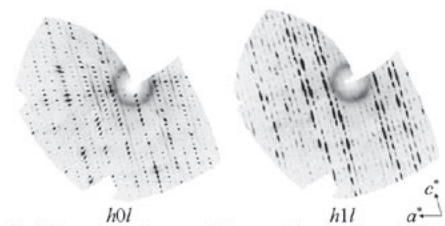


Fig.1 Precession images of observed intensities at 100 K

Keywords: chlorine complex of BEDT-TTF, hydrate, disordered structure

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**Observation of micrometric correlations in sliding incommensurate charge density waves**

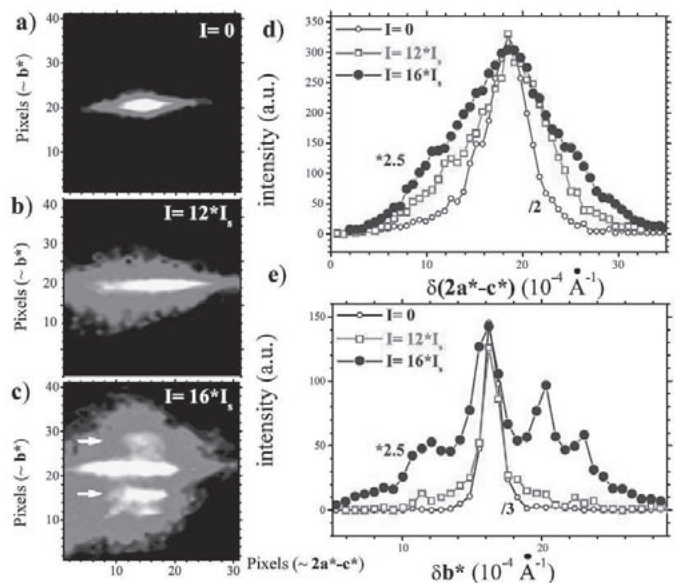
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We present a high resolution coherent diffraction experiment performed on the charge density wave (CDW) compound  $K_{0.3}MoO_3$ . The incommensurate satellite reflections associated with the CDW have been measured as a function of external direct currents. When the current exceeds a threshold value  $I_s$ , the CDW slides as a whole. In this sliding regime, the very high resolution allows one to evidence secondary satellite reflections flanking the CDW reflections. The relative position of the secondary satellite is found to depend on the non-ohmic current, and corresponds to a long range order extending up to micrometers. We discuss the origin of this novel type of incommensurate structure.

D. Le Bolloc'h et al., *Phys. Rev. Lett.* 100, 096403 (2008).



Keywords: incommensurate structures, charge density waves, high-resolution X-ray diffraction

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**Pair distribution function analysis of nanosized materials**

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The pair distribution function analysis method is a powerful tool for the study of glasses, liquids and amorphous materials, as well as crystalline or partly crystalline materials. Recently, this method has found many applications in the study of local structure in crystalline materials, yielding crucial information about atomic-scale structures of nanosized materials. As traditional crystallography breaks down on the nanoscale, we need tools such as PDF to elucidate the structures of nanostructured materials.

Keywords: pdf analysis, nanomaterials, powder x-ray diffraction