

[2] Y. Kubota, M. Takata, T. C. Kobayashi, S. Kitagawa, Coord. Chem. Rev., 251 (2007) 2510.

Keywords: mesoporous materials, adsorption, charge density

### P11.15.111

*Acta Cryst.* (2008). A64, C541

#### Nanoporous metal phosphates with photoluminescence property

Ya-Ching Yang, Sue-Lein Wang

National Tsing Hua University, Chemistry, 101, Section 2, Kuang-Fu Road, Hsinchu, Taiwan, 30013, Taiwan, E-mail: d927434@gmail.com

For the past two decades, research about metal silicate and phosphate with microporous structure has always played an important role in the field of materials chemistry due to their wide application potential from traditional catalyst, molecular sieve and ion exchange to recently developed low-k materials and zeolitic dye laser. In recent years, we have discovered several gallium phosphates containing transition metal with pore size around 1 nm and intriguing photoluminescence property. For example, 24-member ring NTHU-11 and the first organo-metallo phosphates NTHU-2,2 can emit blue light when excited with UV light. The photoluminescence phenomenon is a new property of nanoporous metal phosphate with emission mechanism apparently different from that of existing inorganic phosphor since the later is doped with metal activator or added with sensitizer in host lattice in order to illuminate. At present, the photoluminescence property of nanoporous metal phosphate is substantiated. Besides blue light, zinc gallophosphate that can emit yellow light or even white light have been synthesized. In this presentation, we are going to present a series of nanoporous gallophosphates and zinc gallophosphates via the synthetic strategy of employing the large 4,4'-trimethylenedipyridine (tmdp) amine as a template. Their structures will be described and photoluminescence property will be examined.

References

[1] Lin, C. H.; Wang, S. L.; Lii, K. H. *J. Am. Chem. Soc.* 2001, 123, 4649.

[2] Liao, Y. C.; Liao, F. L.; Chang, W. K.; Wang, S. L. *J. Am. Chem. Soc.* 2004, 126, 1320.

Keywords: metal phosphate, photoluminescence, nanoporous

### P11.16.112

*Acta Cryst.* (2008). A64, C541

#### Crystal growth, structure and physical properties of $Ln(\text{CuGa})_{13}$ compounds ( $Ln = \text{La-Nd, Eu}$ )

Jung Young Cho<sup>1</sup>, Cigdem Capan<sup>2</sup>, Amar B Karki<sup>2</sup>, D. P. Young<sup>2</sup>, Evan L. Thomas<sup>3</sup>, W. Wong-Ng<sup>3</sup>, Yusuke Nambu<sup>4</sup>, Satoru Nakatsuji<sup>4</sup>, Julia Y. Chan<sup>1</sup>

<sup>1</sup>Department of Chemistry, Chemistry, Louisiana State University, Baton Rouge, LA, 70803, USA, <sup>2</sup>Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA, USA, <sup>3</sup>Materials Science and Engineering Laboratory, National Institute of Standards and Technology, Gaithersburg, Maryland 20899, USA, <sup>4</sup>Institute for Solid State Physics, University of Tokyo, Kashiwa 277-8581, Japan, E-mail: jcho1@lsu.edu

Single crystals of  $Ln(\text{CuGa})_{13}$  ( $Ln = \text{La-Nd, Eu}$ ) compounds have been synthesized by flux-growth methods and characterized by single

crystal X-ray diffraction.  $Ln(\text{CuGa})_{13}$  ( $Ln = \text{La-Nd, Eu}$ ), which are isostructural to  $\text{NaZn}_{13}$ , crystallize in the cubic  $Fm-3c$  (No. 226) space group, with  $Z = 8$  and lattice parameters  $a \sim 11.8 \text{ \AA}$ . Magnetic susceptibility data show paramagnetic behavior down to 2 K for Ce, Pr, Nd, and Eu compound, respectively. Metallic behavior is observed below 300 K for each compound. A large positive magnetoresistance up to 154 % at 9 T is also observed for  $\text{Pr}(\text{CuGa})_{13}$ . The structure, magnetic, heat capacity and transport properties of these compounds will be presented and compared to  $Ln(\text{CuGa})_{12}$  ( $Ln = \text{Y, Gd-Er, Yb}$ ) family of compounds.

Keywords: magnetism, magnetoresistance, flux growth

### P11.16.113

*Acta Cryst.* (2008). A64, C541

#### Structure and magnetic properties of a iron(III) spin crossover complex

Ching-yi Wei<sup>1</sup>, Chou-fu Sheu<sup>1</sup>, Yi-hung Liu<sup>2</sup>, Yu Wang<sup>1</sup>

<sup>1</sup>National Taiwan University, Chemistry, No.1, Sec. 4, Roosevelt Road, Taipei, 101, 20348, Taiwan, <sup>2</sup>Instrumentation Center National Taiwan University, No.1, Sec. 4, Roosevelt Road, Taipei, Taiwan, E-mail: b90203043@ntu.edu.tw

New complex,  $[\text{Fe}(\text{3-OMe-salMen})_2]_2[\text{Ni}(\text{mnt})_2]\text{CH}_3\text{CN}$ , (3-OMe-salMen=2-([2-(methyl-amino)ethyl]imino)methyl)-3-methoxyphenol; mnt=maleonitriledithiolate) is synthesized and characterized. (at 298 K, triclinic  $P-1$ , cell parameters  $a = 9.402(2)$ ,  $b = 10.476(2)$ ,  $c = 16.636(3) \text{ \AA}$ ,  $\alpha = 87.17(3)$ ,  $\beta = 77.38(3)$  and  $\gamma = 75.21(3)^\circ$ ). The Fe (III) is an octahedrally coordinated ( $\text{N}_4\text{O}_2$ ) by two tridentate ligand. The bond lengths of Fe-N and Fe-O suggests the Fe(III) is in a low spin (LS) state configuration. From the thermally dependent magnetic measurements, the title complex is in the LS state ( $S=1/2$ ) at temperature range of 5~350K. As the temperature higher than 350 K, the compound becomes at HS state (high spin,  $S=5/2$ ) based on the magnetic data. According to the TGA, the spin transition may be due to the removal of the solvent molecule of  $\text{CH}_3\text{CN}$ . The non-solvated species then displays a gradual spin transition between HS and LS with  $T_{1/2}$  of 290K. When the non-solvated compound was treated with water vapor, the magnetic property of this hydrated sample appears to have different spin transition temperature at 122K. It is known that solvent molecules sometimes do play important roles in the spin transition; the title complex did show different spin transition behaviors in the presence of  $\text{CH}_3\text{CN}$  or of water as a solvent; the one with acetonitrile prefers in LS at room temperature, however the non-solvated one is in HS at room temperature. With the presence of water, a spin transition occurs at lower temperature. The process of removing and retaking solvent molecule is reversible by referring to powder pattern and magnetic measurements. The structure and magnetic relationship, especially in the presence or absence of solvent molecules, is currently under investigation.

Keywords: spin crossover, iron (III), reversible

### P11.16.114

*Acta Cryst.* (2008). A64, C541-542

#### The local structure & dielectric properties of the cubic pyrochlore $\text{Bi}_{1.67}\text{M}_{0.75}\text{Nb}_{1.5}\text{O}_7$ ( $\text{M}=\text{Mg}$ and $\text{Ni}$ )

Binh H Nguyen, Lasse Noren, Ray L Withers, Yun Liu

Australian National University, Research School of Chemistry, RSC, Building 35, Australian National University, Canberra, ACT, 0200,