

templating effects. The ccm ligand has also been shown to be conducive in the formation of transition metal and lanthanoid clusters which are of interest in the area of single molecule magnets.

1. Anthony S. R. Chesman, David R. Turner, David J. Price, Boujemaa Moubaraki, Keith S. Murray, Glen B. Deacon and Stuart R. Batten, *Chem. Commun.*, 2007, 3541-3543.

2. Anthony S. R. Chesman, David R. Turner, Ekaterina I. Izgorodina, Stuart R. Batten and Glen B. Deacon, *Dalton Trans.*, 2007, 1371-1373.

Keywords: lanthanide coordination, bimetallics, magnetic materials

### P09.03.33

*Acta Cryst.* (2008). A64, C484

#### Synthesis and characterization of mixed metal ( $\text{UO}_2^{2+}/\text{TM}^{2+}$ ) inorganic/organic framework materials

Karah E Knope<sup>1</sup>, Christopher L Cahill<sup>1,2</sup>

<sup>1</sup>The George Washington University, Chemistry, 725 21st Street, N.W., Washington, DC, 20052, USA, <sup>2</sup>Geophysical Laboratory, Carnegie Institution of Washington, Washington, DC, 20015, USA, E-mail : kknop@gwu.edu

Inorganic materials containing  $\text{UO}_2^{2+}$  comprise a structurally diverse catalog of compounds wherein layered architectures are most commonly observed. The dimensionality of these structures is typically governed by the terminal nature of the uranyl oxo atoms and the propensity for structure propagation to occur almost exclusively in two dimensions. As a result, three-dimensional structures are not only less frequently observed but also a challenge to obtain synthetically. Within purely inorganic systems, researchers have used templates or, alternatively, incorporated main group or transition metal cations to achieve higher dimensional frameworks. These strategies, in addition to flexible organic linkers, have also been applied to hybrid inorganic-organic systems. Presented here is a series of novel, three-dimensional, mixed metal uranium(VI)/transition metal(II) inorganic-organic hybrid materials. A representative example includes the framework structure of  $(\text{UO}_2)_2(\text{O}_3\text{PCH}_2\text{CO}_2)_2\text{Cu}(\text{H}_2\text{O})_3$ , monoclinic,  $P2_1/c$ ,  $a = 7.6358(3)$ ,  $b = 19.2962(3)$ ,  $c = 11.2401(8)$ ,  $\beta = 100.4990(10)$ . This compound exhibits coordination of copper through the nominally terminal uranyl oxygen atoms and illustrates how the addition of transition metal cations can influence the dimensionality, overall topology and luminescent behavior of hexavalent uranium containing architectures.

Keywords: framework structures, uranium(VI), hydrothermal synthesis

### P09.03.34

*Acta Cryst.* (2008). A64, C484

#### A nine-coordinated $\text{Zr}^{\text{IV}}$ complex obtained from a novel supramolecular proton transfer compound

Hossein Aghabozorg<sup>1</sup>, Mohammad Ghadermazi<sup>2</sup>, Shabnam Sheshmani<sup>3</sup>

<sup>1</sup>Tarbiat Moallem University, Chemistry, Faculty of Chemistry, Tarbiat Moallem University, 49 Mofateh Ave., 15614, Tehran, Iran, Tehran, Iran, 15614, Iran, <sup>2</sup>Department of Chemistry, Kurdistan University, Sanandaj, Iran, <sup>3</sup>Department of Chemistry, Islamic Azad University, Shahr-e Rey Branch, Tehran, Iran, E-mail: haghazorg@yahoo.com

In this research, a novel supramolecular proton transfer compound was synthesized from the reaction between pyridine-2,6-dicarboxylic acid,  $\text{C}_7\text{H}_5\text{NO}_4$ , and propane-1,3-diamine,  $\text{C}_3\text{H}_{10}\text{N}_2$ . According to the crystal structure, the resulting compound formulated as  $2(\text{C}_3\text{H}_{12}\text{N}_2)^{2+}(\text{C}_7\text{H}_3\text{NO}_4)^{2-}(\text{C}_7\text{H}_{4.5}\text{NO}_4)^{1.5-}(\text{C}_7\text{H}_{3.5}\text{NO}_4)^{0.5-}(\text{C}_7\text{H}_5\text{NO}_4) \cdot 5\text{H}_2\text{O}$ . This compound crystallizes in the triclinic system and contains two molecules per unit cell. The unit cell dimensions are  $a=7.8355(4)\text{\AA}$ ,  $b=13.5296(6)\text{\AA}$ ,  $c=20.8930(6)\text{\AA}$ ,  $\alpha=106.558(1)^\circ$ ,  $\beta=90.603(1)^\circ$ , and  $\gamma=106.662(1)^\circ$ . The final R value was 0.0427 for 9245 reflections. In anionic fragment, one of fourth hydrogen atoms of hydroxy groups is disordered. In cationic fragment, two carbon and nitrogen atoms, are disordered on two position with occupancies 0.88/0.12. Anion molecules form two independent hydrogen bonded zigzag-type chains. The hydrogen bonds as type  $\text{O}\cdots\text{H}$ ,  $\text{N}\cdots\text{O}$ , and  $\text{N}\cdots\text{N}$  play a role in the construction of supramolecular framework. Interactions between cationic and anionic fragments consist of ion-pairing, hydrogen bonds and  $\pi$ - $\pi$  stacking. The reaction of the proton transfer compound with  $\text{ZrCl}_4$  was carried out. This complex formulated as  $(\text{C}_3\text{H}_{12}\text{N}_2)[\text{Zr}(\text{C}_7\text{H}_3\text{NO}_4)_3] \cdot 4\text{H}_2\text{O}$ . The  $\text{Zr}^{\text{IV}}$  complex crystallizes in the space group  $P2_1/c$  of the monoclinic system with four molecules per unit cell. The unit cell dimensions are  $a=10.0246(6)\text{\AA}$ ,  $b=17.1883(10)\text{\AA}$ ,  $c=17.8643(10)\text{\AA}$ , and  $\beta=97.2970(10)^\circ$ . The metal ion is ninecoordinated by three pyridine-2,6-dicarboxylate as tridentate ligand. The  $\text{Zr}^{\text{IV}}$  atom is located in the center of a distorted tricapped trigonal prism arrangement. The crystal-packing diagram indicates the layered structure for this complex. This complex arises from ion pairing and the extensive hydrogen bonding.

Keywords: zirconium, supramolecular compounds, crystal structures

### P09.03.35

*Acta Cryst.* (2008). A64, C484-485

#### Binuclear Sn(VI) complex obtained from benzene-1,3-diaminium bis(hydrogen pyridine-2,6-carboxylate)

Jafar Attar Gharamaleki<sup>1</sup>, Shabnam Sheshmani<sup>2</sup>, Zahra Hasanpour<sup>3</sup>, Mohammad Ghadermazi<sup>4</sup>, Hossein Aghabozorg<sup>5</sup>, Guido Kickelbick<sup>6</sup>

<sup>1</sup>Tarbiat Moallem University, Chemistry, Faculty of Chemistry, Tarbiat Moallem University, 49 Mofateh Ave., 15614, Tehran, Iran, Tehran, Iran, 15614, Iran, <sup>2</sup>Department of Chemistry, Islamic Azad University, Shahr-e Rey Branch, Tehran, Iran, <sup>3</sup>Department of Chemistry, Islamic Azad University, Shahr-e Rey Branch, Tehran, Iran, <sup>4</sup>Department of Chemistry, Faculty of Science, Kurdistan University, Sanandaj, Iran, <sup>5</sup>Faculty of Chemistry, Tarbiat Moallem University, Tehran, Iran, <sup>6</sup>Institute of Materials Chemistry, Vienna University of Technology, Wien, Austria, E-mail: attar\_jafar@yahoo.com

In recent years, our research group have studied and worked on several bi- or trivalent metal complexes with several proton transfer ion pairs containing pyridine-2,6-dicarboxylic acid,  $\text{pydcH}_2$ . In resulting complexes, some fragments of ion pairs coordinate to metal ions and some other fragments act as counter ions in the structure. Here we wish to report the molecular structure of the Sn(VI) complex, which obtained from a novel proton transfer compound  $(\text{bdaH}_2)(\text{pydcH})_2 \cdot 2\text{H}_2\text{O}$ . The proton transfer compound  $(\text{bdaH}_2)(\text{pydcH})_2 \cdot 2\text{H}_2\text{O}$ , has been prepared from the reaction between benzene-1,3-diamine, bda, and pyridine-2,6-dicarboxylic acid,  $\text{pydcH}_2$ . The reaction of this adduct with  $\text{Sn}(\text{CH}_3)_2\text{Cl}_2$  gives complex with stoichiometry  $[\text{Sn}(\text{pydc})(\text{OC}_2\text{H}_5)(\text{CH}_3)_2(\mu\text{-O})_2]$ . This complex was characterized by IR, NMR spectroscopy and X-ray crystallography. This complex crystallizes in the monoclinic system, space group  $P2_1/c$ , with four molecules per unit cell. The unit cell dimensions are  $a=11.5924(14)\text{\AA}$ ,  $b=13.2674(17)\text{\AA}$ ,  $c=7.7566(10)\text{\AA}$