

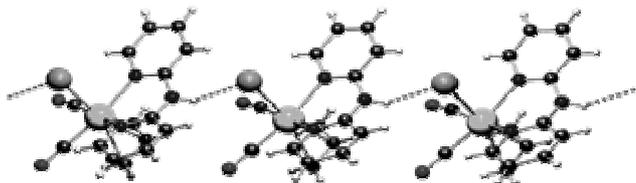
**P.09.04.8***Acta Cryst.* (2005). A61, C360**Polynuclear Core [Mn<sub>6</sub>(O)<sub>2</sub>Piv<sub>10</sub>] in the Molecular Magnets Design**Galina Romanenko, Elena Fursova, Kseniya Nosova, Victor Ovcharenko, *International Tomography Center SB RAS, Novosibirsk, Russia*. E-mail: romanenk@tomo.nsc.ru

Mixed-valence manganese clusters, in particular, polynuclear oxocarboxylate clusters of manganese, [Mn<sup>II</sup><sub>x</sub>Mn<sup>III(IV)</sup><sub>y</sub>O<sub>z</sub>], display a non-typical magnetic behavior - slow relaxation of magnetization at low temperatures. This led to the creation of a specific family of magnets, so-called single-molecule magnets. Single-molecule magnets are of particular interest because of these are magnetic domains of strict definite dimensions. Therefore, using multinuclear manganese compounds shows great promise in design of heterospin complexes. We synthesized a large group of such complexes based on [Mn<sub>6</sub>(O)<sub>2</sub>Piv<sub>10</sub>(Thf)<sub>4</sub>] core with 2-R-4,4,5,5-tetramethyl-4,5-dihydro-1*H*-imidazolyl-3-oxide-1-oxyl (NIT-R, R = H, Me, Et, *p*-Py, *n*-butylpyrazole). Both chain polymer [Mn<sub>6</sub>(O)<sub>2</sub>Piv<sub>10</sub>(Thf)<sub>2</sub>(NIT-Me)Mn<sub>6</sub>(O)<sub>2</sub>Piv<sub>10</sub>(Thf)(CH<sub>2</sub>Cl<sub>2</sub>)(NIT-Me)] and [Mn<sub>6</sub>(O)<sub>2</sub>Piv<sub>10</sub>(NIT-Me)<sub>2</sub>], possessing a diamondlike frame structure, and dumbbelllike [(EtOAc)<sub>3</sub>Mn<sub>6</sub>(O)<sub>2</sub>Piv<sub>10</sub>(NIT-Me)Mn<sub>6</sub>(O)<sub>2</sub>Piv<sub>10</sub>(EtOAc)<sub>3</sub>] molecules contain [Mn<sub>6</sub>(O)<sub>2</sub>Piv<sub>10</sub>] cluster fragments linked by NIT-Me bridging molecules. Among the latter a new molecular magnet [Mn<sub>6</sub>(O)<sub>2</sub>Piv<sub>10</sub>(Thf)<sub>2</sub>(NIT-Me)Mn<sub>6</sub>(O)<sub>2</sub>Piv<sub>10</sub>(Thf)(CH<sub>2</sub>Cl<sub>2</sub>)(NIT-Me)] with T<sub>c</sub>=3.5 K has been found [1]. It was shown that the formation of high dimensional crystal structure has the exacting requirements for structure complementary of [Mn<sub>6</sub>(O)<sub>2</sub>Piv<sub>10</sub>] and NIT-R, which can be realized only for R = CH<sub>3</sub>.

[1] Ovcharenko V., Fursova E., Romanenko G., Ikorskii V., *Inorg. Chem.*, 2004, **43**, 13332.**Keywords:** molecular magnets, radicals, clusters**P.09.04.9***Acta Cryst.* (2005). A61, C360**Crystal Structures of Mo(II) Complexes with 2,2'-Dipyridylamine**Susana Quintal<sup>a,b</sup>, Patrícia Pinto<sup>a</sup>, Vítor Félix<sup>c</sup>, Michael Drew<sup>d</sup>, Maria José Calhorda<sup>a,b</sup>, <sup>a</sup>CQB, Universidade de Lisboa, Portugal. <sup>b</sup>ITQB, Oeiras, Portugal. <sup>c</sup>Universidade de Aveiro, Portugal, <sup>d</sup>University of Reading, UK. E-mail: smquintal@fc.ul.pt

Organometallic complexes are interesting building blocks in the design and synthesis of functional solids. Derivatives of the conical fragment Mo(II)(η<sup>3</sup>-C<sub>3</sub>H<sub>5</sub>)(CO)<sub>2</sub> are useful precursors to build solids.

In this work, we describe the synthesis and characterization of new Mo(II) complexes with the 2,2'-dipyridylamine (dipa) ligand, [MoBr(η<sup>3</sup>-C<sub>3</sub>H<sub>5</sub>)(CO)<sub>2</sub>(dipa)] **1**, [MoBr(η<sup>3</sup>-C<sub>3</sub>H<sub>5</sub>)(CO)<sub>2</sub>(dipa)]<sub>2</sub>(4,4'-bipy)](PF<sub>6</sub>)<sub>2</sub> **2**, and [Mo(CH<sub>3</sub>CN)(η<sup>3</sup>-C<sub>3</sub>H<sub>5</sub>)(CO)<sub>2</sub>(dipa)]OTf **3**. The crystal structures of all compounds were determined by single crystal X-ray diffraction. The dipa ligand is always bonded to Mo(II) through the heterocyclic nitrogen atoms. The presence of the NH group in the dipa ligand may lead to intermolecular hydrogen bond interactions, as shown in the figure for complex **1**.

**Keywords:** molybdenum compounds, crystal structures, dipyridylamine**P.09.05.1***Acta Cryst.* (2005). A61, C360**Highly Symmetrical Hydrogen-bonded Networks**Marissa G. Haywood, Brendan F. Abrahams, Timothy A. Hudson, Richard Robson, *School of Chemistry, University of Melbourne, 3010, Victoria, Australia*. E-mail: m.haywood@pgrad.unimelb.edu.au

Metal/ligand covalent bonds and hydrogen bonds are the two major types of interactions that supramolecular chemists exploit to engineer both finite and infinite networks, for possible use in functional materials. The guanidinium cation, [C(NH<sub>2</sub>)<sub>3</sub>]<sup>+</sup>, has exerted powerful structure-determining effects on numerous coordination and hydrogen-bonding networks. The 3 pairs of hydrogen-bonds of the trigonal cation are positioned perfectly to interact with a variety of oxyanions to act as a 3-connecting node, in this case to create two new families of 3-dimensional hydrogen-bonding networks of cubic symmetry. One family are of the composition, XO<sub>4</sub>[C(NH<sub>2</sub>)<sub>3</sub>][Me<sub>4</sub>N], where X=S, Cr and Mo, and have the (10,3)-a net topology. The second family are of the composition [B(OMe)<sub>3</sub>]<sub>4</sub>[C(NH<sub>2</sub>)<sub>3</sub>]<sub>4</sub><sup>+</sup>X<sup>-</sup>.solvate, where X=Cl, PF<sub>6</sub>, NO<sub>3</sub>, BF<sub>4</sub>, Br, and I, and crystallise with the borocite topology. Single crystal X-ray studies have been conducted to characterise all compounds.

**Keywords:** crystal engineering, guanidinium cation, hydrogen-bonded networks**P.09.05.2***Acta Cryst.* (2005). A61, C360**Supramolecular Approach to Generation and Stabilization of Labile Organic Anions**Thomas C. W. Mak, Chi-Keung Lam, *Department of Chemistry, The Chinese University of Hong Kong, Shatin, New Territories, Hong Kong SAR, P. R. China*. E-mail: tcwmak@cuhk.edu.hk

Urea and its derivatives interact with various anions to generate hydrogen-bonded host lattices that may incorporate water or other uncharged hydrophilic molecules, forming crystalline inclusion compounds with bulky hydrophobic organic cations as the guest species.<sup>[1]</sup> Some elusive anions such as dihydrogen borate,<sup>[2]</sup> allophanate,<sup>[3]</sup> and 3-thioallophanate<sup>[4]</sup> have been generated *in situ* and stabilized as a host component. This strategy has led to successful isolation of the non-benzenoid aromatic D<sub>nh</sub> and enediolate C<sub>2v</sub> valence tautomers of rhodizonate C<sub>6</sub>O<sub>6</sub><sup>2-</sup> [5] and croconate C<sub>5</sub>O<sub>5</sub><sup>2-</sup>.<sup>[6]</sup>

Our recent studies in the supramolecular assembly of hydrogen-bonded infinite arrays based on preconceived cogwheel, rosette-tape,<sup>[7]</sup> and rosette-layer structural motifs will also be presented.

This work is supported by the Hong Kong Research Grants Council (Project Ref. No. CUHK 402003).

[1] Mak T.C.W., Li Q. in *Advances in Molecular Structure and Research*, (Eds.: M. Hargittai, I. Hargittai), JAI Press, Stamford, Connecticut, 1998, Vol. IV, pp. 151-225. [2] Li Q., Xue F., Mak T.C.W., *Inorg. Chem.* 1999, **38**, 4142. [3] Mak T. C.W., Yip W.H., Li Q., *J. Am. Chem. Soc.* 1995, **117**, 11995. [4] Lam C.-K., Chan T.-L., Mak T.C.W., *CrystEngComm.* **2004**, **6**, 290. [5] Lam C.-K., Mak T.C.W., *Angew. Chem. Int. Ed.* 2001, **40**, 3453. [6] Lam C.-K., Cheng M.-F., Li C.-L., Zhang J.-P., Chen X.-M., Li W.-K., Mak T.C.W., *Chem. Commun.* **2004**, 448. [7] Mak T.C.W., Xue F., *J. Am. Chem. Soc.* 2000, **122**, 9860.

**Keywords:** labile organic anions, supramolecular assemblies, urea inclusion compounds