MS13 P05

Synthesis, Structure and Magnetic Properties of New 1D and 2D Manganese Azido Complexes

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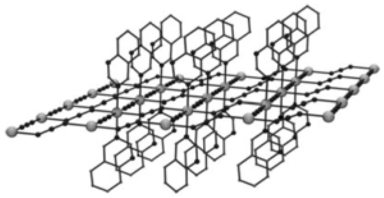
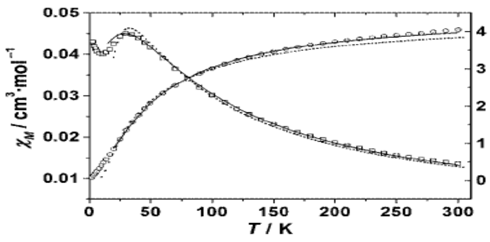
The use of azide ion as extremely versatile ligand in coordination chemistry is very interesting due to its ability to coordinate to transition metal atoms in different ways, for example as a terminal, or as a bridging ligand between metal atoms. Azide can bridge two paramagnetic centers either in an 'end-on' μ-(1, 1-N$_3$) fashion or an 'end-to-end' μ-(1, 3-N$_3$) fashion, depending on the steric and electronic requirements of the other co-ligands present in the complex. Generally, the μ-(1,3-N$_3$) azide bridge is known for its strong antiferromagnetic interaction while the μ-(1,1- N$_3$) connection mode shows a strong ferromagnetic interaction. Recently we have synthesized a number of new polymeric derivatives of the (azido) Mn^{II} system which have been structurally and magnetically characterized. The magnetic analysis for **1D**- $[Mn(H_2O)(\mu\text{-}N_3)(N_3)(quinaz)_2]_n$ (**1**), **2D**- $[Mn(\mu\text{-}N_3)_2(quinaz)_2]_n$ (**2**) and **1D**- $[Mn_2(3\text{-ampy})4(\mu\text{-}N_3)_2(N_3)_2(H_2O)_2]_n$, (**3**) (quinaz = quinazoline and 3-ampy = 3- aminopyridine) reveals moderate antiferromagnetic coupling, while the magnetic susceptibility measurements show weak ferromagnetic interactions for the **1D**- $[Mn(\mu\text{-}N_3)_2(pyzamid)_2]_n$ (**4**) (pyzamid = pyrazineamide). [1, 2]



$[Mn(\mu\text{-}N_3)_2(quinaz)_2]_n$ (**2**).

Antiferromagetic interaction in (**2**)



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MS13 P06

Synthesis, Structure and Supramolecular Architecture of Bis(Perfluoroaryl) Zinc(II) Adducts of Pyridines and Benzonitriles :Towards Directing Non-Centrosymmetric Assembly Without Recourse to Coordination Polymers

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Keywords: Zinc(II), Fourfold Embraces, Perfluoroaryl-aryl Interactions.

Two series of adducts between benzonitriles (L = C_6H_5CN, p-C_6H_5-C_6H_4CN, p-C_4H_4N-C_6H_4CN) or pyridines (L = C_5H_5N, p-$C_6H_5C_5H_4N$, p-C_4H_4N-C_5H_4N) and the highly Lewis acidic perfluoroaryl zinc compounds $(C_6F_5)_2Zn$ and $(p\text{-}C_6F_5C_6F_4)_2Zn$ have been prepared and structurally characterised. In all but one case the expected tetrahedral adduct was obtained exclusively. When L = p-C_4H_4N-C_6H_4CN a remarkable solvent dependence on the coordination geometry was observed; when crystallised from 1,2-difluorobenzene the expected tetrahedral geometry was formed, whilst from dichloromethane a three coordinate complex was obtained, apparently as a result of an intermolecular Zn-π interaction.

The supramolecular structures of the tetrahedral adducts present a number of surprises. Not least, the perfluoroaryl-aryl interaction, although present in a number of the lattices, does not predominate and the most significant supramolecular synthons appear to be fourfold aryl and biaryl embraces (Figure 1).

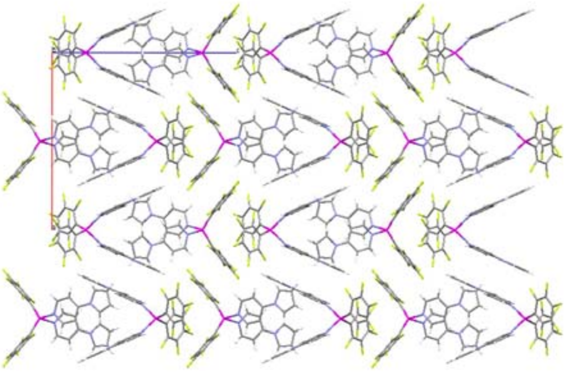

Figure 1. View of the packing of $(p\text{-}C_4H_4N\text{-}C_5H_4N)_2Zn(C_6F_5)_2$, illustrating the opposing columns.

We are currently exploring whether these columns are conserved in co-crystalline materials and whether manipulation of structures of this type can be used to engender non-centrosymmetric architectures.

MS13 P07

Isostructurality in trivalent metal tris(benzoylacetonates)

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Keywords: isostructurality, pseudopolymorphism, metal diketonates

Isostructurality is a similarity of the spatial arrangement of molecules off different compounds in their crystal structures. A prerequisite for isostructurality of two compounds is isometry of their molecules. This is best achieved for molecules which differ only in one or few core atoms, while the surface of the molecule remains mostly unchanged [1]. A very good example of such