conference abstracts

s9'.m1.p11 Polymeric Cu(II)-Complexes with 1,4,5,8,9,12-Hexaazatriphenylene(HAT) as Bridging Ligand H. Grove and J. Sletten, *Department of Chemistry, University of Bergen, N-5007 Bergen, Norway*
Keywords: molecular solids.

X-ray crystallographic structure determinations of hat-bridged Cu(II) complexes have been performed. $[Cu_4(hat)_2Cl_8]\cdot6H_2O$ (**1**), $[Cu(hat)(H_2O)_2](NO_3)_2$ (**2**) and $[Cu_2(hat)(H_2O)_6](SO_4)_2]\cdot2H_2O$ (**3**). Crystal data; **1**: P-1, a = 6.7729(3) Å, b = 11.7016(5) Å, c =11.7080(5) Å, α = 85.725(2)º, β = 78.736(2) º, γ = 78.559(1)º, **2**: $P2_1/n$, a = 9.3161(3) Å, b= 15.9239(4) Å, c = 10.1922(3) Å, β = 91.854(1)°, **3**: $Pca2_1$, a = 13.5778(4) Å, b = 9.4149(1) Å, c = 17.8842(4) Å.

In **1** tetranuclear entities with a central dichloro-bridge between copper atoms and two outer hat-bridges (Cu-hat-Cu-Cl_2-Cu-hat-Cu units) are found. These units are linked into sheets through weak axial Cu···Cl bonds between the outer copper atoms and chlorine atoms of neighbour units. The central copper atoms have square pyramidal coordination geometries, while the outer ones are elongated octahedral. The hat ligands coordinate in the equatorial planes of both copper atoms, while the bridging chlorine atoms coordinate in equatorial position on one side and in axial position on the other side.

In **2** bis-bidentate hat bridges copper atoms forming a zig-zag shaped chain with hat on one side chelating to copper (Cu having elongated octahedral surroundings) at one equatorial and one axial position, and on the other side at two equatorial positions. Water molecules are in the remaining axial and equatorial position.

In **3** hat coordinates in the tris-bidentate mode. One of the symmetry independent copper atoms participates in the chain formation, coordinating to two hat molecules, while the other copper atom is externally bound to only one hat. Water molecules completes the elongated octahedral coordination spheres in both cases.

Temperature dependent magnetic susceptibility measurements will be performed to study the propagation of magnetic interaction through the hat-ligand.

s9'.m1.p12 Oxalato-bridged Dimer **[Fe₂oxF₄(DMSO)₄]** and Double-Chain (imidH)₂[Fe₂oxF₆]: Structures and Magnetism. W. Massa, R. Leo, J. Pebler, *Department of Chemistry, Philipps-University, D-35032 Marburg, Germany.*
Keywords: oxalato-fluoro-ferrate(III), iron(III) double-chain, magnetism.

The crystal structure of a new Fe(III) dimer obtained by fluorination of $FeCl_3$ with Me_3SnF in the presence of oxalic acid and crystallization from DMSO (dimethyl sulfoxide) has been determined on a 4-circle diffracto-meter: **[Fe₂oxF₄(DMSO)₄] 1**, Space group $P2_1/n$, Z=2, a = 7.259(2), b = 11.409(3), c = 13.374(2) Å, β = 97.26(1)°, R = 4.47%. It shows a tetradentate bridging oxalato anion, equatorial *cis* fluorine and axial *trans* DMSO ligands.

From an aqueous solution of $FeF_3\cdot3H_2O$, oxalic acid, and imidazolium fluoride, crystals of **(imidH)₂[Fe₂oxF₆] 2** could be precipitated. Space group Pban, Z = 2, a = 9.143(2), b = 20.837(6), c = 3.890(1) Å, R = 2.51%. The structure shows anionic chains formed by bridging *trans* fluorine ligands connected, like in the dimer above, by oxalate anions to a double chain. The bridge angle at F is 173.7°. The double chains are connected by H - bonds N-H···F (N···F 2.70 Å) to form layers parallel (010). The terminal Fe–F distances are extremely short (1.851(2) Å), the bridging bond lengths Fe–F are 1.948(1) Å.

1   **2**
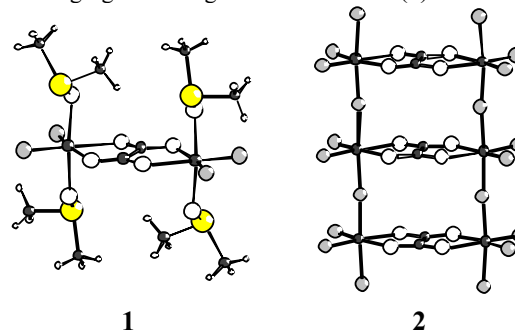
The magnetic properties of both compounds have been studied using a SQUID magnetometer down to T = 1.8 K. **1** shows the typical behaviour of an antiferromagne-tic dimer, a fit based on the Heisenberg model (S = 5/2, L = 0) yielded an exchange energy of J/k = -3.5 K, similar to that in the double fluorine-bridged complex anion $[Fe_2F_8(H_2O)_2]^{2-}$ (J/k = -3.2 K) [1].

The double chain structure **2** (spin ladder) revealed a complex magnetic behaviour including a strong 1D exchange energy along the chain (J_1/k = -17.3(3) K), a weaker second exchange energy over the oxalato bridges ($|J_2/k|$ = 0.6(1) K) and a third very weak inter-chain exchange coupling with $|J_3/k|$ = 0.04(1) K leading to 3D ordering at a Néel temperature of 14.5(3) K. An anisotropy constant of D_x/k= +0.15(1) K was estimated. The dynamic properties in the regime of 1D behaviour are interpreted based on Mössbauer spin-relaxation spectra.[2].

[1] J.Pebler et al., to be published
[2] J.Pebler, C.Frommen, M.Mangold, W.Treutmann, Z.Naturforsch. 54a, 317 (1999)