

In I-III and secondary glyoxylamides in the CSD the amide resonance makes the average  $\alpha$  C=O longer than the  $\beta$  C=O, but by  $<0.01$  Å, suggesting fairly similar abilities as hydrogen bond acceptors. From a secondary indol-2-ylglyoxylamide structure Black et al. [1] inferred that a set of 3 hydrogen-bonded rings, S(5) from amide H to  $\beta$ -O,  $R_2^2(10)$  involving the same atoms intermolecularly, and S(6) from indole NH to  $\alpha$ -O could be a robust supramolecular synthon. In a series of indol-3-yl analogues we find that the S(5) persists, and the S(6) replaces the indole NH with the adjacent CH as donor but remains fairly strong. However, C(4) chains linking amide H to  $\alpha$ -O occur as often as the  $R_2^2(10)$  motif.

[1] Black, D.St.C., Craig, D.C., McConnell, D.B., *J. Am. Chem. Soc.*, 1996, 118, 8148.

#### MS19 P06

**Reaction of 1,3,5-triazacyclohexane with copper : formation of other complex** Saida Latreche<sup>a\*</sup>, Ahcène Bouchemma<sup>b</sup>, Abdelhamid Mousser<sup>a</sup>, Randolph D.Köhn<sup>c</sup>, Gabriel K Köhn<sup>c</sup>. <sup>a</sup>*Département de Chimie, Centre Universitaire Larbi Tebessi Tebessa, Algérie.* <sup>b</sup>*Laboratoire de Chimie Appliquée et Technologie des Matériaux, Centre Universitaire Larbi Ben M'hidi, Oum El Bouaghi.* <sup>c</sup>*Department of Chemistry, University of Bath, Bath, BA2 7AY, UK.* E-mail:latrechesouad@yahoo.fr

**Keywords:** Triazacyclohexane , copper complexes , X-ray.

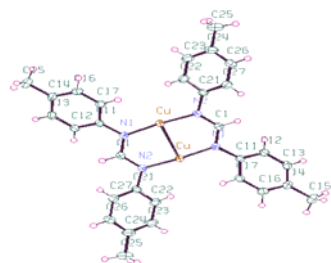
Copper complexes with three facially coordinating nitrogen atoms play an important role in the biological binding and activation of dioxygen<sup>[1]</sup>. They are used, for example, as bioinorganic model systems, reagents with high metal ion selectivity or as olefin polymerisation catalysts.

Many complexes containing triazacyclohexane and larger macrocyclic amines are known<sup>[2,3]</sup>.

The title complex 1,3,5-(4-methylphenyl)-1,3,5-triazacyclohexane **1** is prepared by reaction of formaldehyde with primary amine (4-methyl aniline)<sup>[4]</sup>. The complexation of 1,3,5-(4-methylphenyl)-1,3,5-triazacyclohexane **1** give a bimetallic complex in which the ligand is fragmented ( Fig 1).

As the coordination number of these copper complexes is two short bonds between (1.879 and 1.881Å).

The Para magnetism of this complex made it difficult to get useful H-or C-NMR. The ligand and complex were characterized by X-ray crystallography.



**Figure 1:** X- ray structure of (p-tol)NCHNH(p-tol)

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[2] P.Chaudhuri, K. Wieghard, *Prog. Inorg. Chem.* 1987, 35, 329.

[3] R.D.Kohn, P.Kampe, G.K.Kohn. *Eur. J. Inorg.Chem.* 2005, 3217-3223.

[4] A. Bouchemma, P.H.McCabe, G.A. Sim. *Acta Cryst.* 1990. C46, 674-676.

#### MS19 P07

**The Structural Class Concept, an Extension** Ake Oskarsson, *Department of Chemistry, Lund University, P.O. Box 124, SE-221 00 Lund, Sweden.* E-mail: [ake.oskarsson@inorg.lu.se](mailto:ake.oskarsson@inorg.lu.se)

**Keywords:** structural-class, symmetry , packing

Novacki [1] was the first to study space group frequencies at a time when the space groups were only known for about 3000 crystal structures. Since then a number of studies has appeared. An important improvement in this field was introduced by Belsky et al. [2,3] with the structural class concept, which beside the space group also includes the Z value and the distribution of molecules over equivalent positions. Implicit in this notation is also unoccupied special positions, which is of importance in discussing crystal packing, since every unoccupied position is a waste of space [4]. Therefore it is suggested that these positions should be added to the structural class notation in the following way: a semicolon shows the end of the structural class and then the unoccupied special positions are given within brackets. No unoccupied special positions are denoted ;[0]. An obvious notation would be  $P2_1/c, Z=2(-1);[(-1^3)]$  and  $P2_1/c, Z=4(1);[(-1^4)]$  etc. This notation will thus explicit give an overview of all Wyckoff positions, occupied or not, and will be helpfull in addressing questions like *i)* which molecular symmetries are retained and avoided in the solid state and *ii)* which Wyckoff positions are unoccupied. A few examples regarding complexes *cis/trans*-PtX<sub>2</sub>L<sub>2</sub> and *cis/trans*-PtX<sub>4</sub>L<sub>2</sub>, where X=halogen and L=neutral ligand, will be discussed.

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[4] Brock, C.P., Dunitz, J.D. *Chem. Mater.* 1994, 6, 1118.

#### MS19 P08

**Unusual tin(II)-iron complexes (RO)<sub>2</sub>Sn-Fe(CO)<sub>4</sub> and {[Li]((RO)<sub>3</sub>Sn-Fe(CO)<sub>4</sub>)}<sub>2</sub> (R = CH<sub>2</sub>CH<sub>2</sub>NMe<sub>2</sub>)** Victor N. Khrustalev, *A.N.Nesmeyanov Institute of Organoelement Compounds RAS, Moscow, Russia* E-mail: [vkx@xray.ineos.ac.ru](mailto:vkx@xray.ineos.ac.ru)

**Keywords:** tin(II), transition-metal complexes, X-ray diffraction analysis

Two new tin(II)-iron complexes (RO)<sub>2</sub>Sn-Fe(CO)<sub>4</sub> (**3**) and {[Li]((RO)<sub>3</sub>Sn-Fe(CO)<sub>4</sub>)}<sub>2</sub> (**4**) (R = CH<sub>2</sub>CH<sub>2</sub>NMe<sub>2</sub>) have been structurally characterized. Unusual types of heteronuclear bonding between heavier Group 14 elements and transition metals have been revealed. The iron atoms both in **3** and **4** have a trigonal-bipyramidal coordination typical for FeL<sub>5</sub>-fragments. The “stannylene” ligand in **3** occupies the equatorial position, whereas the stannate ligand in **4** is axially disposed. The structures of **3** and **4** indicate that the monomeric tin(II) compound (RO)<sub>2</sub>Sn (**1**) [1] is a better  $\pi$ -acceptor than a  $\sigma$ -donor toward iron [2] and thus displays the stannylene-like properties, while the