

bonds in the crystal structure but crystal packing is stabilized by eight C-H $\cdots\pi$  and four  $\pi\cdots\pi$  interactions. Some of the C-H $\cdots\pi$  interactions are with the H $\cdots$ Cg distance shorter than 2.70Å (Cg is the centroid of five- or six-membered ring with delocalized  $\pi$  bonds). Two of the C-H $\cdots\pi$  interactions are intramolecular and play a very significant role in the orientation of phenyl rings and -OCH<sub>2</sub>CH<sub>3</sub> fragments.

**Keywords:** C-H $\cdots\pi$  interaction, Ni(II) complex, thiosemicarbazide

#### P.07.01.10

*Acta Cryst.* (2005). A61, C297

#### Isolation and Characterization of a Ferromagnetic Gadolinium(III) Citrate Chain

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Novel lanthanide citrate chains have been hydrothermally synthesized from Ln<sub>2</sub>O<sub>3</sub> (Ln = Gd, Nd) and citric acid at pH = 2 and 120 °C. Their structure, crystal packing, network topology, hydrogen bonds, metal ligand interactions, TG and DTA measurements and magnetic susceptibility properties are examined. Two new isostructural compounds are described in detail: [Ln(Hcit)(H<sub>2</sub>O)<sub>2</sub>.H<sub>2</sub>O]<sub>n</sub> (Ln: Gd (1), Nd (2), Hcit = C(OH)(COO-)(CH<sub>2</sub>COO)<sub>2</sub>). They are monoclinic, P2<sub>1</sub>/n, and crystallize as linear polymers. The multidentate citrate anion coordinates through six out of its seven oxygen atoms, five of them acting as simple donors and the remaining one in a bridging mode. Two aqua molecules complete a LnO<sub>9</sub> coordination environment. Each citrate links to 3 lanthanide metal centers leading to the formation of "ladder like" chains parallel to [100] where the steps are defined by the Ln-O-Ln bridges (Ln...Ln: 4.321(4)/4.389(2)Å, for Gd/Nd respectively), connected to each other by longer citrate-based "linkers" (Ln...Ln : 6.145(4)/6.230(2)Å).

The inter-linkage of chains is achieved through H-bonding to which the three water molecules provide five donor hydrogens.

Magnetic susceptibility measurements in (1) show that ferromagnetic interactions are operative between the Gd(III) centers below 10 K.

**Keywords:** lanthanides, structures, ferromagnetism

#### P.07.01.11

*Acta Cryst.* (2005). A61, C297

#### Novel Water-soluble Peroxo Complexes of Nb(V) and Ta(V)

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In recent years, multimetallic Nb-based oxides have generated considerable interest in many fields: these oxides are mainly described as ferroelectrics, ion conductors and oxidation catalysts. In the frame of research aimed at developing new synthetic procedures of these Nb-containing oxides, water-soluble peroxo complexes of niobium(V) and tantalum(V) have been prepared and investigated spectroscopically and structurally.

The compounds studied are of two types: peroxo-carboxylato and peroxo-polyaminocarboxylato (PAC) complexes, the latter ones will be described. The peroxo-PAC complexes were synthesized in the presence excess hydrogen peroxide. These conditions led to the oxidation *in situ* of the nitrogen atoms of the ligands into N-oxides. Two PAC ligands were selected: ethylenediaminetetraacetic acid (H<sub>4</sub>edta) and propylenediaminetetraacetic acid (H<sub>4</sub>pdta).

The crystal structures of the guanidinium derivatives of the (edta)- and (pdta) Nb and also of the (edta)-Ta complexes have been determined at 100K. In all the three compounds, the metal exhibits an eightfold coordination by two bidentate peroxo ligands and a tetradentate bis(N-oxido) PAC ligand resulting in a distorted dodecahedral geometry. The coordination Nb-O and Ta-O bond

lengths are very similar.

**Keywords:** niobium complexes, peroxo compounds, polyaminocarboxylate acids

#### P.07.01.12

*Acta Cryst.* (2005). A61, C297

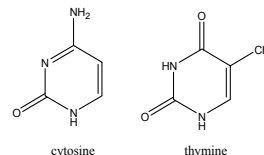
#### Studies in the Structural Chemistry of Complexes between Nucleobases and s-Block Metals

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In the past years, it has been found that interaction of biomolecules with metal ions are of interest in studies of biological functions of metal ions, especially alkali and alkaline earth metals, because they have abundant distribution in the human body. In addition it is known that s-block metal ions interact with the negatively charged phosphate group of nucleic acids and thus stabilise the DNA and RNA structures.

The study of the structural chemistry of nucleobases with transition metals is well known and many complexes have been synthesized and characterised. By contrast, the literature does not show many structures containing nucleobases and s-block metals and only little information is provided on the subject [1].

To rectify this imbalance, part of our research concentrates on the synthesis and crystallographic characterisation of complexes of the five nucleobases (cytosine and thymine for example) with the Group I metal ions lithium, sodium, potassium, rubidium and caesium. We will present some examples of these new complexes and discuss the structural features observed in each case (coordination, hydrogen bonding etc.).



[1] Lippert B., *Coordination Chemistry Reviews*, 2000, **200-202**, 487-516.

**Keywords:** nucleobases, s-block metals, coordination

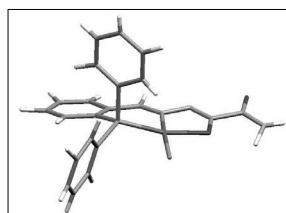
#### P.07.01.13

*Acta Cryst.* (2005). A61, C297

#### Structure of Pd(II) Complex with a 2-(diphenylphosphino)benzaldehyde Derivative

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A Pd(II) complex with 2-{{(2E)-2-[2-(diphenylphosphino)benzylidene]hydrazino}-2-oxoacetamide was obtained from K<sub>2</sub>[PdCl<sub>4</sub>] and the ligand in ethanol.



The complex crystallizes in the monoclinic P2<sub>1</sub>/n space group. The chelate ligand is monodeprotonated at the hydrazonic nitrogen, and behaves as a PNO tridentate, generating a six-membered and a five-membered ring upon coordination. A chloride atom completes the square planar coordination geometry, which is slightly distorted, with the P atom deviating from the N, O, Pd, Cl best plane, due to the puckering of the six-membered chelation ring. Despite the presence of several hydrogen bond donors and acceptors on the complex molecule, the only evident directional interaction in the crystal packing is a very weak intermolecular contact N-H...N (N...N=3.405(6)Å, N-H...N=150(6)°).

**Keywords:** Pd(II) complex, hydrazone, PNO tridentate