s13.m38.p9 Facile Oxidation of Metal Cations by Complexation with an Easy-to-prepare Ligand. Gaël Labat, Gilles Gasser, Antonia Neels, Helen Stoeckli-Evans, Institute of Chemistry, University of Neuchâtel, Switzerland. E-mail: gael.labat@unine.ch

## Keywords: N,O-ligand; Oxidation; Powder-diffraction

A new ligand, pyridine-2-carboxylic acid (3-hydroxy-pyridine-2-carbonyl)-amide, has been synthesized by a one-step reaction and in a quantitative manner. Complexations with different transition metal cations gave very interesting results [1]. For example, oxidations of the metal cations were observed with Fe(II) and Co(III) to give respectively, Fe(III) and Co(III) complexes. It was possible to form 2 polymorphs of the Fe(III) complex via 2 different synthetic methods.

Comparisons of our single crystal (fig.1) and powder X-Ray diffraction structure solutions with the structures of the complexes formed with the similar ligand, bis(2-pyridylcarbonyl)amine[2,3], will be discussed.

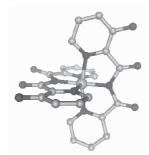


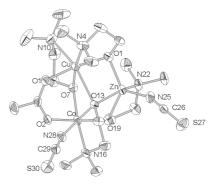
Fig. 1: Structure of the Co(III) complex

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S13.m38.p10 Novel Heterotrimetallic Cu<sup>II</sup>/Co<sup>III</sup>/Zn<sup>II</sup>
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## Keywords: Direct synthesis; Heterotrimetallic complex; Crystal structure

Heterotrimetallic complexes is a novel class of heteronuclear systems that may offer potential applications as new materials that exhibit exciting physical and magnetic properties. Despite the impressive progress in the preparation of mixed-metal complexes the field of heterotrimetallic compounds remains largely unexplored. The reaction of zerovalent copper, zinc oxide, cobalt(II) acetate and 2-(dimethylamino)ethanol (HMe<sub>2</sub>Ea) in the presence of ammoniun thiocyanate in air yielded the novel heterotrimetallic compound [CuCoZn(Me<sub>2</sub>Ea)<sub>4</sub>(NCS)<sub>2</sub>(CH<sub>3</sub>COO)] that has been characterized by a range of spectroscopic methods and structurally. The complex features a trinuclear unit with an incomplete cube-like core CuZnCoO<sub>4</sub> (Fig).



The coordination environmental of the cobalt atom is completed by four O atoms (average 1.907 Å) and two N atoms (av. 1.947 Å) of three Me<sub>2</sub>Ea, NCS- and acetate groups in a distorted octahedral geometry. The copper atom adopts a distorted octahedral coordinational sphere with a {CuN<sub>2</sub>O<sub>4</sub>} chromophore. The four copper-O(N) bonds in the equatorial plane vary between 1.946(9) and 2.063(11) Å, the axial bonds are elongated (av. 2.409 Å). The zinc atom forms three quite short bonds with N and O atoms, O(1), O(19), N(25), and a longer bonding distance to O(13) and N(22), making a distored trigonal bipyramidal geometry. The amino alkoxo- and acetate-bridges between metal centres result in the copper-cobalt, copper-zinc and cobalt-zinc separations of 3.054(9), 3.023(3) and 2.975(3) Å, respectively. The trinuclear units show no significant intermolecular contacts in the solid state.  $C_{20}H_{43}CoCuN_6O_6S_2Zn$ , M = 715.56, monoclinic, a =11.247(6) Å, b = 11.185(4) Å, c = 25.641(13) Å,  $\beta = 100.18(3)^{\circ}$ ,  $U = 3175(3) \text{ Å}^3$ , T = 173(2) K, P = 23.071(15)/1, P = 103.15(5),  $U = 3175(3) \text{ Å}^3$ , T = 173(2) K, P = 1.54178mm<sup>-1</sup>, 6763 reflection measured, 6428 unique, 2689 observed (I  $> 2\sigma(I)$ , R = 0.0861. This work was supported in part by INTAS Grant 03-51-4532.