

Cell parameters using Nonius Kappa CCD at 173 K (Å and °) are: (I) 14.071(2), 14.071(2), 39.993(4), 90.0, 90.0 and 90.0; (II) 21.114(4), 4.972(1), 25.710(4), 90.0, 94.27(3) and 90.0; (III) 10.708(3), 19.143(3), 29.027(4), 90.0, 94.70(3) and 90.0; (IV) 10.937(2), 27.320(5), 15.120(3), 90.0, 105.23(3) and 90.0.

Slightly distorted coordination spheres are tetrahedral in four-coordinated compounds (I) and (II) and octahedral in six-coordinated compounds (III) and (IV). Bond distances (Å) within the coordination spheres for Co-O vary from 1.927(3) to 1.947(3) in (I), from 1.889(3) to 1.906(3) in (II), 1.897(2) in (III) and from 1.878(2) to 1.901(2) in (IV) and for Co-N from 1.940(4) to 2.019(4) in (I), from 1.982(4) to 1.984(4) in (II), from 1.962(2) to 1.994(2) in (III) and from 1.947(2) to 1.963(2) in (IV). The values are comparable to those found in some similar compounds [1-3].

Salicylaldehydes can be prepared from salicylaldehyde and respective aliphatic or aromatic amines heating overnight.

[1] De, R.L., Samanta, K., Maiti, K., Keller, E., *Inorg. Chim. Acta*, 2001, 316, 113.

[2] Iyere, P., Boadi, W., Ross, L., *Acta Cryst. E*, 2004, E60, m304.

[3] Li, X., Huang, L., Dong, S., Li, M., Sun, H., *Acta Cryst. E*, 2005, E61, o465.

MS16 P06

Organic-Donor Inorganic-Acceptor Salts:

$[(TTF)_6(XMO_{12}O_{40})(Et_4N)]$, X=Si and P.

A. M'hanni*, L. Ouahab**, * Laboratoire de Thermodynamique et Modélisation Moléculaire, USTHB, Faculté de Chimie, BP : 32 El-Alia, Bab -Ezzouar, Alger 16111, Algérie. Email: mhannia@yahoo.fr ** Laboratoire de Chimie du Solide et Inorganique Moléculaire URA 254 CNRS, Université de Rennes I, F35042 Rennes

Key words: Donor Acceptor compound, Magnetism, Crystallography

The preparation, X-ray crystal structure, optical and magnetic properties of two Organic-Donor Inorganic-Acceptor (ODIA) salts: $[(TTF)_6(XMO_{12}O_{40})(Et_4N)]$, X= Si (1) and P(2) are presented.

The two materials are isostructural. Their X-ray crystal structures are characterized by 1-D TTF chains lying inside the channels formed by the inorganic anions and isolated TTF molecules. Magnetic experiments for both salts are compared: they are different and suggest, in particular, the presence of one non-interacting electron in 2, in contrast with the diamagnetic behaviour of 1. The optical absorption measurements of the two compounds are essentially identical. They show the presence of both intense charge transfer bands around 4800 cm⁻¹ and vibronic modes in the middle IR range (1300-1400 cm⁻¹), characteristic of mixed valence salts.

MS16 P07

Crystal structure and magnetic properties of mononuclear Co(II) and Ni(II) complexes

B. Papánková^a, I. Svoboda^b, R. Boča^a, H. Fuess^b ^aInstitute of Inorganic Chemistry, Technology and Materials, Slovak Technical University, SK-812 37 Bratislava, Slovakia.

^bInstitut für Materials Science, Darmstadt University of Technology, D - 64289 Darmstadt, Germany.

E-mail: blazena.papankova@stuba.sk

Keywords: Metal complexes-1, Magnetism-2, ZFS - 3

There has recently been great interest in the study of the properties of molecular magnets. In the last two decades many molecular magnetic compounds have been synthesized [1]. Our interest is an investigation of interesting coordinating properties of Co(II) and Ni(II) with N - donor base and carboxylate ligand. The heteroleptic complexes with the $\{MeN_2O_2O_2\}$ [2, 3], $\{MeN_4O_2\}$ [4, 5], $\{MeN_6\}$ [6] chromophore, where M = Ni and Co have been prepared, structurally characterized and subjected to magnetochemical investigation down to 2 K (susceptibility and magnetization measurement). They show magnetic behavior typical for zero-field splitting (ZFS) systems. The axial parameter of the ZFS, *D*, adopts either positive or negative values and correlates with axial distortion of the coordination polyhedra.

[1] Sato O., Tao J., Zhang Y-Z., *Angew.Chem.Int.Ed.*, 2007, 46, 2152.

[2] Ivaníková R., Boča R., Dlháň L., Fuess H., Mašlejová A., Mrázová V., Svoboda I., Titiš J., *Polyhedron* 2006, 25 3261.

[3] Papánková B., Svoboda I., Fuess H., *Acta Cryst.E62*, 2006, m1916.

[4] Boča R., Dlháň L., Haase W., Herchel R., Mašlejová A., Papánková B., *Chem. Phys. Lett.* 2003, 373, 402.

[5] Papánková B., Svoboda I., Fuess H., Šintálová K., *Acta Cryst.E61*, 2005, m2036.

[6] Mašlejová A., Ivaníková R., Svoboda I., Papánková B., Dlháň L., Mikloš D., Fuess H., Boča R., *Polyhedron*, 2006, 25, 1823.

MS16 P08

Triphenylguanidinium benzoate: Crystal structure and

DFT calculations P. S. Pereira da Silva^a, M. Ramos Silva^b, C. Cardoso^c, S. R. Domingos^b, J. A. Paixão^b, A.

Matos Beja,^a *Escola Superior Agrária, Instituto Politécnico de Castelo Branco, Quinta da Senhora de Mércules, Apartado 119, 6001-909 Castelo Branco, Portugal* ^bCEMDRX, Physics Department, University of Coimbra, 3004-516 Coimbra, Portugal ^cCFC, Physics Department, University of Coimbra, 3004-516 Coimbra, Portugal. E-mail: manuela@pollux.fis.uc.pt

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Triphenylguanidine (TPG) is an octupolar molecule. Such molecules are particularly interesting from the point of view of nonlinear optics. Their null dipole moment does not stand as a drawback for its crystallization and still allows the crystal to present large third order susceptibilities if some symmetry requirements are fulfilled. A non-centrosymmetric crystal was obtained mixing an ethanolic solution of benzoic acid with TPG. In the resulting salt, the anions and cations are linked in chains via hydrogen bonds. Although none of the molecules is chiral, the propeller like arrangement of the phenyl rings of TPG⁺ promotes such chiral crystallization (space group Cc). In the cation, the dihedral angles between the phenyl rings and the plane defined by the central guanidinium fragment are very similar, in the range 57.73(13)-59.94(14)°. The corresponding angles for other TPG⁺ salts reported in the literature are within the range 32.6(3)-70.2(3)° [1-5], a variability that attests the