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

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MS16 P06

Organic-Donor Inorganic-Acceptor Sats: $[(TTF)_6(XMo_{12}O_{40})(Et_4N)]$, X=Si and P.

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Key words: Donor Acceptor compound, Magnetism, Crystallography

The preparation, X-ray crystal structure, optical and magnetic properties of two Organic-Donor Inorganic-Accepter (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] [a]*Institute of Inorganic Chemistry, Technology and Materials, Slovak Technical University, SK-812 37 Bratislava, Slovakia.* [b]*Institut for Materials Science, Darmstadt University of Technology, D - 64289 Darmstadt, Germany*.
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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.

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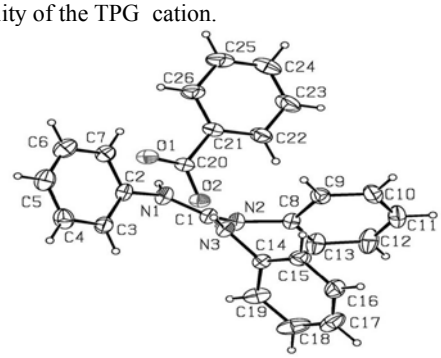
MS16 P08

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[b,a] *Escola Superior Agrária, Instituto Politécnico de Castelo Branco, Quinta da Senhora de Mércules, Apartado 119, 6001-909 Castelo Branco, Portugal* [b]*CEMDRX, Physics Department, University of Coimbra, 3004-516 Coimbra, Portugal* [c]*CFC, Physics Department, University of Coimbra, 3004-516 Coimbra, Portugal.* E-mail: manuela@pollux.fis.uc.pt

Keywords; DFT calculations, optical activity, structure determination

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-centrossymmetric crystal was obtained mixing a 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)º. The corresponding angles for other TPG^+ salts reported in the literature are within the range 32.6(3)-70.2(3)º [1-5], a variability that attests the

flexibility of the TPG^{+} cation.



We also performed density functional theory calculations within the local density approximation using the code Abinit [6].

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MS16 P09

Crystallographic and conformational analyses of (*E*) 2-[(4iodophenylimino)metyhl]-5-methoxyphenol

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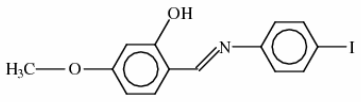
Keywords: Crystal structure; PM3; Conformational analysis

(E)-2-[4iodophenylimino)methyl]-5-methoxyphenol ($C_{14}H_{12}INO_2$) was synthesized and its crystal structure determined. It crystallizes in the orthorhombic space group, $Pna2_1$, with a = 6.2833(4), b = 7.1334(4), c = 29.0321(14) Å, $R(F^2)$ = 0.0238 for 2560 independent reflections.



The intramolecular hydrogen bond occurs between the pairs of atom O1 and N1 [2.609(4)Å] and the hydrogen atom is essentially bonded to the oxygen atom. There are two intermolecular C-H· · ·O hydrogen bonds between neighbouring molecules. The aromatic phenyl rings are an acceptor of four intermolecular C-H· · ·Ph hydrogen bonds. Conformations of the title compound were investigated by semi-empirical quantum mechanical PM3 calculations.

MS16 P10

Comparison of ferredoxins from *Ps. aeruginosa, E. coli* and an *Al. vinosum* mutant E. Saridakis[a], P. Giastas[a], G. Efthymiou[c], J.-M. Moulis[b], P. Kyritsis[c], I. M. Mavridis[a], [a]*National Center for Scientific Research "Demokritos", Athens, Greece,* [b]*DRDC/BMC, CEA-GRENOBLE, France,* [c]*Department of Chemistry, University of Athens, Greece*
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Keywords: ferredoxins; redox proteins; electron transfer proteins

The 2[4Fe-4S] Ferredoxins (Fds) are a type of electron transfer proteins found in anaerobic microorganisms. Two main families can be distinguished: The first includes the clostridial Fds with two isopotential [4Fe-4S] clusters (~ –400 mV). The second includes Fds characterized by very negative and widely different reduction potentials of the two clusters (~ -670 to ~ -430 mV). The 2[4Fe-4S] *Allochromatium vinosum* ferredoxin (AlvinFd) is the prototype of the second family and its structure has already been solved to a resolution of 2.1Å [1]. A characteristic member of the AlvinFd family from *Pseudomonas aeruginosa* has recently been determined to 1.32Å resolution [2]. Presently, the V13G mutant AlvinFd crystal structure has been solved to 1.65Å. It was crystallized in space group $P3_12$, a = b = 51.42, c = 76.55Å. The structure of another member of the family, the *E. coli* 2[4Fe-4S] ferredoxin (EcFd), was also determined to a resolution of 1.65Å. The latter, which exhibits merohedral twinning, was crystallized in space group $P3_2$, a = b = 65.35, c = 132.34Å. The comparison of the three members of the Fd family (detailed structural information, precise geometry of the clusters, conformation around and between the two clusters) will be presented. The structural studies are expected to shed more light on the unusual redox properties of these ferredoxins.

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MS16 P11

Non-traditional Bonding Interactions via Experimental Charge Density Nav S. Dhaliwal[1], Lee M. Daniels[1], T. Stanley Cameron[2] and Joseph D. Ferrara[1], [1]Rigaku Americas Corp., 9009 New Trails Dr., The Woodlands, TX 77381 USA and [2]Department of Chemistry, Dalhousie University, Halifax, Nova Scotia, Canada B3H 4J3.

Years ago, crystallography revolutionized a lot of thought about Important Science, and provided perhaps the most powerful tool for the study of chemical bonding. Precise positional information giving exact bond distances became routine; more recently advances in charge density studies have provided extensive views of bonding once available only in theory. Direct observation of covalent bonding is now possible, and extension of the analysis provides detailed information about *intermolecular* interactions. Using the criteria proposed by Koch and Popelier, a "bond path" can be constructed between any two atoms or groups in a structure, allowing one to distinguish "bonding" interactions from van der Waals contacts. In this work interactions such as H-H bonding, F-F bonding, I-S bonding, P-N ring bonding, etc. are considered.