

Keywords: Benzamides, Isomers, *ab initio*

FA4-MS33-P09

Planarity of tuberculostatic (aryl)heteroaryl- and heteroarocarbonimidoyl-dithiocarbazonic acid esters

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A rise of the mortality rates and spread of tuberculosis also in developed countries, attributed to the emergence of multi-drug resistant strains, resulted in a search for new lead compounds. Several dithiocarbazonic acid esters obtained by Foks [1-3] have shown high activity against standard and resistant strains of *Mycobacterium tuberculosis*.

Our early crystallographic studies on type A structures (Scheme, X=N,CH) showed all of them to maintain planarity in the crystal state due to two intramolecular hydrogen bonds and extensive conjugation. Therefore we have assumed that their planarity is a prerequisite for tuberculostatic activity [4-6]. At that time the question could not be answered by inspection of CSD, as structures incapable of adopting planar conformation, for example N⁻-substituted, were not known.

Now, as we have solved more similar structures (Scheme), including compounds with forced twist at N-N bond through their substitution or with free ring orientation due to lack of ortho N atom, more specific conclusions have been drawn.

[1] Foks, H., et al., Phosphorus, Sulfur, and Silicon, 2000, 158, 107. [2] Gobis K., et al., *ibid.*, 2006, 181, 965. [3] Gobis K., et al., *Heterocycles*, 2006, 68, 2615. [4] Orlewska C., et al., *Polish J. Chem.*, 2001, 75, 1237. [5] Główka M.L., et al., *J. Chem. Cryst.*, 2005, 35, 477. [6] Olczak A., et al., *J. Mol. Struct.*, 2007, 830, 171.

Keywords: tuberculostatics, intramolecular interactions, SAR

FA4-MS33-P10

Structure and Magnetic properties of Manganese (III)-Schiff-Base-Hexacyanoferrate-Polymeric Compound.

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A cyano-bridged Mn(III)-Fe(III) complex, [Mn(L)]₂Fe(CN)₆(NEt₃)(MeOH)₂ (**1**) (L=N,N-bis(5-bromo salicylidene)-2,2-dimethyl-1,3-diaminopropane) was prepared and characterized. The compound **1** crystallizes in Trigonal space group *P3(2)* with *a*= 28.5554, *b*= 28.5554, *c*= 19.2155 Å, γ= 120.00°. Single crystal X-ray analysis reveals that the complex assumes a cyano-bridged Mn₄Fe unit. The four CN in the equatorial plane of the [Fe(CN)₆]³⁻ moiety bridge four Mn

ions, each in the *cis* position, which results in a 3D neutral layered structure giving a [-Mn-NC-Fe-CN-Mn-] linkage. The Mn ion assumes an elongated octahedral geometry, in which the equatorial sites are occupied by N₂O₂ donor atoms of the Schiff base ligand, and the two axial positions are filled by two cyanide ion of [Fe(CN)₆]³⁻. The magnetic measurement showed this complex to exhibit ferromagnetic behavior.

Keywords: cyanide complexes, molecular magnets, crystal engineering

FA4-MS33-P11

Structural and magnetic transitions in ionic fullerene complexes with metalloporphyrins. Salavat Khasanov^a, Leokadia Zorina^a, Dmitry Konarev^b, ^aInstitute of Solid State Physics, RAS, Russia, ^bInstitute of Problem of Chemical Physics, RAS, Russia

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Ionic complexes containing C₆₀^{•-} radical anions and metalloporphyrins coordinatively bound to *N,N'*-trimethylpiperazinium cations, {(TMP⁺)₂M^{II}TTP}·(C₆₀^{•-})₂·(C₆H₄Cl₂)₂·(C₆H₅CN)₂ (M = Zn (**1**) and Mn (**2**)), have been obtained [1]. The crystal structures of **1** and **2** solved at 250 and 270 K, respectively, show layered packing in which fullerene layers alternate with the (TMP⁺)₂M^{II}TTP ones. Fullerenes form pairs in the layer with short center-to-center distance of 10.044 and 10.077 Å, respectively. The structures of **1** and **2** solved at 100 K showed the formation of singly bonded (C₆₀^{•-})₂ dimers. That results in the transition of **1** from paramagnetic to diamagnetic state accompanied by the disappearance of the EPR signal of C₆₀^{•-} at 220-150 K. Dimerization in **2** results in decrease in magnetic moment from 6.36 to 6.00 μ_B at 200-150 K and change in the shape of EPR signal. The room-temperature EPR signal shows a major broad component at g = 2.0678 (ΔH = 111.6 mT) attributed to both paramagnetic C₆₀^{•-} and high-spin (TMP⁺)₂Mn^{II}TTP species having strong exchange interaction. After dimerization the signal is characteristic of isolated high-spin Mn^{II}TTP (g_⊥ = 6 with |A| = 7.3 mT and g_∥ ≈ 2). Two TMP⁺ cations can coordinate to M^{II} in (TMP⁺)₂M^{II}TTP. However, a weak coordination bond is formed only with one cation with the M^{II}...N(TMP⁺) distances of 2.489(2)-2.688(3) Å. As a result, metal atoms displace by ± 0.232(3) (**1**, 250 K), ± 0.231(1) (**1**, 100 K) and ± 0.4684(7) Å (**2**, 270 K) out of the porphyrin plane to be located above and below the porphyrin plane with equal occupancies for both positions. Symmetry of the crystal structure of **2** lowers from monoclinic to triclinic under cooling. That results in unequal 0.85/0.15 occupation of the Mn^{II} positions at 100 K with the displacement of metal by 0.391(2) and 0.554(4) Å, respectively.

[1] Dmitri V. Konarev, Salavat S. Khasanov, Guzeliya R. Mukhamadiyeva, Leokadia V. Zorina, Akihiro Otsuka, Hideki Yamochi, Gunzi Saito, and Rimma N. Lyubovskaya, *Inorg. Chem.* 2010

Keywords: fullerenes, low-temperature structures, magnetic structural phase transitions