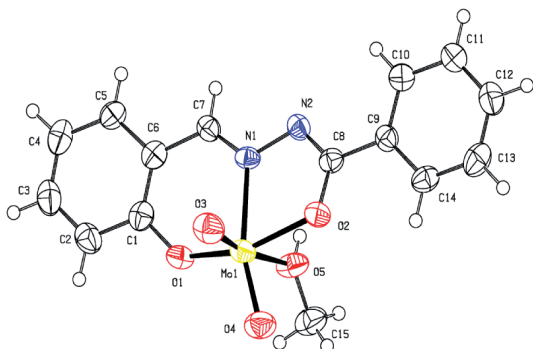


MS61.P18

Acta Cryst. (2011) A67, C611**X-ray structure of methanol {E-N/(2-hydroxybenzylidene)benzohydrazido}dioxidomolybdenum(VI)**

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In the structure of the title compound, [Mo(C₁₄H₁₀N₂O₄)(CH₃OH)], the Mo^{VI} ion is octahedrally coordinated by two oxido atoms, the N atom and two deprotonated OH groups of the tridentate Schiff base ligand(E)-N/(2-hydroxybenzylidene)benzohydrazid and by a methanol O atom. Its crystal data: C₁₅H₁₄MoN₂O₅ Triclinic, P, a = 7.8478 (13) Å, b = 9.7989 (16) Å, c = 10.3766 (17) Å, α = 10.3766 (17)°, β = 94.315 (13)°, γ = 107.834 (13)°, Z = 2, μ = 0.89 mm⁻¹ T = 233 (2) K, 0.40 × 0.15 × 0.15 mm.



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Keywords: Dioxidomolybdenum(VI) complex

MS61.P19

Acta Cryst. (2011) A67, C611**Polymeric manganese(II) complex with isophthalate ion and 2,2'-dipyridylamine**

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In the past decade the design and synthesis of metal-organic coordination polymers with anions of isophthalic (1,3-benzenedicarboxylic) acid, ipht, have become a growing field in crystal engineering due to their structural diversity and potential application as functional materials [1]. We have been continually interested in synthesis and characterisation of ternary transition metal complexes containing polycarboxylate anions and some aromatic N-containing ligands [2,3]. As a continuation of our research, the polymeric complex, [Mn(dipya)(ipht)]_n, where dipya is 2,2'-dipyridylamine, represents a novel example.

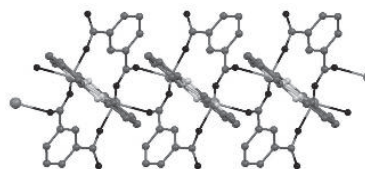
In [Mn(dipya)(ipht)]_n, ipht anion bridges three Mn atoms with bidentate-bridging and monodentate COO groups. In this way

centrosymmetric double chains extending along *c*-axis are formed (Figure). Mn(II) ions are in a deformed square pyramidal environment consisting of two N atoms from chelating dipya ligand and three O atoms from three different ipht ligands. The shortest intrachain Mn–Mn distance of only 3.76 Å could be the cause of possible strong magnetic interactions. Two crystallographically different Mn atoms are linked by two bridging ipht ligands to construct eight-membered [Mn₂O₄C₂] rings. Similar rings are already found in the ipht structures where at least one bidentate-bridging COO exist [3].

Double chains are stacked by face to face π-π interactions at centroid-centroid distances of 3.67 and 3.79 Å. Uncoordinated O atoms from monodentate COO groups and the amine H atoms of dipya build hydrogen bonds, which connect adjacent chains. Therefore through π-π interactions and hydrogen bonds the chains are packed into a three-dimensional framework.

The compound was hydrothermally synthesized in a Teflon-lined steel autoclave (T = 433 K, 5 days) starting from an aqueous solution containing Mn(NO₃)₂, dipya and sodium isophthalate. The structure was refined using single-crystal X-ray diffraction data (Oxford diffractometer, CCD detector, θ_{max} = 25.7°, 6711 measured reflections, R_{int} = 0.018, T = 293 K).

Crystal data: C₁₈H₁₃MnN₃O₄, M_r = 390.25, monoclinic, space group C2/c, a = 14.8320(6), b = 21.9325(6), c = 11.9995(5) Å, β = 122.916(6)°, V = 3276.8(2) Å³, Z = 8, F(000) = 1592, ρ_x = 1.582 g cm⁻³, μ(Mo Kα) = 0.836 mm⁻¹. The refinement on F² (287 parameters) yielded R₁ = 0.037, wR₂ = 0.067, S = 0.97 for all data, and R₁ = 0.027 for 2478 observed reflections with I ≥ 2σ(I).



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Keywords: complex, carboxylate ligand, crystal structure

MS61.P20

Acta Cryst. (2011) A67, C611–C612**Isonicotinic acid [1-(2,3 hydroxy phenyl) methylidene] hydrazide**

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In the title compound, C₁₃H₁₁N₃O₃, crystallizes with two molecules in the asymmetric unit which differ significantly in the conformation of hydrogen bonds, dihedral and torsion angle. The compound crystallizes in the monoclinic spacegroup P 2₁/c with a=7.7781(2)Å, b=30.0719(8)Å, c=10.5116(3)Å, α=90°, β=101.551(2)°, γ=90° and Z=8. The crystal structure is stabilized by intermolecular hydrogen bonds.

Schiff bases are typically formed by the condensation of a primary amine and an aldehyde. Also, schiff bases are a functional group that contains a carbon-nitrogen (C=N) double bond (an imine group). These