MS61.P18

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X-ray structure of methanol {E-N/-(2- hydroxybenzlidene)benzoh ydrazido}dioxidomolybdenum(VI)

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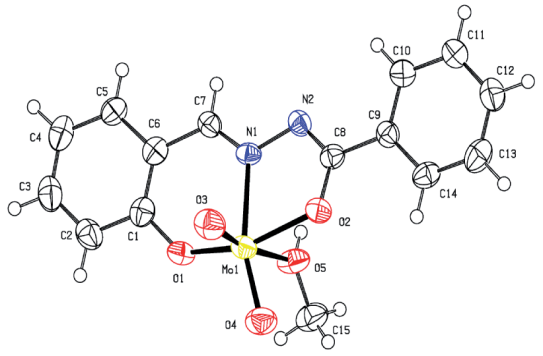
In the structure of the title compound, $[Mo(C_{14}H_{10}N_2O_4)(CH_3OH)]$, the Mo^{VI} ion is octahedrally coordinated by two oxido atoms, the N atom and two deprotonated OH groups of the tridentate Schiff base ligand(E)-N/-(2-hydroxybenzylidene)benzohydrazid and by a methanol O atom. Its crystal data: C15H14MoN2O5 Triclinic, P, a = 7.8478 (13) Å, b = 9.7989 (16) Å, c = 10.3766 (17) Å, c = 10.3766 (17) Å, α = 94.315 (13)°, β = 107.834 (13)°, γ = 90.565 (13)°, Z = 2, μ = 0.89 mm−1 T = 233 (2)anf K, 0.40 × 0.15 × 0.15 mm.



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Kewyords: Dioxidomolybdenum(VI) complex

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Polymeric manganese(II) complex with isophthalate ion and 2,2'-dipyridylamine

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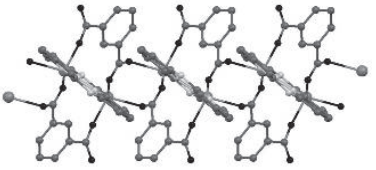
In the past decade the design and synthesis of metal-organic coordination polymers with anions of isophthalic (1,3-benzenedicarboxylic) acid, ipht, have become a growing field in crystal engineering due to their structural diversity and potential application as functional materials [1]. We have been 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 squere 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 $[Mn_2O_4C_2]$ 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 $Mn(NO_3)_2$, 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: $C_{18}H_{13}MnN_3O_4$, M_r = 390.25, monoclinic, space group *C*2/*c*, a = 14.8320(6), b = 21.9325(6), c = 11.9995(5) Å, β = 122.916(6) °, V = 3276.8(2) Å^3, Z = 8, $F(000)$ = 1592, ρ_x = 1.582 g cm^{-3}, μ(Mo Kα) = 0.836 mm^{-1}. The refinement on F^2 (287 parameters) yielded R_1 = 0.037, wR_2 = 0.067, S = 0.97 for all data, and R_1 = 0.027 for 2478 observed reflections with $I \geq 2\sigma(I)$.



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Keywords: complex, carboxylate ligand, crystal structure

MS61.P20

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Isonicotinic acid [1- (2,3 hydroxy phenyl) methylldene] hydrazide

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In the title compound, $C_{13}H_{11}N_3O_3$, 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 2_1/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