Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Diaquabis(1,2-di-4-pyridylethane-κ*N*)-bis(2-nitrobenzoate-κ*O*)manganese(II)

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Received 5 December 2006
Accepted 11 December 2006

In the title mixed-ligand complex, $[Mn(C_7H_4NO_4)_2(C_{12}H_{12}N_2)_2(H_2O)_2]$, was synthesized and its crystal structure was studied. The Mn atom is six-coordinated in slightly distorted octahedral coordination geometry by two N atoms of two 1,2-di-4-pyridylethane ligands (*L*), two O atoms of monodentate 2-nitrobenzoate ligands and two O atoms of water molecules. The Mn atom is located on a centre of inversion. A one-dimensional structure is formed in the [101] direction by intermolecular hydrogen bonds between the aqua ligands and N atoms of *L*. An intramolecular hydrogen bond between the other aqua ligand and a neighbouring O atom of a carboxylate group is also observed.

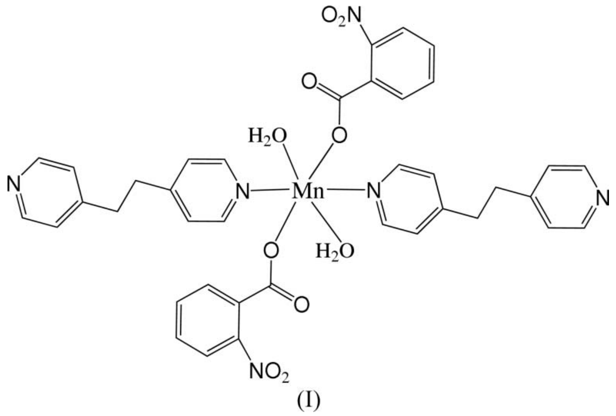
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.052
wR factor = 0.073
Data-to-parameter ratio = 11.6

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

1,2-Di-4-pyridylethane (*L*) is a very popular ligand because of its structural versatility and hydrogen bonding in the construction of crystal engineering materials (Hong *et al.*, 1999). However, only seven mono-coordinated *L* ligands have been reported (Rochon *et al.*, 1998; Nel *et al.*, 2000; Hong *et al.*, 1999; Vollenhoven & Laubacher, 1976; Fu *et al.*, 2004; Girginova *et al.*, 2005; Ferbinteanu *et al.*, 1999) in 158 complexes (Cambridge Structural Database, Version 5.27, update of August 2006; Allen, 2002) constructed from the *L* ligand. We have now combined Mn^{II} cations with 2-nitrobenzoate anion and *L* as a secondary ligand, forming the title complex, $[Mn(C_7H_4NO_4)_2(C_{12}H_{12}N_2)_2(H_2O)_2]$, (I), which is reported here.



(I)

Each carboxylate coordinates in a monodentate fashion and the Mn^{II} atom lies on a centre of symmetry. Fig. 1 shows the molecular structure of (I). The central Mn^{II} atom in (I) is coordinated by two O atoms from different 2-nitrobenzoate ligands, two N atoms from two ligands *L* and two O atoms of water molecules, resulting in a slightly distorted octahedral

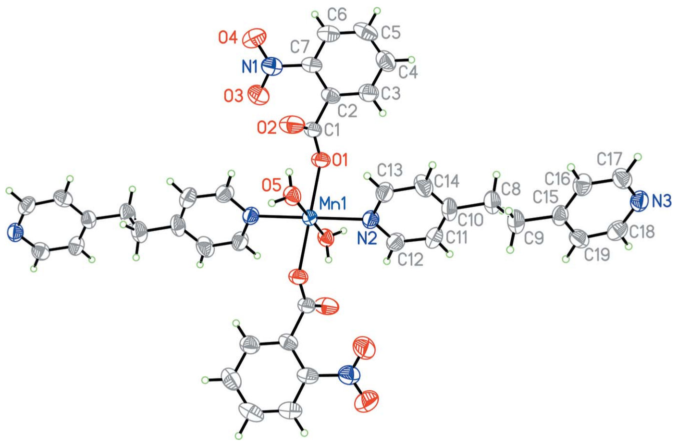


Figure 1
Molecular structure of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are represented by spheres of arbitrary radii. (Symmetry operation used to generate equivalent atoms: $-x$, $-y$, $-z$.)

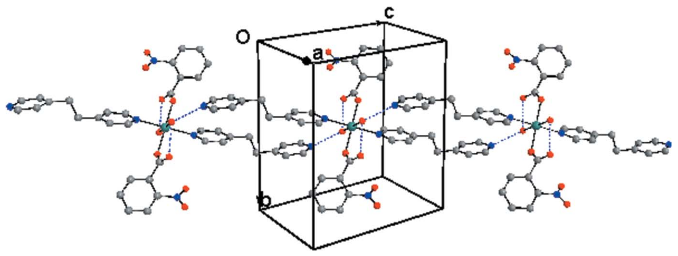


Figure 2
One-dimensional supramolecular structure of (I). Blue dashed lines indicate the hydrogen-bonding interactions.

coordination environment. Both *L* ligands act in a monocoordination mode and show an *anti* configuration. The Mn—O and Mn—N distances are comparable to the corresponding distances in related complexes (Ma *et al.*, 2004; Zhang *et al.*, 2002; Table 1). The *cis* angles at the central Mn^{II} atom are all close to 90°, with a maximum deviation of 3.92 (8)°. It is interesting to note that one O atom from a water molecule bonds with an adjacent N atom of *L* through a strong intermolecular hydrogen bond, and a one-dimensional supramolecular chain is formed in the [101] direction (Fig. 2). An intramolecular hydrogen bond between the other aqua ligand and a neighbouring O atom of a carboxylate groups is also observed (Table 2).

Experimental

A water–ethanol (1:1 *v*/*v*) solution (5 ml) of $\text{Mn(OAc)}_2\cdot 4\text{H}_2\text{O}$ (0.0490 g, 0.2 mmol) was added to a water–ethanol (1:1 *v*/*v*) solution (5 ml) of 2-nitrobenzoic acid (0.0668 g, 0.4 mmol), NaOH (0.0160 g, 0.4 mmol) and 1,2-di-4-pyridylethane (0.0736 g, 0.4 mmol). A light-yellow powder was obtained after a week. The powder was recrystallized from a mixed solvent composed of dimethylformamide, ethanol and water (1:1:1 *v*/*v*/*v*) by slow evaporation at room temperature; light-yellow block-shaped crystals of (I) were obtained after several days (yield 57.2%). Analysis calculated for $\text{C}_{38}\text{H}_{36}\text{MnN}_6\text{O}_{10}$: C 57.65, H 4.58, N 10.62%; found: C 57.39, H 4.67, N 10.45%.

Crystal data

$[\text{Mn}(\text{C}_7\text{H}_4\text{NO}_4)_2(\text{C}_{12}\text{H}_{12}\text{N}_2)_2(\text{H}_2\text{O})_2]$
$M_r = 791.67$
Monoclinic, $P2_1/n$
$a = 10.4669$ (16) Å
$b = 13.256$ (2) Å
$c = 14.019$ (2) Å
$\beta = 110.918$ (4)°

$V = 1817.0$ (5) Å^3
$Z = 2$
$D_x = 1.447$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.43$ mm^{-1}
$T = 293$ (2) K
Block, light yellow
0.20 × 0.15 × 0.10 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{\min} = 0.92$, $T_{\max} = 0.96$

10007 measured reflections
3751 independent reflections
2104 reflections with $I > 2\sigma(I)$
$R_{\text{int}} = 0.065$
$\theta_{\max} = 26.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.073$
$S = 0.84$
3751 reflections
322 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0078P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.41$ e Å^{-3}
$\Delta\rho_{\min} = -0.48$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Mn1—O5	2.1822 (17)	Mn1—N2	2.281 (2)
Mn1—O1	2.2100 (18)		
O5—Mn1—O1	86.42 (7)	O1—Mn1—N2	86.08 (8)
O5—Mn1—N2	89.13 (8)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5*B*···O2	0.85	1.83	2.666 (3)	166
O5—H5*A*···N3$^{\text{i}}$	0.85	1.91	2.756 (3)	172

Symmetry code: (i) $x-1, y, z-1$.

All the H atoms were placed at calculated positions and refined with a riding model; C—H = 0.93-0.97 Å, $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for aromatic and CH_2, and O—H = 0.85 Å for water H atoms; $U_{\text{iso}}(\text{H})$ values of water H atoms were refined.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 2000); program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

The authors thank the Programme for Excellent Talents in Huaiyin Teachers College and Technological Research Foundation of Huai'an City for financial support.

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