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Key indicators

Single-crystal X-ray study
 T = 173 K
 Mean $\sigma(\text{C}-\text{C}) = 0.002 \text{ \AA}$
 R factor = 0.027
 wR factor = 0.079
 Data-to-parameter ratio = 18.7

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

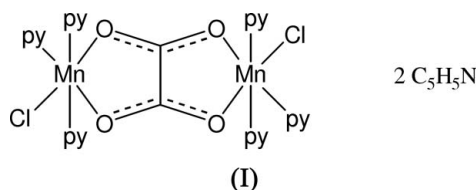
**μ -Oxalato-bis[chlorotripyridinemanganese(II)]
 pyridine disolvate**

The Mn complex of the title compound, $[\text{Mn}_2(\text{C}_2\text{O}_4)\text{Cl}_2(\text{C}_5\text{H}_5\text{N})_6] \cdot 2\text{C}_5\text{H}_5\text{N}$, is located on a crystallographic centre of inversion. The pyridine solvent molecules are located on general positions. Each Mn centre is octahedrally coordinated by three pyridine ligands, one Cl atom and a chelating oxalate dianion which bridges the two Mn centres.

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Comment

In a previous paper (Bolte, 2006), the structure of μ -oxalato-bis[chlorotripyridinecobalt(II)]pyridine disolvate has been described. In order to find out whether the exchange of the metal would lead to the same structure, the title compound, (I), had been synthesized. A perspective view of the title compound, (I), is shown in Fig. 1. Bond lengths and angles can be regarded as normal (Cambridge Structural Database, Version 5.27, updated January 2006; *MOGUL* Version 1.1; Allen, 2002).



The Mn atoms are octahedrally coordinated by three pyridine ligands, one Cl atom and a chelating oxalate dianion which bridges the two Mn centres. The three Mn–N bond lengths are significantly different. Those which are mutually

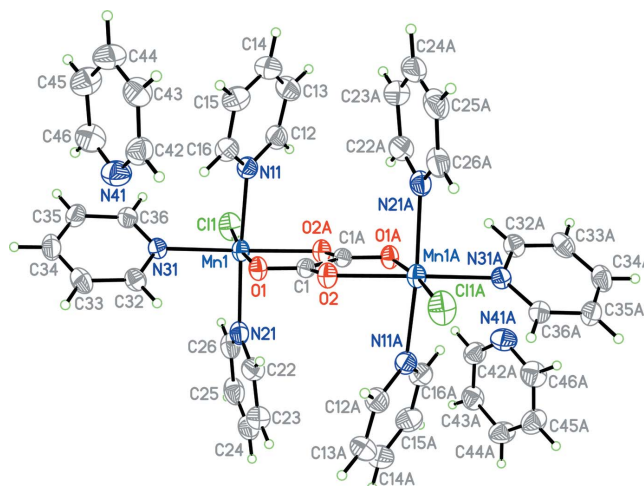


Figure 1
 Perspective view of the title compound with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Atoms with the suffix A are generated by the symmetry code $(1 - x, -y, 1 - z)$.

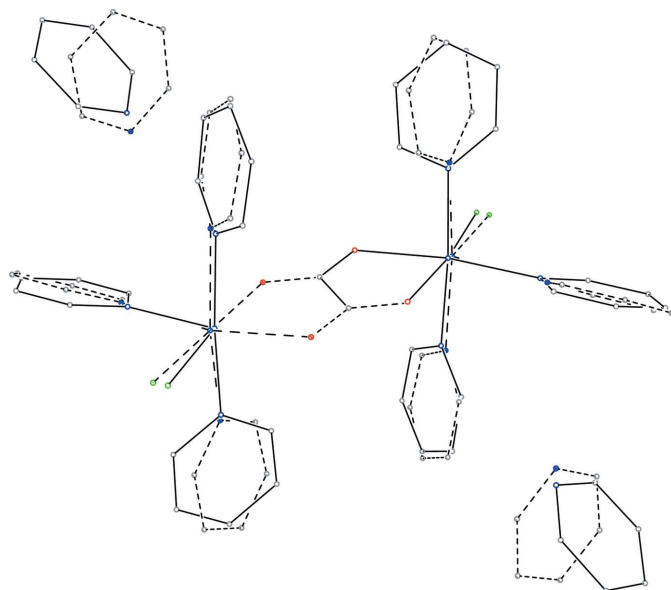


Figure 2

Least-squares fit of (I) (dashed lines) with the Co compound (solid lines); the r.m.s. deviation of the metal atoms and the oxalate bridges is 0.056 Å.

trans are longer than that which is *trans* to an Mn—O bond (Table 1). The two Mn—O bonds have the same length within standard uncertainty. The space between the complexes is filled by pyridine solvent molecules.

It is remarkable that (I) is not isostructural with the Co complex (Bolte, 2006). The molecules are rather similar (Fig. 2) and even the pyridine solvent molecules occupy almost the same positions. Both complexes are located on a centre of inversion, but the space groups are different, *viz.* $P\bar{1}$ for (I) and $P2_1/c$ for the Co complex.

Experimental

The title compound was synthesized according to the procedure described by Chattopadhyay *et al.* (2002) and crystallized from pyridine.

Crystal data

$[\text{Mn}_2(\text{C}_2\text{O}_4)\text{Cl}_2(\text{C}_5\text{H}_5\text{N})_6]\cdot 2\text{C}_5\text{H}_5\text{N}$
 $M_r = 901.60$
 Triclinic, $P\bar{1}$
 $a = 9.7867$ (8) Å
 $b = 10.1883$ (9) Å
 $c = 10.9221$ (9) Å
 $\alpha = 79.096$ (7)°
 $\beta = 82.110$ (7)°
 $\gamma = 89.374$ (7)°
 $V = 1059.13$ (15) Å³

$Z = 1$
 $D_x = 1.414$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 15958 reflections
 $\theta = 2.6\text{--}27.2^\circ$
 $\mu = 0.77$ mm⁻¹
 $T = 173$ (2) K
 Needle, colourless
 $0.42 \times 0.14 \times 0.12$ mm

Data collection

Stoe IPDS-II two-circle diffractometer
 ω scans
 Absorption correction: multi-scan (MULABS; Blessing, 1995; Spek, 2003)
 $T_{\min} = 0.737$, $T_{\max} = 0.913$
 15958 measured reflections

4899 independent reflections
 4456 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.041$
 $\theta_{\max} = 27.7^\circ$
 $h = -12 \rightarrow 12$
 $k = -13 \rightarrow 13$
 $l = -14 \rightarrow 13$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.028$
 $wR(F^2) = 0.079$
 $S = 1.03$
 4899 reflections
 262 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0473P)^2 + 0.1483P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.31$ e Å⁻³
 $\Delta\rho_{\min} = -0.45$ e Å⁻³

Table 1

Selected bond lengths (Å).

Mn1—O2 ⁱ	2.1980 (8)	Mn1—N21	2.3068 (11)
Mn1—O1	2.2081 (8)	Mn1—N11	2.3267 (11)
Mn1—N31	2.2754 (10)	Mn1—Cl1	2.4418 (4)

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

H atoms were located in a difference map, but were geometrically positioned and refined with fixed individual displacement parameters [$U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$] using a riding model (C—H = 0.95 Å).

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2003).

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