Poly[di-μ-chloro-bis(1,10-phenanthroline)-μ_4-terephthalato-dimanganese(II)]

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.007 Å
R factor = 0.045
wR factor = 0.092
Data-to-parameter ratio = 12.8

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

In the structure of the title complex, [Mn$_2$(C$_8$H$_4$O$_4$)Cl$_2$-(C$_{12}$H$_8$N$_2$)$_2$], each Mn^{II} cation is surrounded by two O atoms from two terephthalate dianions, two bridging Cl atoms and two N atoms from a 1,10-phenanthroline molecule in a distorted octahedral geometry. Each terephthalate dianion functions as a μ_4-bridging ligand to form a zigzag chain. Neighbouring chains are held together by μ-chloro bridges, which create a three-dimensional architecture.

Comment

The formation reactions of coordination polymers are mainly controlled and modified by the coordination geometry of the central metals, the structural chemistry of the organic ligands, the nature of the solvents and the molar ratio of the central metal to the organic ligand (Eddaoudi *et al.*, 2001). In this field, popular bridging organic ligands are terephthalic acid and its derivatives (Sun *et al.*, 2001; Zhu *et al.*, 2002, 2004; Baeg & Lee, 2003; Wang *et al.*, 2003; Xiao & Zhu, 2003; Hong & You, 2004). With the aim of searching for novel metal coordination polymers, we studied the reaction of MnCl$_2$ with terephthalic acid in *N,N*-dimethylacetamide as solvent and obtained the title complex, (I).

(I)
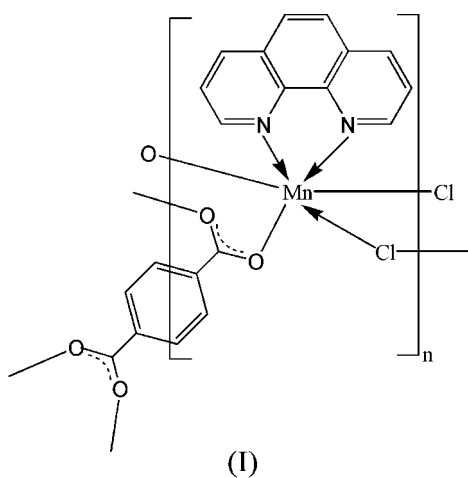
In (I), each Mn^{II} cation is coordinated by two O atoms from two terephthalate dianions, two bridging Cl atoms and two N atoms from a 1,10-phenanthroline molecule to form a highly distorted octahedral geometry (Fig. 1 and Table 1). The dihedral angle between the benzene ring of the terephthalate dianion and the 1,10-phenanthroline ring system is 102.8 (3)°. In the crystal structure, the terephthalate dianion functions as a μ_4-bridging ligand linking four different Mn^{II} atoms, and the 1,10-phenanthroline as a chelating ligand, resulting in a zigzag

metal-organic papers
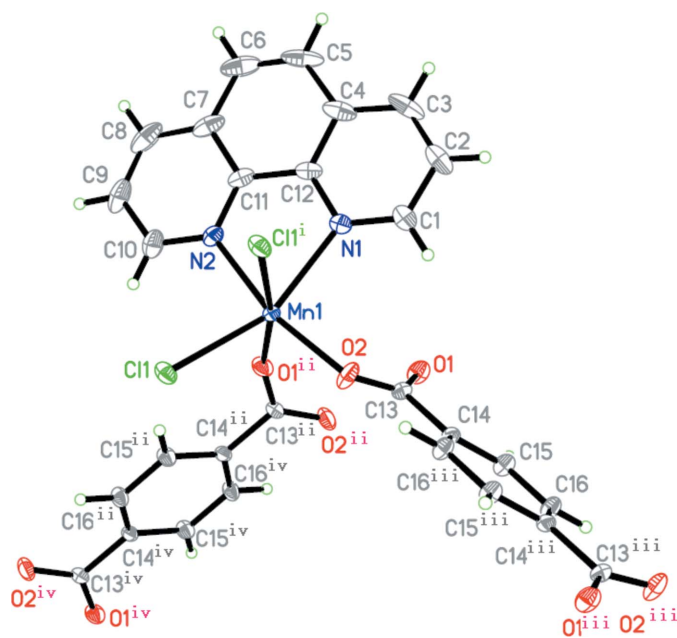
Figure 1
The coordination environment of the Mn^{II} atom in (I) with the atom numbering, showing displacement ellipsoids at the 30% probability level [symmetry codes: (i) $-x$, $-y$, $1-z$; (ii) $-x$, y, $\frac{3}{2}-z$; (iii) $\frac{1}{2}-x$, $-\frac{1}{2}-y$, $2-z$; (iv) $x-\frac{1}{2}$, $-\frac{1}{2}-y$, $z-\frac{1}{2}$].

chain (Fig. 2). Neighbouring chains are held together by μ-chloro bridges, which create a three-dimensional architecture (Fig. 3).

Experimental

A solution (10 ml) of *N,N*-dimethylacetamide containing MnCl$_2$·4H$_2$O (0.5 mmol, 0.099 g) and terephthalic acid (0.5 mmol, 0.083 g) was added slowly to an *N,N*-dimethylacetamide solution (10 ml) of 1,10-phenanthroline (0.5 mmol, 0.091 g). The mixture was stirred for a few minutes. Yellow crystals suitable for X-ray analysis were obtained when the solution was allowed to stand at room temperature for about three months.

Crystal data

[Mn$_2$(C$_8$H$_4$O$_4$)Cl$_2$(C$_{12}$H$_8$N$_2$)$_2$]	$Z = 4$
$M_r = 705.30$	$D_x = 1.672$ Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
$a = 22.997$ (2) Å	$\mu = 1.14$ mm^{-1}
$b = 10.4104$ (9) Å	$T = 298$ (2) K
$c = 16.2512$ (18) Å	Prism, yellow
$\beta = 133.949$ (3)°	$0.34 \times 0.25 \times 0.18$ mm
$V = 2801.2$ (5) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	10077 measured reflections
	2553 independent reflections
φ and ω scans	2409 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)	$R_{int} = 0.029$
	$\theta_{max} = 25.3°$
$T_{min} = 0.698$, $T_{max} = 0.821$	
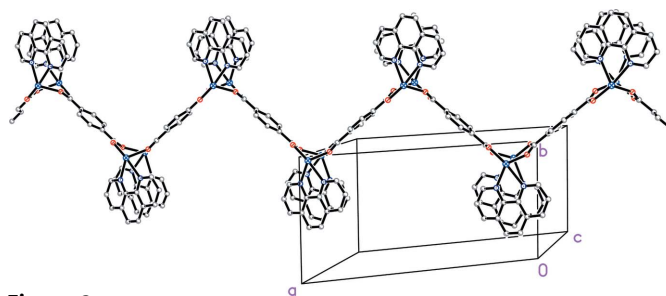
Figure 2
A partial packing view, showing a molecular zigzag chain of (I) running along the *a* axis. H atoms have been omitted.
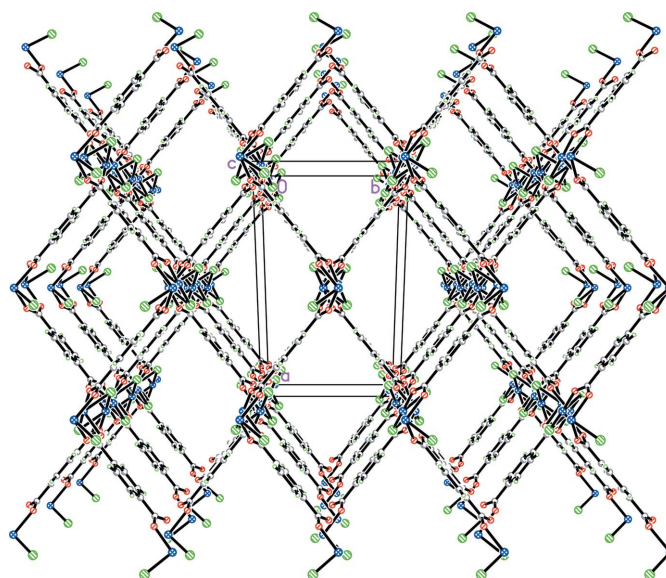
Figure 3
A packing diagram of (I), viewed along the *c* axis, showing the three-dimensional network structure. For clarity, 1,10-phenanthroline molecules have been omitted.

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0266P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.045$	$+ 8.647P]$
$wR(F^2) = 0.092$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.19$	$(\Delta/\sigma)_{max} = 0.001$
2553 reflections	$\Delta\rho_{max} = 0.53$ e Å^{-3}
199 parameters	$\Delta\rho_{min} = -0.40$ e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Mn1—Cl1	2.5448 (9)	Mn1—O1^{ii}	2.140 (2)
Mn1—Cl1^i	2.6024 (9)	Mn1—N2	2.277 (3)
Mn1—O2	2.096 (2)	Mn1—N1	2.344 (3)
O2—Mn1—O1^{ii}	93.98 (9)	N2—Mn1—Cl1	93.15 (7)
O2—Mn1—N2	165.70 (10)	N1—Mn1—Cl1	156.19 (7)
O1^{ii}—Mn1—N2	85.03 (9)	O2—Mn1—Cl1^i	91.77 (7)
O2—Mn1—N1	95.37 (10)	O1^{ii}—Mn1—Cl1^i	169.82 (6)
O1^{ii}—Mn1—N1	107.07 (9)	N2—Mn1—Cl1^i	91.44 (7)
N2—Mn1—N1	71.43 (10)	N1—Mn1—Cl1^i	80.70 (7)
O2—Mn1—Cl1	101.09 (7)	Cl1—Mn1—Cl1^i	81.71 (3)
O1^{ii}—Mn1—Cl1	88.94 (6)	Mn1—Cl1—Mn1^i	98.29 (3)

Symmetry codes: (i) $-x$, $-y$, $-z+1$; (ii) $-x$, y, $-z+\frac{3}{2}$.

All H atoms were positioned geometrically (C—H = 0.93 Å) and refined as riding, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2002); software used to prepare material for publication: *SHELXTL* (Bruker, 2002).

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