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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.007 Å
R factor = 0.048
wR factor = 0.099
Data-to-parameter ratio = 15.5

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

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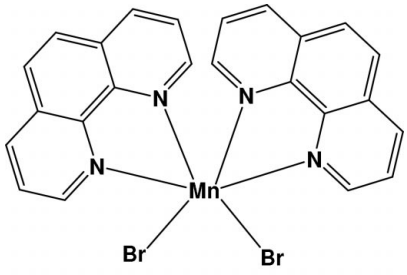
In the title complex, $[MnBr_2(C_{24}H_{16}N_4)]$, there is a weak C—H···Br intermolecular interaction in the crystal structure, giving rise to molecular chains along the *a* axis.

Comment

In recent years, simple metal complexes of phenanthroline and its derivatives have attracted great interest because they can be used to study the hydrolysis of biologically important phosphate diesters with poor leaving groups, *e.g.* DNA (Wall *et al.*, 1999). These complexes can also be used to develop new diagnostic and therapeutic agents in DNA binding and cleavage (Barton, 1986; Naing *et al.*, 1995). We report here the title complex, (I), a new metal complex of phenanthroline. A search of the January 2004 Cambridge Structural Database (Allen, 2002; Bruno *et al.*, 2002) found no report of (I).



(I)

Compound (I) has expected values for bond lengths and angles. The dihedral angle between the two phenanthroline planes is 84.74 (6)° and the average Mn—Br bond length is 2.535 (2) Å, within the range of previously reported values [2.496 (2) (Kienitz *et al.*, 2000) and 2.677 (2) Å (Goodgame *et al.*, 1999)]. There is a weak intermolecular interaction, C13—

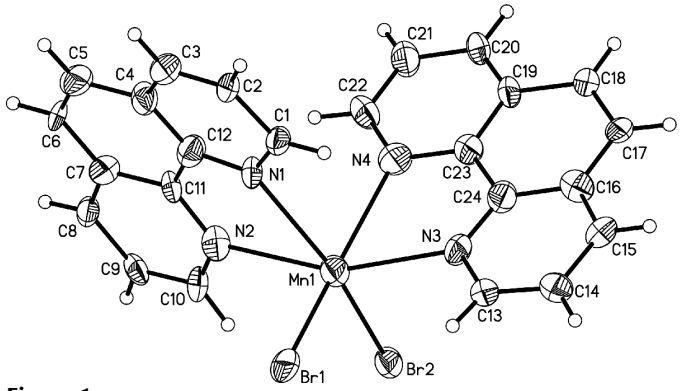


Figure 1
The molecular structure of (I), shown with 30% probability displacement ellipsoids.

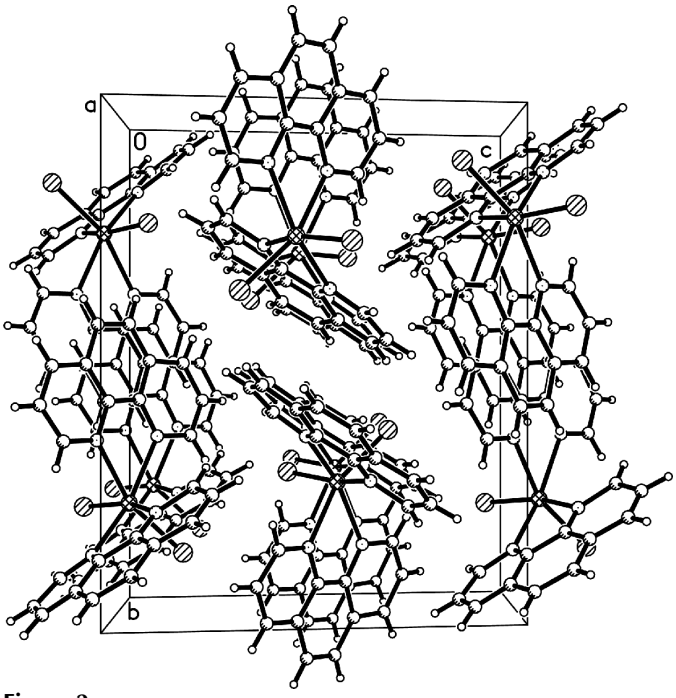


Figure 2
The packing of (I), viewed down the *a* axis.

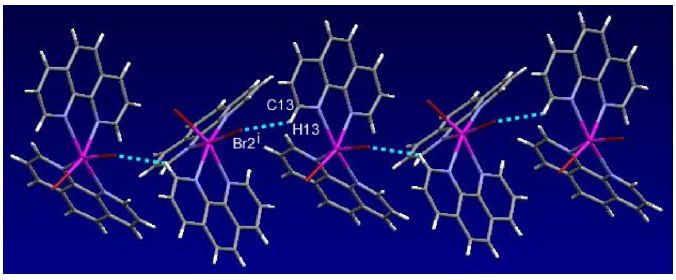


Figure 3
The molecular chains formed by the weak intermolecular interaction (dashed lines) of C13—H13···Br2^{i} [symmetry code: (i) $x, \frac{3}{2}-y, \frac{1}{2}+z$.]

H13···Br2^{i} [symmetry code: (i) $x, \frac{3}{2}-y, \frac{1}{2}+z$], in the structure, giving one-dimensional molecular chains arranged along the *a* axis, as shown in Figs. 2 and 3.

Experimental

To a warm solution of 1,10-phenanthroline (0.344 g, 2 mmol) in CH_3OH (20 ml) was added $MnBr_2{\cdot}4H_2O$ (0.265 g, 1 mmol) with slow heating and stirring. The mixture was refluxed for 2 h, then cooled to room temperature. After about two weeks, yellow single crystals suitable for X-ray crystallographic analysis were obtained. Analysis calculated for $C_{24}H_{16}Br_2MnN_4$: C 50.11, H 2.80, N 9.74%; found: C 50.05, H 2.76, N 9.69%.

Crystal data

$[MnBr_2(C_{24}H_{16}N_4)]$
M_r = 575.17
Monoclinic, $P2_1/c$
a = 10.423 (3) Å
b = 16.223 (3) Å
c = 13.244 (3) Å
β = 99.62 (2)°
V = 2208.0 (9) Å^3
Z = 4
D_x = 1.730 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1225 reflections
θ = 2.5–20.4°
μ = 4.24 mm^{-1}
T = 293 (2) K
Block, yellow
0.20 × 0.10 × 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} = 0.61, T_{max} = 0.66
9269 measured reflections
4334 independent reflections
3284 reflections with $I > 2\sigma(I)$
R_{int} = 0.042
θ_{max} = 26.0°
$h = -12 \rightarrow 12$
$k = -20 \rightarrow 20$
$l = -16 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.099
S = 1.02
4334 reflections
280 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.05P)^2 + 1.55P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.96 e Å^{-3}
$\Delta\rho_{min}$ = −0.73 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Br1—Mn1	2.5313 (10)	Mn1—N3	2.429 (4)
Br2—Mn1	2.5268 (11)	Mn1—N2	2.445 (4)
Mn1—N4	2.391 (4)	Mn1—N1	2.448 (4)
N4—Mn1—N3	67.06 (13)	N2—Mn1—Br2	99.86 (9)
N4—Mn1—N2	95.51 (13)	N1—Mn1—Br2	160.63 (9)
N3—Mn1—N2	161.56 (12)	N4—Mn1—Br1	161.29 (11)
N4—Mn1—N1	80.27 (13)	N3—Mn1—Br1	99.77 (9)
N3—Mn1—N1	107.97 (12)	N2—Mn1—Br1	95.62 (10)
N2—Mn1—N1	61.13 (12)	N1—Mn1—Br1	92.04 (9)
N4—Mn1—Br2	99.19 (11)	Br2—Mn1—Br1	93.66 (3)
N3—Mn1—Br2	89.27 (9)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H13···Br2^{i}	0.93	2.78	3.466 (5)	131

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

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 2000); program(s) used to solve and refine structure: *SHELXTL* (Bruker, 2000); molecular graphics: *SHELXTL* and *MERCURY* (Version 1.2.1; Bruno *et al.*, 2002).

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