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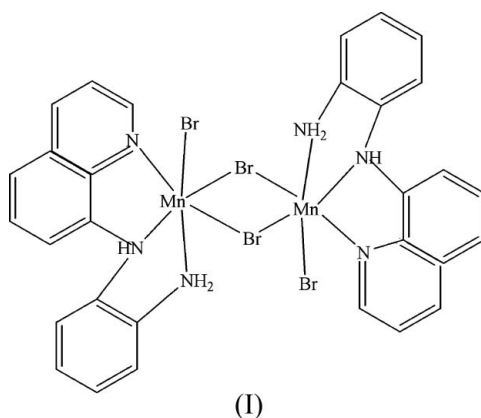
Key indicators

Single-crystal X-ray study
 $T = 120$ K
Mean $\sigma(\text{C}-\text{C}) = 0.005$ Å
 R factor = 0.033
 wR factor = 0.071
Data-to-parameter ratio = 20.2For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Di- μ -bromo-bis{bromo[*N*-(8-quinolyl)-*o*-phenyl-
enediamine- $\kappa^3 N, N', N''$]manganese(II)}

The title compound, $[\text{Mn}_2\text{Br}_4(\text{C}_{15}\text{H}_{13}\text{N}_3)_2]$, is the first crystallographically characterized metal complex of the *N*-(8-quinolyl)-*o*-phenylenediamine ligand. The centre of the molecule lies on a crystallographic inversion centre, so the $\text{Mn}_2(\mu\text{-Br})_2$ four-membered ring is planar with $\text{Mn}-\text{Br}$ bond lengths of 2.6210 (5) and 2.7147 (6) Å.

Comment

Although the tridentate ligand *N*-(8-quinolyl)-*o*-phenylenediamine (8-Q-phen) has been known for a long time (Jensen & Nielsen, 1964), no crystallographic data of any metal complex of this ligand have been published; the title compound, (I) (Fig. 1), represents the first example of this type. The centre of the molecule lies on a crystallographic inversion centre, so that the Mn_2Br_2 ring is planar. The Mn atom has a slightly distorted octahedral coordination involving the two bromide bridges, a terminal bromide and the three N-atom donors from an 8-Q-phen ligand with each N atom *trans* to a Br^- anion. Similar $\text{XM}(\mu_2\text{-X})_2\text{MX}$ core geometries are known, for example, Cambridge Structural Database (CSD, *MOGUL* Version 1.7; Allen, 2002) refcodes AZULOW (Wu *et al.*, 2004), QAMBEM (Davies *et al.*, 2004) and QEMREF (Romero *et al.*, 2001).



As in the crystal structure of the free ligand (Seshadri *et al.*, 2004), (II), the mean planes of the quinolyl system (atoms N1/C1–C9) and the benzene ring (atoms C10–C15) are almost perpendicular, with a dihedral angle of 71.57 (8)° between the planes. In the Mn_2Br_2 four-membered ring, the $\text{Mn}-\text{Br}$ distances are 2.6210 (5) and 2.7147 (6) Å (Table 1). For the terminal Br atom (Br2), the $\text{Mn1}-\text{Br2}$ bond length is, as expected, shorter [2.6096 (6) Å]. In other complexes exhibiting $\text{Mn}-\mu\text{-Br}$ units, the corresponding distances range from 2.581 Å (fourfold Mn coordination in GAYWIM; Pohl *et al.*, 1988) to 2.753 Å (sixfold coordination in XEJFIB; Gillon *et*

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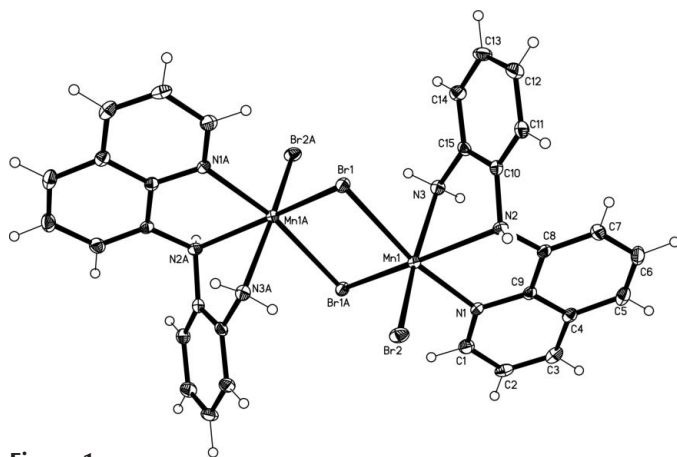


Figure 1
View of (I), showing the atom labeling scheme and displacement ellipsoids at the 50% probability level. Unlabeled atoms (and atoms marked by letter A) are related to the labeled atoms by the symmetry operator $(1 - x, -y, 2 - z)$.

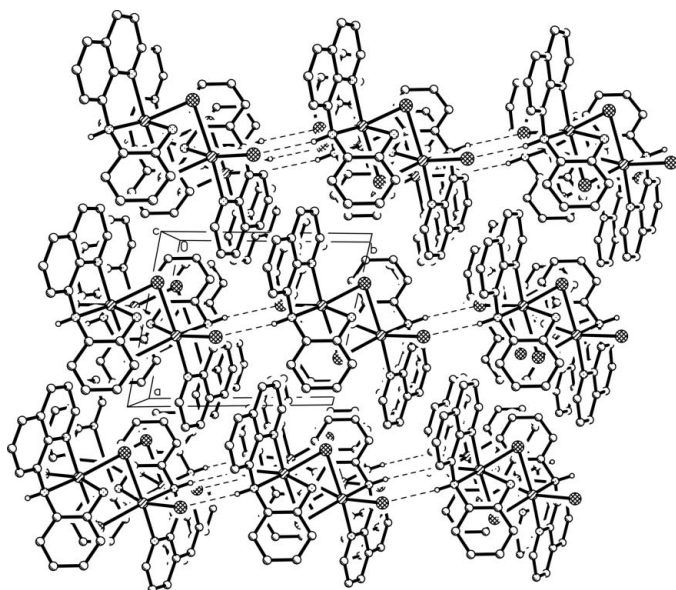


Figure 2
The crystal packing viewed approximately along the c axis. The intermolecular hydrogen bonds are shown as dashed lines. H atoms not involved in bridging have been omitted.

al., 2000); the terminal Mn—Br bonds in these compounds are 2.456 and 2.645 Å, respectively. In (I), the Mn—N(amine) bond length [2.340 (2) Å] is considerably longer than the Mn—N(quinolyl) bond [2.245 (2) Å], which is *trans* to the long Mn— μ -Br bond.

In the ligand, the C—N bond lengths in (I) (Table 1) and (II) are slightly different for atoms N2 [1.448 (4)/1.460 (4) Å in (I) *versus* 1.384/1.425 Å in (II)] and N3 [1.439 (4) Å in (I) *versus* 1.381 (3) Å in (II)]. The C—N distances for quinolyl atom N1 are, however, essentially the same in (I) and (II). The crystal packing (Fig. 2) displays an intermolecular N2—H2 \cdots Br2ⁱⁱ hydrogen bond [symmetry code: (ii) $-x + 1, -y + 1, -z + 2$], with H \cdots Br = 2.68 Å and N—H \cdots Br = 152° (values corrected for N—H = 1.03 Å), running along the [010] direction.

Experimental

The title compound was obtained by the reaction of equimolar amounts of MnBr₂ (0.5 mmol) and 8-Q-phen in acetonitrile (15 ml). This solution was stirred for 30 min, refluxed for a further 30 mins and then filtered; the Mn complex was crystallized using the vapor pressure equalization method in the presence of diethyl ether. IR (KBr, cm⁻¹): ν strong 1498, 1380, 953, 831, 800, 777, 757; medium 3321, 3257, 3186, 1563, 1458, 1311, 1245, 1198, 1085, 1066, 902, 867, 744, 705, 511, 490.

Crystal data

[Mn₂Br₄(C₁₅H₁₃N₃)₂]
 $M_r = 900.09$
 Triclinic, $P\bar{1}$
 $a = 8.8833$ (7) Å
 $b = 9.8725$ (8) Å
 $c = 9.9162$ (8) Å
 $\alpha = 103.055$ (2)°
 $\beta = 110.397$ (2)°
 $\gamma = 97.351$ (2)°
 $V = 773.45$ (11) Å³

$Z = 1$
 $D_x = 1.932$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 2034 reflections
 $\theta = 2.5\text{--}24.9^\circ$
 $\mu = 6.01$ mm⁻¹
 $T = 120$ (2) K
 Prism, colorless
 $0.20 \times 0.10 \times 0.08$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Bruker, 2002)
 $T_{\min} = 0.379$, $T_{\max} = 0.645$
 10807 measured reflections

3837 independent reflections
 3167 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.040$
 $\theta_{\max} = 28.3^\circ$
 $h = -11 \rightarrow 11$
 $k = -13 \rightarrow 13$
 $l = -13 \rightarrow 13$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.033$
 $wR(F^2) = 0.071$
 $S = 1.01$
 3837 reflections
 190 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0281P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.002$
 $\Delta\rho_{\max} = 0.59$ e Å⁻³
 $\Delta\rho_{\min} = -0.47$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Br1—Mn1 ⁱ	2.6210 (5)	N1—C1	1.326 (4)
Br1—Mn1	2.7147 (6)	N1—C9	1.372 (4)
Br2—Mn1	2.6096 (6)	N2—C10	1.448 (4)
Mn1—N1	2.245 (2)	N2—C8	1.460 (4)
Mn1—N2	2.340 (2)	N3—C15	1.439 (4)
Mn1—N3	2.340 (2)		
Mn1 ⁱ —Br1—Mn1	89.813 (17)	Br1 ⁱ —Mn1—Br1	90.187 (17)
N1—Mn1—N2	74.48 (9)		

Symmetry code: (i) $-x + 1, -y, -z + 2$.

The H atoms were positioned geometrically and allowed to ride on their parent atoms, with N—H = 0.92–0.93 Å, C—H = 0.95 Å and $U_{\text{iso}} = 1.2U_{\text{eq}}$ (parent atom).

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

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