metal-organic compounds

Bis{2,4-dibromo-6-[(2-oxidoethylimino)methyl]phenolato-$\kappa^3 O,N,O'$}-manganese(IV) methanol hemisolvate monohydrate

Gang-Biao Jiang,[a,b] Shu-Hua Zhang[a] and Ming-Hua Zeng[a]*

[a]School of Chemistry and Chemical Engineering, Guangxi Normal University, Guilin 541004, People's Republic of China, and [b]College of Resources and Environment, South China Agriculture University, Guangzhou 510642, People's Republic of China
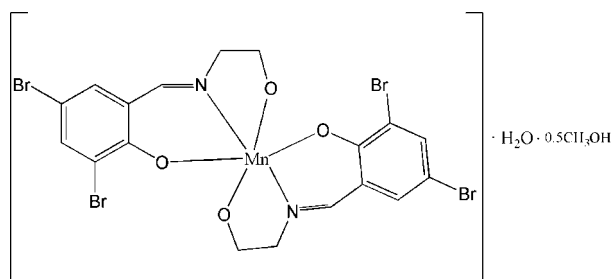Correspondence e-mail: zmh@mailbox.gxnu.edu.cn

In the title compound, $[Mn(C_9H_7Br_2NO_2)_2] \cdot 0.5CH_4O \cdot H_2O$, the Mn^{IV} atom is coordinated in a distorted octahedral geometry by two N and four O atoms from two different tridentate 2,4-dibromo-6-[(2-oxidoethylimino)methyl]phenolate ligands. In the crystal structure, the methanol solvent molecule is disordered over two positions with equal occupancies. The crystal packing reveals a three-dimensional network generated by short Br···Br interactions [Br···Br = 3.555 (5)–3.742 (5) Å], and O—H···O and O—H···Br hydrogen bonds.

Related literature

A similar manganese(II) complex also has a distorted octahedral geometry (Kessissoglou *et al.*, 1986). For related literature, see: Cohen *et al.* (1964); Zordan *et al.* (2005); Desiraju (1989); Zaman *et al.* (2004); Sarma & Desiraju (1986).

Experimental

Crystal data

$C_{18}H_{14}Br_4MnN_2O_4 \cdot 0.5CH_4O \cdot H_2O$	V = 9661 (2) Å³
M_r = 730.89	Z = 16
Orthorhombic, $Fdd2$	Mo $K\alpha$ radiation
a = 26.286 (4) Å	μ = 7.20 mm⁻¹
b = 32.908 (5) Å	T = 293 (2) K
c = 11.1681 (17) Å	0.18 × 0.14 × 0.13 mm

Data collection

Bruker SMART CCD area-detector diffractometer	8149 measured reflections
	4075 independent reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	3143 reflections with $I > 2\sigma(I)$
T_{min} = 0.357, T_{max} = 0.455	R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051	H-atom parameters constrained
$wR(F^2)$ = 0.133	$\Delta\rho_{max}$ = 1.09 e Å⁻³
S = 1.05	$\Delta\rho_{min}$ = −0.39 e Å⁻³
4075 reflections	Absolute structure: Flack (1983), 1669 Friedel pairs
290 parameters	Flack parameter: 0.045 (19)
20 restraints	

Table 1
Selected geometric parameters (Å, °).

Mn1—O2	1.871 (7)	Mn1—O3	2.027 (7)
Mn1—O1	1.906 (7)	Mn1—N2	2.094 (7)
Mn1—N1	1.984 (7)	Mn1—O4	2.324 (6)
O2—Mn1—O1	174.3 (3)	N1—Mn1—N2	162.6 (3)
O2—Mn1—N1	83.9 (3)	O3—Mn1—N2	86.2 (3)
O1—Mn1—N1	90.6 (3)	O2—Mn1—O4	92.3 (3)
O2—Mn1—O3	92.7 (3)	O1—Mn1—O4	85.9 (3)
O1—Mn1—O3	90.6 (3)	N1—Mn1—O4	87.3 (3)
N1—Mn1—O3	110.2 (3)	O3—Mn1—O4	162.2 (3)
O2—Mn1—N2	89.9 (3)	N2—Mn1—O4	76.7 (3)
O1—Mn1—N2	95.0 (3)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5A···Br1ⁱ	0.85	3.04	3.893 (18)	179
O1W—H1WA···O5	0.85	1.52	2.19 (2)	134

Symmetry code: (i) $x - \frac{1}{4}, -y + \frac{3}{4}, z + \frac{1}{4}$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); 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, 1997); software used to prepare material for publication: *SHELXTL*.

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supplementary materials

Bis{2,4-dibromo-6-[(2-oxidoethylimino)methyl]phenolato-κ^3O,N,O'}manganese(IV) methanol hemisolvate monohydrate

G.-B. Jiang, S.-H. Zhang and M.-H. Zeng

Comment

Interest on packing arrangements of halogenated compounds goes back many years to what Schmidt called the 'chloro effect', where the presence of chloro substituents on aromatic compounds frequently results in stacking arrangements with a short (*ca* 4 Å) crystallographic axis (Cohen *et al.*, 1964; Zordan *et al.*, 2005; Desiraju, 1989). The title compound, (I), contains the dibrominated ligand L^- with two Br atoms accessible at the periphery of each ligand.

In (I) the Mn^{IV} atom is coordinated by two N and four O atoms from two different tridentate ligands L^{2-} forming a distorted octahedral geometry (Fig. 1 and Table 1). The shortest Br···Br contacts (Zordan *et al.*, 2005; Zaman *et al.*, 2004; Sarma & Desiraju, 1986) are Br3^i···Br3^{ii} = 3.555 (5) Å, Br3^i···Br4^{iii} = 3.742 (5) Å, and Br4^i···Br2^{iv} = 3.631 (5) Å, [symmetry codes: (i) $1/2 - x, -1/2 - y, z$; (ii) $x, -1 + y, z$; (iii) $1/4 + x, -1/4 - y, -1/4 + z$; (iv) $1/4 - x, -3/4 - y, 1/4 + z$]. The molecules of (I) are connected into a 3-D network through short Br···Br interactions, very strong O–H···O hydrogen bond and O–H···Br hydrogen bond (Table 2 and Fig. 2).

Experimental

A solution of 2-amino-ethanol (0.061 g, 1 mmol) and caustic potash (0.112 g, 2 mmol) in methanol (10 ml) was added slowly to a solution of 3,5-dibromo-2-hydroxybenzaldehyde (1 mmol, 0.280 g) in methanol (20 ml). The mixture was stirred for 1 h at 323 K, then added slowly to a solution of MnCl$_2$ (2 mmol, 0.396 g) in methanol (10 ml). This mixture was stirred and refluxed for 2 h at 323 K. The solution was filtered and the filtrate was left to stand at room temperature. Deep purple suitable for X-ray diffraction were obtained in a yield of 38% (based on manganese).

Refinement

H atoms of the water molecule were located in a difference Fourier map. The O—H distances were normalized to 0.85 Å and the H atoms were allowed to ride on the O atom, with $U_{iso}(H) = 1.5 U_{eq}(O)$. All other H atoms were positioned geometrically and refined as riding, with C–H distances of 0.93–0.97 Å and $U_{iso}(H) = 1.2 U_{eq}(C)$.
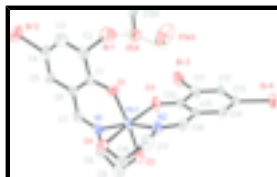
Figures

Fig. 1. The asymmetric unit of (I) with displacement ellipsoids drawn at the 30% probability level. Non-solution H atoms have been omitted.
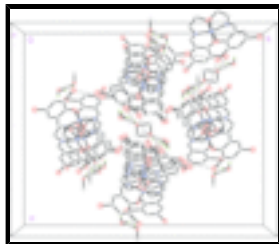
Fig. 2. The 3-D network of (I): dashed lines denote hydrogen bonds and Br···Br interactions. Non-solution H atoms have been omitted.

Bis{2,4-dibromo-6-[(2-oxidoethylimino)methyl]phenolato-$\kappa^3 O,N,O'$}manganese(IV) methanol hemisolvate monohydrate

Crystal data

$C_{18}H_{14}Br_4MnN_2O_4 \cdot 0.5CH_4O \cdot H_2O$	$D_x = 2.010$ Mg m^{-3}
$M_r = 730.89$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Orthorhombic, $Fdd2$	Cell parameters from 4075 reflections
$a = 26.286$ (4) Å	$\theta = 2.5–26.0º$
$b = 32.908$ (5) Å	$\mu = 7.20$ mm^{-1}
$c = 11.1681$ (17) Å	$T = 293$ (2) K
$V = 9661$ (2) Å^3	Block, deep purple
$Z = 16$	$0.18 \times 0.14 \times 0.13$ mm
$F_{000} = 5632$	

Data collection

Bruker SMART CCD area-detector diffractometer	4075 independent reflections
Radiation source: fine-focus sealed tube	3143 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.029$
$T = 293(2)$ K	$\theta_{max} = 26.0º$
φ and ω scans	$\theta_{min} = 2.5º$
Absorption correction: multi-scan SADABS (Sheldrick, 1996)	$h = -32 \rightarrow 14$
$T_{min} = 0.357$, $T_{max} = 0.455$	$k = -38 \rightarrow 38$
8149 measured reflections	$l = -13 \rightarrow 12$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.051$	$w = 1/[\sigma^2(F_o^2) + (0.0654P)^2 + 43.5887P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.133$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.05$	$\Delta\rho_{max} = 1.09$ e Å^{-3}
4075 reflections	$\Delta\rho_{min} = -0.38$ e Å^{-3}

290 parameters	Extinction correction: none	
20 restraints	Absolute structure: Flack (1983), 1669 Friedel pairs	
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.045 (19)	
Secondary atom site location: difference Fourier map		

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	y	z	$U_{iso}*/U_{eq}$	Occ. (<1)
Mn1	0.04388 (5)	0.25185 (4)	0.55027 (13)	0.0418 (3)	
Br1	0.14995 (5)	0.31726 (4)	0.25588 (13)	0.0797 (4)	
Br2	0.21088 (5)	0.16499 (5)	0.07739 (14)	0.1024 (5)	
Br3	0.18568 (5)	0.26672 (3)	0.84250 (12)	0.0769 (4)	
Br4	0.09302 (5)	0.40746 (4)	1.02880 (13)	0.0909 (5)	
C1	0.1120 (3)	0.2418 (3)	0.3450 (9)	0.045 (2)	
C2	0.1451 (4)	0.2600 (3)	0.2601 (11)	0.063 (3)	
C3	0.1729 (4)	0.2370 (4)	0.1815 (12)	0.074 (3)	
H3	0.1939	0.2493	0.1253	0.089*	
C4	0.1690 (5)	0.1956 (4)	0.1872 (11)	0.073 (3)	
C5	0.1366 (3)	0.1763 (3)	0.2602 (10)	0.058 (3)	
H5	0.1323	0.1483	0.2543	0.070*	
C6	0.1091 (3)	0.1988 (3)	0.3463 (9)	0.048 (2)	
C7	0.0781 (3)	0.1767 (3)	0.4321 (10)	0.049 (2)	
H7	0.0756	0.1487	0.4238	0.059*	
C8	0.0263 (4)	0.1681 (3)	0.6026 (11)	0.062 (3)	
H8A	0.0481	0.1606	0.6690	0.075*	
H8B	0.0142	0.1435	0.5642	0.075*	
C9	−0.0180 (3)	0.1932 (3)	0.6464 (11)	0.059 (3)	
H9A	−0.0444	0.1944	0.5857	0.071*	
H9B	−0.0323	0.1813	0.7183	0.071*	
C10	0.0955 (3)	0.3013 (3)	0.7461 (9)	0.046 (2)	
C11	0.1330 (4)	0.3063 (3)	0.8315 (10)	0.059 (3)	
C12	0.1339 (4)	0.3363 (3)	0.9175 (8)	0.052 (2)	
H12	0.1592	0.3375	0.9758	0.062*	
C13	0.0937 (4)	0.3656 (3)	0.9116 (10)	0.061 (3)	
C14	0.0584 (3)	0.3634 (3)	0.8245 (9)	0.051 (2)	
H14	0.0334	0.3834	0.8202	0.061*	

C15	0.0581 (3)	0.3327 (3)	0.7422 (8)	0.045 (2)	
C16	0.0194 (3)	0.3353 (3)	0.6506 (9)	0.046 (2)	
H16	−0.0019	0.3579	0.6536	0.055*	
C17	−0.0327 (4)	0.3176 (3)	0.4826 (10)	0.063 (3)	
H17A	−0.0575	0.3347	0.5224	0.075*	
H17B	−0.0207	0.3317	0.4117	0.075*	
C18	−0.0569 (3)	0.2783 (3)	0.4473 (10)	0.057 (3)	
H18A	−0.0751	0.2671	0.5153	0.069*	
H18B	−0.0813	0.2831	0.3838	0.069*	
N1	0.0543 (2)	0.1932 (2)	0.5168 (8)	0.0453 (17)	
N2	0.0111 (3)	0.3096 (2)	0.5650 (7)	0.0466 (17)	
O1	0.0876 (2)	0.26594 (18)	0.4206 (6)	0.0494 (15)	
O2	0.0007 (2)	0.23280 (19)	0.6711 (6)	0.0564 (17)	
O3	0.0963 (3)	0.2718 (2)	0.6697 (7)	0.0630 (19)	
O4	−0.0208 (2)	0.2505 (2)	0.4085 (6)	0.0536 (16)	
O5	−0.0213 (4)	0.4752 (5)	0.7733 (17)	0.081 (4)	0.50
H5A	−0.0383	0.4657	0.7150	0.121*	0.50
C19	0.0282 (5)	0.4748 (6)	0.759 (2)	0.068 (6)	0.50
H19A	0.0378	0.4953	0.7022	0.102*	0.50
H19B	0.0388	0.4487	0.7305	0.102*	0.50
H19C	0.0444	0.4803	0.8346	0.102*	0.50
O1W	−0.0549 (6)	0.4146 (5)	0.7965 (13)	0.172 (6)	
H1WA	−0.0572	0.4403	0.8021	0.257*	
H1WB	−0.0857	0.4111	0.7760	0.257*	

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0489 (6)	0.0388 (7)	0.0378 (7)	0.0059 (6)	−0.0051 (6)	−0.0072 (6)
Br1	0.0789 (7)	0.0729 (8)	0.0871 (9)	−0.0109 (6)	0.0038 (6)	0.0148 (7)
Br2	0.0957 (9)	0.1375 (13)	0.0739 (10)	0.0320 (8)	0.0151 (7)	−0.0354 (9)
Br3	0.0814 (7)	0.0637 (7)	0.0855 (9)	0.0061 (6)	−0.0389 (6)	−0.0095 (6)
Br4	0.0996 (8)	0.0844 (8)	0.0886 (11)	−0.0175 (7)	0.0070 (7)	−0.0550 (8)
C1	0.040 (4)	0.055 (6)	0.041 (5)	0.003 (4)	−0.003 (4)	−0.017 (5)
C2	0.080 (7)	0.062 (6)	0.046 (7)	0.002 (5)	−0.002 (5)	0.004 (5)
C3	0.061 (6)	0.108 (11)	0.054 (8)	−0.008 (6)	−0.013 (5)	0.003 (7)
C4	0.085 (8)	0.092 (9)	0.043 (7)	0.018 (7)	−0.013 (6)	−0.026 (6)
C5	0.050 (5)	0.075 (7)	0.049 (6)	0.012 (5)	0.008 (5)	−0.020 (6)
C6	0.035 (4)	0.060 (6)	0.050 (6)	0.001 (4)	0.003 (4)	−0.013 (5)
C7	0.056 (5)	0.029 (5)	0.063 (7)	0.008 (4)	−0.003 (5)	−0.011 (5)
C8	0.069 (6)	0.059 (6)	0.059 (7)	−0.012 (5)	0.002 (5)	0.003 (5)
C9	0.048 (5)	0.062 (7)	0.067 (7)	−0.008 (5)	−0.004 (5)	0.010 (5)
C10	0.050 (5)	0.032 (5)	0.055 (6)	−0.006 (4)	−0.001 (4)	−0.001 (4)
C11	0.077 (6)	0.041 (5)	0.058 (7)	−0.005 (4)	−0.012 (5)	−0.002 (5)
C12	0.065 (6)	0.052 (6)	0.039 (6)	−0.018 (5)	−0.007 (4)	−0.012 (4)
C13	0.064 (6)	0.068 (7)	0.050 (6)	−0.019 (5)	0.010 (5)	−0.028 (5)
C14	0.056 (5)	0.047 (5)	0.050 (6)	0.006 (4)	0.009 (4)	−0.011 (4)
C15	0.054 (5)	0.037 (5)	0.043 (6)	−0.012 (4)	0.009 (4)	−0.010 (4)

C16	0.058 (5)	0.034 (5)	0.045 (6)	0.006 (4)	0.000 (4)	0.003 (4)
C17	0.072 (6)	0.061 (7)	0.056 (7)	0.023 (5)	−0.018 (5)	−0.003 (5)
C18	0.043 (5)	0.080 (7)	0.050 (6)	0.008 (5)	−0.002 (4)	0.001 (5)
N1	0.034 (3)	0.051 (4)	0.050 (5)	0.000 (3)	−0.005 (3)	−0.005 (4)
N2	0.054 (4)	0.044 (4)	0.042 (5)	0.009 (3)	−0.009 (3)	−0.004 (4)
O1	0.044 (3)	0.047 (4)	0.057 (4)	0.002 (3)	0.006 (3)	0.001 (3)
O2	0.071 (4)	0.055 (4)	0.043 (4)	0.008 (3)	−0.004 (3)	−0.005 (3)
O3	0.074 (4)	0.054 (4)	0.061 (5)	0.013 (3)	−0.020 (3)	−0.028 (4)
O4	0.049 (3)	0.057 (4)	0.055 (4)	0.012 (3)	−0.009 (3)	−0.007 (3)
O5	0.057 (7)	0.105 (10)	0.080 (11)	0.003 (7)	−0.002 (8)	0.013 (9)
C19	0.042 (9)	0.074 (11)	0.088 (14)	0.019 (8)	0.050 (9)	0.032 (11)
O1W	0.214 (12)	0.196 (12)	0.105 (11)	−0.067 (10)	0.020 (9)	0.009 (9)

Geometric parameters (Å, °)

Mn1—O2	1.871 (7)	C9—H9B	0.9700
Mn1—O1	1.906 (7)	C10—O3	1.292 (11)
Mn1—N1	1.984 (7)	C10—C11	1.381 (14)
Mn1—O3	2.027 (7)	C10—C15	1.426 (12)
Mn1—N2	2.094 (7)	C11—C12	1.377 (14)
Mn1—O4	2.324 (6)	C12—C13	1.432 (14)
Br1—C2	1.888 (10)	C12—H12	0.9300
Br2—C4	1.931 (11)	C13—C14	1.348 (14)
Br3—C11	1.905 (10)	C14—C15	1.367 (13)
Br4—C13	1.900 (9)	C14—H14	0.9300
C1—O1	1.326 (10)	C15—C16	1.446 (13)
C1—C6	1.415 (13)	C16—N2	1.295 (12)
C1—C2	1.419 (15)	C16—H16	0.9300
C2—C3	1.370 (17)	C17—C18	1.494 (14)
C3—C4	1.368 (18)	C17—N2	1.496 (12)
C3—H3	0.9300	C17—H17A	0.9700
C4—C5	1.339 (17)	C17—H17B	0.9700
C5—C6	1.414 (13)	C18—O4	1.388 (11)
C5—H5	0.9300	C18—H18A	0.9700
C6—C7	1.453 (14)	C18—H18B	0.9700
C7—N1	1.257 (12)	O5—C19	1.312 (9)
C7—H7	0.9300	O5—H5A	0.8501
C8—N1	1.464 (13)	C19—H19A	0.9600
C8—C9	1.508 (14)	C19—H19B	0.9600
C8—H8A	0.9700	C19—H19C	0.9600
C8—H8B	0.9700	O1W—H1WA	0.8500
C9—O2	1.419 (11)	O1W—H1WB	0.8500
C9—H9A	0.9700		
O2—Mn1—O1	174.3 (3)	H9A—C9—H9B	108.5
O2—Mn1—N1	83.9 (3)	O3—C10—C11	122.4 (8)
O1—Mn1—N1	90.6 (3)	O3—C10—C15	122.2 (8)
O2—Mn1—O3	92.7 (3)	C11—C10—C15	115.2 (8)
O1—Mn1—O3	90.6 (3)	C12—C11—C10	125.5 (9)
N1—Mn1—O3	110.2 (3)	C12—C11—Br3	115.6 (8)

O2—Mn1—N2	89.9 (3)	C10—C11—Br3	118.7 (7)
O1—Mn1—N2	95.0 (3)	C11—C12—C13	115.9 (8)
N1—Mn1—N2	162.6 (3)	C11—C12—H12	122.0
O3—Mn1—N2	86.2 (3)	C13—C12—H12	122.0
O2—Mn1—O4	92.3 (3)	C14—C13—C12	120.4 (8)
O1—Mn1—O4	85.9 (3)	C14—C13—Br4	122.0 (8)
N1—Mn1—O4	87.3 (3)	C12—C13—Br4	117.6 (7)
O3—Mn1—O4	162.2 (3)	C13—C14—C15	121.9 (9)
N2—Mn1—O4	76.7 (3)	C13—C14—H14	119.0
O1—C1—C6	124.4 (9)	C15—C14—H14	119.0
O1—C1—C2	117.9 (8)	C14—C15—C10	120.8 (8)
C6—C1—C2	117.6 (8)	C14—C15—C16	115.7 (8)
C3—C2—C1	121.4 (10)	C10—C15—C16	123.5 (8)
C3—C2—Br1	119.9 (9)	N2—C16—C15	126.9 (8)
C1—C2—Br1	118.7 (8)	N2—C16—H16	116.5
C4—C3—C2	118.7 (12)	C15—C16—H16	116.5
C4—C3—H3	120.6	C18—C17—N2	109.8 (7)
C2—C3—H3	120.6	C18—C17—H17A	109.7
C5—C4—C3	123.2 (11)	N2—C17—H17A	109.7
C5—C4—Br2	120.1 (9)	C18—C17—H17B	109.7
C3—C4—Br2	116.6 (10)	N2—C17—H17B	109.7
C4—C5—C6	119.4 (10)	H17A—C17—H17B	108.2
C4—C5—H5	120.3	O4—C18—C17	111.2 (7)
C6—C5—H5	120.3	O4—C18—H18A	109.4
C5—C6—C1	119.2 (9)	C17—C18—H18A	109.4
C5—C6—C7	118.3 (9)	O4—C18—H18B	109.4
C1—C6—C7	122.5 (8)	C17—C18—H18B	109.4
N1—C7—C6	124.0 (8)	H18A—C18—H18B	108.0
N1—C7—H7	118.0	C7—N1—C8	119.9 (8)
C6—C7—H7	118.0	C7—N1—Mn1	129.1 (7)
N1—C8—C9	107.0 (8)	C8—N1—Mn1	110.8 (6)
N1—C8—H8A	110.3	C16—N2—C17	118.0 (7)
C9—C8—H8A	110.3	C16—N2—Mn1	125.6 (6)
N1—C8—H8B	110.3	C17—N2—Mn1	115.3 (6)
C9—C8—H8B	110.3	C1—O1—Mn1	129.1 (6)
H8A—C8—H8B	108.6	C9—O2—Mn1	112.2 (6)
O2—C9—C8	107.3 (7)	C10—O3—Mn1	131.9 (6)
O2—C9—H9A	110.3	C18—O4—Mn1	105.9 (5)
C8—C9—H9A	110.3	C19—O5—H5A	115.3
O2—C9—H9B	110.3	H1WA—O1W—H1WB	94.9
C8—C9—H9B	110.3		

Hydrogen-bond geometry (Å, °)

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5A···Br1[i]	0.85	3.04	3.893 (18)	179
O1W—H1WA···O5	0.85	1.52	2.19 (2)	134

Symmetry codes: (i) $x-1/4$, $-y+3/4$, $z+1/4$.

Fig. 1

Fig. 2