metal-organic compounds

μ-Fumarato-κ⁴O,O′;O″,O‴-bis[aqua(2,9-dimethyl-1,10-phenanthroline-κ²N,N)-(nitrato-κ²O,O′)manganese(II)]

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In the centrosymmetric title compound, $[Mn_2(C_4H_2O_4)(NO_3)_2(C_{14}H_{12}N_2)_2(H_2O)_2]$, each Mn atom is six-coordinate in a distorted octahedral geometry. Molecules form stacks by π–π interactions (centroid–centroid distances of 3.826, 3.708 and 3.719 Å). The water molecules act as donors to form O—H···O hydrogen bonds. Moreover, the molecules are linked into chains along the a axis by C—H···O intermolecular hydrogen bonds.

Related literature

For details of the DNA electrochemical biosensors of metal–phenanthroline complexes, see: Wang *et al.* (1996). For bond-length data, see: Allen *et al.* (1987).
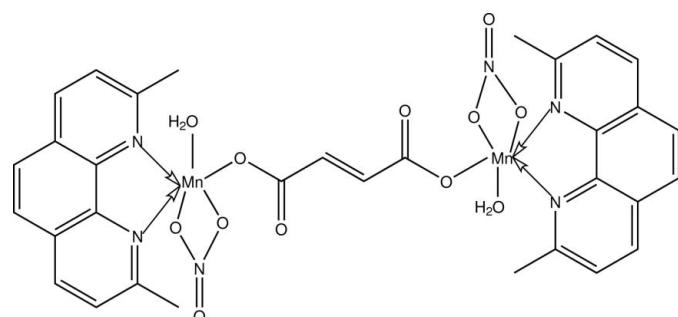
Experimental

Crystal data

$[Mn_2(C_4H_2O_4)(NO_3)_2(C_{14}H_{12}N_2)_2(H_2O)_2]$
$M_r = 800.50$
Monoclinic, $P2_1/c$
$a = 12.034$ (2) Å
$b = 9.1824$ (16) Å
$c = 16.416$ (2) Å
$\beta = 113.532$ (10)°
$V = 1663.1$ (4) Å³
$Z = 2$
Mo $K\alpha$ radiation
$\mu = 0.83$ mm⁻¹
$T = 293$ (2) K
$0.42 \times 0.33 \times 0.20$ mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.723$, $T_{max} = 0.852$
8963 measured reflections
3266 independent reflections
2951 reflections with $I > 2\sigma(I)$
$R_{int} = 0.013$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.134$
$S = 1.06$
3266 reflections
230 parameters
H-atom parameters constrained
$\Delta\rho_{max} = 0.77$ e Å⁻³
$\Delta\rho_{min} = -0.86$ e Å⁻³

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1W1···O2^i	0.82	2.23	2.978 (4)	151
O1W—H2W1···O4^{ii}	0.82	1.87	2.677 (3)	170
C6—H6A···O4^{iii}	0.93	2.57	3.353 (4)	142
C9—H9A···O1^{iv}	0.93	2.56	3.439 (5)	157

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997a); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997a); molecular graphics: *SHELXTL* (Sheldrick, 1997b); software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

References

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supplementary materials

μ-Fumarato-$\kappa^4O,O';O'',O'''$-bis[aqua(2,9-dimethyl-1,10-phenanthroline-κ^2N,N)(nitrato-κ^2O,O')manganese(II)]

L. Li, H. Zhang, M.-L. Zhang and S. Bi

Comment

Metal-phenanthroline complexes are good indicators for hydridization detection in DNA electrochemical biosensors (Wang *et al.*, 1996). In our search for new indicators, the title complex was synthesized and its structure is presented here.

The binuclear manganese complex in (I) possesses a crystallographically imposed centre of symmetry (Fig. 1). Each Mn^{II} atom is six-coordinated by two N atoms from one 9,10-dimethyl-phennathroline ligand, one O atoms from water, one O atom from fumaric acid, and two O atom from nitrate anion in a distorted octahedral environment. The axial position is occupied by water molecule O atom and one N atom from 9,10-dimethyl-phennathroline ligand, with an O1W—Mn1—N1 bond angle of 167.68 (1)°.

In the crystal structure, the short interplanar distances between the phenanthroline moieties suggest strong $\pi\cdots\pi$ interactions. The distances between benzene rings are $Cg1\cdots Cg2^{iii}$ = 3.826, $Cg1\cdots Cg3^{iii}$ = 3.708 and $Cg3\cdots Cg3^{iii}$ = 3.719 Å, where $Cg1$, $Cg2$ and $Cg3$ denote the centroids of N1/C2—C5/C13, N2/C8—C12 and C5—C8/C12/C13 rings, respectively, which contribute to the crystal packing [symmetry code: (i) $-x + 1, -y, -z + 1$]. The water molecules act as donors to form O—H$\cdots$O hydrogen bonds (Table 2). Moreover, the molecules are linked into chains along the *a* axis by C6—H6A$\cdots$O4 and C9—H9A$\cdots$O1 intermolecular hydrogen bonds.

Experimental

To a solution of 2,9-dimethyl-1,10-phenanthroline (0.21 g, 1 mmol) and fumaric acid (0.058 g, 0.5 mmol) in ethanol (10 ml) was added a solution of Mn(Ac)$_2$ (0.11 g, 1 mmol) in distilled water (10 ml). The mixture was stirred and then refluxed for 2 h. The hot solution was then filtered into another flask containing ethanol-water. Brown crystals appeared over a period of one week by slow evaporation at room temperature.

Refinement

All H atoms were located in difference Fourier map. Water H atoms were refined with O1W—H1W1 and O1W—H2W1 distance restrains of 0.82 Å [1.5 U_{eq}(O)]. The remaining H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.96 Å, and with U_{iso}(H) = 1.2 U_{eq}(C) and 1.5 U_{eq}(methyl C) H atoms.

supplementary materials

Figures
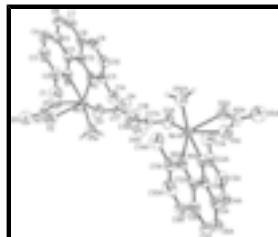
Fig. 1. The structure of the compound (I) showing 50% probability displacement ellipsoids and the atom numbering scheme. H atoms have been omitted for clarity.
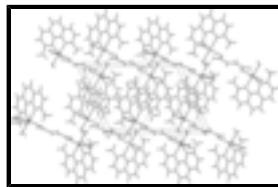

Fig. 2. A packing diagram of (I), viewed down the *b* axis. Hydrogen bonds are indicated by dashed lines.

μ-Fumarato-$\kappa^4 O,O';O'',O'''$-bis[aqua(2,9- dimethyl-1,10-phenanthroline-$\kappa^2 N,N$)(nitrato-$\kappa^2 O,O'$)manganese(II)]
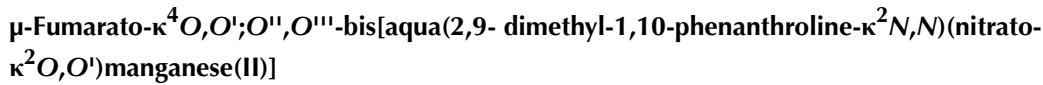
Crystal data

$[Mn_2(C_4H_2O_4)(NO_3)_2(C_{14}H_{12}N_2)_2(H_2O)_2]$	$F_{000} = 820$
$M_r = 800.50$	$D_x = 1.587$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 5923 reflections
$a = 12.034$ (2) Å	$\theta = 2.2–26.0º$
$b = 9.1824$ (16) Å	$\mu = 0.83$ mm^{-1}
$c = 16.416$ (2) Å	$T = 293$ (2) K
$\beta = 113.532$ (10)º	Block, colourless
$V = 1663.1$ (4) Å^3	$0.42 \times 0.33 \times 0.20$ mm
$Z = 2$	

Data collection

Siemens SMART 1000 CCD area-detector diffractometer	3266 independent reflections
Radiation source: fine-focus sealed tube	2951 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.013$
Detector resolution: 8.33 pixels mm^{-1}	$\theta_{max} = 26.1º$
$T = 293(2)$ K	$\theta_{min} = 1.9º$
ω scans	$h = -14 \rightarrow 13$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$k = -10 \rightarrow 11$
$T_{min} = 0.723$, $T_{max} = 0.852$	$l = -20 \rightarrow 18$
8963 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.043$	H-atom parameters constrained
$wR(F^2) = 0.134$	$w = 1/[\sigma^2(F_o^2) + (0.0858P)^2 + 1.1575P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} = 0.001$
3266 reflections	$\Delta\rho_{max} = 0.77$ e Å^{-3}
230 parameters	$\Delta\rho_{min} = -0.86$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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	$U_{iso}*/U_{eq}$
Mn1	0.17583 (3)	0.18538 (4)	0.32962 (2)	0.03045 (16)
O2	0.1578 (2)	0.4355 (3)	0.31837 (15)	0.0611 (6)
C13	0.4425 (3)	0.1767 (3)	0.43220 (19)	0.0417 (6)
C17	0.0603 (2)	0.0233 (3)	0.40796 (17)	0.0428 (6)
N1	0.3457 (2)	0.2379 (3)	0.44183 (15)	0.0428 (5)
O1	0.2395 (2)	0.3349 (2)	0.2384 (2)	0.0683 (7)
O3	0.0941 (2)	0.1538 (2)	0.41663 (15)	0.0567 (5)
N2	0.3019 (2)	0.0450 (2)	0.30670 (14)	0.0397 (5)
N3	0.2067 (2)	0.4487 (2)	0.26373 (17)	0.0484 (6)
O4	0.07726 (19)	−0.0591 (2)	0.35325 (14)	0.0544 (5)
C12	0.4195 (2)	0.0740 (3)	0.36088 (18)	0.0414 (6)
C18	0.0025 (2)	−0.0354 (3)	0.46628 (18)	0.0441 (6)
H18A	−0.0319	−0.1278	0.4539	0.066*
C2	0.3652 (3)	0.3286 (3)	0.5095 (2)	0.0511 (7)
C8	0.5185 (3)	0.0068 (3)	0.3506 (2)	0.0504 (7)
C7	0.6398 (3)	0.0422 (4)	0.4098 (3)	0.0644 (9)
H7A	0.7047	−0.0016	0.4023	0.077*
C9	0.4917 (3)	−0.0945 (4)	0.2813 (2)	0.0600 (8)

H9A	0.5539	−0.1406	0.2713	0.072*
C5	0.5638 (3)	0.2069 (3)	0.4898 (2)	0.0528 (7)
C10	0.3740 (3)	−0.1249 (3)	0.2288 (2)	0.0565 (8)
H10A	0.3560	−0.1941	0.1839	0.068*
C3	0.4854 (3)	0.3626 (4)	0.5702 (2)	0.0635 (9)
H3A	0.4976	0.4256	0.6174	0.076*
C14	0.1502 (3)	−0.0849 (4)	0.1806 (2)	0.0568 (7)
H14A	0.0965	−0.0275	0.1979	0.085*
H14B	0.1336	−0.1864	0.1843	0.085*
H14C	0.1380	−0.0613	0.1207	0.085*
C4	0.5817 (3)	0.3042 (4)	0.5597 (2)	0.0633 (9)
H4A	0.6599	0.3284	0.5989	0.076*
C11	0.2793 (3)	−0.0527 (3)	0.24174 (18)	0.0442 (6)
C1	0.2607 (4)	0.3946 (4)	0.5233 (2)	0.0686 (9)
H1A	0.1862	0.3616	0.4776	0.103*
H1B	0.2652	0.4988	0.5210	0.103*
H1C	0.2634	0.3657	0.5803	0.103*
C6	0.6609 (3)	0.1381 (4)	0.4763 (2)	0.0626 (9)
H6A	0.7404	0.1597	0.5140	0.075*
O1W	0.0156 (2)	0.1824 (2)	0.21622 (17)	0.0578 (6)
H1W1	−0.0327	0.1265	0.2237	0.069*
H2W1	−0.0054	0.2661	0.1999	0.087*
O5	0.2199 (2)	0.5687 (3)	0.23736 (19)	0.0756 (7)*

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0309 (2)	0.0322 (2)	0.0326 (2)	−0.00011 (12)	0.01727 (17)	0.00015 (13)
O2	0.0537 (12)	0.0752 (16)	0.0575 (13)	−0.0015 (11)	0.0255 (10)	0.0064 (11)
C13	0.0423 (14)	0.0407 (14)	0.0415 (14)	−0.0010 (10)	0.0162 (11)	0.0109 (10)
C17	0.0358 (12)	0.0532 (15)	0.0381 (13)	−0.0041 (11)	0.0136 (10)	0.0003 (11)
N1	0.0481 (12)	0.0426 (12)	0.0398 (11)	−0.0047 (10)	0.0198 (9)	0.0004 (9)
O1	0.0637 (15)	0.0486 (13)	0.102 (2)	0.0047 (10)	0.0423 (14)	−0.0012 (12)
O3	0.0667 (14)	0.0573 (12)	0.0567 (12)	−0.0170 (10)	0.0358 (11)	−0.0034 (10)
N2	0.0453 (12)	0.0376 (11)	0.0415 (11)	−0.0011 (9)	0.0228 (9)	0.0032 (9)
N3	0.0459 (12)	0.0379 (12)	0.0585 (14)	−0.0027 (9)	0.0178 (11)	0.0094 (10)
O4	0.0573 (12)	0.0651 (13)	0.0474 (11)	0.0009 (10)	0.0278 (9)	−0.0037 (10)
C12	0.0426 (13)	0.0400 (13)	0.0451 (13)	0.0035 (10)	0.0213 (11)	0.0132 (11)
C18	0.0422 (13)	0.0474 (15)	0.0442 (13)	−0.0074 (11)	0.0189 (11)	−0.0016 (11)
C2	0.0658 (19)	0.0458 (16)	0.0423 (15)	−0.0082 (13)	0.0223 (14)	−0.0016 (11)
C8	0.0516 (15)	0.0492 (15)	0.0602 (17)	0.0110 (12)	0.0327 (14)	0.0188 (13)
C7	0.0453 (16)	0.074 (2)	0.078 (2)	0.0169 (15)	0.0287 (15)	0.0304 (19)
C9	0.068 (2)	0.0586 (18)	0.070 (2)	0.0212 (15)	0.0448 (17)	0.0157 (16)
C5	0.0458 (15)	0.0536 (17)	0.0506 (16)	−0.0047 (13)	0.0104 (13)	0.0191 (13)
C10	0.080 (2)	0.0460 (16)	0.0567 (17)	0.0093 (15)	0.0415 (17)	0.0026 (14)
C3	0.079 (2)	0.0575 (18)	0.0435 (16)	−0.0178 (17)	0.0134 (15)	−0.0053 (14)
C14	0.0668 (19)	0.0561 (17)	0.0536 (17)	−0.0095 (15)	0.0304 (15)	−0.0129 (14)
C4	0.0570 (19)	0.064 (2)	0.0495 (18)	−0.0160 (15)	0.0014 (15)	0.0098 (14)

C11	0.0577 (16)	0.0393 (13)	0.0441 (14)	−0.0016 (12)	0.0293 (12)	0.0020 (11)
C1	0.084 (2)	0.070 (2)	0.063 (2)	−0.0124 (18)	0.0406 (19)	−0.0252 (17)
C6	0.0400 (15)	0.071 (2)	0.068 (2)	0.0019 (15)	0.0119 (14)	0.0243 (18)
O1W	0.0517 (12)	0.0504 (13)	0.0666 (14)	−0.0075 (9)	0.0186 (11)	0.0087 (9)

Geometric parameters (Å, °)

Mn1—O3	2.053 (2)	C8—C9	1.404 (5)
Mn1—O1W	2.078 (2)	C8—C7	1.430 (5)
Mn1—N2	2.136 (2)	C7—C6	1.345 (6)
Mn1—N1	2.191 (2)	C7—H7A	0.9300
Mn1—O2	2.307 (3)	C9—C10	1.361 (5)
Mn1—O1	2.372 (3)	C9—H9A	0.9300
O2—N3	1.260 (3)	C5—C4	1.401 (5)
C13—N1	1.358 (4)	C5—C6	1.422 (5)
C13—C5	1.415 (4)	C10—C11	1.406 (4)
C13—C12	1.441 (4)	C10—H10A	0.9300
C17—O3	1.255 (4)	C3—C4	1.349 (6)
C17—O4	1.251 (3)	C3—H3A	0.9300
C17—C18	1.491 (4)	C14—C11	1.505 (4)
N1—C2	1.333 (4)	C14—H14A	0.9600
O1—N3	1.246 (3)	C14—H14B	0.9600
N2—C11	1.336 (4)	C14—H14C	0.9600
N2—C12	1.364 (3)	C4—H4A	0.9300
N3—O5	1.217 (4)	C1—H1A	0.9600
C12—C8	1.411 (4)	C1—H1B	0.9600
C18—C18[i]	1.306 (5)	C1—H1C	0.9600
C18—H18A	0.9300	C6—H6A	0.9300
C2—C3	1.425 (5)	O1W—H1W1	0.8200
C2—C1	1.493 (5)	O1W—H2W1	0.8199
O3—Mn1—O1W	95.18 (10)	C9—C8—C12	117.1 (3)
O3—Mn1—N2	127.51 (9)	C9—C8—C7	122.9 (3)
O1W—Mn1—N2	107.74 (9)	C12—C8—C7	120.0 (3)
O3—Mn1—N1	89.52 (9)	C6—C7—C8	120.8 (3)
O1W—Mn1—N1	167.68 (8)	C6—C7—H7A	119.6
N2—Mn1—N1	77.92 (9)	C8—C7—H7A	119.6
O3—Mn1—O2	98.08 (8)	C10—C9—C8	119.6 (3)
O1W—Mn1—O2	85.28 (8)	C10—C9—H9A	120.2
N2—Mn1—O2	129.58 (8)	C8—C9—H9A	120.2
N1—Mn1—O2	82.78 (9)	C13—C5—C4	116.9 (3)
O3—Mn1—O1	152.37 (9)	C13—C5—C6	120.1 (3)
O1W—Mn1—O1	81.98 (9)	C4—C5—C6	123.0 (3)
N2—Mn1—O1	78.87 (8)	C9—C10—C11	120.6 (3)
N1—Mn1—O1	88.57 (9)	C9—C10—H10A	119.7
O2—Mn1—O1	54.35 (8)	C11—C10—H10A	119.7
N3—O2—Mn1	95.62 (18)	C4—C3—C2	120.5 (3)
N1—C13—C5	123.0 (3)	C4—C3—H3A	119.8
N1—C13—C12	118.1 (2)	C2—C3—H3A	119.8
C5—C13—C12	118.9 (3)	C11—C14—H14A	109.5

O3—C17—O4	121.4 (3)	C11—C14—H14B	109.5
O3—C17—C18	119.0 (3)	H14A—C14—H14B	109.5
O4—C17—C18	119.6 (3)	C11—C14—H14C	109.5
C13—N1—C2	118.8 (3)	H14A—C14—H14C	109.5
C13—N1—Mn1	111.50 (18)	H14B—C14—H14C	109.5
C2—N1—Mn1	129.3 (2)	C3—C4—C5	119.9 (3)
N3—O1—Mn1	92.88 (18)	C3—C4—H4A	120.0
C17—O3—Mn1	106.22 (18)	C5—C4—H4A	120.0
C11—N2—C12	118.6 (2)	N2—C11—C10	121.2 (3)
C11—N2—Mn1	127.84 (19)	N2—C11—C14	119.4 (2)
C12—N2—Mn1	113.10 (17)	C10—C11—C14	119.4 (3)
O5—N3—O1	122.5 (3)	C2—C1—H1A	109.5
O5—N3—O2	120.3 (3)	C2—C1—H1B	109.5
O1—N3—O2	117.1 (2)	H1A—C1—H1B	109.5
N2—C12—C13	118.0 (2)	C2—C1—H1C	109.5
N2—C12—C8	122.9 (3)	H1A—C1—H1C	109.5
C13—C12—C8	119.1 (3)	H1B—C1—H1C	109.5
C18^i—C18—C17	123.8 (3)	C7—C6—C5	121.1 (3)
C18^i—C18—H18A	118.1	C7—C6—H6A	119.4
C17—C18—H18A	118.1	C5—C6—H6A	119.4
N1—C2—C3	120.8 (3)	Mn1—O1W—H1W1	109.5
N1—C2—C1	120.1 (3)	Mn1—O1W—H2W1	109.6
C3—C2—C1	119.1 (3)	H1W1—O1W—H2W1	119.4
O3—Mn1—O2—N3	−178.89 (17)	Mn1—O2—N3—O5	−179.0 (2)
O1W—Mn1—O2—N3	−84.32 (17)	Mn1—O2—N3—O1	1.4 (3)
N2—Mn1—O2—N3	24.9 (2)	C11—N2—C12—C13	−178.3 (2)
N1—Mn1—O2—N3	92.62 (17)	Mn1—N2—C12—C13	8.5 (3)
O1—Mn1—O2—N3	−0.82 (16)	C11—N2—C12—C8	0.9 (4)
C5—C13—N1—C2	−1.4 (4)	Mn1—N2—C12—C8	−172.3 (2)
C12—C13—N1—C2	177.4 (2)	N1—C13—C12—N2	0.4 (3)
C5—C13—N1—Mn1	172.5 (2)	C5—C13—C12—N2	179.2 (2)
C12—C13—N1—Mn1	−8.8 (3)	N1—C13—C12—C8	−178.8 (2)
O3—Mn1—N1—C13	138.51 (18)	C5—C13—C12—C8	0.0 (4)
O1W—Mn1—N1—C13	−108.9 (4)	O3—C17—C18—C18^i	−8.6 (5)
N2—Mn1—N1—C13	9.86 (17)	O4—C17—C18—C18^i	169.5 (4)
O2—Mn1—N1—C13	−123.29 (18)	C13—N1—C2—C3	0.9 (4)
O1—Mn1—N1—C13	−69.06 (18)	Mn1—N1—C2—C3	−171.7 (2)
O3—Mn1—N1—C2	−48.5 (2)	C13—N1—C2—C1	−178.3 (3)
O1W—Mn1—N1—C2	64.2 (5)	Mn1—N1—C2—C1	9.1 (4)
N2—Mn1—N1—C2	−177.1 (3)	N2—C12—C8—C9	−0.4 (4)
O2—Mn1—N1—C2	49.7 (2)	C13—C12—C8—C9	178.8 (2)
O1—Mn1—N1—C2	104.0 (2)	N2—C12—C8—C7	−180.0 (2)
O3—Mn1—O1—N3	4.9 (3)	C13—C12—C8—C7	−0.8 (4)
O1W—Mn1—O1—N3	90.76 (19)	C9—C8—C7—C6	−178.8 (3)
N2—Mn1—O1—N3	−159.3 (2)	C12—C8—C7—C6	0.7 (5)
N1—Mn1—O1—N3	−81.31 (19)	C12—C8—C9—C10	−0.9 (4)
O2—Mn1—O1—N3	0.82 (16)	C7—C8—C9—C10	178.6 (3)
O4—C17—O3—Mn1	−1.0 (3)	N1—C13—C5—C4	0.5 (4)

C18—C17—O3—Mn1	176.98 (19)	C12—C13—C5—C4	−178.2 (2)
O1W—Mn1—O3—C17	72.8 (2)	N1—C13—C5—C6	179.6 (3)
N2—Mn1—O3—C17	−44.2 (2)	C12—C13—C5—C6	0.8 (4)
N1—Mn1—O3—C17	−118.6 (2)	C8—C9—C10—C11	1.8 (5)
O2—Mn1—O3—C17	158.80 (19)	N1—C2—C3—C4	0.5 (5)
O1—Mn1—O3—C17	155.4 (2)	C1—C2—C3—C4	179.7 (3)
O3—Mn1—N2—C11	97.9 (2)	C2—C3—C4—C5	−1.3 (5)
O1W—Mn1—N2—C11	−13.5 (2)	C13—C5—C4—C3	0.8 (5)
N1—Mn1—N2—C11	177.8 (2)	C6—C5—C4—C3	−178.2 (3)
O2—Mn1—N2—C11	−112.3 (2)	C12—N2—C11—C10	0.0 (4)
O1—Mn1—N2—C11	−91.3 (2)	Mn1—N2—C11—C10	172.1 (2)
O3—Mn1—N2—C12	−89.66 (18)	C12—N2—C11—C14	−179.3 (2)
O1W—Mn1—N2—C12	158.93 (16)	Mn1—N2—C11—C14	−7.2 (4)
N1—Mn1—N2—C12	−9.73 (16)	C9—C10—C11—N2	−1.4 (4)
O2—Mn1—N2—C12	60.2 (2)	C9—C10—C11—C14	177.9 (3)
O1—Mn1—N2—C12	81.19 (17)	C8—C7—C6—C5	0.1 (5)
Mn1—O1—N3—O5	179.0 (3)	C13—C5—C6—C7	−0.9 (5)
Mn1—O1—N3—O2	−1.4 (3)	C4—C5—C6—C7	178.1 (3)

Symmetry codes: (i) −x, −y, −z+1.

Hydrogen-bond geometry (Å, °)

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O1W—H1W1⋯O2[ii]	0.82	2.23	2.978 (4)	151
O1W—H2W1⋯O4[iii]	0.82	1.87	2.677 (3)	170
C6—H6A⋯O4[iv]	0.93	2.57	3.353 (4)	142
C9—H9A⋯O1[v]	0.93	2.56	3.439 (5)	157

Symmetry codes: (ii) −x, y−1/2, −z+1/2; (iii) −x, y+1/2, −z+1/2; (iv) −x+1, −y, −z+1; (v) −x+1, y−1/2, −z+1/2.

Fig. 1

Fig. 2