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(Acetylacetonato-κ^2O,O')aqua[salicylaldehyde nicotinoylhydrazonato(2−)-κ^3O,N,O']manganese(III)

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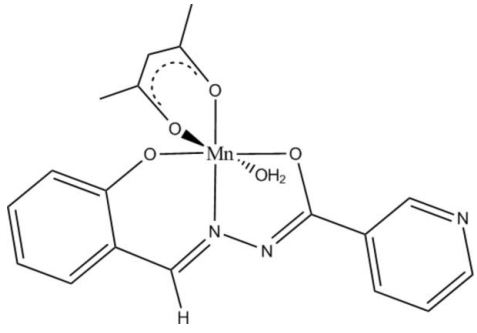
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.039; wR factor = 0.105; data-to-parameter ratio = 17.1.

The Mn^{III} atom in the title complex, $[Mn(C_{13}H_9N_3O_2)(C_5H_7O_2)(H_2O)]$, is coordinated by three donors from a dianionic ligand, salicylaldehyde nicotylhydrazone, two O atoms from an acetylacetonate anion and a water molecule in a distorted octahedral geometry. There is an extended two-dimensional supramolecular motif resulting from O—H···N hydrogen bonds between the coordinated water molecule and a hydrazine N or pyridine N atom, and from C—H···O hydrogen bonds between a CH group and the phenolate O atom.

Related literature

For general background, see: Janiak (2003); Kitagawa *et al.* (2004); Graham & Pike (2000); Niu *et al.* (2005); Adams *et al.* (2000); Ranford *et al.* (1998); Batten & Robson (1998); Hagrman *et al.* (1999). For related structures, see: Kessissoglou *et al.* (2002); Sailaja *et al.* (2003); Zhang *et al.* (2001); Clérac *et al.* (2002); Mitra *et al.* (2006); Hoshino *et al.* (2003); Nakamura *et al.* (2001); Liu *et al.* (2001).



Experimental

Crystal data

$[Mn(C_{13}H_9N_3O_2)(C_5H_7O_2)(H_2O)]$
M_r = 411.29
Monoclinic, $P2_1/c$
a = 17.462 (2) Å
b = 9.5286 (18) Å
c = 11.529 (3) Å
β = 106.798 (5)°
V = 1836.4 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.75 mm^{-1}
T = 293 (2) K
0.58 × 0.49 × 0.10 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Absorption correction: multi-scan (*TEXRAY*; Molecular Structure Corporation, 1999)
T_{min} = 0.598, T_{max} = 0.932
17468 measured reflections
4203 independent reflections
3380 reflections with $I > 2\sigma(I)$
R_{int} = 0.047

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.105
S = 1.06
4203 reflections
246 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5B···N2^{i}	0.90	2.14	3.013 (2)	164
O5—H5C···N1^{ii}	0.88	1.92	2.784 (3)	165
C7—H7A···O2^{iii}	0.93	2.27	3.160 (2)	160
C13—H13A···O2^{iii}	0.93	2.59	3.390 (3)	145

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

Data collection: *TEXRAY* (Molecular Structure Corporation, 1999); cell refinement: *TEXRAY*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1999); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEX* (McArdle, 1995); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2362).

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(Acetylacetonato-κ^2O,O')aqua[salicylaldehyde nicotinoylhydrazonato(2−)-κ^3O,N,O']manganese(III)

Zeng-You Wang, Shi-Xiong Liu and Zhong-Wu Fu

S1. Comment

Metal-organic supramolecular complexes with various fascinating topologies have been studied widely for their versatile chemical and physical properties and potential applications as functional materials (Janiak, 2003; Kitagawa *et al.*, 2004). Self-assembly based on molecular building blocks has become an effective approach to construct these functional materials. In the development of supramolecular chemistry, hydrogen-bonding plays an important role in selfassembling multi-dimensional metal-organic supramolecular frameworks or networks (Graham & Pike, 2000). Some nicotylhydrazone derivatives and aroylhydrazone derivatives had led to a number of complexes with multidimensional structures or extended multidimensional structures. (Niu *et al.*, 2005; Adams *et al.*, 2000; Ranford *et al.*, 1998). The syntheses and characterization of these complexes has been an area of rapid growth in recent years.(Batten & Robson, 1998; Hagrman *et al.*, 1999). Herein, we report the synthesis and crystal structure of the title manganese(III) complex.

Complex (I) crystallizes in the space group $P2_1/c$. The crystal structure reveals that complex (I) consists of a neutral $Mn(C_{13}H_9N_3O_2)(C_5H_7O_2)(H_2O)$ unit. As shown in Fig. 1, compound (I) is composed of one salicylaldehyde-nicotylhydrazone dianion, one acetylacetone anion, one coordinated water molecule and one Mn^{III} cations. The manganese(III) atom exists in a distorted octahedral environment defined by one carbonyl oxygen atom O1, one hydrazine nitrogen atom N3 and one phenolate oxygen atom O2 of the deprotonated Schiff base ligand, the two oxygen atoms (O3 and O4) of the acetylacetonate (acac) anion and one oxygen atom O5 of the coordinated water molecule. O1, N3, O2 and O4 atoms are located in the equatorial plane, while O3 and O5 occupy the axial positions. The bond length of Mn1—O1 (carbonyl oxygen) in complex (I) is 1.935 (2) Å, while the corresponding values in the similar known complexes are between 1.959 (2) and 1.971 (1)Å (Kessissoglou *et al.*, 2002). The bond length of Mn1—O2(phenolic oxygen) in complex (I) is 1.886 (2) Å, while the corresponding values in the known complexes are between 1.844 (3) and 1.923 (3)Å (Sailaja *et al.*, 2003; Zhang *et al.*, 2001; Clérac *et al.*, 2002) The bond length of Mn1—N3(hydrazone nitrogen) in complex (I) is 1.972 (2) Å, which is similar to the corresponding values 1.968 (4)–1.999 (7)Å of the known complexes (Mitra *et al.*, 2006; Hoshino *et al.*, 2003). The bond distance of axial Mn1—O3 ($acac^-$) (2.122 (2) Å) is 0.20 Å longer than that of the equatorial Mn1—O4($acac^-$) (1.920 (1) Å), O3 and O4 being from the same $acac^-$ ligand. This typical Jahn-Teller elongation along the *z* axis of the manganese(III) ion was also observed in some manganese(III) compounds (Nakamura *et al.*, 2001; Liu *et al.*, 2001). The title complex molecules are linked by hydrogen bonds (Table 1) into a two-dimensional supramolecular network. As illustrated in Fig. 2, one complex molecule connected to two neighboring complex molecules *via* hydrogen bonds of O—H(H_2O)···N(hydrazine) type and C—H···O(phenolate) type, resulting in an extended chain along the *c* axis. These hydrogen bonds are marked with green color in Fig. 2. A t the same time, the neighboring extended chains are combined by *O*—*H*(H_2O)···*N*(pyridine) hydrogen bonds with pink color, forming an extended two-dimensional network.

S2. Experimental

A DMF solution of salicylaldehyde-nicotylhydrazone ligand (24 mg, 0.1 mmol) and a methanol solution of $Mn(acac)_3$ (35 mg, 0.1 mmol) were mixed and stirred for 3 h. The resulting solution was then left for aerial evaporation at room temperature. Black block crystals of (I), suitable in size for single-crystal X-ray diffraction, appeared after two weeks.

S3. Refinement

Water H atoms and the H atom attached to C16 in $acac^-$ group were founded in a difference Fourier map, and then allowed to ride on the O and C16 atoms with U_{iso}=1.5U_{eq}(O) and U_{iso}=1.2U_{eq}(C), respectively. The other H atoms were placed in idealized positions and treated as riding with C—H = 0.93 Å, U_{iso}(H) = 1.2U_{eq}(C) for aromatic and 0.96 Å, U_{iso}(H) = 1.5U_{eq}(C) for CH_3 atoms.

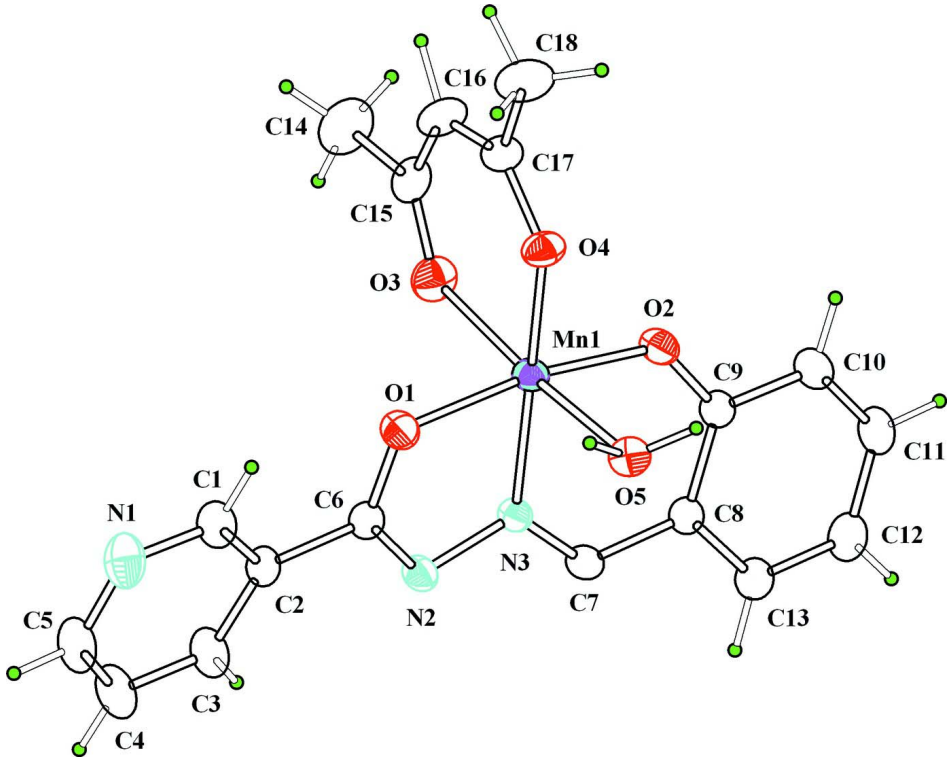

Figure 1

The molecular structure of (I), with the atom-numbering scheme and 30% probability displacement ellipsoids.

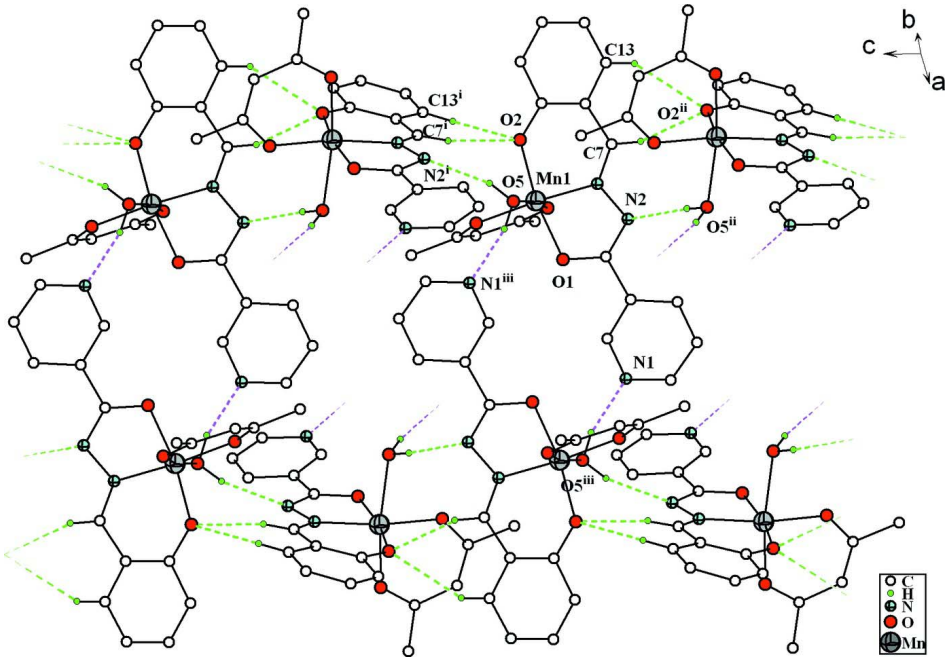

Figure 2

A plot illustrating extended two-dimensional structure of (I), hydrogen bonds are drawn as dashed lines. H atoms not-involved in hydrogen bonding have been omitted.

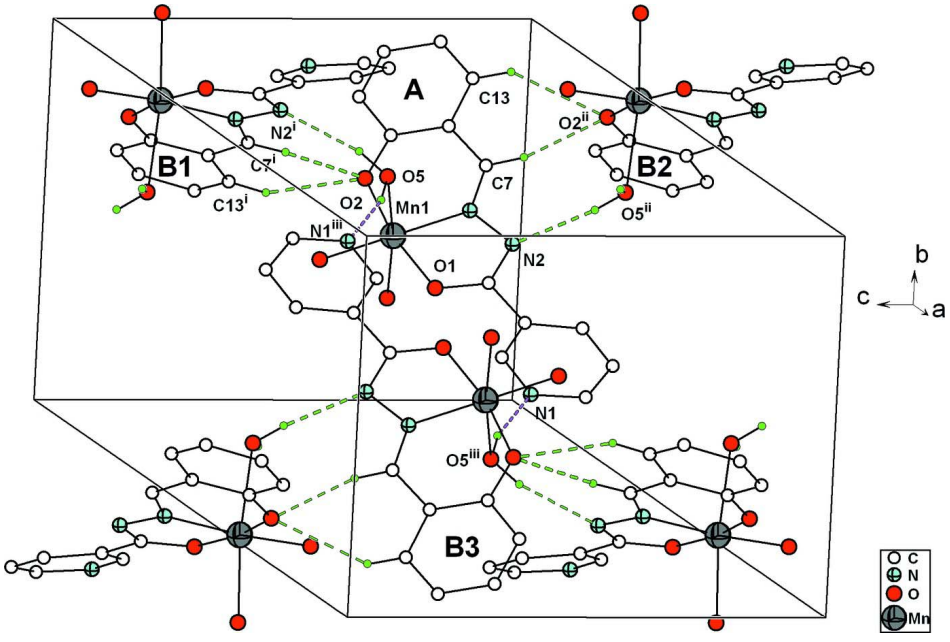

Figure 3

The extended two-dimensional net-work connected by hydrogen bonds, which are drawn as dashed lines. H atoms not-involved in hydrogen bonding have been omitted.

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Crystal data

$[Mn(C_{13}H_9N_3O_2)(C_5H_7O_2)(H_2O)]$
$M_r = 411.29$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 17.462$ (2) Å
$b = 9.5286$ (18) Å
$c = 11.529$ (3) Å
$\beta = 106.798$ (5)°
$V = 1836.4$ (6) Å^3
$Z = 4$
$F(000) = 848$
$D_x = 1.488$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 17468 reflections
$\theta = 3.2$–$27.5°$
$\mu = 0.75$ mm^{-1}
$T = 293$ K
Block, black
0.58 × 0.49 × 0.10 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*TEXRAY*; Molecular Structure Corporation, 1999)
$T_{min} = 0.598$, $T_{max} = 0.932$
17468 measured reflections
4203 independent reflections
3380 reflections with $I > 2\sigma(I)$
$R_{int} = 0.047$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.2°$
$h = -22 \rightarrow 22$
$k = -12 \rightarrow 12$
$l = -12 \rightarrow 14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.105$
$S = 1.06$
4203 reflections
246 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.056P)^2 + 0.2426P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.40$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ e Å^{-3}

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	0.249798 (18)	0.57337 (3)	0.43657 (2)	0.03214 (11)
O1	0.34284 (9)	0.48904 (15)	0.40574 (12)	0.0409 (3)
O2	0.15564 (9)	0.67021 (14)	0.43678 (12)	0.0384 (3)

O3	0.19055 (11)	0.37673 (16)	0.40212 (15)	0.0509 (4)
O4	0.27874 (10)	0.52725 (15)	0.60578 (12)	0.0419 (3)
O5	0.32467 (9)	0.77095 (14)	0.50465 (13)	0.0405 (3)
H5B	0.3069	0.8261	0.5550	0.061*
H5C	0.3709	0.7356	0.5472	0.061*
N1	0.53617 (13)	0.3198 (2)	0.3250 (2)	0.0579 (5)
N2	0.29071 (10)	0.57484 (16)	0.21251 (15)	0.0343 (4)
N3	0.23512 (10)	0.63091 (16)	0.26725 (13)	0.0302 (3)
C1	0.47353 (14)	0.3815 (2)	0.3467 (2)	0.0463 (5)
H1B	0.4732	0.3895	0.4269	0.056*
C2	0.40938 (13)	0.43433 (19)	0.25884 (19)	0.0373 (4)
C3	0.41031 (18)	0.4214 (3)	0.1385 (2)	0.0572 (7)
H3A	0.3677	0.4534	0.0753	0.069*
C4	0.4756 (2)	0.3604 (3)	0.1159 (3)	0.0716 (9)
H4A	0.4781	0.3518	0.0367	0.086*
C5	0.53676 (18)	0.3125 (3)	0.2098 (3)	0.0658 (7)
H5A	0.5810	0.2730	0.1928	0.079*
C6	0.34313 (12)	0.50249 (19)	0.29342 (17)	0.0343 (4)
C7	0.18497 (12)	0.7207 (2)	0.20497 (17)	0.0337 (4)
H7A	0.1885	0.7435	0.1283	0.040*
C8	0.12392 (12)	0.78839 (19)	0.24536 (17)	0.0332 (4)
C9	0.11051 (12)	0.75715 (18)	0.35741 (17)	0.0331 (4)
C10	0.04471 (14)	0.8204 (2)	0.3828 (2)	0.0440 (5)
H10A	0.0341	0.8006	0.4556	0.053*
C11	−0.00431 (15)	0.9108 (2)	0.3023 (2)	0.0490 (6)
H11A	−0.0482	0.9499	0.3207	0.059*
C12	0.01056 (15)	0.9450 (2)	0.1939 (2)	0.0511 (6)
H12A	−0.0224	1.0081	0.1407	0.061*
C13	0.07387 (14)	0.8852 (2)	0.1662 (2)	0.0436 (5)
H13A	0.0843	0.9086	0.0939	0.052*
C14	0.1360 (2)	0.1594 (3)	0.4358 (3)	0.0801 (9)
H14A	0.1246	0.1535	0.3493	0.120*
H14B	0.0867	0.1641	0.4569	0.120*
H14C	0.1655	0.0779	0.4724	0.120*
C15	0.18474 (15)	0.2891 (2)	0.4808 (2)	0.0499 (6)
C16	0.22056 (18)	0.3043 (2)	0.6060 (2)	0.0586 (7)
H16A	0.2100	0.2300	0.6570	0.070*
C17	0.26526 (15)	0.4158 (2)	0.6601 (2)	0.0449 (5)
C18	0.3042 (2)	0.4170 (3)	0.7940 (2)	0.0728 (9)
H18A	0.3610	0.4275	0.8098	0.109*
H18B	0.2930	0.3304	0.8284	0.109*
H18C	0.2836	0.4940	0.8297	0.109*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.03229 (18)	0.03714 (17)	0.02695 (16)	0.00286 (12)	0.00849 (12)	0.00486 (11)
O1	0.0407 (9)	0.0492 (8)	0.0326 (7)	0.0147 (7)	0.0103 (6)	0.0088 (6)

O2	0.0359 (8)	0.0488 (8)	0.0325 (7)	0.0063 (6)	0.0132 (6)	0.0050 (6)
O3	0.0556 (11)	0.0453 (8)	0.0487 (9)	−0.0095 (7)	0.0102 (8)	−0.0057 (7)
O4	0.0515 (10)	0.0417 (7)	0.0303 (7)	−0.0014 (7)	0.0081 (6)	0.0076 (6)
O5	0.0358 (8)	0.0441 (7)	0.0390 (7)	−0.0016 (6)	0.0068 (6)	0.0023 (6)
N1	0.0410 (12)	0.0618 (12)	0.0654 (13)	0.0187 (10)	0.0068 (10)	−0.0026 (11)
N2	0.0316 (9)	0.0408 (8)	0.0320 (8)	0.0060 (7)	0.0114 (7)	0.0021 (7)
N3	0.0281 (9)	0.0343 (7)	0.0285 (7)	0.0030 (6)	0.0085 (7)	0.0023 (6)
C1	0.0413 (13)	0.0515 (11)	0.0425 (12)	0.0088 (10)	0.0065 (10)	−0.0033 (10)
C2	0.0362 (11)	0.0349 (9)	0.0403 (11)	0.0063 (8)	0.0105 (9)	−0.0002 (8)
C3	0.0633 (17)	0.0670 (15)	0.0411 (12)	0.0315 (13)	0.0148 (12)	0.0041 (11)
C4	0.082 (2)	0.0829 (19)	0.0559 (15)	0.0405 (17)	0.0301 (15)	0.0051 (14)
C5	0.0575 (18)	0.0671 (15)	0.0785 (19)	0.0266 (13)	0.0286 (15)	−0.0014 (14)
C6	0.0331 (11)	0.0338 (9)	0.0349 (10)	0.0011 (8)	0.0083 (8)	−0.0006 (8)
C7	0.0321 (10)	0.0404 (9)	0.0286 (9)	0.0020 (8)	0.0085 (8)	0.0036 (8)
C8	0.0309 (10)	0.0344 (9)	0.0334 (9)	0.0025 (8)	0.0079 (8)	0.0000 (8)
C9	0.0298 (10)	0.0333 (9)	0.0350 (9)	−0.0024 (7)	0.0077 (8)	−0.0033 (8)
C10	0.0406 (13)	0.0499 (11)	0.0453 (11)	0.0033 (10)	0.0187 (10)	−0.0017 (9)
C11	0.0386 (13)	0.0503 (12)	0.0609 (14)	0.0122 (10)	0.0188 (11)	−0.0025 (11)
C12	0.0458 (14)	0.0495 (12)	0.0545 (14)	0.0175 (10)	0.0088 (11)	0.0057 (10)
C13	0.0438 (13)	0.0443 (10)	0.0417 (11)	0.0098 (9)	0.0108 (10)	0.0044 (9)
C14	0.083 (2)	0.0524 (14)	0.104 (2)	−0.0233 (15)	0.026 (2)	−0.0089 (15)
C15	0.0479 (14)	0.0353 (10)	0.0687 (15)	−0.0019 (9)	0.0199 (12)	−0.0020 (10)
C16	0.0756 (19)	0.0434 (11)	0.0589 (15)	−0.0054 (12)	0.0228 (14)	0.0148 (11)
C17	0.0494 (14)	0.0463 (11)	0.0412 (11)	0.0074 (10)	0.0166 (10)	0.0130 (9)
C18	0.101 (3)	0.0729 (17)	0.0410 (14)	−0.0015 (16)	0.0143 (15)	0.0194 (12)

Geometric parameters (Å, º)

Mn1—O2	1.8860 (14)	C5—H5A	0.9300
Mn1—O4	1.9195 (14)	C7—C8	1.434 (3)
Mn1—O1	1.9354 (14)	C7—H7A	0.9300
Mn1—N3	1.9718 (16)	C8—C9	1.410 (3)
Mn1—O3	2.1216 (16)	C8—C13	1.410 (3)
Mn1—O5	2.2971 (14)	C9—C10	1.401 (3)
O1—C6	1.303 (2)	C10—C11	1.370 (3)
O2—C9	1.315 (2)	C10—H10A	0.9300
O3—C15	1.259 (3)	C11—C12	1.388 (3)
O4—C17	1.289 (2)	C11—H11A	0.9300
O5—H5B	0.9021	C12—C13	1.361 (3)
O5—H5C	0.8812	C12—H12A	0.9300
N1—C1	1.327 (3)	C13—H13A	0.9300
N1—C5	1.333 (4)	C14—C15	1.505 (3)
N2—C6	1.300 (3)	C14—H14A	0.9600
N2—N3	1.407 (2)	C14—H14B	0.9600
N3—C7	1.285 (2)	C14—H14C	0.9600
C1—C2	1.370 (3)	C15—C16	1.405 (4)
C1—H1B	0.9300	C16—C17	1.358 (3)
C2—C3	1.398 (3)	C16—H16A	0.9713

C2—C6	1.478 (3)	C17—C18	1.497 (4)
C3—C4	1.370 (4)	C18—H18A	0.9600
C3—H3A	0.9300	C18—H18B	0.9600
C4—C5	1.361 (4)	C18—H18C	0.9600
C4—H4A	0.9300		

O2—Mn1—O4	94.83 (6)	O1—C6—C2	116.94 (17)
O2—Mn1—O1	169.05 (6)	N3—C7—C8	124.64 (17)
O4—Mn1—O1	95.92 (6)	N3—C7—H7A	117.7
O2—Mn1—N3	90.07 (6)	C8—C7—H7A	117.7
O4—Mn1—N3	172.13 (7)	C9—C8—C13	119.71 (18)
O1—Mn1—N3	79.02 (6)	C9—C8—C7	122.60 (17)
O2—Mn1—O3	93.11 (7)	C13—C8—C7	117.64 (17)
O4—Mn1—O3	87.65 (6)	O2—C9—C10	119.25 (17)
O1—Mn1—O3	89.36 (7)	O2—C9—C8	123.10 (17)
N3—Mn1—O3	98.24 (6)	C10—C9—C8	117.64 (18)
O2—Mn1—O5	90.51 (6)	C11—C10—C9	121.3 (2)
O4—Mn1—O5	83.32 (6)	C11—C10—H10A	119.4
O1—Mn1—O5	88.73 (6)	C9—C10—H10A	119.4
N3—Mn1—O5	90.50 (6)	C10—C11—C12	121.0 (2)
O3—Mn1—O5	170.53 (6)	C10—C11—H11A	119.5
C6—O1—Mn1	112.73 (12)	C12—C11—H11A	119.5
C9—O2—Mn1	130.91 (12)	C13—C12—C11	119.3 (2)
C15—O3—Mn1	125.99 (15)	C13—C12—H12A	120.3
C17—O4—Mn1	130.61 (15)	C11—C12—H12A	120.3
Mn1—O5—H5B	115.4	C12—C13—C8	121.0 (2)
Mn1—O5—H5C	102.5	C12—C13—H13A	119.5
H5B—O5—H5C	107.1	C8—C13—H13A	119.5
C1—N1—C5	117.0 (2)	C15—C14—H14A	109.5
C6—N2—N3	108.27 (16)	C15—C14—H14B	109.5
C7—N3—N2	116.70 (15)	H14A—C14—H14B	109.5
C7—N3—Mn1	127.66 (13)	C15—C14—H14C	109.5
N2—N3—Mn1	115.42 (11)	H14A—C14—H14C	109.5
N1—C1—C2	124.5 (2)	H14B—C14—H14C	109.5
N1—C1—H1B	117.8	O3—C15—C16	124.6 (2)
C2—C1—H1B	117.8	O3—C15—C14	116.8 (2)
C1—C2—C3	117.4 (2)	C16—C15—C14	118.6 (2)
C1—C2—C6	119.89 (19)	C17—C16—C15	125.3 (2)
C3—C2—C6	122.7 (2)	C17—C16—H16A	118.4
C4—C3—C2	118.3 (2)	C15—C16—H16A	116.2
C4—C3—H3A	120.8	O4—C17—C16	125.7 (2)
C2—C3—H3A	120.8	O4—C17—C18	113.7 (2)
C5—C4—C3	119.7 (2)	C16—C17—C18	120.6 (2)
C5—C4—H4A	120.1	C17—C18—H18A	109.5
C3—C4—H4A	120.1	C17—C18—H18B	109.5
N1—C5—C4	123.0 (2)	H18A—C18—H18B	109.5
N1—C5—H5A	118.5	C17—C18—H18C	109.5
C4—C5—H5A	118.5	H18A—C18—H18C	109.5

N2—C6—O1	124.14 (18)	H18B—C18—H18C	109.5
N2—C6—C2	118.88 (17)		
O2—Mn1—O1—C6	−10.2 (4)	C3—C4—C5—N1	1.1 (5)
O4—Mn1—O1—C6	−179.52 (14)	N3—N2—C6—O1	−1.1 (3)
N3—Mn1—O1—C6	−5.61 (13)	N3—N2—C6—C2	−178.91 (16)
O3—Mn1—O1—C6	92.91 (14)	Mn1—O1—C6—N2	5.6 (3)
O5—Mn1—O1—C6	−96.37 (14)	Mn1—O1—C6—C2	−176.53 (13)
O4—Mn1—O2—C9	164.44 (17)	C1—C2—C6—N2	167.1 (2)
O1—Mn1—O2—C9	−4.9 (4)	C3—C2—C6—N2	−12.4 (3)
N3—Mn1—O2—C9	−9.40 (17)	C1—C2—C6—O1	−10.8 (3)
O3—Mn1—O2—C9	−107.66 (17)	C3—C2—C6—O1	169.6 (2)
O5—Mn1—O2—C9	81.10 (17)	N2—N3—C7—C8	179.71 (17)
O2—Mn1—O3—C15	−92.8 (2)	Mn1—N3—C7—C8	−6.0 (3)
O4—Mn1—O3—C15	1.9 (2)	N3—C7—C8—C9	−3.1 (3)
O1—Mn1—O3—C15	97.8 (2)	N3—C7—C8—C13	179.7 (2)
N3—Mn1—O3—C15	176.63 (19)	Mn1—O2—C9—C10	−177.10 (14)
O2—Mn1—O4—C17	95.0 (2)	Mn1—O2—C9—C8	4.3 (3)
O1—Mn1—O4—C17	−87.0 (2)	C13—C8—C9—O2	−178.60 (19)
O3—Mn1—O4—C17	2.1 (2)	C7—C8—C9—O2	4.2 (3)
O5—Mn1—O4—C17	−175.0 (2)	C13—C8—C9—C10	2.8 (3)
C6—N2—N3—C7	171.09 (17)	C7—C8—C9—C10	−174.42 (19)
C6—N2—N3—Mn1	−3.94 (19)	O2—C9—C10—C11	−179.5 (2)
O2—Mn1—N3—C7	10.08 (18)	C8—C9—C10—C11	−0.8 (3)
O1—Mn1—N3—C7	−169.04 (18)	C9—C10—C11—C12	−1.3 (4)
O3—Mn1—N3—C7	103.23 (18)	C10—C11—C12—C13	1.4 (4)
O5—Mn1—N3—C7	−80.43 (18)	C11—C12—C13—C8	0.6 (4)
O2—Mn1—N3—N2	−175.53 (13)	C9—C8—C13—C12	−2.7 (3)
O1—Mn1—N3—N2	5.34 (12)	C7—C8—C13—C12	174.6 (2)
O3—Mn1—N3—N2	−82.38 (13)	Mn1—O3—C15—C16	−3.4 (4)
O5—Mn1—N3—N2	93.96 (13)	Mn1—O3—C15—C14	176.78 (19)
C5—N1—C1—C2	1.7 (4)	O3—C15—C16—C17	1.0 (4)
N1—C1—C2—C3	0.2 (4)	C14—C15—C16—C17	−179.2 (3)
N1—C1—C2—C6	−179.3 (2)	Mn1—O4—C17—C16	−4.8 (4)
C1—C2—C3—C4	−1.6 (4)	Mn1—O4—C17—C18	175.20 (19)
C6—C2—C3—C4	178.0 (2)	C15—C16—C17—O4	3.3 (4)
C2—C3—C4—C5	1.0 (5)	C15—C16—C17—C18	−176.7 (3)
C1—N1—C5—C4	−2.4 (5)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5*B*···N2^{i}	0.90	2.14	3.013 (2)	164
O5—H5*C*···N1^{ii}	0.88	1.92	2.784 (3)	165
C7—H7*A*···O2^{iii}	0.93	2.27	3.160 (2)	160
C13—H13*A*···O2^{iii}	0.93	2.59	3.390 (3)	145

Symmetry codes: (i) *x*, −*y*+3/2, *z*+1/2; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) *x*, −*y*+3/2, *z*−1/2.