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## Structure Reports

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# Azido(methanol)[*N,N'*-(*o*-phenylene)-bis(pyridine-2-carboxamidato)]-manganese(III)

Yuhua Feng<sup>a,b</sup> and Daizheng Liao<sup>a\*</sup>

<sup>a</sup>Department of Chemistry, Nankai University, Tianjin 300071, People's Republic of China, and <sup>b</sup>Department of Chemistry, Tonghua Teachers College, Tonghua 134002, People's Republic of China

Correspondence e-mail: coord@nankai.edu.cn

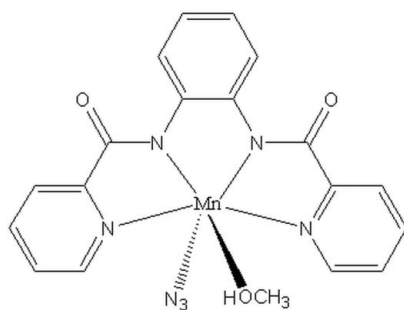
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Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.006$  Å;  $R$  factor = 0.060;  $wR$  factor = 0.159; data-to-parameter ratio = 12.7.

In the title complex,  $[\text{Mn}(\text{C}_{18}\text{H}_{12}\text{N}_4\text{O}_2)(\text{N}_3)(\text{CH}_4\text{O})]$ , the  $\text{Mn}^{\text{III}}$  ion is in a distorted octahedral coordination environment. In the crystal structure, intermolecular  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds connect molecules into centrosymmetric dimers.

## Related literature

For general background, see: Ni, Kou, Zheng *et al.* (2005); Ni, Kou, Zhang *et al.* (2005); Ni, Kou, Zhao *et al.* (2005); Colacio *et al.* (2005); Dominguez-Vera *et al.* (2005); For bond-length data, see: Havranek *et al.* (1999); Lin *et al.* (2003); Liang *et al.* (2007). For related literature, see: Lecren *et al.* (2007); Zhang *et al.* (2006).



## Experimental

### Crystal data

 $[\text{Mn}(\text{C}_{18}\text{H}_{12}\text{N}_4\text{O}_2)(\text{N}_3)(\text{CH}_4\text{O})]$ 
 $M_r = 445.33$ Monoclinic,  $P2_1/c$  $a = 12.115$  (2) Å $b = 9.4987$  (19) Å $c = 16.748$  (3) Å $\beta = 95.94$  (3)° $V = 1917.0$  (6) Å<sup>3</sup> $Z = 4$ Mo  $K\alpha$  radiation $\mu = 0.73$  mm<sup>-1</sup> $T = 293$  (2) K

0.14 × 0.14 × 0.14 mm

### Data collection

Rigaku Saturn diffractometer  
Absorption correction: multi-scan  
(Jacobson, 1998)

 $T_{\min} = 0.905$ ,  $T_{\max} = 0.905$ 

15658 measured reflections  
3406 independent reflections  
2957 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.061$

### Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.060$  $wR(F^2) = 0.159$  $S = 1.07$ 

3406 reflections

269 parameters

7 restraints

H atoms treated by a mixture of independent and constrained refinement

 $\Delta\rho_{\text{max}} = 0.47$  e Å<sup>-3</sup> $\Delta\rho_{\text{min}} = -0.52$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O3}-\text{H}\cdots\text{O2}^i$	0.849 (10)	1.88 (2)	2.696 (4)	162 (6)

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

Data collection: *CrystalClear* (Rigaku, 2001); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; 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: *CrystalStructure* (Rigaku, 2001).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2555).

## References

- Bruker (1997). *SHELXTL*, Bruker Axis Inc., Madison, Wisconsin, USA.
- Colacio, E., Costes, J. P., Dominguez-Vera, J. M., Maimoun, I. B. & Suarez-Varela, J. (2005). *Chem. Commun.* pp. 534–536.
- Dominguez-Vera, J. M., Suarez-Varela, J., Maimoun, I. B. & Colacio, E. (2005). *Eur. J. Inorg. Chem.* pp. 1907–1912.
- Havranek, M., Singh, A. & Sames, D. (1999). *J. Am. Chem. Soc.* **121**, 8965–8966.
- Jacobson, R. (1998). Private communication to the Rigaku Corporation.
- Lecren, L., Wernsdorfer, W., Li, Y. G., Vindigni, A., Miyasaka, H. & Clerac, R. (2007). *J. Am. Chem. Soc.* **129**, 5045–5051.
- Liang, L., Qu, Y.-Y., Yang, L. & Zhou, X.-G. (2007). *Acta Cryst.* **E63**, m1503–m1505.
- Lin, J., Tu, C., Lin, H., Jiang, P. J., Ding, J. & Guo, Z. J. (2003). *Inorg. Chem. Commun.* **6**, 262–265.
- Ni, Z. H., Kou, H. Z., Zhang, L. F., Ge, C. H., Cui, A. L., Wang, R. J., Li, Y. D. & Sato, O. (2005). *Angew. Chem. Int. Ed.* **44**, 7742–7745.
- Ni, Z. H., Kou, H. Z., Zhao, Y. H., Zheng, L., Wang, R. J., Cui, A. L. & Sato, O. (2005). *Inorg. Chem.* **44**, 2050–2059.
- Ni, Z. H., Kou, H. Z., Zheng, L., Zhao, Y. H., Zhang, L. F., Wang, R. J., Cui, A. L. & Sato, O. (2005). *Inorg. Chem.* **44**, 4728–4736.
- Rigaku (2001). *CrystalClear* (Version 13) and *CrystalStructure* (Version 3.7.0). Rigaku Corporation, Tokyo, Japan.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
- Zhang, B., Ni, Z. H., Cui, A. L. & Kou, H. Z. (2006). *New J. Chem.* **30**, 1327–1332.

## supporting information

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## Azido(methanol)[*N,N'*-(*o*-phenylene)bis(pyridine-2-carboxamidato)]manganese(III)

Yuhua Feng and Daizheng Liao

### S1. Comment

The planar tetradentate ligand bpb<sup>2-</sup>, bpb = 1,2-bis(pyridine-2-carboxamido)benzene, can coordinate four equatorial sites of six-coordinated paramagnetic cations, leaving two free axial positions to be occupied by bridging ligands. It is hence, one of the ideal candidates to act as a co-ligand for constructing expanded structures (Colacio *et al.*, 2005; Ni, Kou, Zheng *et al.*, 2005; Ni, Kou, Zhang *et al.*, 2005; Ni, Kou, Zhao *et al.*, 2005; Dominguez-Vera *et al.*, 2005; Havranek *et al.*, 1999; Lin *et al.*, 2003; Liang *et al.*, 2007; Zhang *et al.*, 2006). Mn(III) compounds, with a high-spin ground state related to the Mn(III) ion ( $S = 2$ ) and an apparent magnetic anisotropy of hexacoordinated Mn(III) centres due to Jahn–Teller distortion, usually display appealing magnetic properties (Lecren *et al.*, 2007).

We originally attempted to synthesize complexes featuring azido-bridged Mn(III) metal chains by reaction of the [Mn(III)(bpb)]<sup>2-</sup> building blocks with NaN<sub>3</sub>. But, we fortuitously obtained title compound (I), and we report herein its crystal structure.

### S2. Experimental

To a solution of [Mn(bpb)Cl(H<sub>2</sub>O)] (0.425 g, 1 mmol) in 20 ml of methanol was added a solution of NaN<sub>3</sub> (0.065 g, 1 mmol) in a minimum volume of H<sub>2</sub>O. After stirring for 30 min at room temperature, the dark brown solution was filtered and allowed to stand for about one month at room temperature to form dark brown crystals of 1, [Mn(bpb)(N<sub>3</sub>)(CH<sub>3</sub>OH)]. The crystals were collected by suction filtration, washed with a minimum amount of water, and dried *in vacuo*. Elemental analysis: C<sub>19</sub>H<sub>16</sub>MnN<sub>7</sub>O<sub>2</sub>, Calcd: C 51.25%, H 3.62%, N 22.02%, Found: C 51.68%, H 3.87%, N 22.35%. IR (KBr): 2035 cm<sup>-1</sup> (N<sub>3</sub><sup>-</sup>), 1622 cm<sup>-1</sup> (C=O).

### S3. Refinement

The H atom bonded to the O atom was located in a difference map and refined isotropically with a distance restraints of O—H = 0.84 (2) Å. Other H atoms were positioned geometrically and refined using a riding model (including free rotation about the ethanol C—C bond), with C—H = 0.93–0.96 Å and with  $U_{\text{iso}}(\text{H}) = 1.2$  (1.5 for methyl group) times  $U_{\text{eq}}(\text{C})$ .

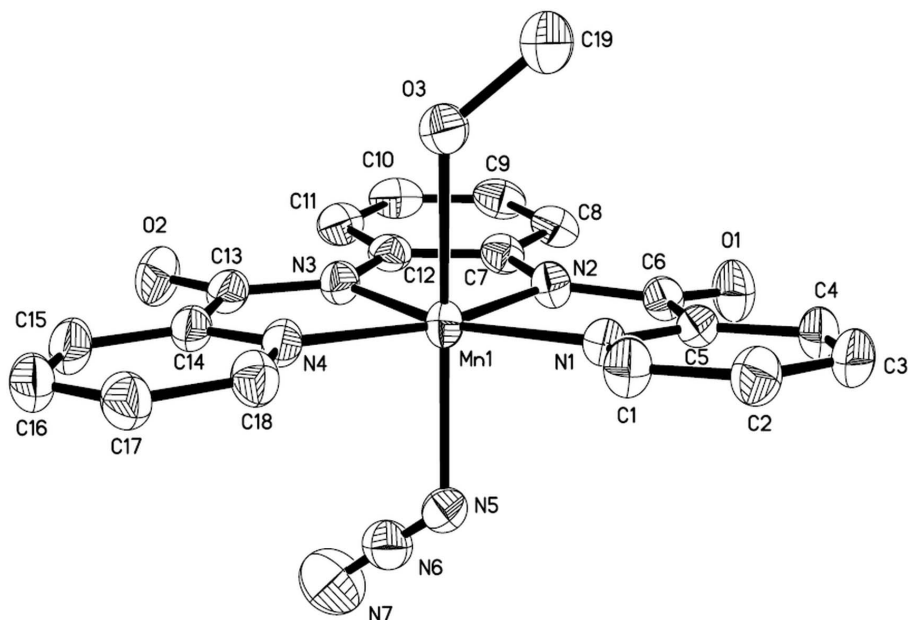


Figure 1

The molecular structure with atom labels and 30% probability displacement ellipsoids for non-H atoms.

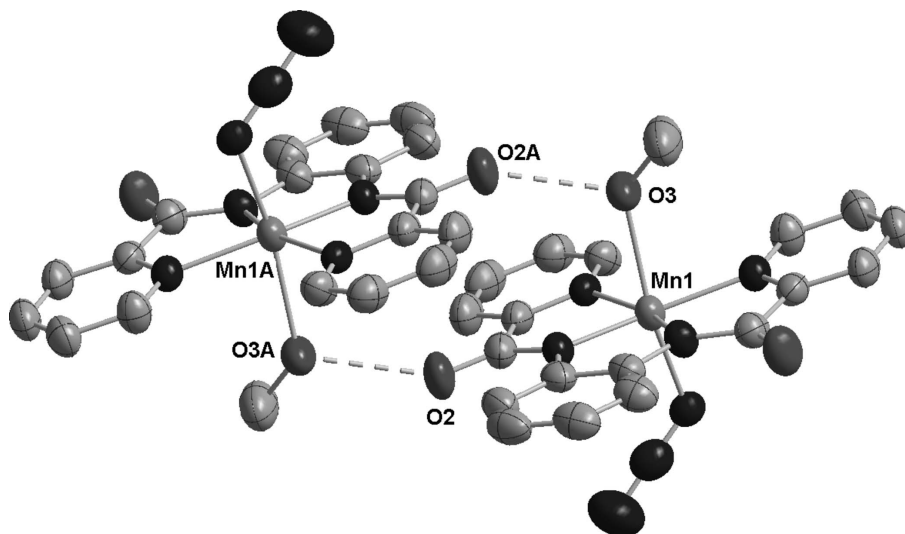


Figure 2

A centrosymmetric hydrogen-bonded dimer with the donor-acceptor distances shown as dashed lines [symmetry code: (A)  $-x, -y + 1, -z$ ].

### Azido(methanol)[*N,N'*-(*o*-phenylene)bis(pyridine-2-carboxamidato)]manganese(III)

#### Crystal data

$[\text{Mn}(\text{C}_{18}\text{H}_{12}\text{N}_4\text{O}_2)(\text{N}_3)(\text{CH}_4\text{O})]$

$M_r = 445.33$

Monoclinic,  $P2_1/c$

Hall symbol:  $-P\ 2_1/c$

$a = 12.115\ (2)\ \text{\AA}$

$b = 9.4987\ (19)\ \text{\AA}$

$c = 16.748\ (3)\ \text{\AA}$

$\beta = 95.94\ (3)^\circ$

$V = 1917.0\ (6)\ \text{\AA}^3$

$Z = 4$

$F(000) = 912$

$D_x = 1.543\ \text{Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71070 \text{ \AA}$   
 Cell parameters from 3879 reflections  
 $\theta = 1.2\text{--}27.8^\circ$   
 $\mu = 0.73 \text{ mm}^{-1}$

$T = 293 \text{ K}$   
 Prim, red  
 $0.14 \times 0.14 \times 0.14 \text{ mm}$

*Data collection*

Rigaku Saturn  
 diffractometer  
 Radiation source: fine-focus sealed tube  
 Graphite monochromator  
 Detector resolution: 7.31 pixels  $\text{mm}^{-1}$   
 $\omega$  scans  
 Absorption correction: multi-scan  
 (Jacobson, 1998)  
 $T_{\min} = 0.905$ ,  $T_{\max} = 0.905$

15658 measured reflections  
 3406 independent reflections  
 2957 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.061$   
 $\theta_{\max} = 25.1^\circ$ ,  $\theta_{\min} = 2.5^\circ$   
 $h = -14 \rightarrow 14$   
 $k = -11 \rightarrow 11$   
 $l = -19 \rightarrow 19$

*Refinement*

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.060$   
 $wR(F^2) = 0.159$   
 $S = 1.07$   
 3406 reflections  
 269 parameters  
 7 restraints  
 Primary atom site location: structure-invariant  
 direct methods

Secondary atom site location: difference Fourier  
 map  
 Hydrogen site location: inferred from  
 neighbouring sites  
 H atoms treated by a mixture of independent  
 and constrained refinement  
 $w = 1/[\sigma^2(F_o^2) + (0.0859P)^2 + 0.7977P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.47 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -0.52 \text{ e \AA}^{-3}$

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Mn1	0.28436 (4)	0.43236 (5)	0.07581 (3)	0.0426 (2)
N1	0.4102 (2)	0.2866 (3)	0.09158 (17)	0.0457 (7)
N2	0.2637 (2)	0.3704 (3)	0.18327 (17)	0.0475 (7)
N3	0.1504 (2)	0.5370 (3)	0.08979 (18)	0.0457 (7)
N4	0.2560 (2)	0.5208 (3)	-0.03746 (17)	0.0446 (7)
N5	0.4047 (3)	0.5963 (4)	0.10720 (19)	0.0547 (6)
N6	0.3766 (3)	0.7072 (4)	0.12232 (18)	0.0547 (6)
N7	0.3505 (5)	0.8221 (5)	0.1379 (3)	0.1030 (15)
O1	0.3481 (3)	0.2476 (3)	0.29189 (17)	0.0692 (8)
O2	0.0275 (2)	0.7020 (3)	0.03047 (18)	0.0723 (9)
O3	0.1885 (3)	0.2409 (3)	0.01209 (19)	0.0651 (8)
H	0.1217 (19)	0.269 (7)	0.008 (4)	0.14 (3)*
C19	0.1894 (5)	0.0937 (5)	0.0353 (4)	0.0912 (17)
H19A	0.1415	0.0413	-0.0031	0.137*
H19B	0.1637	0.0848	0.0874	0.137*
H19C	0.2636	0.0575	0.0369	0.137*
C17	0.2895 (4)	0.5841 (4)	-0.1701 (2)	0.0584 (10)
H17A	0.3309	0.5721	-0.2134	0.070*
C14	0.1715 (3)	0.6137 (4)	-0.0417 (2)	0.0479 (9)
C9	0.0439 (4)	0.4628 (4)	0.3157 (3)	0.0624 (11)

H9A	0.0212	0.4431	0.3659	0.075*
C2	0.5578 (3)	0.1396 (4)	0.0584 (3)	0.0574 (10)
H2A	0.6032	0.1086	0.0204	0.069*
C4	0.5005 (3)	0.1313 (4)	0.1897 (2)	0.0536 (10)
H4A	0.5073	0.0953	0.2416	0.064*
C8	0.1394 (4)	0.4006 (4)	0.2927 (3)	0.0579 (10)
H8A	0.1815	0.3406	0.3276	0.069*
C6	0.3408 (3)	0.2842 (4)	0.2216 (2)	0.0479 (9)
C10	-0.0179 (4)	0.5543 (4)	0.2643 (3)	0.0638 (12)
H10A	-0.0815	0.5957	0.2803	0.077*
C16	0.2034 (4)	0.6788 (5)	-0.1744 (3)	0.0659 (12)
H16A	0.1859	0.7320	-0.2206	0.079*
C15	0.1430 (4)	0.6940 (4)	-0.1093 (3)	0.0629 (11)
H15A	0.0842	0.7572	-0.1110	0.075*
C3	0.5692 (3)	0.0850 (4)	0.1344 (3)	0.0592 (11)
H3A	0.6230	0.0171	0.1487	0.071*
C18	0.3139 (3)	0.5069 (4)	-0.1007 (2)	0.0519 (9)
H18A	0.3725	0.4433	-0.0978	0.062*
C12	0.1084 (3)	0.5218 (4)	0.1652 (2)	0.0470 (8)
C1	0.4782 (3)	0.2411 (4)	0.0387 (2)	0.0543 (10)
H1A	0.4714	0.2791	-0.0127	0.065*
C11	0.0140 (3)	0.5842 (4)	0.1899 (3)	0.0577 (10)
H11A	-0.0275	0.6464	0.1560	0.069*
C13	0.1080 (3)	0.6216 (4)	0.0299 (2)	0.0518 (9)
C7	0.1716 (3)	0.4288 (4)	0.2169 (2)	0.0463 (9)
C5	0.4215 (3)	0.2321 (4)	0.1666 (2)	0.0438 (8)

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Mn1	0.0434 (4)	0.0411 (4)	0.0427 (4)	0.0090 (2)	0.0012 (2)	0.0035 (2)
N1	0.0429 (16)	0.0452 (17)	0.0479 (17)	0.0029 (13)	-0.0007 (13)	0.0035 (14)
N2	0.0507 (18)	0.0436 (17)	0.0488 (17)	0.0073 (14)	0.0079 (14)	0.0056 (14)
N3	0.0446 (16)	0.0414 (16)	0.0502 (17)	0.0054 (13)	0.0002 (13)	0.0015 (13)
N4	0.0480 (17)	0.0396 (16)	0.0438 (16)	0.0042 (13)	-0.0074 (13)	0.0001 (13)
N5	0.0579 (14)	0.0584 (15)	0.0468 (13)	-0.0053 (13)	0.0012 (10)	0.0014 (13)
N6	0.0579 (14)	0.0584 (15)	0.0468 (13)	-0.0053 (13)	0.0012 (10)	0.0014 (13)
N7	0.125 (3)	0.075 (3)	0.111 (3)	0.007 (3)	0.020 (3)	-0.013 (2)
O1	0.079 (2)	0.076 (2)	0.0525 (17)	0.0197 (16)	0.0103 (14)	0.0191 (15)
O2	0.0586 (18)	0.075 (2)	0.081 (2)	0.0288 (16)	-0.0044 (15)	0.0049 (16)
O3	0.0572 (18)	0.0463 (16)	0.088 (2)	0.0060 (14)	-0.0097 (15)	0.0000 (14)
C19	0.073 (3)	0.066 (3)	0.128 (5)	0.010 (3)	-0.019 (3)	0.010 (3)
C17	0.072 (3)	0.055 (2)	0.047 (2)	-0.004 (2)	-0.0016 (19)	0.0044 (18)
C14	0.050 (2)	0.0401 (19)	0.051 (2)	0.0023 (16)	-0.0084 (16)	0.0009 (16)
C9	0.064 (3)	0.056 (2)	0.071 (3)	-0.010 (2)	0.026 (2)	-0.011 (2)
C2	0.050 (2)	0.054 (2)	0.069 (3)	0.0123 (19)	0.0077 (18)	0.001 (2)
C4	0.054 (2)	0.047 (2)	0.056 (2)	0.0082 (18)	-0.0080 (18)	0.0097 (18)
C8	0.064 (3)	0.048 (2)	0.064 (3)	-0.0072 (19)	0.017 (2)	-0.0005 (19)

C6	0.052 (2)	0.043 (2)	0.048 (2)	0.0008 (17)	0.0005 (16)	0.0045 (17)
C10	0.056 (3)	0.060 (3)	0.079 (3)	-0.005 (2)	0.022 (2)	-0.021 (2)
C16	0.079 (3)	0.060 (3)	0.054 (2)	-0.002 (2)	-0.014 (2)	0.014 (2)
C15	0.062 (3)	0.055 (2)	0.066 (3)	0.010 (2)	-0.014 (2)	0.010 (2)
C3	0.050 (2)	0.053 (2)	0.073 (3)	0.0150 (18)	-0.003 (2)	0.005 (2)
C18	0.062 (2)	0.048 (2)	0.044 (2)	0.0049 (18)	-0.0006 (17)	-0.0006 (17)
C12	0.046 (2)	0.0369 (18)	0.057 (2)	-0.0031 (16)	0.0029 (16)	-0.0060 (17)
C1	0.054 (2)	0.059 (2)	0.050 (2)	0.0104 (19)	0.0058 (17)	0.0071 (18)
C11	0.052 (2)	0.050 (2)	0.072 (3)	0.0041 (18)	0.007 (2)	-0.012 (2)
C13	0.043 (2)	0.045 (2)	0.064 (2)	0.0045 (17)	-0.0071 (17)	0.0008 (18)
C7	0.048 (2)	0.041 (2)	0.052 (2)	-0.0008 (15)	0.0109 (16)	-0.0039 (15)
C5	0.0442 (19)	0.0398 (19)	0.0458 (19)	-0.0010 (15)	-0.0032 (15)	0.0020 (15)

*Geometric parameters (Å, °)*

Mn1—N2	1.934 (3)	C14—C15	1.379 (5)
Mn1—N3	1.937 (3)	C14—C13	1.493 (6)
Mn1—N1	2.056 (3)	C9—C10	1.387 (6)
Mn1—N4	2.070 (3)	C9—C8	1.390 (6)
Mn1—N5	2.161 (3)	C9—H9A	0.9300
Mn1—O3	2.354 (3)	C2—C3	1.369 (6)
N1—C1	1.341 (5)	C2—C1	1.380 (5)
N1—C5	1.353 (4)	C2—H2A	0.9300
N2—C6	1.352 (5)	C4—C3	1.380 (6)
N2—C7	1.414 (5)	C4—C5	1.380 (5)
N3—C13	1.345 (5)	C4—H4A	0.9300
N3—C12	1.417 (5)	C8—C7	1.392 (5)
N4—C18	1.336 (5)	C8—H8A	0.9300
N4—C14	1.348 (5)	C6—C5	1.496 (5)
N5—N6	1.143 (4)	C10—C11	1.371 (6)
N6—N7	1.174 (5)	C10—H10A	0.9300
O1—C6	1.222 (4)	C16—C15	1.382 (6)
O2—C13	1.239 (4)	C16—H16A	0.9300
O3—C19	1.451 (5)	C15—H15A	0.9300
O3—H	0.849 (10)	C3—H3A	0.9300
C19—H19A	0.9600	C18—H18A	0.9300
C19—H19B	0.9600	C12—C11	1.389 (5)
C19—H19C	0.9600	C12—C7	1.408 (5)
C17—C16	1.374 (6)	C1—H1A	0.9300
C17—C18	1.380 (5)	C11—H11A	0.9300
C17—H17A	0.9300		
N2—Mn1—N3	81.55 (13)	C8—C9—H9A	119.8
N2—Mn1—N1	80.87 (12)	C3—C2—C1	119.2 (4)
N3—Mn1—N1	161.63 (13)	C3—C2—H2A	120.4
N2—Mn1—N4	161.93 (12)	C1—C2—H2A	120.4
N3—Mn1—N4	80.85 (12)	C3—C4—C5	118.8 (4)
N1—Mn1—N4	116.19 (12)	C3—C4—H4A	120.6

N2—Mn1—N5	98.16 (13)	C5—C4—H4A	120.6
N3—Mn1—N5	98.81 (13)	C9—C8—C7	119.4 (4)
N1—Mn1—N5	88.92 (13)	C9—C8—H8A	120.3
N4—Mn1—N5	88.53 (12)	C7—C8—H8A	120.3
N2—Mn1—O3	94.67 (13)	O1—C6—N2	127.4 (4)
N3—Mn1—O3	94.08 (12)	O1—C6—C5	120.8 (3)
N1—Mn1—O3	82.11 (11)	N2—C6—C5	111.8 (3)
N4—Mn1—O3	82.57 (11)	C11—C10—C9	120.6 (4)
N5—Mn1—O3	162.99 (13)	C11—C10—H10A	119.7
C1—N1—C5	118.7 (3)	C9—C10—H10A	119.7
C1—N1—Mn1	129.0 (2)	C17—C16—C15	119.2 (4)
C5—N1—Mn1	112.3 (2)	C17—C16—H16A	120.4
C6—N2—C7	125.6 (3)	C15—C16—H16A	120.4
C6—N2—Mn1	118.4 (2)	C14—C15—C16	118.8 (4)
C7—N2—Mn1	115.8 (2)	C14—C15—H15A	120.6
C13—N3—C12	125.4 (3)	C16—C15—H15A	120.6
C13—N3—Mn1	118.5 (3)	C2—C3—C4	119.6 (4)
C12—N3—Mn1	116.0 (2)	C2—C3—H3A	120.2
C18—N4—C14	118.8 (3)	C4—C3—H3A	120.2
C18—N4—Mn1	129.4 (3)	N4—C18—C17	122.1 (4)
C14—N4—Mn1	111.5 (2)	N4—C18—H18A	119.0
N6—N5—Mn1	120.6 (3)	C17—C18—H18A	119.0
N5—N6—N7	178.3 (5)	C11—C12—C7	119.8 (4)
C19—O3—Mn1	129.3 (3)	C11—C12—N3	127.2 (4)
C19—O3—H	108 (5)	C7—C12—N3	112.9 (3)
Mn1—O3—H	102 (4)	N1—C1—C2	122.0 (4)
O3—C19—H19A	109.5	N1—C1—H1A	119.0
O3—C19—H19B	109.5	C2—C1—H1A	119.0
H19A—C19—H19B	109.5	C10—C11—C12	120.0 (4)
O3—C19—H19C	109.5	C10—C11—H11A	120.0
H19A—C19—H19C	109.5	C12—C11—H11A	120.0
H19B—C19—H19C	109.5	O2—C13—N3	127.1 (4)
C16—C17—C18	119.1 (4)	O2—C13—C14	120.5 (4)
C16—C17—H17A	120.4	N3—C13—C14	112.3 (3)
C18—C17—H17A	120.4	C8—C7—C12	119.8 (4)
N4—C14—C15	122.0 (4)	C8—C7—N2	126.5 (4)
N4—C14—C13	116.3 (3)	C12—C7—N2	113.7 (3)
C15—C14—C13	121.7 (4)	N1—C5—C4	121.8 (3)
C10—C9—C8	120.4 (4)	N1—C5—C6	115.8 (3)
C10—C9—H9A	119.8	C4—C5—C6	122.4 (3)
N2—Mn1—N1—C1	174.5 (3)	C10—C9—C8—C7	-1.2 (6)
N3—Mn1—N1—C1	157.5 (4)	C7—N2—C6—O1	-4.0 (6)
N4—Mn1—N1—C1	0.8 (4)	Mn1—N2—C6—O1	171.2 (3)
N5—Mn1—N1—C1	-87.1 (3)	C7—N2—C6—C5	175.3 (3)
O3—Mn1—N1—C1	78.4 (3)	Mn1—N2—C6—C5	-9.6 (4)
N2—Mn1—N1—C5	-5.0 (2)	C8—C9—C10—C11	0.3 (6)
N3—Mn1—N1—C5	-22.0 (5)	C18—C17—C16—C15	-0.3 (6)

N4—Mn1—N1—C5	-178.7 (2)	N4—C14—C15—C16	-0.2 (6)
N5—Mn1—N1—C5	93.5 (2)	C13—C14—C15—C16	-178.2 (4)
O3—Mn1—N1—C5	-101.0 (2)	C17—C16—C15—C14	0.2 (6)
N3—Mn1—N2—C6	-177.0 (3)	C1—C2—C3—C4	0.6 (6)
N1—Mn1—N2—C6	8.3 (3)	C5—C4—C3—C2	0.0 (6)
N4—Mn1—N2—C6	169.9 (3)	C14—N4—C18—C17	-0.3 (6)
N5—Mn1—N2—C6	-79.3 (3)	Mn1—N4—C18—C17	-173.8 (3)
O3—Mn1—N2—C6	89.5 (3)	C16—C17—C18—N4	0.4 (6)
N3—Mn1—N2—C7	-1.4 (3)	C13—N3—C12—C11	3.5 (6)
N1—Mn1—N2—C7	-176.1 (3)	Mn1—N3—C12—C11	-179.5 (3)
N4—Mn1—N2—C7	-14.5 (6)	C13—N3—C12—C7	-178.3 (3)
N5—Mn1—N2—C7	96.4 (3)	Mn1—N3—C12—C7	-1.4 (4)
O3—Mn1—N2—C7	-94.9 (3)	C5—N1—C1—C2	0.8 (6)
N2—Mn1—N3—C13	178.7 (3)	Mn1—N1—C1—C2	-178.6 (3)
N1—Mn1—N3—C13	-164.4 (3)	C3—C2—C1—N1	-1.0 (6)
N4—Mn1—N3—C13	-5.4 (3)	C9—C10—C11—C12	0.6 (6)
N5—Mn1—N3—C13	81.7 (3)	C7—C12—C11—C10	-0.6 (6)
O3—Mn1—N3—C13	-87.2 (3)	N3—C12—C11—C10	177.5 (4)
N2—Mn1—N3—C12	1.5 (3)	C12—N3—C13—O2	1.6 (6)
N1—Mn1—N3—C12	18.5 (5)	Mn1—N3—C13—O2	-175.3 (3)
N4—Mn1—N3—C12	177.5 (3)	C12—N3—C13—C14	179.9 (3)
N5—Mn1—N3—C12	-95.5 (3)	Mn1—N3—C13—C14	3.1 (4)
O3—Mn1—N3—C12	95.7 (3)	N4—C14—C13—O2	-178.5 (3)
N2—Mn1—N4—C18	-166.4 (4)	C15—C14—C13—O2	-0.4 (6)
N3—Mn1—N4—C18	-179.5 (3)	N4—C14—C13—N3	3.0 (5)
N1—Mn1—N4—C18	-6.7 (4)	C15—C14—C13—N3	-178.8 (3)
N5—Mn1—N4—C18	81.3 (3)	C9—C8—C7—C12	1.2 (6)
O3—Mn1—N4—C18	-84.1 (3)	C9—C8—C7—N2	-177.5 (4)
N2—Mn1—N4—C14	19.8 (5)	C11—C12—C7—C8	-0.3 (5)
N3—Mn1—N4—C14	6.7 (2)	N3—C12—C7—C8	-178.6 (3)
N1—Mn1—N4—C14	179.4 (2)	C11—C12—C7—N2	178.5 (3)
N5—Mn1—N4—C14	-92.5 (3)	N3—C12—C7—N2	0.2 (4)
O3—Mn1—N4—C14	102.1 (3)	C6—N2—C7—C8	-4.9 (6)
N2—Mn1—N5—N6	-85.4 (3)	Mn1—N2—C7—C8	179.8 (3)
N3—Mn1—N5—N6	-2.8 (3)	C6—N2—C7—C12	176.3 (3)
N1—Mn1—N5—N6	-166.0 (3)	Mn1—N2—C7—C12	1.1 (4)
N4—Mn1—N5—N6	77.7 (3)	C1—N1—C5—C4	-0.2 (5)
O3—Mn1—N5—N6	136.0 (4)	Mn1—N1—C5—C4	179.3 (3)
N2—Mn1—O3—C19	-39.4 (4)	C1—N1—C5—C6	-178.1 (3)
N3—Mn1—O3—C19	-121.2 (4)	Mn1—N1—C5—C6	1.4 (4)
N1—Mn1—O3—C19	40.7 (4)	C3—C4—C5—N1	-0.3 (6)
N4—Mn1—O3—C19	158.6 (4)	C3—C4—C5—C6	177.5 (4)
N5—Mn1—O3—C19	99.5 (5)	O1—C6—C5—N1	-175.8 (3)
C18—N4—C14—C15	0.3 (6)	N2—C6—C5—N1	4.9 (5)
Mn1—N4—C14—C15	174.8 (3)	O1—C6—C5—C4	6.3 (6)
C18—N4—C14—C13	178.4 (3)	N2—C6—C5—C4	-173.0 (3)
Mn1—N4—C14—C13	-7.1 (4)		



*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
O3—H $\cdots$ O2 <sup>i</sup>	0.85 (1)	1.88 (2)	2.696 (4)	162 (6)

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