Acta Crystallographica Section E
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Retraction of articles

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This article reports the retraction of 11 articles published in *Acta Crystallographica Section E* between 2005 and 2009.

After further thorough investigation (see Harrison *et al.*, 2010), 11 additional articles are retracted by the authors or by the journal as a result of problems with the data sets or incorrect atom assignments. Full details of all the articles are given in Table 1.

Table 1
Details of articles to be retracted, in order of publication.

Title	Reference	DOI	Refcode
[N,N′-Bis(2-hydroxynaphthylmethylene)-1,2-ethanediaminato]zinc(II)	Chen *et al.* (2005)	10.1107/S1600536805026796	YAWZOM
Diazidobis(2,2′-biimidazole)copper(II)	Liu *et al.* (2007)	10.1107/S1600536807047873	SILZIX
Dichlorido(1,10-phenanthroline)copper(II)	Liu (2007)	10.1107/S1600536807056735	MISSAJ
Diazidobis(2,2′-biimidazole)cobalt(II)	Li *et al.* (2008)	10.1107/S1600536807062873	MIRYAO
Diazidobis(2,2′-biimidazole)manganese(II)	Zhang *et al.* (2008)	10.1107/S1600536808017984	MODBUD
Diazidobis(2,2′-biimidazole)iron(II)	Hao *et al.* (2008*a*)	10.1107/S1600536808018539	MODFOB
Bis(pentane-2,4-dionato)bis[2-(4-pyridyl)-4,4,5,5-tetramethylimidazoline-1-oxyl 3-oxide]nickel(II)	Hao *et al.* (2008*b*)	10.1107/S1600536808018552	MODFUH
Bis(pentane-2,4-dionato-κ^2O,O')bis[4,4,5,5-tetramethyl-2-(4-pyridyl)imidazoline-1-oxyl 3-oxide-κN^2]manganese(II)	Liu, Zhang *et al.* (2008)	10.1107/S1600536808022952	MODLUN
Bis[2,4-pentanedionato(1−)]bis[4,4,5,5-tetramethyl-2-(4-pyridyl)imidazoline-1-oxyl 3-oxide]manganese(II)	Liu, He *et al.* (2008)	10.1107/S1600536808038440	MODLUN01
Di-μ-chlorido-bis[chlorido(1,10-phenanthroline-κ^2N,N')zinc(II)]	Yang *et al.* (2009)	10.1107/S1600536809014482	JOLBOC
Tris(ethylenediamine)manganese(II) sulfate	Lu (2009)	10.1107/S1600536809034874	YUCZEC

References

Chen, G., Zhao, B., Sun, M. & Qi, W. (2005). *Acta Cryst.* E**61**, m1869–m1870.
Hao, L., Mu, C. & Kong, B. (2008*a*). *Acta Cryst.* E**64**, m956.
Hao, L., Mu, C. & Kong, B. (2008*b*). *Acta Cryst.* E**64**, m957.
Harrison, W. T. A., Simpson, J. & Weil, M. (2010). *Acta Cryst.* E**66**, e1–e2.
Li, S., Wang, S.-B., Zhang, F.-L. & Tang, K. (2008). *Acta Cryst.* E**64**, m76.
Liu, Y.-Q. (2007). *Acta Cryst.* E**63**, m2991.
Liu, Y., Dou, J., Li, D. & Zhang, X. (2007). *Acta Cryst.* E**63**, m2661.
Liu, Y., He, Q., Zhang, X., Xue, Z. & Lv, C. (2008). *Acta Cryst.* E**64**, m1604.
Liu, Y., Zhang, X., Xue, Z., He, Q. & Zhang, Y. (2008). *Acta Cryst.* E**64**, m1077.
Lu, J. (2009). *Acta Cryst.* E**65**, m1187.
Yang, X.-M., Leng, Q.-B., Chen, Y., He, Y.-G. & Luo, S.-W. (2009). *Acta Cryst.* E**65**, m567.
Zhang, X., Wei, P. & Li, B. (2008). *Acta Cryst.* E**64**, m934.

  doi:10.1107/S1600536810053882

Acta Crystallographica Section E
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Bis(pentane-2,4-dionato-κ^2O,O')-bis[4,4,5,5-tetramethyl-2-(4-pyridyl)-imidazoline-1-oxyl 3-oxide-κN^2]-manganese(II)

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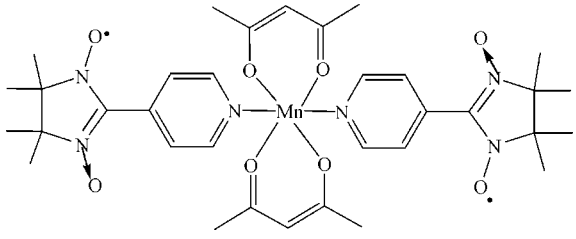
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.041; wR factor = 0.115; data-to-parameter ratio = 14.7.

The title compound, $[Mn(C_5H_7O_2)_2(C_{12}H_{16}N_3O_2)_2]$, is isostructural with its Ni^{II}-containing analogue [Hao, Mu & Kong (2008). *Acta Cryst.* E**64**, m957]. The asymmetric unit comprises one-half of the molecule and the Mn^{II} ion is located on an inversion centre. The coordination geometry around the Mn^{II} ion is slightly distorted octahedral, comprised of four O and two N atoms, in which the four O atoms in the equatorial plane come from two pentane-2,4-dionate ligands and the two N atoms in the axial coordination sites from 4,4,5,5-tetramethyl-2-(4-pyridyl)imidazoline-1-oxyl 3-oxide.

Related literature

For related literature, see: Eddaoudi *et al.* (2000); Hye & Myunghyun (1998); Li *et al.* (1999); Tabares *et al.* (2001). For the isostructural Ni^{II}-containing compound, see: Hao *et al.* (2008).



Experimental

Crystal data

$[Mn(C_5H_7O_2)_2(C_{12}H_{16}N_3O_2)_2]$
M_r = 721.71
Triclinic, $P\overline{1}$
a = 7.107 (2) Å
b = 10.018 (2) Å
c = 12.786 (2) Å
α = 98.16 (3)°
β = 103.20 (3)°
γ = 92.76 (3)°
V = 874.3 (3) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.44 mm^{-1}
T = 298 (2) K
0.39 × 0.28 × 0.17 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.848, T_{max} = 0.929
6447 measured reflections
3371 independent reflections
2590 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.114
S = 1.00
3371 reflections
229 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.50 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Mn1—O2	2.0151 (17)	Mn1—N3	2.178 (2)
Mn1—O1	2.0386 (17)		
O2^i—Mn1—O2	180	O1—Mn1—N3^i	91.90 (7)
O2^i—Mn1—O1	90.98 (7)	O2—Mn1—N3	89.00 (7)
O2—Mn1—O1	89.02 (7)	O1—Mn1—N3	88.10 (7)
O1^i—Mn1—O1	180	N3^i—Mn1—N3	180
O2—Mn1—N3^i	91.00 (7)		

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2160).

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Hao, L., Mu, C. & Kong, B. (2008). *Acta Cryst.* E**64**, m957.
Hye, J. C. & Myunghyun, P. S. (1998). *J. Am. Chem. Soc.* **120**, 10622–10628.
Li, H., Eddaoudi, M., O'Keeffe, M. & Yaghi, O. M. (1999). *Nature (London)*, **402**, 276–279.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Tabares, L. C., Navarro, J. A. R. & Salas, J. M. (2001). *J. Am. Chem. Soc.* **123**, 383–387.

supporting information

Acta Cryst. (2008). E**64**, m1077 [doi:10.1107/S1600536808022952]

Bis(pentane-2,4-dionato-κ^2O,O')bis[4,4,5,5-tetramethyl-2-(4-pyridyl)-imidazoline-1-oxyl 3-oxide-κN^2]manganese(II)

Ying Liu, Xianxi Zhang, Zechun Xue, Qingpeng He and Yu Zhang

S1. Comment

Due to the interesting structures from supramolecular assemblies as well as potential applications on smart optoelectronic, magnetic and porous materials, the design and synthesis of metal–organic coordination polymers have attracted considerable attention (Eddaoudi *et al.*, 2000; Hye & Myunghyun, 1998; Li *et al.*, 1999; Tabares *et al.*, 2001). In this paper, we report the structure of the title compound, (I).

As shown in Fig. 1, the asymmetric unit comprises a half of the molecule and Mn^{II} ion locates on an inversion centre. The coordination geometry around Mn^{II} is slightly distorted octahedral, comprised of four O and two N atoms. In which, the four oxygen atoms in the equatorial plane come from two pentane-2,4-dionate and the two nitrogen atoms in the axial coordination sites from 2-(4-pyridyl)-4,4,5,5-tetramethylimidazoline-1-oxyl-3-oxide. The Mn—N and Mn—O bond lengths are in the range of 2.178 (2)–2.178 (2) and 2.0151 (17)–2.0386 (17) Å, respectively.

S2. Experimental

A mixture of Manganese(II) acetylacetonate (0.5 mmol) and 2-(4-pyridyl)-4,4,5,5-tetramethylimidazoline-1-oxyl-3-oxide (1 mmol) in 20 ml methanol was refluxed for one day. The resulted solution was filtered. The filtrate was kept in the open flask and evaporated naturally at room temperature. Several days later, pink blocks of (I) were obtained with a high yield of *ca* 67% based on Mn^{II}. Anal. Calc. for $C_{34}H_{46}MnN_6O_8$: C 56.53, H 6.37, N 11.64%; Found: C 56.45, H 6.29, N 11.58%.

S3. Refinement

All H atoms were placed in calculated positions with C—H = 0.93 Å and C—H = 0.96 distances and refined as riding with U_{iso}(H) = 1.2 and 1.5 U_{eq}(carrier).

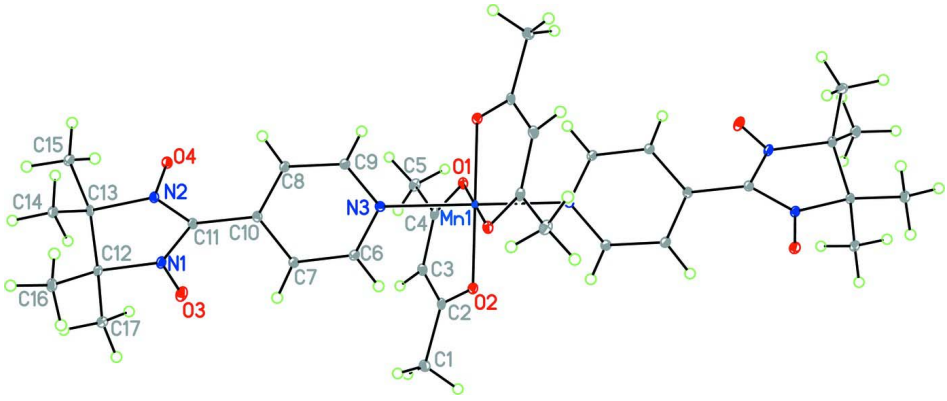

Figure 1

The molecular structure of (I) around Mn^{II}, drawn with 30% probability displacement ellipsoids for the non-hydrogen atoms.

Bis(pentane-2,4-dionato-κ^2O,O′)bis[4,4,5,5-tetramethyl-2-(4- pyridyl)imidazoline-1-oxyl 3-oxide-κN^2]manganese(II)

Crystal data

$[Mn(C_5H_7O_2)_2(C_{12}H_{16}N_3O_2)_2]$
$M_r = 721.71$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.107$ (2) Å
$b = 10.018$ (2) Å
$c = 12.786$ (2) Å
$\alpha = 98.16$ (3)°
$\beta = 103.20$ (3)°
$\gamma = 92.76$ (3)°
$V = 874.3$ (3) Å^3
$Z = 1$
$F(000) = 381$
$D_x = 1.371$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3371 reflections
$\theta = 3.0$–$26.1°$
$\mu = 0.44$ mm^{-1}
$T = 298$ K
Block, pink
0.39 × 0.28 × 0.17 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min} = 0.848$, $T_{max} = 0.930$
6447 measured reflections
3371 independent reflections
2590 reflections with $I > 2\sigma(I)$
$R_{int} = 0.033$
$\theta_{max} = 26.1°$, $\theta_{min} = 3.0°$
$h = -6 \rightarrow 8$
$k = -12 \rightarrow 12$
$l = -11 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.114$
$S = 1.00$
3371 reflections
229 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
$w = 1/[\sigma^2(F_o^2) + (0.066P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.56$ e Å^{-3}
$\Delta\rho_{min} = -0.50$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Mn1	0.0000	0.0000	0.0000	0.0281 (7)
C1	−0.1322 (4)	0.3856 (3)	0.1293 (2)	0.0310 (6)
H1A	−0.2696	0.3835	0.1006	0.046*
H1B	−0.0731	0.4742	0.1305	0.046*
H1C	−0.1069	0.3644	0.2019	0.046*
C2	−0.0486 (3)	0.2828 (2)	0.05829 (19)	0.0231 (5)
C3	0.1138 (4)	0.3209 (3)	0.0230 (2)	0.0257 (6)
H3	0.1665	0.4100	0.0456	0.031*
C4	0.2049 (3)	0.2369 (2)	−0.0433 (2)	0.0241 (6)
C5	0.3726 (4)	0.2934 (3)	−0.0814 (2)	0.0327 (6)
H5A	0.4879	0.2528	−0.0507	0.049*
H5B	0.3914	0.3896	−0.0585	0.049*
H5C	0.3458	0.2740	−0.1593	0.049*
C6	0.1702 (3)	0.1166 (2)	0.23876 (19)	0.0219 (5)
H6	0.0386	0.1239	0.2339	0.026*
C7	0.2971 (3)	0.1613 (2)	0.3372 (2)	0.0220 (5)
H7	0.2520	0.1980	0.3969	0.026*
C8	0.5527 (4)	0.0957 (3)	0.2535 (2)	0.0243 (6)
H8	0.6833	0.0870	0.2560	0.029*
C9	0.4137 (3)	0.0539 (2)	0.1579 (2)	0.0229 (5)
H9	0.4544	0.0177	0.0964	0.027*
C10	0.4945 (3)	0.1510 (2)	0.3462 (2)	0.0214 (5)
C11	0.6317 (3)	0.1984 (3)	0.45046 (19)	0.0220 (5)
C12	0.7429 (3)	0.2985 (3)	0.63433 (19)	0.0228 (5)
C13	0.9183 (3)	0.2690 (2)	0.58648 (18)	0.0206 (5)
C14	1.0771 (3)	0.3830 (3)	0.6102 (2)	0.0254 (6)
H14A	1.1718	0.3589	0.5696	0.038*
H14B	1.1380	0.3985	0.6866	0.038*
H14C	1.0221	0.4638	0.5896	0.038*
C15	1.0021 (4)	0.1370 (3)	0.6128 (2)	0.0248 (6)
H15A	0.8995	0.0657	0.5955	0.037*
H15B	1.0644	0.1474	0.6888	0.037*
H15C	1.0952	0.1146	0.5706	0.037*
C16	0.7505 (4)	0.2552 (3)	0.7443 (2)	0.0304 (6)
H16A	0.6337	0.2761	0.7667	0.046*

H16B	0.8603	0.3025	0.7970	0.046*
H16C	0.7622	0.1595	0.7388	0.046*
C17	0.6888 (4)	0.4436 (3)	0.6351 (2)	0.0320 (6)
H17A	0.6873	0.4698	0.5656	0.048*
H17B	0.7823	0.5025	0.6907	0.048*
H17C	0.5626	0.4502	0.6496	0.048*
N1	0.5857 (3)	0.2135 (2)	0.54865 (16)	0.0248 (5)
N2	0.8187 (3)	0.2418 (2)	0.46656 (16)	0.0217 (5)
N3	0.2243 (3)	0.06280 (19)	0.14902 (16)	0.0206 (4)
O1	0.1568 (2)	0.11188 (17)	−0.07682 (13)	0.0249 (4)
O2	−0.1367 (2)	0.16521 (17)	0.03802 (13)	0.0245 (4)
O3	0.4265 (2)	0.1723 (2)	0.56890 (14)	0.0353 (5)
O4	0.9121 (2)	0.25076 (18)	0.39302 (14)	0.0274 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0255 (17)	0.0255 (17)	0.0309 (19)	−0.0021 (13)	0.0044 (15)	−0.0037 (14)
C1	0.0354 (15)	0.0245 (14)	0.0295 (15)	0.0070 (11)	0.0010 (12)	0.0017 (11)
C2	0.0253 (13)	0.0220 (13)	0.0173 (13)	0.0039 (10)	−0.0057 (10)	0.0043 (10)
C3	0.0297 (14)	0.0208 (13)	0.0232 (14)	0.0009 (10)	−0.0009 (11)	0.0043 (10)
C4	0.0228 (13)	0.0245 (13)	0.0215 (14)	0.0001 (10)	−0.0047 (10)	0.0090 (10)
C5	0.0275 (14)	0.0306 (14)	0.0399 (17)	0.0000 (11)	0.0039 (12)	0.0122 (12)
C6	0.0186 (12)	0.0260 (13)	0.0220 (14)	0.0034 (10)	0.0049 (10)	0.0061 (10)
C7	0.0218 (13)	0.0276 (13)	0.0171 (13)	0.0031 (10)	0.0051 (10)	0.0035 (10)
C8	0.0196 (13)	0.0308 (14)	0.0223 (14)	0.0033 (10)	0.0045 (11)	0.0037 (11)
C9	0.0229 (13)	0.0268 (13)	0.0192 (13)	0.0041 (10)	0.0046 (10)	0.0044 (10)
C10	0.0213 (13)	0.0240 (12)	0.0184 (13)	0.0009 (10)	0.0033 (10)	0.0042 (10)
C11	0.0210 (13)	0.0293 (13)	0.0155 (13)	0.0018 (10)	0.0046 (10)	0.0025 (10)
C12	0.0204 (13)	0.0301 (14)	0.0162 (13)	0.0044 (10)	0.0004 (10)	0.0032 (10)
C13	0.0190 (12)	0.0291 (13)	0.0119 (12)	0.0009 (10)	0.0007 (10)	0.0023 (10)
C14	0.0231 (13)	0.0284 (14)	0.0233 (14)	0.0013 (10)	0.0030 (11)	0.0033 (11)
C15	0.0209 (13)	0.0279 (13)	0.0253 (14)	0.0037 (10)	0.0037 (11)	0.0057 (11)
C16	0.0259 (14)	0.0444 (17)	0.0200 (14)	0.0032 (12)	0.0030 (11)	0.0062 (12)
C17	0.0271 (14)	0.0388 (16)	0.0284 (16)	0.0112 (12)	0.0039 (12)	0.0015 (12)
N1	0.0158 (11)	0.0388 (13)	0.0188 (12)	0.0004 (9)	0.0032 (9)	0.0036 (9)
N2	0.0179 (11)	0.0298 (11)	0.0171 (11)	0.0011 (8)	0.0038 (9)	0.0039 (9)
N3	0.0222 (11)	0.0214 (10)	0.0184 (11)	0.0028 (8)	0.0049 (9)	0.0036 (8)
O1	0.0256 (9)	0.0244 (9)	0.0219 (10)	0.0001 (7)	0.0009 (7)	0.0030 (7)
O2	0.0238 (9)	0.0245 (9)	0.0230 (10)	0.0043 (7)	0.0005 (7)	0.0037 (7)
O3	0.0183 (10)	0.0617 (14)	0.0272 (11)	−0.0016 (9)	0.0067 (8)	0.0113 (10)
O4	0.0218 (9)	0.0406 (11)	0.0204 (10)	0.0010 (8)	0.0078 (8)	0.0032 (8)

Geometric parameters (Å, º)

Mn1—O2^{i}	2.0151 (17)	C9—N3	1.333 (3)
Mn1—O2	2.0151 (17)	C9—H9	0.9300
Mn1—O1^{i}	2.0386 (17)	C10—C11	1.461 (3)

Mn1—O1	2.0386 (17)	C11—N2	1.339 (3)
Mn1—N3^{i}	2.178 (2)	C11—N1	1.358 (3)
Mn1—N3	2.178 (2)	C12—N1	1.503 (3)
C1—C2	1.509 (3)	C12—C16	1.520 (3)
C1—H1A	0.9600	C12—C17	1.520 (3)
C1—H1B	0.9600	C12—C13	1.533 (3)
C1—H1C	0.9600	C13—N2	1.514 (3)
C2—O2	1.271 (3)	C13—C14	1.513 (3)
C2—C3	1.388 (4)	C13—C15	1.526 (3)
C3—C4	1.395 (4)	C14—H14A	0.9600
C3—H3	0.9300	C14—H14B	0.9600
C4—O1	1.268 (3)	C14—H14C	0.9600
C4—C5	1.502 (3)	C15—H15A	0.9600
C5—H5A	0.9600	C15—H15B	0.9600
C5—H5B	0.9600	C15—H15C	0.9600
C5—H5C	0.9600	C16—H16A	0.9600
C6—N3	1.342 (3)	C16—H16B	0.9600
C6—C7	1.372 (3)	C16—H16C	0.9600
C6—H6	0.9300	C17—H17A	0.9600
C7—C10	1.391 (3)	C17—H17B	0.9600
C7—H7	0.9300	C17—H17C	0.9600
C8—C9	1.382 (3)	N1—O3	1.279 (3)
C8—C10	1.394 (3)	N2—O4	1.279 (2)
C8—H8	0.9300		

O2^{i}—Mn1—O2	180.00 (10)	N2—C11—N1	108.0 (2)
O2^{i}—Mn1—O1^{i}	89.02 (7)	N2—C11—C10	127.1 (2)
O2—Mn1—O1^{i}	90.98 (7)	N1—C11—C10	124.8 (2)
O2^{i}—Mn1—O1	90.98 (7)	N1—C12—C16	109.9 (2)
O2—Mn1—O1	89.02 (7)	N1—C12—C17	105.8 (2)
O1^{i}—Mn1—O1	180.00 (9)	C16—C12—C17	110.7 (2)
O2^{i}—Mn1—N3^{i}	89.00 (7)	N1—C12—C13	99.99 (19)
O2—Mn1—N3^{i}	91.00 (7)	C16—C12—C13	115.7 (2)
O1^{i}—Mn1—N3^{i}	88.10 (7)	C17—C12—C13	113.8 (2)
O1—Mn1—N3^{i}	91.90 (7)	N2—C13—C14	110.88 (19)
O2^{i}—Mn1—N3	91.00 (7)	N2—C13—C15	105.76 (19)
O2—Mn1—N3	89.00 (7)	C14—C13—C15	110.9 (2)
O1^{i}—Mn1—N3	91.90 (7)	N2—C13—C12	99.71 (17)
O1—Mn1—N3	88.10 (7)	C14—C13—C12	115.9 (2)
N3^{i}—Mn1—N3	180.00 (8)	C15—C13—C12	112.7 (2)
C2—C1—H1A	109.5	C13—C14—H14A	109.5
C2—C1—H1B	109.5	C13—C14—H14B	109.5
H1A—C1—H1B	109.5	H14A—C14—H14B	109.5
C2—C1—H1C	109.5	C13—C14—H14C	109.5
H1A—C1—H1C	109.5	H14A—C14—H14C	109.5
H1B—C1—H1C	109.5	H14B—C14—H14C	109.5
O2—C2—C3	126.0 (2)	C13—C15—H15A	109.5
O2—C2—C1	114.5 (2)	C13—C15—H15B	109.5

C3—C2—C1	119.5 (2)	H15A—C15—H15B	109.5
C4—C3—C2	125.6 (2)	C13—C15—H15C	109.5
C4—C3—H3	117.2	H15A—C15—H15C	109.5
C2—C3—H3	117.2	H15B—C15—H15C	109.5
O1—C4—C3	125.0 (2)	C12—C16—H16A	109.5
O1—C4—C5	114.8 (2)	C12—C16—H16B	109.5
C3—C4—C5	120.1 (2)	H16A—C16—H16B	109.5
C4—C5—H5A	109.5	C12—C16—H16C	109.5
C4—C5—H5B	109.5	H16A—C16—H16C	109.5
H5A—C5—H5B	109.5	H16B—C16—H16C	109.5
C4—C5—H5C	109.5	C12—C17—H17A	109.5
H5A—C5—H5C	109.5	C12—C17—H17B	109.5
H5B—C5—H5C	109.5	H17A—C17—H17B	109.5
N3—C6—C7	124.0 (2)	C12—C17—H17C	109.5
N3—C6—H6	118.0	H17A—C17—H17C	109.5
C7—C6—H6	118.0	H17B—C17—H17C	109.5
C6—C7—C10	118.9 (2)	O3—N1—C11	127.0 (2)
C6—C7—H7	120.5	O3—N1—C12	121.8 (2)
C10—C7—H7	120.5	C11—N1—C12	111.0 (2)
C9—C8—C10	119.1 (2)	O4—N2—C11	126.4 (2)
C9—C8—H8	120.5	O4—N2—C13	121.89 (18)
C10—C8—H8	120.5	C11—N2—C13	111.45 (18)
N3—C9—C8	123.4 (2)	C9—N3—C6	116.9 (2)
N3—C9—H9	118.3	C9—N3—Mn1	124.82 (16)
C8—C9—H9	118.3	C6—N3—Mn1	118.27 (16)
C7—C10—C8	117.7 (2)	C4—O1—Mn1	121.54 (16)
C7—C10—C11	119.6 (2)	C2—O2—Mn1	121.01 (16)
C8—C10—C11	122.7 (2)		

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