

## Retraction of articles

## IUCr Editorial Office

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

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- Hao, L., Mu, C. & Kong, B. (2008a). *Acta Cryst.* **E64**, m956.
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- Li, S., Wang, S.-B., Zhang, F.-L. & Tang, K. (2008). *Acta Cryst.* **E64**, m76.
- Liu, Y.-Q. (2007). *Acta Cryst.* **E63**, m2991.
- Liu, Y., Dou, J., Li, D. & Zhang, X. (2007). *Acta Cryst.* **E63**, m2661.
- Liu, Y., He, Q., Zhang, X., Xue, Z. & Lv, C. (2008). *Acta Cryst.* **E64**, m1604.
- Liu, Y., Zhang, X., Xue, Z., He, Q. & Zhang, Y. (2008). *Acta Cryst.* **E64**, m1077.
- Lu, J. (2009). *Acta Cryst.* **E65**, m1187.
- Yang, X.-M., Leng, Q.-B., Chen, Y., He, Y.-G. & Luo, S.-W. (2009). *Acta Cryst.* **E65**, m567.
- Zhang, X., Wei, P. & Li, B. (2008). *Acta Cryst.* **E64**, m934.

**Bis[2,4-pentanedionato(1-)]bis[4,4,5,5-tetramethyl-2-(4-pyridyl)-imidazoline-1-oxyl 3-oxide]manganese(II)**

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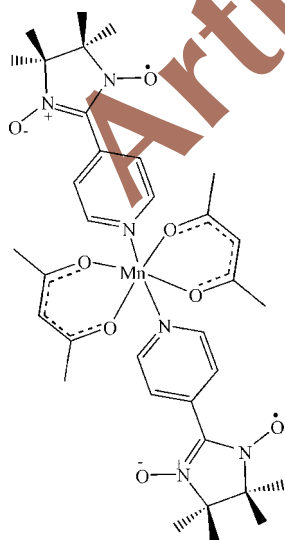
Received 9 November 2008; accepted 18 November 2008

Key indicators: single-crystal X-ray study; *T* = 293 K; mean  $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$ ; *R* factor = 0.041; *wR* factor = 0.118; data-to-parameter ratio = 14.3.

In the title compound,  $[\text{Mn}(\text{C}_5\text{H}_7\text{O}_2)_2(\text{C}_{12}\text{H}_{16}\text{N}_3\text{O}_2)]$ , the manganese(II) cation (site symmetry  $\bar{1}$ ) is hexacoordinated by four O and two N atoms in a distorted trans- $\text{MnN}_2\text{O}_4$  octahedral geometry. The four O atoms belonging to two 2,4-pentanedionate anions lie in the equatorial plane and the two N atoms occupy the axial coordination sites.

**Related literature**

For related structures, see: Caruso *et al.* (2005); Iskander *et al.* (2001); Rajak *et al.* (2000); Sangeetha *et al.* (2000); Sutradhar *et al.* (2006).



**Experimental**

*Crystal data*

$[\text{Mn}(\text{C}_5\text{H}_7\text{O}_2)_2(\text{C}_{12}\text{H}_{16}\text{N}_3\text{O}_2)]$   
 $M_r = 721.71$   
 Triclinic,  $P\bar{1}$   
 $a = 7.277 (3) \text{ \AA}$   
 $b = 9.7167 (15) \text{ \AA}$   
 $c = 13.2643 (15) \text{ \AA}$   
 $\alpha = 97.978 (10)^\circ$   
 $\beta = 103.342 (10)^\circ$   
 $\gamma = 92.869 (10)^\circ$   
 $V = 900.4 (4) \text{ \AA}^3$   
 $Z = 1$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.42 \text{ mm}^{-1}$   
 $T = 293 (2) \text{ K}$   
 $0.12 \times 0.10 \times 0.08 \text{ mm}$

*Data collection*

Bruker APEXII CCD area-detector diffractometer  
 Absorption correction: multi-scan (*SADABS*; Bruker, 2001)  
 $T_{\text{min}} = 0.951, T_{\text{max}} = 0.970$   
 6210 measured reflections  
 3264 independent reflections  
 2511 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.033$

*Refinement*

$R[F^2 > 2\sigma(F^2)] = 0.041$   
 $wR(F^2) = 0.118$   
 $S = 1.00$   
 3264 reflections  
 229 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.58 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.51 \text{ e \AA}^{-3}$

**Table 1**

Selected bond lengths ( $\text{\AA}$ ).

Mn1—O1	1.9964 (17)	Mn1—N1	2.242 (2)
Mn1—O3	2.0597 (17)		

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: HB2842).

**References**

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 Sangeetha, N. R. & Pal, S. (2000). *Bull. Chem. Soc. Jpn.*, **73**, 357–361.  
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 Sutradhar, M., Mukherjee, G., Drew, M. G. B. & Ghosh, S. (2006). *Inorg. Chem.* **45**, 5150–5158.

## supporting information

*Acta Cryst.* (2008). E64, m1604 [doi:10.1107/S1600536808038440]

**Bis[2,4-pentanedionato(1-)]bis[4,4,5,5-tetramethyl-2-(4-pyridyl)-imidazoline-1-oxyl 3-oxide]manganese(II)**

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**S1. Comment**

To design different kinds of metal-based coordination architectures with appropriate organic radicals and co-ligands has been an important subject during the last decade because of its potential usages for molecule-based magnetic materials and optical devices. Varying the organic units, such as tridentate nitronyl nitroxide radical, and bidentate nitroxide radical could results in a large number of building blocks with the potential applications. In this paper, we report the structure of the title compound, (I).

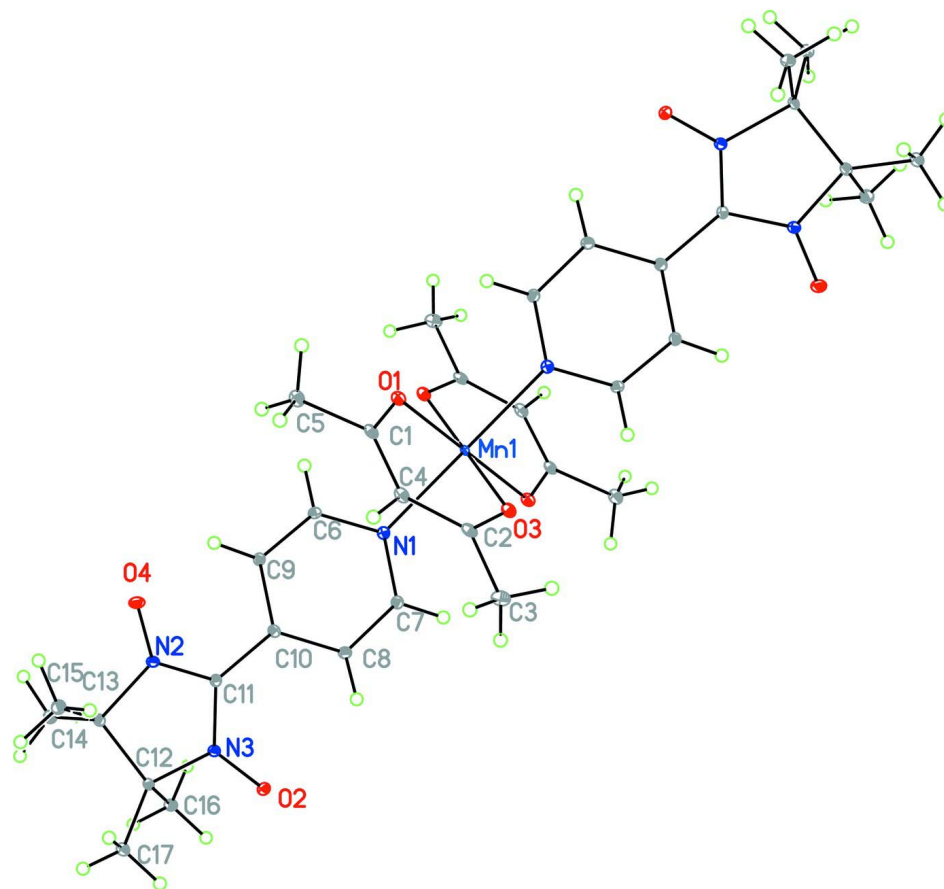
As shown in Fig. 1, the manganese(II) cation is hexacoordinated with four O and two N atoms showing a slightly distorted octahedral geometry. The Mn(II) cation lies on an inversion centre. The four oxygen atoms belonging to two 2,4-pentanedionate lie in the equatorial plane and the two nitrogen atoms lie in the axial coordination sites (Table 1).

**S2. Experimental**

A mixture of manganese(II) acetylacetonate (1 mmol) and 2-(4-pyridyl)-4,4,5,5-tetramethylimidazoline-1-oxyl-3-oxide (1 mmol) in 20 ml methanol was refluxed for several hours. The above cooled solution was filtered and the filtrate was kept in an ice box. One week later, brown blocks of (I) were obtained with a yield of *ca* 3%. Anal. Calc. for  $C_{34}H_{46}N_6MnO_8$ : C 56.48, H 6.31, N 11.55%; Found: C 56.53, H 6.37, N 11.64%.

**S3. Refinement**

All H atoms were placed in calculated positions with C—H = 0.93–0.96 Å and refined as riding with  $U_{iso}(H) = 1.2U_{eq}(C)$  or  $1.5U_{eq}(\text{methyl C})$ .



**Figure 1**

The molecular structure of (I) around Mn(II), drawn with 30% probability displacement ellipsoids for the non-hydrogen atoms. The unlabelled atoms are generated by the symmetry operation  $(-x, -y, -z)$ .

**Bis[2,4-pentanedionato(1-)]bis[4,4,5,5-tetramethyl-2-(4-pyridyl)imidazoline-1-oxyl 3-oxide]manganese(II)**

*Crystal data*

$[\text{Mn}(\text{C}_5\text{H}_7\text{O}_2)_2(\text{C}_{12}\text{H}_{16}\text{N}_3\text{O}_2)]$

$M_r = 721.71$

Triclinic,  $P\bar{1}$

Hall symbol:  $-P\ 1$

$a = 7.277\ (3)\ \text{\AA}$

$b = 9.7167\ (15)\ \text{\AA}$

$c = 13.2643\ (15)\ \text{\AA}$

$\alpha = 97.978\ (10)^\circ$

$\beta = 103.342\ (10)^\circ$

$\gamma = 92.869\ (10)^\circ$

$V = 900.4\ (4)\ \text{\AA}^3$

$Z = 1$

$F(000) = 381$

$D_x = 1.331\ \text{Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 3264 reflections

$\theta = 2.9\text{--}25.5^\circ$

$\mu = 0.42\ \text{mm}^{-1}$

$T = 293\ \text{K}$

Block, brown

$0.12 \times 0.10 \times 0.08\ \text{mm}$

*Data collection*

Bruker APEXII CCD area-detector  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan  
(*SADABS*; Bruker, 2001)

$T_{\min} = 0.951$ ,  $T_{\max} = 0.970$

6210 measured reflections

3264 independent reflections

2511 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.033$   
 $\theta_{\text{max}} = 25.5^\circ$ ,  $\theta_{\text{min}} = 2.9^\circ$

$h = -6 \rightarrow 8$   
 $k = -11 \rightarrow 11$   
 $l = -11 \rightarrow 16$

### Refinement

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.041$   
 $wR(F^2) = 0.118$   
 $S = 1.00$   
 3264 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  
 $w = 1/[\sigma^2(F_o^2) + (0.07P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.007$   
 $\Delta\rho_{\text{max}} = 0.58 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.51 \text{ e } \text{\AA}^{-3}$

### 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 ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Mn1	0.0000	0.0000	0.0000	0.0236 (6)
C1	-0.0486 (4)	0.2828 (3)	0.0582 (2)	0.0237 (6)
C2	0.2048 (4)	0.2371 (3)	-0.0432 (2)	0.0249 (6)
C3	0.3726 (4)	0.2936 (3)	-0.0812 (2)	0.0343 (7)
H3A	0.4838	0.2496	-0.0522	0.052*
H3B	0.3946	0.3926	-0.0589	0.052*
H3C	0.3449	0.2741	-0.1564	0.052*
C4	0.1139 (4)	0.3210 (3)	0.0232 (2)	0.0264 (6)
H4	0.1672	0.4122	0.0467	0.032*
C5	-0.1320 (4)	0.3856 (3)	0.1294 (2)	0.0319 (7)
H5A	-0.2665	0.3830	0.1019	0.048*
H5B	-0.0754	0.4781	0.1327	0.048*
H5C	-0.1066	0.3607	0.1985	0.048*
C6	0.1703 (4)	0.1166 (3)	0.2387 (2)	0.0220 (6)
H6	0.0417	0.1238	0.2338	0.026*
C7	0.4138 (4)	0.0539 (3)	0.1578 (2)	0.0232 (6)
H7	0.4539	0.0187	0.0984	0.028*
C8	0.5526 (4)	0.0956 (3)	0.2535 (2)	0.0246 (6)
H8	0.6802	0.0871	0.2560	0.030*
C9	0.2971 (4)	0.1612 (3)	0.3371 (2)	0.0222 (6)
H9	0.2526	0.1967	0.3950	0.027*
C10	0.4944 (4)	0.1510 (3)	0.3461 (2)	0.0222 (6)

C11	0.6315 (4)	0.1986 (3)	0.4507 (2)	0.0222 (6)
C12	0.9181 (3)	0.2690 (3)	0.58642 (19)	0.0210 (6)
C13	0.7430 (4)	0.2984 (3)	0.6343 (2)	0.0232 (6)
C14	0.7504 (4)	0.2549 (3)	0.7443 (2)	0.0307 (7)
H14A	0.6361	0.2770	0.7652	0.046*
H14B	0.8576	0.3046	0.7948	0.046*
H14C	0.7620	0.1564	0.7404	0.046*
C15	0.6888 (4)	0.4434 (3)	0.6352 (2)	0.0328 (7)
H15A	0.6878	0.4715	0.5685	0.049*
H15B	0.7786	0.5045	0.6894	0.049*
H15C	0.5648	0.4483	0.6483	0.049*
C16	1.0020 (4)	0.1369 (3)	0.6128 (2)	0.0254 (6)
H16A	0.9033	0.0623	0.5969	0.038*
H16B	1.0634	0.1492	0.6861	0.038*
H16C	1.0930	0.1147	0.5722	0.038*
C17	1.0770 (4)	0.3830 (3)	0.6102 (2)	0.0260 (6)
H17A	1.1689	0.3565	0.5711	0.039*
H17B	1.1363	0.3975	0.6838	0.039*
H17C	1.0271	0.4677	0.5908	0.039*
N1	0.2243 (3)	0.0629 (2)	0.14911 (16)	0.0214 (5)
N2	0.5856 (3)	0.2134 (2)	0.54863 (17)	0.0250 (5)
N3	0.8188 (3)	0.2417 (2)	0.46660 (17)	0.0221 (5)
O1	-0.1368 (2)	0.16513 (17)	0.03794 (14)	0.0254 (4)
O2	0.9120 (3)	0.25072 (19)	0.39302 (14)	0.0277 (4)
O3	0.1567 (2)	0.11183 (18)	-0.07693 (14)	0.0259 (4)
O4	0.4265 (3)	0.1723 (2)	0.56899 (15)	0.0351 (5)

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Mn1	0.0270 (15)	0.0192 (14)	0.0214 (15)	0.0067 (11)	0.0002 (11)	0.0001 (11)
C1	0.0267 (14)	0.0198 (13)	0.0197 (14)	0.0041 (10)	-0.0057 (11)	0.0045 (10)
C2	0.0244 (14)	0.0214 (13)	0.0246 (15)	0.0003 (10)	-0.0055 (11)	0.0087 (11)
C3	0.0301 (16)	0.0276 (15)	0.0445 (19)	-0.0007 (12)	0.0041 (14)	0.0122 (13)
C4	0.0316 (15)	0.0180 (13)	0.0256 (15)	0.0005 (11)	-0.0013 (12)	0.0040 (11)
C5	0.0373 (17)	0.0220 (14)	0.0327 (17)	0.0074 (12)	0.0012 (13)	0.0017 (12)
C6	0.0193 (13)	0.0234 (13)	0.0245 (15)	0.0035 (10)	0.0056 (11)	0.0061 (11)
C7	0.0246 (14)	0.0242 (13)	0.0212 (15)	0.0045 (10)	0.0052 (11)	0.0045 (11)
C8	0.0208 (14)	0.0270 (14)	0.0258 (16)	0.0026 (10)	0.0051 (11)	0.0044 (11)
C9	0.0238 (14)	0.0234 (13)	0.0199 (14)	0.0033 (10)	0.0055 (11)	0.0038 (10)
C10	0.0233 (14)	0.0217 (13)	0.0209 (15)	0.0006 (10)	0.0035 (11)	0.0045 (10)
C11	0.0230 (14)	0.0260 (13)	0.0178 (14)	0.0022 (10)	0.0051 (11)	0.0030 (11)
C12	0.0201 (13)	0.0256 (14)	0.0151 (14)	0.0009 (10)	0.0007 (10)	0.0026 (10)
C13	0.0224 (14)	0.0268 (14)	0.0185 (14)	0.0038 (11)	0.0009 (11)	0.0029 (11)
C14	0.0270 (15)	0.0405 (17)	0.0236 (16)	0.0033 (12)	0.0035 (12)	0.0060 (12)
C15	0.0292 (16)	0.0346 (16)	0.0330 (18)	0.0106 (12)	0.0046 (13)	0.0017 (13)
C16	0.0225 (14)	0.0250 (14)	0.0284 (16)	0.0034 (10)	0.0040 (12)	0.0058 (11)
C17	0.0254 (14)	0.0254 (14)	0.0254 (16)	0.0013 (11)	0.0031 (12)	0.0034 (11)

N1	0.0236 (12)	0.0185 (11)	0.0221 (13)	0.0025 (8)	0.0051 (10)	0.0039 (9)
N2	0.0175 (12)	0.0340 (13)	0.0225 (13)	0.0003 (9)	0.0038 (9)	0.0040 (10)
N3	0.0192 (11)	0.0260 (11)	0.0206 (12)	0.0014 (9)	0.0038 (10)	0.0041 (9)
O1	0.0261 (10)	0.0207 (9)	0.0268 (11)	0.0038 (7)	0.0006 (8)	0.0039 (8)
O2	0.0235 (10)	0.0367 (11)	0.0239 (11)	0.0013 (8)	0.0087 (8)	0.0033 (8)
O3	0.0280 (10)	0.0210 (9)	0.0258 (11)	-0.0002 (7)	0.0011 (8)	0.0031 (8)
O4	0.0205 (10)	0.0555 (14)	0.0309 (12)	-0.0011 (9)	0.0076 (9)	0.0113 (10)

Geometric parameters ( $\text{\AA}$ ,  $^\circ$ )

Mn1—O1 <sup>i</sup>	1.9964 (17)	C9—C10	1.422 (4)
Mn1—O1	1.9964 (17)	C9—H9	0.9300
Mn1—O3	2.0597 (17)	C10—C11	1.508 (4)
Mn1—O3 <sup>i</sup>	2.0597 (17)	C11—N3	1.365 (3)
Mn1—N1	2.242 (2)	C11—N2	1.405 (3)
Mn1—N1 <sup>i</sup>	2.242 (2)	C12—C16	1.498 (3)
C1—O1	1.246 (3)	C12—C17	1.507 (3)
C1—C4	1.417 (4)	C12—N3	1.566 (3)
C1—C5	1.524 (4)	C12—C13	1.571 (4)
C2—O3	1.241 (3)	C13—C15	1.482 (4)
C2—C4	1.415 (4)	C13—N2	1.527 (3)
C2—C3	1.530 (4)	C13—C14	1.564 (4)
C3—H3A	0.9600	C14—H14A	0.9600
C3—H3B	0.9600	C14—H14B	0.9600
C3—H3C	0.9600	C14—H14C	0.9600
C4—H4	0.9300	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—N1	1.379 (3)	C16—H16B	0.9600
C6—C9	1.412 (4)	C16—H16C	0.9600
C6—H6	0.9300	C17—H17A	0.9600
C7—N1	1.364 (3)	C17—H17B	0.9600
C7—C8	1.421 (4)	C17—H17C	0.9600
C7—H7	0.9300	N2—O4	1.304 (3)
C8—C10	1.434 (4)	N3—O2	1.320 (3)
C8—H8	0.9300		
O1 <sup>i</sup> —Mn1—O1	180.0	N3—C11—N2	108.1 (2)
O1 <sup>i</sup> —Mn1—O3	87.80 (7)	N3—C11—C10	126.2 (2)
O1—Mn1—O3	92.20 (7)	N2—C11—C10	125.6 (2)
O1 <sup>i</sup> —Mn1—O3 <sup>i</sup>	92.20 (7)	C16—C12—C17	108.1 (2)
O1—Mn1—O3 <sup>i</sup>	87.80 (7)	C16—C12—N3	106.9 (2)
O3—Mn1—O3 <sup>i</sup>	180.0	C17—C12—N3	110.9 (2)
O1 <sup>i</sup> —Mn1—N1	90.40 (7)	C16—C12—C13	112.5 (2)
O1—Mn1—N1	89.60 (7)	C17—C12—C13	117.4 (2)
O3—Mn1—N1	89.56 (7)	N3—C12—C13	100.45 (18)
O3 <sup>i</sup> —Mn1—N1	90.44 (7)	C15—C13—N2	103.7 (2)

O1 <sup>i</sup> —Mn1—N1 <sup>i</sup>	89.60 (7)	C15—C13—C14	109.2 (2)
O1—Mn1—N1 <sup>i</sup>	90.40 (7)	N2—C13—C14	112.0 (2)
O3—Mn1—N1 <sup>i</sup>	90.44 (7)	C15—C13—C12	114.0 (2)
O3 <sup>i</sup> —Mn1—N1 <sup>i</sup>	89.56 (7)	N2—C13—C12	100.01 (19)
N1—Mn1—N1 <sup>i</sup>	180.0	C14—C13—C12	116.9 (2)
O1—C1—C4	125.9 (2)	C13—C14—H14A	109.5
O1—C1—C5	112.3 (2)	C13—C14—H14B	109.5
C4—C1—C5	121.8 (2)	H14A—C14—H14B	109.5
O3—C2—C4	123.9 (2)	C13—C14—H14C	109.5
O3—C2—C3	113.3 (2)	H14A—C14—H14C	109.5
C4—C2—C3	122.8 (2)	H14B—C14—H14C	109.5
C2—C3—H3A	109.5	C13—C15—H15A	109.5
C2—C3—H3B	109.5	C13—C15—H15B	109.5
H3A—C3—H3B	109.5	H15A—C15—H15B	109.5
C2—C3—H3C	109.5	C13—C15—H15C	109.5
H3A—C3—H3C	109.5	H15A—C15—H15C	109.5
H3B—C3—H3C	109.5	H15B—C15—H15C	109.5
C2—C4—C1	127.8 (2)	C12—C16—H16A	109.5
C2—C4—H4	116.1	C12—C16—H16B	109.5
C1—C4—H4	116.1	H16A—C16—H16B	109.5
C1—C5—H5A	109.5	C12—C16—H16C	109.5
C1—C5—H5B	109.5	H16A—C16—H16C	109.5
H5A—C5—H5B	109.5	H16B—C16—H16C	109.5
C1—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
N1—C6—C9	124.4 (2)	C12—C17—H17C	109.5
N1—C6—H6	117.8	H17A—C17—H17C	109.5
C9—C6—H6	117.8	H17B—C17—H17C	109.5
N1—C7—C8	123.1 (2)	C7—N1—C6	116.8 (2)
N1—C7—H7	118.5	C7—N1—Mn1	124.50 (17)
C8—C7—H7	118.5	C6—N1—Mn1	118.67 (16)
C7—C8—C10	119.5 (2)	O4—N2—C11	127.6 (2)
C7—C8—H8	120.2	O4—N2—C13	120.6 (2)
C10—C8—H8	120.2	C11—N2—C13	111.6 (2)
C6—C9—C10	118.6 (2)	O2—N3—C11	126.1 (2)
C6—C9—H9	120.7	O2—N3—C12	122.78 (18)
C10—C9—H9	120.7	C11—N3—C12	110.91 (19)
C9—C10—C8	117.6 (2)	C1—O1—Mn1	118.40 (17)
C9—C10—C11	119.2 (2)	C2—O3—Mn1	119.22 (17)
C8—C10—C11	123.2 (2)		

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