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Crystal structure of poly[(*N*,*N*-dimethylacetamide-κO)(μ_4-5-methylisophthalato-$\kappa^5 O$:O,O':O'':O''')manganese(II)]

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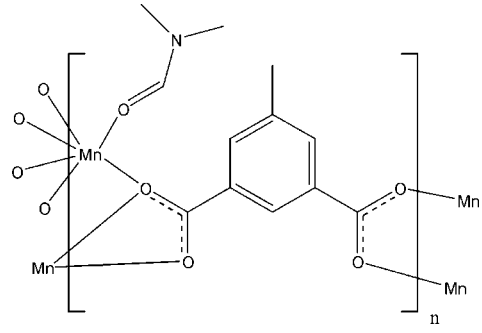
The title compound, poly[(*N*,*N*-dimethylacetamide-κO)(μ_4-5-methylisophthalato-$\kappa^5 O$,O':O',O'':O'')manganese(II)], $[Mn(C_9H_6O_4)(C_3H_7NO)]_n$, was obtained from a mixture containing $MnCl_2{\cdot}4H_2O$ and 5-methylisophthalic acid in *N*,*N*-dimethylacetamide solution. The Mn^{2+} ion is coordinated by five O atoms from four bridging 5-methylisophthalate ligands and one O atom from one *N*,*N*-dimethylacetamide ligand, defining a considerably distorted coordination polyhedron with one very long Mn—O bond of 2.623 (2) Å. The Mn^{2+} ions are joined by carboxylate groups, forming rod-shaped secondary building units along the *a* axis. The rods are further connected by 5-methylisophthalate ligands to form the pcu (primitive cubic net) structure.

Keywords: crystal structure; manganese(II) coordination polymer; pcu structure; *N*,*N*-dimethylacetamide; 5-methylisophthalate.

CCDC reference: 1035658

1. Related literature

For the structures of coordination polymers comprising first-row transition metal ions and benzene dicarboxylates, see: Deng *et al.* (2013); Jin *et al.* (2012); Li *et al.* (2010); Yang *et al.* (2013); Zhou *et al.* (2009). For the nomenclature for metal-organic frameworks, see: Rosi *et al.* (2005);. A very closely related crystal structure, poly[(dimethylformamide)(5-methoxybenzene-1,3-dicarboxylato)manganese(II)], was reported recently (Huang, 2013). The author described the structure in a PtS (cooperite) topology according to a different analytical approach (Carlucci *et al.*, 2003; Hill *et al.*, 2005).



2. Experimental

2.1. Crystal data

$[Mn(C_9H_6O_4)(C_3H_7NO)]$
M_r = 306.17
Orthorhombic, $Pna2_1$
a = 7.281 (5) Å
b = 15.148 (11) Å
c = 10.903 (8) Å
V = 1202.5 (15) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.11 mm^{-1}
T = 200 K
0.15 × 0.10 × 0.10 mm

2.2. Data collection

Bruker APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.851, T_{max} = 0.897
10159 measured reflections
2874 independent reflections
2768 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.059
S = 1.07
2874 reflections
175 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}
Absolute structure: Flack (1983), 0 Friedel pairs
Absolute structure parameter: 0.025 (14)

Table 1
Selected geometric parameters (Å, °).

Mn1—O4^{i}	2.0609 (19)	Mn1—O5	2.1342 (18)
Mn1—O3^{ii}	2.0855 (15)	Mn1—O2^{iii}	2.1378 (16)
Mn1—O1	2.0885 (16)		
O4^{i}—Mn1—O3^{ii}	131.59 (6)	O1—Mn1—O5	166.04 (5)
O4^{i}—Mn1—O1	83.59 (6)	O4^{i}—Mn1—O2^{iii}	135.70 (6)
O3^{ii}—Mn1—O1	98.77 (7)	O3^{ii}—Mn1—O2^{iii}	92.23 (7)
O4^{i}—Mn1—O5	83.95 (6)	O1—Mn1—O2^{iii}	97.51 (7)
O3^{ii}—Mn1—O5	84.88 (7)	O5—Mn1—O2^{iii}	95.80 (7)

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

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *DIAMOND* (Brandenburg, 2007); software used to prepare material for publication: *SHELXTL*.

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: FK2084).

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supporting information

Acta Cryst. (2015). E**71**, m1–m2 [doi:10.1107/S2056989014025626]

Crystal structure of poly[(*N*,*N*-dimethylacetamide-κO)(μ_4-5-methylisophthalato-$\kappa^5 O$:O,O':O'':O''')manganese(II)]

Lan Jin, Li-Li Zha, San Gao, Shi-Yao Yang and Rong-Bin Huang

S1. Chemical context

S2. Structural commentary

We have reported the structures of dozens of coordination polymers comprising first-row transition metal ions and benzene dicarboxylates (Deng *et al.*, 2013; Jin *et al.*, 2012; Li *et al.* 2010; Yang *et al.*, 2013; Zhou *et al.*, 2009). We found that metal ion is the most important factor that influences the structure of coordination polymer.

The title compound, $[Mn(C_9H_6O_4)(C_3H_7O)]_n$, (I) was obtained with the same method reported in our previous paper (Yang *et al.*, 2013). The structure feature of I is quite similar to those manganese analogs reported in that paper. The Mn^{2+} ions are joined by carboxyl groups to form rod-shaped secondary building units (SBUs) along the *a* axis. Each rod is further connected to four adjacent rods by 5-methylisophthalates to form the rod packing type 2 **pcu** (primitive cubic net) structure according to the nomenclature for metal-organic frameworks (Rosi *et al.*, 2005). A very closely related molecular structure, poly[(dimethylformamide)(5-methoxybenzene-1,3-dicarboxylato)manganese(II)], was reported recently (Huang, 2013). The author described the structure in **PtS** (cooperite) topology according to a different analysis approach (Carlucci *et al.*, 2003; Hill *et al.*, 2005).

S3. Supramolecular features

S4. Database survey

S5. Synthesis and crystallization

A mixture containing $MnCl_2.4H_2O$ (0.039 g, 0.20 mmol) and 5-methylisophthalic acid (H_2mip, 0.036 g, 0.20 mmol) in 10 mL *N*,*N*-dimethylacetamide (DMF) was heated at 100 °C for 5000 min. Colourless block crystals were generated (0.025 g, 41%).

S6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. H atoms bonded to C atoms were positioned geometrically and refined using a riding model (including free rotation about the C—C bond), with C—H = 0.95–0.99 Å and with U_{iso}(H) = 1.2 (1.5 for methyl groups) times U_{eq}(C).

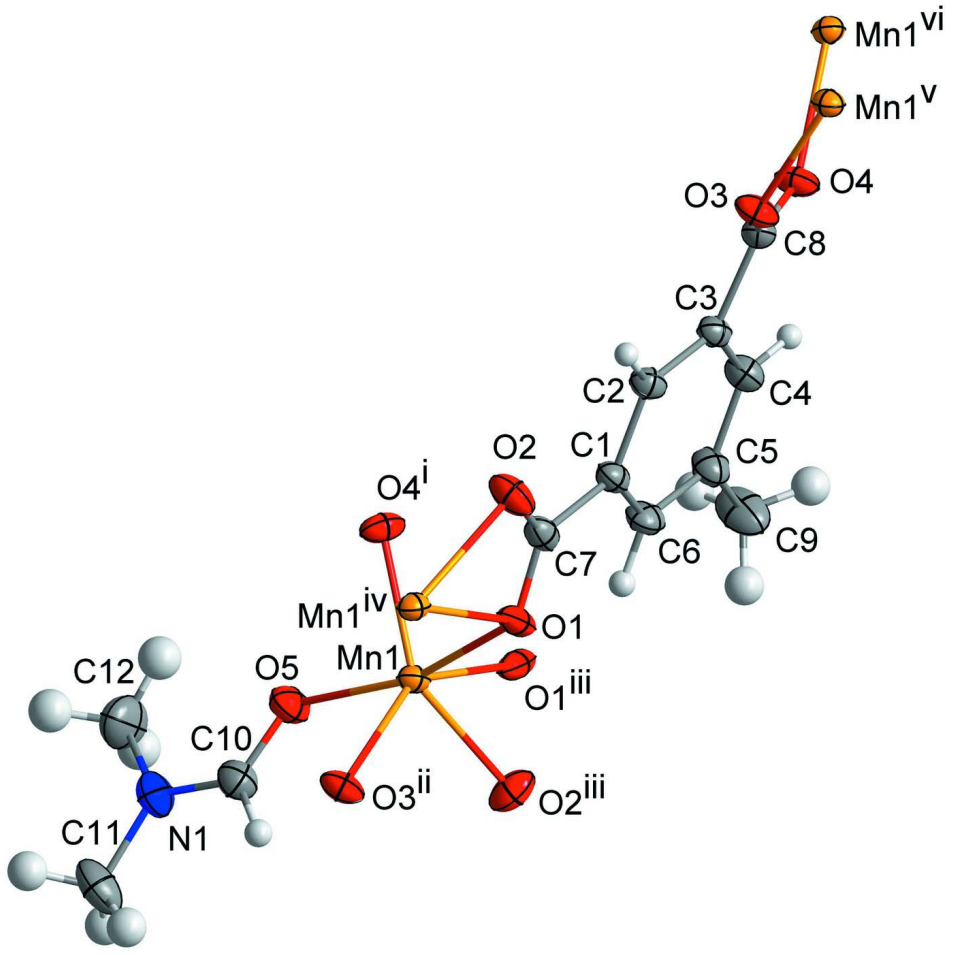

Figure 1

Coordination modes in (I). Anisotropic displacement ellipsoids are drawn at the 50% probability level. Symmetry codes: i -*x*, -*y* + 2, *z* + 1/2; ii -*x* + 1/2, *y* - 1/2, *z* + 1/2; iii *x* - 1/2, -*y* + 3/2, *z*; iv *x* + 1/2, -*y* + 3/2, *z*; v -*x* + 1/2, *y* + 1/2, *z* - 1/2; vi -*x*, -*y* + 2, *z* - 1/2.

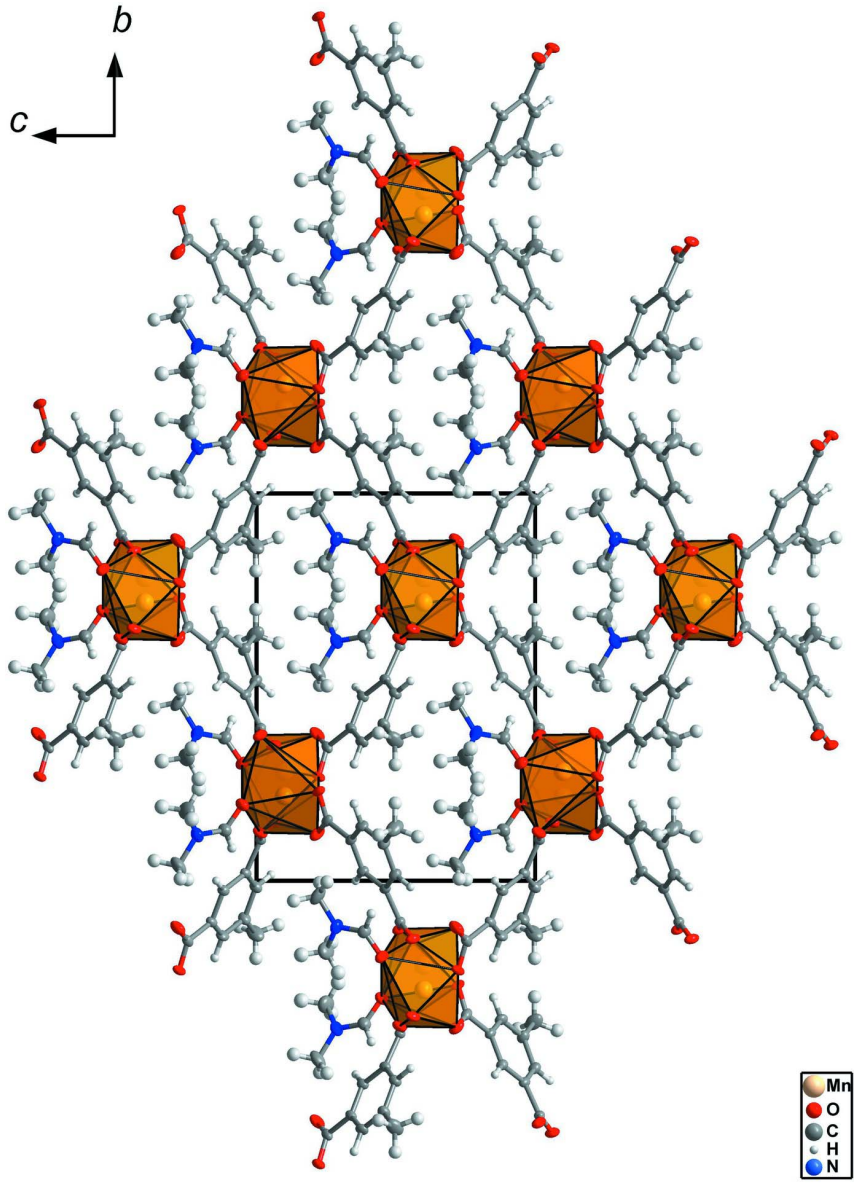

Figure 2

The packing of (I), viewed down the *a* axis, showing MnO_6 in polyhedra.

Poly[(*N*,*N*-dimethylacetamide-κO)(μ_4-5-methylisophthalato-$\kappa^5 O$:*O*,*O*′:*O*″:*O*‴)manganese(II)]

Crystal data

$[Mn(C_9H_6O_4)(C_3H_7NO)]$
M_r = 306.17
Orthorhombic, $Pna2_1$
Hall symbol: P 2c -2n
a = 7.281 (5) Å
b = 15.148 (11) Å
c = 10.903 (8) Å
V = 1202.5 (15) Å^3
Z = 4
$F(000)$ = 628
D_x = 1.691 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 6647 reflections
θ = 2.3–28.7°
μ = 1.11 mm^{-1}
T = 200 K
Rod, colorless
0.15 × 0.10 × 0.10 mm

Data collection

Bruker APEX area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scan
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.851, T_{max} = 0.897
10159 measured reflections
2874 independent reflections
2768 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 29.0°, θ_{min} = 2.3°
h = −9→9
k = −19→19
l = −13→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.059
S = 1.07
2874 reflections
175 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0316P)^2 + 0.1079P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}
Absolute structure: Flack (1983), 0 Friedel pairs
Absolute structure parameter: 0.025 (14)

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	0.02668 (3)	0.718473 (13)	0.40075 (4)	0.01733 (7)
O1	0.21890 (19)	0.76885 (7)	0.27699 (13)	0.0264 (3)
O2	0.40794 (19)	0.87833 (8)	0.28213 (14)	0.0320 (3)
O3	0.30783 (16)	1.12474 (7)	−0.01315 (13)	0.0244 (3)
O4	0.02059 (16)	1.15017 (8)	−0.06146 (13)	0.0254 (3)
O5	−0.15683 (19)	0.69631 (9)	0.55025 (14)	0.0301 (3)
N1	−0.2451 (2)	0.61847 (11)	0.71232 (16)	0.0323 (4)
C1	0.1457 (2)	0.89377 (11)	0.16063 (16)	0.0210 (3)
C2	0.1976 (2)	0.97512 (10)	0.11805 (18)	0.0208 (3)
H2A	0.3104	1.0003	0.1442	0.025*
C3	0.0878 (2)	1.02002 (10)	0.03817 (16)	0.0196 (3)
C4	−0.0754 (2)	0.98383 (11)	0.00205 (17)	0.0237 (3)
H4A	−0.1529	1.0157	−0.0523	0.028*
C5	−0.1290 (3)	0.90257 (12)	0.04273 (18)	0.0269 (4)
C6	−0.0157 (3)	0.85839 (12)	0.12133 (19)	0.0261 (4)

H6A	−0.0505	0.8014	0.1494	0.031*
C7	0.2643 (2)	0.84485 (11)	0.24625 (17)	0.0236 (4)
C8	0.1438 (2)	1.10570 (10)	−0.01549 (17)	0.0197 (3)
C9	−0.3076 (3)	0.86426 (15)	0.0039 (3)	0.0448 (6)
H9A	−0.2980	0.7997	0.0020	0.067*
H9B	−0.3392	0.8861	−0.0780	0.067*
H9C	−0.4034	0.8817	0.0623	0.067*
C10	−0.1507 (3)	0.63087 (12)	0.61313 (19)	0.0282 (4)
H10A	−0.0704	0.5849	0.5880	0.034*
C11	−0.2297 (3)	0.53842 (16)	0.7799 (2)	0.0459 (6)
H11A	−0.1283	0.5032	0.7469	0.069*
H11B	−0.3446	0.5050	0.7731	0.069*
H11C	−0.2057	0.5520	0.8664	0.069*
C12	−0.3792 (4)	0.68114 (17)	0.7505 (3)	0.0545 (7)
H12A	−0.3596	0.7369	0.7069	0.082*
H12B	−0.3680	0.6911	0.8390	0.082*
H12C	−0.5022	0.6586	0.7319	0.082*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.01845 (11)	0.01338 (10)	0.02015 (12)	0.00142 (7)	0.00145 (16)	0.00084 (12)
O1	0.0343 (7)	0.0170 (5)	0.0279 (7)	0.0074 (5)	0.0119 (6)	0.0068 (5)
O2	0.0262 (7)	0.0330 (7)	0.0368 (8)	−0.0002 (6)	−0.0060 (6)	0.0145 (6)
O3	0.0188 (6)	0.0207 (5)	0.0336 (7)	−0.0019 (4)	0.0012 (5)	0.0087 (5)
O4	0.0232 (6)	0.0172 (6)	0.0359 (8)	0.0006 (4)	−0.0074 (5)	0.0059 (5)
O5	0.0333 (7)	0.0266 (6)	0.0305 (8)	0.0002 (6)	0.0079 (6)	0.0069 (6)
N1	0.0328 (9)	0.0366 (9)	0.0274 (10)	−0.0036 (7)	0.0051 (7)	0.0065 (7)
C1	0.0227 (8)	0.0191 (7)	0.0211 (8)	0.0021 (6)	0.0043 (6)	0.0043 (6)
C2	0.0192 (8)	0.0193 (7)	0.0240 (8)	0.0002 (6)	0.0026 (6)	0.0021 (6)
C3	0.0202 (8)	0.0175 (7)	0.0212 (8)	0.0010 (6)	0.0047 (7)	0.0019 (6)
C4	0.0217 (8)	0.0230 (8)	0.0264 (9)	0.0006 (6)	0.0005 (7)	0.0053 (7)
C5	0.0267 (9)	0.0274 (9)	0.0267 (9)	−0.0067 (7)	−0.0001 (7)	0.0044 (7)
C6	0.0295 (9)	0.0201 (8)	0.0286 (10)	−0.0051 (6)	0.0048 (7)	0.0040 (7)
C7	0.0262 (8)	0.0235 (8)	0.0213 (9)	0.0070 (7)	0.0060 (7)	0.0051 (7)
C8	0.0223 (8)	0.0168 (7)	0.0199 (8)	0.0008 (6)	0.0000 (6)	0.0005 (6)
C9	0.0371 (12)	0.0452 (12)	0.0521 (14)	−0.0188 (9)	−0.0127 (10)	0.0132 (11)
C10	0.0253 (9)	0.0291 (9)	0.0303 (10)	−0.0008 (7)	0.0022 (8)	0.0026 (8)
C11	0.0445 (13)	0.0526 (13)	0.0407 (14)	−0.0074 (10)	0.0018 (11)	0.0222 (11)
C12	0.0674 (17)	0.0524 (14)	0.0437 (15)	0.0092 (13)	0.0238 (13)	−0.0037 (12)

Geometric parameters (Å, º)

Mn1—O4^{i}	2.0609 (19)	C2—C3	1.364 (2)
Mn1—O3^{ii}	2.0855 (15)	C2—H2A	0.9500
Mn1—O1	2.0885 (16)	C3—C4	1.367 (2)
Mn1—O5	2.1342 (18)	C3—C8	1.481 (2)
Mn1—O2^{iii}	2.1378 (16)	C4—C5	1.365 (2)

O1—C7	1.244 (2)	C4—H4A	0.9500
O2—C7	1.226 (2)	C5—C6	1.365 (3)
O2—Mn1^{iv}	2.1378 (16)	C5—C9	1.485 (3)
O3—C8	1.229 (2)	C6—H6A	0.9500
O3—Mn1^{v}	2.0855 (15)	C9—H9A	0.9800
O4—C8	1.228 (2)	C9—H9B	0.9800
O4—Mn1^{vi}	2.0609 (18)	C9—H9C	0.9800
O5—C10	1.206 (2)	C10—H10A	0.9500
N1—C10	1.295 (3)	C11—H11A	0.9800
N1—C11	1.424 (3)	C11—H11B	0.9800
N1—C12	1.424 (3)	C11—H11C	0.9800
C1—C6	1.361 (3)	C12—H12A	0.9800
C1—C2	1.370 (2)	C12—H12B	0.9800
C1—C7	1.472 (2)	C12—H12C	0.9800

O4^{i}—Mn1—O3^{ii}	131.59 (6)	C4—C5—C9	120.65 (19)
O4^{i}—Mn1—O1	83.59 (6)	C1—C6—C5	121.77 (17)
O3^{ii}—Mn1—O1	98.77 (7)	C1—C6—H6A	119.1
O4^{i}—Mn1—O5	83.95 (6)	C5—C6—H6A	119.1
O3^{ii}—Mn1—O5	84.88 (7)	O2—C7—O1	121.56 (17)
O1—Mn1—O5	166.04 (5)	O2—C7—C1	119.62 (16)
O4^{i}—Mn1—O2^{iii}	135.70 (6)	O1—C7—C1	118.76 (17)
O3^{ii}—Mn1—O2^{iii}	92.23 (7)	O4—C8—O3	126.10 (17)
O1—Mn1—O2^{iii}	97.51 (7)	O4—C8—C3	116.16 (16)
O5—Mn1—O2^{iii}	95.80 (7)	O3—C8—C3	117.70 (15)
C7—O1—Mn1	133.66 (12)	C5—C9—H9A	109.5
C7—O2—Mn1^{iv}	104.72 (11)	C5—C9—H9B	109.5
C8—O3—Mn1^{v}	135.39 (11)	H9A—C9—H9B	109.5
C8—O4—Mn1^{vi}	137.13 (12)	C5—C9—H9C	109.5
C10—O5—Mn1	122.70 (13)	H9A—C9—H9C	109.5
C10—N1—C11	120.94 (19)	H9B—C9—H9C	109.5
C10—N1—C12	120.75 (18)	O5—C10—N1	125.04 (18)
C11—N1—C12	118.1 (2)	O5—C10—H10A	117.5
C6—C1—C2	119.04 (17)	N1—C10—H10A	117.5
C6—C1—C7	120.53 (16)	N1—C11—H11A	109.5
C2—C1—C7	120.42 (17)	N1—C11—H11B	109.5
C3—C2—C1	120.22 (17)	H11A—C11—H11B	109.5
C3—C2—H2A	119.9	N1—C11—H11C	109.5
C1—C2—H2A	119.9	H11A—C11—H11C	109.5
C2—C3—C4	119.58 (15)	H11B—C11—H11C	109.5
C2—C3—C8	121.87 (16)	N1—C12—H12A	109.5
C4—C3—C8	118.50 (15)	N1—C12—H12B	109.5
C5—C4—C3	121.09 (17)	H12A—C12—H12B	109.5
C5—C4—H4A	119.5	N1—C12—H12C	109.5
C3—C4—H4A	119.5	H12A—C12—H12C	109.5
C6—C5—C4	118.27 (17)	H12B—C12—H12C	109.5
C6—C5—C9	121.07 (18)		

O4^{i}—Mn1—O1—C7	−2.37 (18)	Mn1^{iv}—O2—C7—O1	−2.1 (2)
O3^{ii}—Mn1—O1—C7	−133.56 (19)	Mn1^{iv}—O2—C7—C1	−179.51 (13)
O5—Mn1—O1—C7	−29.3 (4)	Mn1—O1—C7—O2	104.6 (2)
O2^{iii}—Mn1—O1—C7	132.99 (19)	Mn1—O1—C7—C1	−78.0 (2)
O4^{i}—Mn1—O5—C10	−152.61 (17)	C6—C1—C7—O2	−178.90 (18)
O3^{ii}—Mn1—O5—C10	−19.79 (16)	C2—C1—C7—O2	2.0 (3)
O1—Mn1—O5—C10	−125.7 (2)	C6—C1—C7—O1	3.7 (3)
O2^{iii}—Mn1—O5—C10	71.94 (17)	C2—C1—C7—O1	−175.45 (17)
C6—C1—C2—C3	0.5 (3)	Mn1^{vi}—O4—C8—O3	−26.5 (3)
C7—C1—C2—C3	179.64 (16)	Mn1^{vi}—O4—C8—C3	155.59 (13)
C1—C2—C3—C4	0.8 (3)	Mn1^{v}—O3—C8—O4	−12.1 (3)
C1—C2—C3—C8	−176.42 (16)	Mn1^{v}—O3—C8—C3	165.74 (13)
C2—C3—C4—C5	−1.3 (3)	C2—C3—C8—O4	−163.04 (17)
C8—C3—C4—C5	176.03 (17)	C4—C3—C8—O4	19.7 (2)
C3—C4—C5—C6	0.4 (3)	C2—C3—C8—O3	18.9 (2)
C3—C4—C5—C9	179.3 (2)	C4—C3—C8—O3	−158.37 (17)
C2—C1—C6—C5	−1.4 (3)	Mn1—O5—C10—N1	172.24 (15)
C7—C1—C6—C5	179.47 (18)	C11—N1—C10—O5	179.4 (2)
C4—C5—C6—C1	0.9 (3)	C12—N1—C10—O5	5.1 (3)
C9—C5—C6—C1	−178.0 (2)		

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