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Poly[μ_2-aqua-μ_4-naphthalene-1,8-dicarboxylato-manganese(II)]

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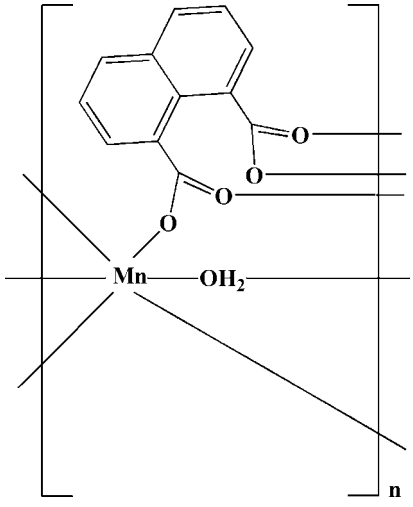
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.005 Å; R factor = 0.040; wR factor = 0.089; data-to-parameter ratio = 11.4.

The asymmetric unit of the title complex, $[Mn(C_{12}H_6O_4)(H_2O)]_n$, contains one Mn^{II} ion, one 1,8-naphthalenedicarboxylate (1,8-NDC) ligand and one water molecule. The Mn^{II} ion is six-coordinated within a distorted octahedral coordination geometry, in which the equatorial sites are occupied by four carboxylate O atoms from four different 1,8-NDC ligands, while the axial positions are occupied by two O atoms of two coordinated water molecules. Adjacent Mn^{II} centres are bridged by one coordinated water and two carboxylate groups in a *syn–syn* mode to form infinite chains along the *b* axis, which are further cross-linked by the naphthalene spacers of the 1,8-NDC ligands to produce a two-dimensional extended network.

Related literature

For general background, see: Chen *et al.* (2005). For related literature, see: Van der Ploeg *et al.* (1979); Hu *et al.* 2006.



Experimental

Crystal data

$[Mn(C_{12}H_6O_4)(H_2O)]$
M_r = 287.12
Monoclinic, $P2_1/c$
a = 15.720 (3) Å
b = 7.2167 (14) Å
c = 9.837 (2) Å
β = 98.87 (3)°
V = 1102.6 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.21 mm^{-1}
T = 294 (2) K
0.20 × 0.20 × 0.16 mm

Data collection

Rigaku R-AXIS RAPID-S diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.794, T_{max} = 0.830
9056 measured reflections
1945 independent reflections
1632 reflections with $I > 2\sigma(I)$
R_{int} = 0.058

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.089
S = 1.09
1945 reflections
171 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.85 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Mn1—O2^{i}	2.115 (2)	Mn1—O3	2.159 (2)
Mn1—O4	2.122 (2)	Mn1—O1*W*	2.214 (2)
Mn1—O1	2.156 (2)	Mn1—O1*W*^{ii}	2.232 (2)
O2^{i}—Mn1—O4	105.32 (8)	O1—Mn1—O1*W*	87.88 (9)
O2^{i}—Mn1—O1	171.04 (8)	O3—Mn1—O1*W*	87.61 (9)
O4—Mn1—O1	83.54 (8)	O2^{i}—Mn1—O1*W*^{ii}	85.20 (9)
O2^{i}—Mn1—O3	83.67 (8)	O4—Mn1—O1*W*^{ii}	86.44 (9)
O4—Mn1—O3	170.82 (8)	O1—Mn1—O1*W*^{ii}	96.86 (8)
O1—Mn1—O3	87.43 (8)	O3—Mn1—O1*W*^{ii}	96.31 (9)
O2^{i}—Mn1—O1*W*	90.70 (9)	O1*W*—Mn1—O1*W*^{ii}	173.97 (6)
O4—Mn1—O1*W*	90.40 (9)		

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

Data collection: *CrystalClear* (Rigaku/MSC, 2005); 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, 1998); software used to prepare material for publication: *SHELXTL*.

The authors thank Tianjin Normal University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2400).

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supporting information

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Poly[μ_2-aqua-μ_4-naphthalene-1,8-dicarboxylato-manganese(II)]

Guo-Ying Zhang, Xin Zhang and Gui-Sheng Yu

S1. Comment

Aromatic carboxylic derivatives as versatile building blocks not only exhibit great potentials in constructing multi-dimensional networks, but also provide various advantages in producing magnetic molecular assemblies with variable size from discrete molecules to nanometer-scale aggregates and infinite solids (Chen *et al.*, 2005). 1,8-Naphthalenedicarboxylate (1,8-NDC), a rigid multi- carboxylate ligand, is of special interest, since its multiple coordination sites, high symmetry and large conjugated structure can allow to construct molecular assemblies with novel structural motifs and physical properties. However, the metal complex of 1,8-NDC is rare so far (Van der Ploeg *et al.*, 1979; Hu *et al.*, 2006). We herein report the crystal structure of the title manganese complex, (I).

The asymmetric unit of (I) contains one Mn^{II} ion, one 1,8-NDC ligand and one water molecule. The Mn^{II} ion is six-coordinated within a distorted octahedral coordination geometry. The equatorial sites are occupied by four carboxylate oxygen atoms from different 1,8-NDC ligands, while the axial positions are occupied by two water molecules. The Mn—O distances are within their normal ranges (Table 1). Adjacent Mn^{II} centers are bridged by two carboxylate groups and one coordination water to form an infinite one-dimensional chain running along the *b* axis, in which the carboxylate groups adopt *syn-syn* bidentate coordination mode (Fig. 2). The intrachain Mn···Mn distance is 3.614 Å. The one-dimensional chains are further cross-linked by the naphthalene spacers of 1,8-NDC to produce a two-dimensional extended network (Fig. 3).

S2. Experimental

For the preparaton of the title complex, a mixture of $MnCl_2$ (1 mmol), 1,8-naphthalenedicarboxylic acid (1 mmol), NaOH (2 mmol) and water (8 ml) in a teflon-lined stainless steel autoclave (15 ml) was kept at 423 K for 2 d. Colorless crystals were obtained after cooling to room temperature (yield; 30%). Anal. Calc. for $C_{12}H_8MnO_5$: C 50.20, H 2.81%; Found: 50.56, H 2.52%.

S3. Refinement

H atom (for H_2O) were located in a difference sythesis and refined isotropically [O—H = 0.89 (4) and 0.80 (4) Å, U_{iso}(H) = 0.055 (13) and 0.045 (12) Å^2]. The remaining H atoms were positioned geometrically, with C—H = 0.93 Å for aromatic H, and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C).

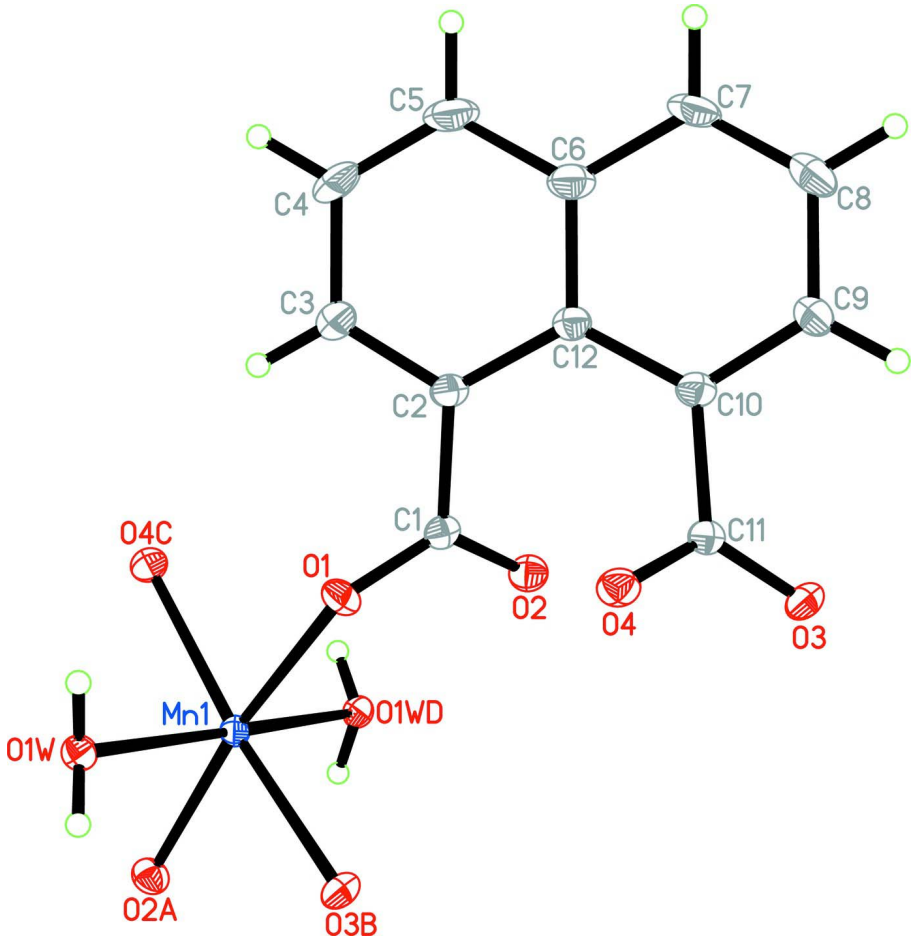

Figure 1

The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. [symmetry codes: (A) 2 - *x*, *y* - 1/2, 1/2 - *z*; (B) 2 - *x*, 1 - *y*,1 - *z*; (C) *x*, 1/2 - *y*, *z* - 1/2; (D) 2 - *x*, 1/2 + *y*, 1/2 - *z*].

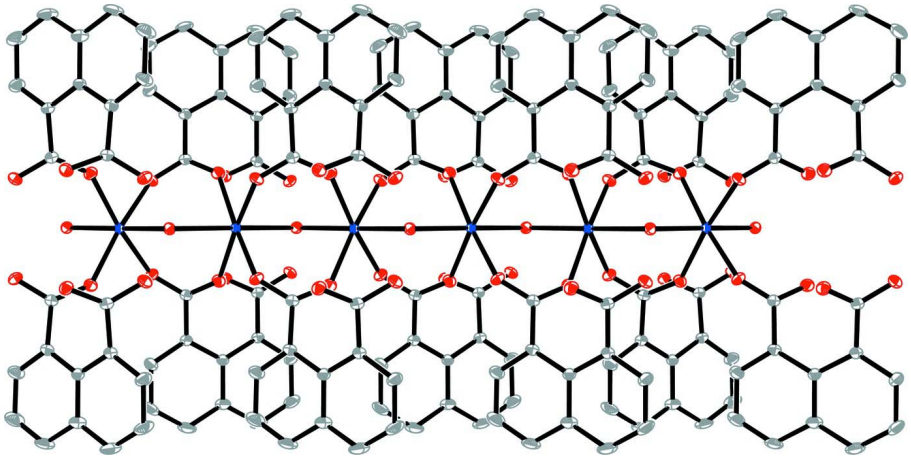

Figure 2

A view of the one-dimensional chain in (I).

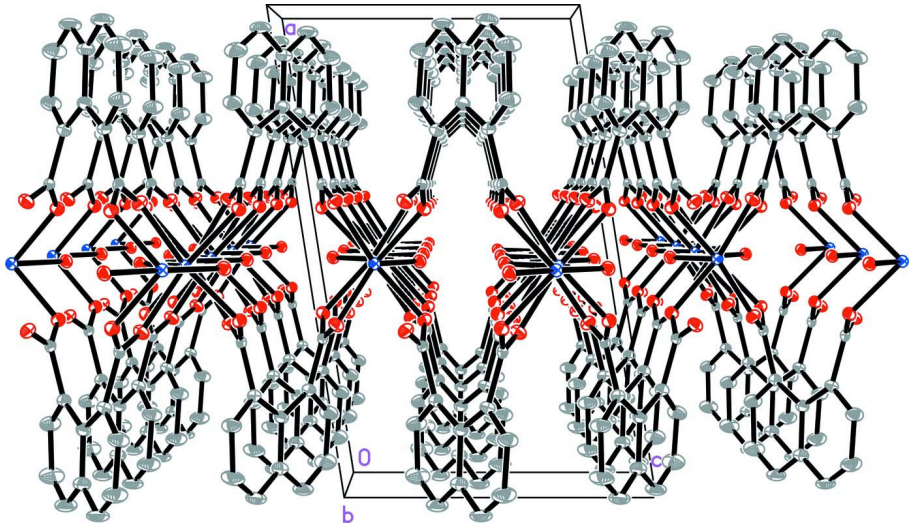

Figure 3

The extended two-dimensional layer structure of (I).

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Crystal data

$[Mn(C_{12}H_6O_4)(H_2O)]$
$M_r = 287.12$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 15.720$ (3) Å
$b = 7.2167$ (14) Å
$c = 9.837$ (2) Å
$\beta = 98.87$ (3)°
$V = 1102.6$ (4) Å^3
$Z = 4$
$F(000) = 580$
$D_x = 1.730$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2641 reflections
$\theta = 3.1$–27.5°
$\mu = 1.21$ mm^{-1}
$T = 294$ K
Block, colourless
0.20 × 0.20 × 0.16 mm

Data collection

Rigaku R-AXIS RAPID-S diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
$T_{min} = 0.794$, $T_{max} = 0.830$
9056 measured reflections
1945 independent reflections
1632 reflections with $I > 2\sigma(I)$
$R_{int} = 0.058$
$\theta_{max} = 25.0°$, $\theta_{min} = 3.1°$
$h = -18 \rightarrow 18$
$k = -8 \rightarrow 8$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.089$
$S = 1.09$
1945 reflections
171 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 atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0445P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.85$ e Å^{-3}
$\Delta\rho_{min} = -0.33$ 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	0.99931 (3)	0.10265 (5)	0.25999 (4)	0.01809 (16)
O1W	0.99998 (17)	−0.1557 (3)	0.3815 (2)	0.0211 (5)
H1WA	0.952 (3)	−0.169 (5)	0.419 (4)	0.055 (13)*
H1WB	1.041 (3)	−0.170 (5)	0.439 (4)	0.045 (12)*
O1	0.90398 (13)	0.2094 (3)	0.3753 (2)	0.0248 (5)
O2	0.89298 (12)	0.5099 (3)	0.3261 (2)	0.0265 (5)
O3	1.09599 (13)	0.2087 (3)	0.4210 (2)	0.0251 (5)
O4	0.89011 (12)	0.0082 (3)	0.1235 (2)	0.0268 (5)
C1	0.86289 (19)	0.3603 (4)	0.3608 (3)	0.0200 (6)
C2	0.76960 (19)	0.3550 (4)	0.3732 (3)	0.0232 (7)
C3	0.7238 (2)	0.2112 (5)	0.3086 (4)	0.0370 (9)
H3	0.7528	0.1119	0.2766	0.044*
C4	0.6336 (2)	0.2110 (6)	0.2897 (4)	0.0509 (11)
H4	0.6032	0.1110	0.2469	0.061*
C5	0.5907 (2)	0.3560 (6)	0.3335 (4)	0.0460 (10)
H5	0.5309	0.3571	0.3169	0.055*
C6	0.63495 (19)	0.5047 (5)	0.4034 (3)	0.0334 (8)
C7	0.5903 (2)	0.6559 (5)	0.4497 (4)	0.0437 (10)
H7	0.5305	0.6576	0.4323	0.052*
C8	0.6326 (2)	0.7975 (6)	0.5184 (4)	0.0501 (10)
H8	0.6021	0.8983	0.5449	0.060*
C9	0.7223 (2)	0.7935 (5)	0.5499 (3)	0.0368 (9)
H9	0.7508	0.8913	0.5990	0.044*
C10	0.7689 (2)	0.6497 (4)	0.5105 (3)	0.0248 (7)
C11	1.13824 (19)	0.3572 (4)	0.4273 (3)	0.0198 (6)
C12	0.72618 (18)	0.5038 (4)	0.4298 (3)	0.0234 (7)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0187 (3)	0.0169 (2)	0.0185 (3)	0.00005 (19)	0.00249 (17)	−0.00056 (18)
O1W	0.0221 (13)	0.0214 (11)	0.0194 (12)	0.0009 (9)	0.0017 (10)	0.0025 (8)

O1	0.0230 (12)	0.0284 (12)	0.0234 (12)	0.0067 (10)	0.0048 (9)	−0.0014 (9)
O2	0.0246 (12)	0.0283 (13)	0.0282 (12)	−0.0030 (10)	0.0091 (9)	0.0008 (9)
O3	0.0230 (12)	0.0288 (12)	0.0232 (12)	−0.0073 (10)	0.0026 (9)	−0.0045 (9)
O4	0.0240 (12)	0.0282 (13)	0.0264 (12)	−0.0009 (9)	−0.0023 (9)	−0.0033 (9)
C1	0.0205 (17)	0.0268 (17)	0.0128 (14)	−0.0021 (13)	0.0027 (11)	−0.0038 (12)
C2	0.0192 (17)	0.0269 (17)	0.0234 (16)	−0.0011 (12)	0.0029 (12)	−0.0009 (13)
C3	0.027 (2)	0.034 (2)	0.050 (2)	−0.0056 (15)	0.0051 (16)	−0.0138 (16)
C4	0.029 (2)	0.051 (3)	0.070 (3)	−0.0170 (18)	−0.0015 (19)	−0.026 (2)
C5	0.0181 (19)	0.063 (3)	0.055 (2)	−0.0063 (17)	0.0005 (16)	−0.0129 (19)
C6	0.0208 (19)	0.044 (2)	0.035 (2)	0.0001 (15)	0.0018 (14)	−0.0031 (16)
C7	0.0168 (19)	0.057 (3)	0.056 (2)	0.0107 (16)	0.0010 (16)	−0.0082 (19)
C8	0.031 (2)	0.052 (3)	0.067 (3)	0.0167 (19)	0.0066 (19)	−0.016 (2)
C9	0.026 (2)	0.037 (2)	0.046 (2)	0.0074 (15)	−0.0002 (15)	−0.0138 (16)
C10	0.0203 (17)	0.0282 (17)	0.0251 (17)	0.0016 (13)	0.0010 (13)	0.0008 (13)
C11	0.0197 (16)	0.0268 (17)	0.0130 (14)	0.0009 (13)	0.0033 (11)	−0.0024 (12)
C12	0.0200 (17)	0.0252 (17)	0.0245 (17)	−0.0003 (13)	0.0017 (12)	0.0010 (13)

Geometric parameters (Å, º)

Mn1—O2^{i}	2.115 (2)	C6—C12	1.418 (4)
Mn1—O4	2.122 (2)	C7—C8	1.343 (5)
Mn1—O1	2.156 (2)	C7—H7	0.9300
Mn1—O3	2.159 (2)	C8—C9	1.396 (5)
Mn1—O1W	2.214 (2)	C8—H8	0.9300
Mn1—O1W^{ii}	2.232 (2)	C9—C10	1.362 (4)
C1—O2	1.247 (3)	C9—H9	0.9300
C1—O1	1.262 (3)	C10—C12	1.423 (4)
C1—C2	1.491 (4)	C10—C11^{iii}	1.494 (4)
C2—C3	1.364 (4)	C11—O4^{ii}	1.252 (3)
C2—C12	1.430 (4)	C11—O3	1.257 (3)
C3—C4	1.401 (5)	C11—C10^{iii}	1.494 (4)
C3—H3	0.9300	O2—Mn1^{ii}	2.115 (2)
C4—C5	1.350 (5)	O4—C11^{i}	1.252 (3)
C4—H4	0.9300	O1W—Mn1^{i}	2.232 (2)
C5—C6	1.400 (5)	O1W—H1WA	0.89 (4)
C5—H5	0.9300	O1W—H1WB	0.80 (4)
C6—C7	1.410 (5)		

O2^{i}—Mn1—O4	105.32 (8)	C5—C6—C12	119.9 (3)
O2^{i}—Mn1—O1	171.04 (8)	C7—C6—C12	118.9 (3)
O4—Mn1—O1	83.54 (8)	C8—C7—C6	121.3 (3)
O2^{i}—Mn1—O3	83.67 (8)	C8—C7—H7	119.4
O4—Mn1—O3	170.82 (8)	C6—C7—H7	119.4
O1—Mn1—O3	87.43 (8)	C7—C8—C9	120.0 (4)
O2^{i}—Mn1—O1W	90.70 (9)	C7—C8—H8	120.0
O4—Mn1—O1W	90.40 (9)	C9—C8—H8	120.0
O1—Mn1—O1W	87.88 (9)	C10—C9—C8	121.5 (3)
O3—Mn1—O1W	87.61 (9)	C10—C9—H9	119.3

O2^{i}—Mn1—O1W^{ii}	85.20 (9)	C8—C9—H9	119.3
O4—Mn1—O1W^{ii}	86.44 (9)	C9—C10—C12	119.6 (3)
O1—Mn1—O1W^{ii}	96.86 (8)	C9—C10—C11^{iii}	116.3 (3)
O3—Mn1—O1W^{ii}	96.31 (9)	C12—C10—C11^{iii}	123.4 (3)
O1W—Mn1—O1W^{ii}	173.97 (6)	O4^{ii}—C11—O3	124.7 (3)
O2—C1—O1	124.6 (3)	O4^{ii}—C11—C10^{iii}	117.3 (3)
O2—C1—C2	117.6 (3)	O3—C11—C10^{iii}	117.8 (3)
O1—C1—C2	117.5 (3)	C6—C12—C10	118.4 (3)
C3—C2—C12	120.2 (3)	C6—C12—C2	117.5 (3)
C3—C2—C1	115.9 (3)	C10—C12—C2	124.0 (3)
C12—C2—C1	123.2 (3)	C1—O1—Mn1	129.36 (18)
C2—C3—C4	120.9 (3)	C1—O2—Mn1^{ii}	138.1 (2)
C2—C3—H3	119.6	C11—O3—Mn1	130.17 (19)
C4—C3—H3	119.6	C11^{i}—O4—Mn1	137.39 (19)
C5—C4—C3	120.1 (3)	Mn1—O1W—Mn1^{i}	108.74 (9)
C5—C4—H4	120.0	Mn1—O1W—H1WA	112 (2)
C3—C4—H4	120.0	Mn1^{i}—O1W—H1WA	105 (2)
C4—C5—C6	121.1 (3)	Mn1—O1W—H1WB	115 (3)
C4—C5—H5	119.5	Mn1^{i}—O1W—H1WB	105 (3)
C6—C5—H5	119.5	H1WA—O1W—H1WB	110 (4)
C5—C6—C7	121.2 (3)		

O2—C1—C2—C3	131.1 (3)	C1—C2—C12—C6	163.6 (3)
O1—C1—C2—C3	−43.2 (4)	C3—C2—C12—C10	173.6 (3)
O2—C1—C2—C12	−39.4 (4)	C1—C2—C12—C10	−16.3 (5)
O1—C1—C2—C12	146.3 (3)	O2—C1—O1—Mn1	−35.5 (4)
C12—C2—C3—C4	3.5 (5)	C2—C1—O1—Mn1	138.5 (2)
C1—C2—C3—C4	−167.3 (3)	O4—Mn1—O1—C1	−84.6 (2)
C2—C3—C4—C5	1.2 (6)	O3—Mn1—O1—C1	97.1 (2)
C3—C4—C5—C6	−2.8 (6)	O1W—Mn1—O1—C1	−175.2 (2)
C4—C5—C6—C7	−179.8 (4)	O1W^{ii}—Mn1—O1—C1	1.0 (3)
C4—C5—C6—C12	−0.4 (6)	O1—C1—O2—Mn1^{ii}	14.5 (5)
C5—C6—C7—C8	179.1 (4)	C2—C1—O2—Mn1^{ii}	−159.4 (2)
C12—C6—C7—C8	−0.3 (6)	O4^{ii}—C11—O3—Mn1	34.3 (4)
C6—C7—C8—C9	−2.5 (6)	C10^{iii}—C11—O3—Mn1	−140.3 (2)
C7—C8—C9—C10	1.2 (6)	O2^{i}—Mn1—O3—C11	83.3 (2)
C8—C9—C10—C12	2.9 (5)	O1—Mn1—O3—C11	−97.7 (3)
C8—C9—C10—C11^{iii}	−168.6 (3)	O1W—Mn1—O3—C11	174.3 (3)
C5—C6—C12—C10	−175.1 (3)	O1W^{ii}—Mn1—O3—C11	−1.1 (3)
C7—C6—C12—C10	4.3 (5)	O2^{i}—Mn1—O4—C11^{i}	55.2 (3)
C5—C6—C12—C2	4.9 (5)	O1—Mn1—O4—C11^{i}	−123.4 (3)
C7—C6—C12—C2	−175.7 (3)	O1W—Mn1—O4—C11^{i}	−35.6 (3)
C9—C10—C12—C6	−5.6 (5)	O1W^{ii}—Mn1—O4—C11^{i}	139.2 (3)
C11^{iii}—C10—C12—C6	165.3 (3)	O2^{i}—Mn1—O1W—Mn1^{i}	−52.06 (11)
C9—C10—C12—C2	174.4 (3)	O4—Mn1—O1W—Mn1^{i}	53.27 (11)

C11^{iii}—C10—C12—C2	−14.7 (5)	O1—Mn1—O1W—Mn1^{i}	136.79 (11)
C3—C2—C12—C6	−6.5 (4)	O3—Mn1—O1W—Mn1^{i}	−135.70 (11)

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