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Diaquabis(4,4′-bipyridine-κN)bis(2,4,5-trifluoro-3-hydroxybenzoato-κO^1)-manganese(II)

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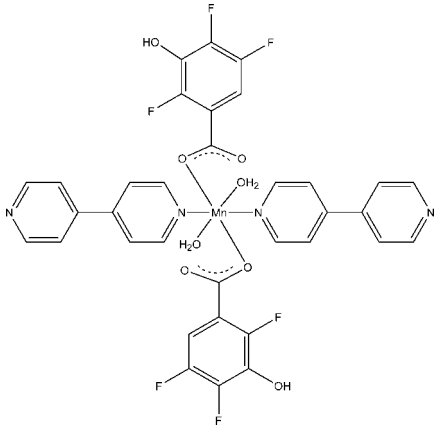
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.038; wR factor = 0.084; data-to-parameter ratio = 11.6.

In the title compound, $[Mn(C_7H_2F_3O_3)_2(C_{10}H_8N_2)_2(H_2O)_2]$, the Mn^{II} ion, situated on a centre of inversion, has a distorted octahedral coordination geometry and is coordinated by two N atoms from two 4,4′-bipyridine ligands, two O atoms from two 2,4,5-trifluoro-3-hydroxybenzoate ligands and two water molecules. Intermolecular O—H···N hydrogen bonds link the molecules into a chain along the a axis. Interactions between neighboring chains occur through O—H···O hydrogen bonds, which link the chains into a two-dimensional supramolecular network parallel to the ac plane. In addition, O—H···O hydrogen bonds between the water molecules and carboxylate groups also exist in the the crystal structure.

Related literature

For general background to the design and synthesis of novel metal-organic coordination polymers based on fluorobenzoic acid, see: Gielen *et al.* (1992); Ma *et al.* (2006); Shi *et al.* (2011). For a related structure, see: Zhu (2009).



Experimental

Crystal data

$[Mn(C_7H_2F_3O_3)_2(C_{10}H_8N_2)_2(H_2O)_2]$
M_r = 785.51
Triclinic, $P\overline{1}$
a = 7.0706 (6) Å
b = 8.2939 (7) Å
c = 13.9856 (12) Å
α = 79.200 (1)°
β = 88.338 (1)°
γ = 79.830 (2)°
V = 792.96 (12) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.51 mm^{-1}
T = 298 K
0.30 × 0.25 × 0.20 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.861, T_{max} = 0.904
4185 measured reflections
2792 independent reflections
2101 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.084
S = 1.01
2792 reflections
241 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H2W···O2	0.85	2.04	2.839 (2)	155
O1W—H1W···O2^{i}	0.84	1.97	2.773 (2)	159
O3—H3···N2^{ii}	0.82	1.89	2.641 (3)	152

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: RN2092).

References

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supporting information

Acta Cryst. (2011). E**67**, m1826 [https://doi.org/10.1107/S1600536811049610]

Diaquabis(4,4′-bipyridine-κN)bis(2,4,5-trifluoro-3-hydroxybenzoato-κO^1)manganese(II)

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S1. Comment

In recent years, the design and synthesis of novel metal-organic coordination polymers based on fluorobenzoic acids have attracted much attention (Gielen *et al.*, 1992; Ma *et al.*, 2006; Zhu, 2009; Shi *et al.*, 2011). We report herein the crystal structure (Fig. 1) of the title compound (I) based on 2,4,5-trifluoro-3-hydroxy-benzoic and 4,4′-bipyridine. In the crystal packing, the adjacent mononuclear units are linked into a linear chain along *a* axis *via* O—H···N hydrogen bonds (Fig. 2). Furthermore, additional interactions within neighboring chains occur through O—H···O hydrogen bonds, thus a two-dimensional supramolecular network parallel to *ac* plane is formed, as shown in Fig. 3. In addition, intramolecular O—H···O hydrogen bonds (O1W—H2W···O2) between the water molecules and carboxylate groups also exist in the the crystal structure.

S2. Experimental

A mixture of $Mn(CH_3COO)_2{\cdot}4H_2O$ (0.1 mmol), 2,4,5-trifluoro-3-hydroxy-benzoic acid (0.2 mmol), Et_3N (0.1 ml), EtOH (3 ml) and H_2O (2 ml) was sealed in a 10 ml Teflon-lined stainless-steel reactor, heated to 393 K for 72 h, and then slowly cooled to room temperature. Light yellow block crystals suitable for X-ray diffraction analysis were collected by filtration.

S3. Refinement

H atoms attached to C atoms were placed in calculated positions (C—H = 0.93 Å) and refined as riding atoms and with U_{iso}(H) = 1.2 U_{eq}(C),respectively. The hydroxyl and water H atoms were located in a difference map and refined with O—H bond length from 0.82 to 0.85 Å and U_{iso}(H) = 1.5 U_{eq}(O).

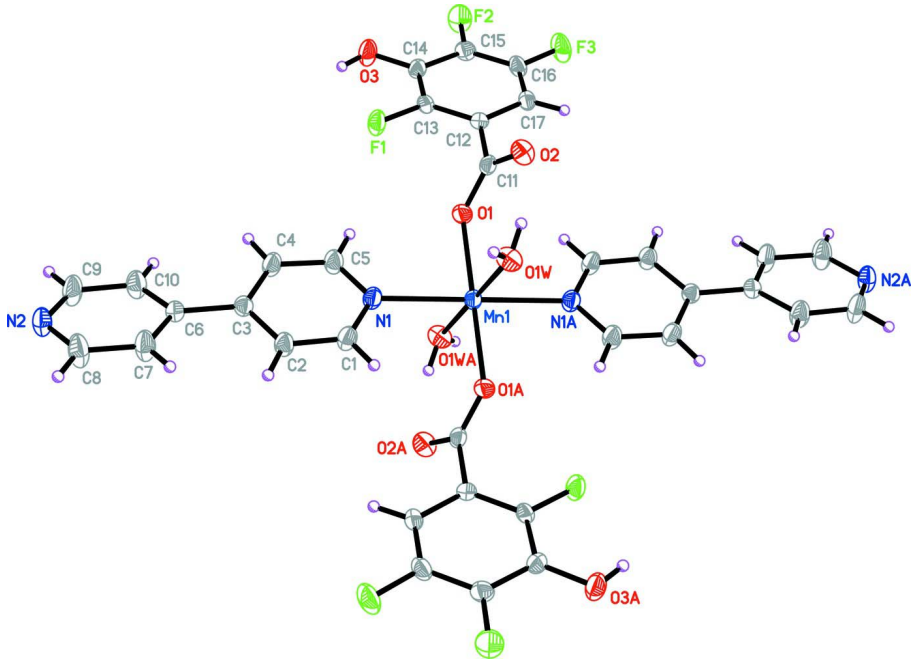

Figure 1

The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level [symmetry codes: (A) -*x*, 1 - *y*, 1 - *z*].

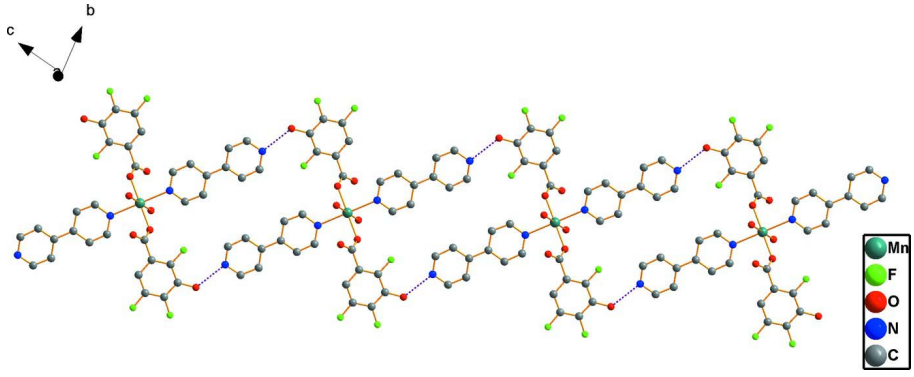

Figure 2

The linear chain of (I). All H atoms have been omitted for clarity

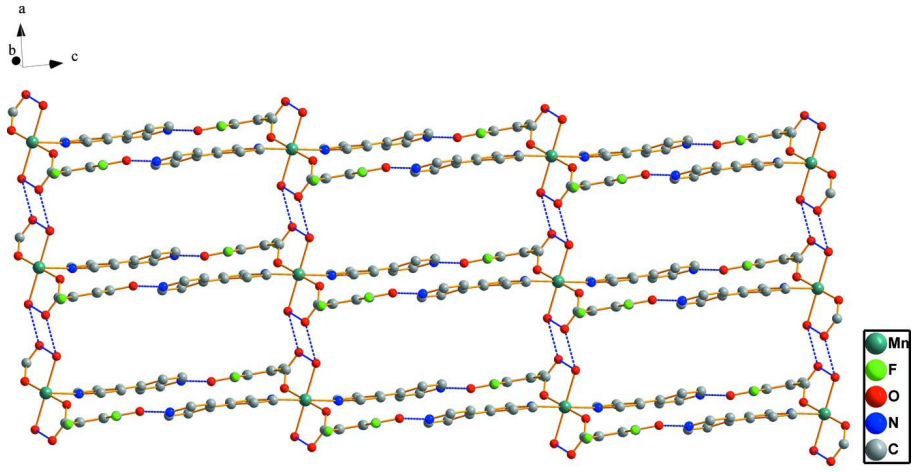

Figure 3

The two-dimensional of (I). All H atoms have been omitted for clarity

Diaquabis(4,4′-bipyridine-κN)bis(2,4,5-trifluoro-3- hydroxybenzoato-κO^1)manganese(II)

Crystal data

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c = 13.9856 (12) Å
α = 79.200 (1)°
β = 88.338 (1)°
γ = 79.830 (2)°
V = 792.96 (12) Å^3
Z = 1
$F(000)$ = 399
D_x = 1.645 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1483 reflections
θ = 2.9–26.6°
μ = 0.51 mm^{-1}
T = 298 K
Block, light yellow
0.30 × 0.25 × 0.20 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.861, T_{max} = 0.904
4185 measured reflections
2792 independent reflections
2101 reflections with $I > 2\sigma(I)$
R_{int} = 0.041
θ_{max} = 25.1°, θ_{min} = 2.5°
h = −8→8
k = −8→9
l = −15→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.084
S = 1.01
2792 reflections
241 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
$w = 1/[\sigma^2(F_o^2) + (0.0281P)^2 + 0.0001P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 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	0.5000	0.5000	0.03192 (17)
F1	0.2679 (2)	0.40469 (16)	0.18986 (10)	0.0502 (4)
F2	0.4119 (2)	−0.13268 (18)	0.11722 (11)	0.0654 (5)
F3	0.4709 (2)	−0.26309 (17)	0.30543 (11)	0.0653 (5)
O1	0.1454 (2)	0.3687 (2)	0.39423 (11)	0.0390 (4)
O1W	0.2747 (2)	0.5272 (2)	0.55884 (12)	0.0481 (5)
H1W	0.3355	0.6075	0.5531	0.072*
H2W	0.3528	0.4491	0.5395	0.072*
O2	0.4427 (2)	0.2766 (2)	0.45383 (12)	0.0452 (5)
O3	0.3067 (3)	0.1957 (2)	0.05414 (12)	0.0541 (5)
H3	0.2740	0.2973	0.0440	0.081*
N1	−0.0323 (3)	0.7434 (2)	0.38644 (14)	0.0371 (5)
N2	−0.2524 (3)	1.4900 (3)	0.03585 (15)	0.0475 (6)
C9	−0.2397 (4)	1.3428 (3)	0.01136 (19)	0.0573 (8)
H9	−0.2601	1.3389	−0.0535	0.069*
C10	−0.1977 (4)	1.1936 (3)	0.07644 (19)	0.0513 (7)
H10	−0.1919	1.0933	0.0549	0.062*
C6	−0.1646 (3)	1.1932 (3)	0.17280 (17)	0.0340 (6)
C7	−0.1801 (4)	1.3478 (3)	0.19819 (19)	0.0562 (8)
H7	−0.1596	1.3557	0.2624	0.067*
C8	−0.2257 (5)	1.4904 (3)	0.1290 (2)	0.0617 (9)
H8	−0.2384	1.5927	0.1488	0.074*
C3	−0.1171 (3)	1.0381 (3)	0.24554 (17)	0.0327 (6)
C4	−0.0622 (4)	0.8826 (3)	0.22071 (18)	0.0458 (7)
H4	−0.0530	0.8736	0.1554	0.055*
C5	−0.0210 (4)	0.7414 (3)	0.29101 (18)	0.0465 (7)
H5	0.0164	0.6394	0.2713	0.056*
C1	−0.0822 (4)	0.8925 (3)	0.41036 (17)	0.0409 (6)
H1	−0.0885	0.8980	0.4762	0.049*
C2	−0.1251 (4)	1.0389 (3)	0.34485 (17)	0.0407 (6)
H2	−0.1597	1.1390	0.3669	0.049*
C11	0.3130 (4)	0.2840 (3)	0.39429 (16)	0.0322 (6)
C12	0.3486 (3)	0.1745 (3)	0.31840 (16)	0.0305 (5)
C13	0.3175 (3)	0.2371 (3)	0.22071 (17)	0.0331 (6)
C15	0.3911 (4)	−0.0307 (3)	0.18248 (18)	0.0396 (6)

C16	0.4213 (3)	−0.0955 (3)	0.27927 (18)	0.0395 (6)
C17	0.4035 (3)	0.0031 (3)	0.34792 (17)	0.0355 (6)
H17	0.4276	−0.0432	0.4132	0.043*
C14	0.3377 (3)	0.1397 (3)	0.14978 (17)	0.0350 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0402 (3)	0.0269 (3)	0.0264 (3)	−0.0019 (2)	−0.0003 (2)	−0.0029 (2)
F1	0.0817 (11)	0.0280 (8)	0.0353 (8)	−0.0021 (7)	0.0036 (8)	0.0012 (6)
F2	0.1059 (14)	0.0421 (10)	0.0487 (10)	0.0014 (9)	−0.0030 (9)	−0.0223 (8)
F3	0.0996 (13)	0.0275 (9)	0.0604 (11)	0.0124 (8)	−0.0129 (9)	−0.0065 (8)
O1	0.0435 (11)	0.0392 (10)	0.0310 (10)	0.0052 (8)	−0.0003 (8)	−0.0096 (8)
O1W	0.0412 (11)	0.0415 (11)	0.0618 (12)	−0.0062 (8)	−0.0004 (9)	−0.0109 (9)
O2	0.0460 (11)	0.0439 (11)	0.0478 (11)	−0.0067 (8)	−0.0111 (9)	−0.0128 (9)
O3	0.0902 (15)	0.0395 (11)	0.0288 (10)	−0.0025 (10)	−0.0028 (10)	−0.0042 (8)
N1	0.0477 (13)	0.0311 (12)	0.0310 (12)	−0.0070 (10)	0.0016 (10)	−0.0018 (9)
N2	0.0673 (16)	0.0354 (13)	0.0365 (13)	−0.0076 (11)	−0.0104 (11)	0.0021 (11)
C9	0.095 (2)	0.0457 (18)	0.0285 (15)	−0.0092 (16)	−0.0113 (15)	0.0005 (13)
C10	0.082 (2)	0.0330 (16)	0.0375 (16)	−0.0059 (14)	−0.0067 (14)	−0.0051 (13)
C6	0.0353 (14)	0.0322 (14)	0.0320 (14)	−0.0039 (11)	−0.0009 (11)	−0.0015 (11)
C7	0.095 (2)	0.0367 (17)	0.0334 (16)	−0.0049 (15)	−0.0119 (15)	−0.0031 (13)
C8	0.107 (3)	0.0311 (16)	0.0451 (18)	−0.0064 (16)	−0.0170 (17)	−0.0033 (14)
C3	0.0331 (14)	0.0309 (14)	0.0329 (14)	−0.0065 (11)	0.0002 (11)	−0.0024 (11)
C4	0.072 (2)	0.0352 (16)	0.0276 (14)	−0.0041 (13)	0.0043 (13)	−0.0038 (12)
C5	0.073 (2)	0.0285 (15)	0.0345 (16)	−0.0011 (13)	0.0019 (14)	−0.0046 (12)
C1	0.0605 (18)	0.0342 (15)	0.0283 (14)	−0.0101 (12)	0.0006 (12)	−0.0046 (12)
C2	0.0596 (17)	0.0270 (14)	0.0339 (15)	−0.0057 (12)	0.0003 (12)	−0.0038 (12)
C11	0.0408 (15)	0.0265 (13)	0.0274 (13)	−0.0059 (11)	0.0026 (12)	−0.0002 (10)
C12	0.0277 (13)	0.0318 (14)	0.0308 (13)	−0.0026 (10)	0.0028 (10)	−0.0061 (11)
C13	0.0363 (14)	0.0219 (13)	0.0371 (14)	−0.0003 (10)	0.0027 (11)	−0.0002 (11)
C15	0.0461 (16)	0.0366 (16)	0.0371 (15)	−0.0008 (12)	0.0003 (12)	−0.0153 (13)
C16	0.0455 (16)	0.0244 (14)	0.0444 (16)	0.0020 (11)	−0.0035 (12)	−0.0030 (12)
C17	0.0385 (14)	0.0330 (14)	0.0307 (14)	0.0009 (11)	−0.0038 (11)	−0.0015 (11)
C14	0.0423 (15)	0.0346 (15)	0.0274 (14)	−0.0040 (11)	0.0009 (11)	−0.0062 (11)

Geometric parameters (Å, º)

Mn1—O1	2.1335 (15)	C10—H10	0.9300
Mn1—O1^{i}	2.1335 (15)	C6—C7	1.378 (3)
Mn1—O1W^{i}	2.1949 (16)	C6—C3	1.476 (3)
Mn1—O1W	2.1949 (16)	C7—C8	1.377 (4)
Mn1—N1	2.3038 (19)	C7—H7	0.9300
Mn1—N1^{i}	2.3038 (19)	C8—H8	0.9300
F1—C13	1.361 (3)	C3—C4	1.385 (3)
F2—C15	1.345 (3)	C3—C2	1.389 (3)
F3—C16	1.354 (3)	C4—C5	1.374 (3)
O1—C11	1.266 (3)	C4—H4	0.9300

O1W—H1W	0.8445	C5—H5	0.9300
O1W—H2W	0.8541	C1—C2	1.369 (3)
O2—C11	1.242 (3)	C1—H1	0.9300
O3—C14	1.342 (3)	C2—H2	0.9300
O3—H3	0.8200	C11—C12	1.510 (3)
N1—C1	1.326 (3)	C12—C13	1.377 (3)
N1—C5	1.338 (3)	C12—C17	1.392 (3)
N2—C9	1.316 (3)	C13—C14	1.382 (3)
N2—C8	1.323 (3)	C15—C16	1.368 (3)
C9—C10	1.383 (4)	C15—C14	1.388 (3)
C9—H9	0.9300	C16—C17	1.363 (3)
C10—C6	1.374 (3)	C17—H17	0.9300

O1—Mn1—O1^{i}	180.0	C7—C8—H8	118.2
O1—Mn1—O1W^{i}	88.91 (6)	C4—C3—C2	115.2 (2)
O1^{i}—Mn1—O1W^{i}	91.09 (6)	C4—C3—C6	123.1 (2)
O1—Mn1—O1W	91.09 (6)	C2—C3—C6	121.7 (2)
O1^{i}—Mn1—O1W	88.91 (6)	C5—C4—C3	121.1 (2)
O1W^{i}—Mn1—O1W	180.00 (8)	C5—C4—H4	119.5
O1—Mn1—N1	89.39 (6)	C3—C4—H4	119.5
O1^{i}—Mn1—N1	90.61 (6)	N1—C5—C4	123.2 (2)
O1W^{i}—Mn1—N1	84.76 (7)	N1—C5—H5	118.4
O1W—Mn1—N1	95.24 (7)	C4—C5—H5	118.4
O1—Mn1—N1^{i}	90.61 (6)	N1—C1—C2	124.6 (2)
O1^{i}—Mn1—N1^{i}	89.39 (6)	N1—C1—H1	117.7
O1W^{i}—Mn1—N1^{i}	95.24 (7)	C2—C1—H1	117.7
O1W—Mn1—N1^{i}	84.76 (7)	C1—C2—C3	120.2 (2)
N1—Mn1—N1^{i}	180.0	C1—C2—H2	119.9
C11—O1—Mn1	130.94 (15)	C3—C2—H2	119.9
Mn1—O1W—H1W	133.3	O2—C11—O1	125.9 (2)
Mn1—O1W—H2W	102.0	O2—C11—C12	118.6 (2)
H1W—O1W—H2W	104.9	O1—C11—C12	115.3 (2)
C14—O3—H3	109.5	C13—C12—C17	118.4 (2)
C1—N1—C5	115.8 (2)	C13—C12—C11	122.2 (2)
C1—N1—Mn1	122.51 (15)	C17—C12—C11	119.3 (2)
C5—N1—Mn1	121.30 (16)	F1—C13—C12	119.4 (2)
C9—N2—C8	116.3 (2)	F1—C13—C14	116.7 (2)
N2—C9—C10	123.8 (2)	C12—C13—C14	123.9 (2)
N2—C9—H9	118.1	F2—C15—C16	119.9 (2)
C10—C9—H9	118.1	F2—C15—C14	118.9 (2)
C6—C10—C9	120.1 (3)	C16—C15—C14	121.2 (2)
C6—C10—H10	119.9	F3—C16—C17	120.4 (2)
C9—C10—H10	119.9	F3—C16—C15	117.6 (2)
C10—C6—C7	115.8 (2)	C17—C16—C15	122.0 (2)
C10—C6—C3	122.7 (2)	C16—C17—C12	118.7 (2)
C7—C6—C3	121.5 (2)	C16—C17—H17	120.6
C8—C7—C6	120.4 (3)	C12—C17—H17	120.6
C8—C7—H7	119.8	O3—C14—C13	125.6 (2)

C6—C7—H7	119.8	O3—C14—C15	118.5 (2)
N2—C8—C7	123.6 (3)	C13—C14—C15	115.9 (2)
N2—C8—H8	118.2		
O1W^{i}—Mn1—O1—C11	−155.2 (2)	Mn1—N1—C1—C2	−171.9 (2)
O1W—Mn1—O1—C11	24.8 (2)	N1—C1—C2—C3	−0.3 (4)
N1—Mn1—O1—C11	120.1 (2)	C4—C3—C2—C1	−0.6 (4)
N1^{i}—Mn1—O1—C11	−59.9 (2)	C6—C3—C2—C1	179.3 (2)
O1—Mn1—N1—C1	−165.93 (19)	Mn1—O1—C11—O2	−10.1 (4)
O1^{i}—Mn1—N1—C1	14.07 (19)	Mn1—O1—C11—C12	165.38 (14)
O1W^{i}—Mn1—N1—C1	105.11 (19)	O2—C11—C12—C13	−128.6 (2)
O1W—Mn1—N1—C1	−74.89 (19)	O1—C11—C12—C13	55.6 (3)
O1—Mn1—N1—C5	21.15 (19)	O2—C11—C12—C17	55.3 (3)
O1^{i}—Mn1—N1—C5	−158.85 (19)	O1—C11—C12—C17	−120.5 (2)
O1W^{i}—Mn1—N1—C5	−67.81 (19)	C17—C12—C13—F1	−178.5 (2)
O1W—Mn1—N1—C5	112.19 (19)	C11—C12—C13—F1	5.4 (3)
C8—N2—C9—C10	−1.1 (5)	C17—C12—C13—C14	0.0 (4)
N2—C9—C10—C6	−0.6 (5)	C11—C12—C13—C14	−176.1 (2)
C9—C10—C6—C7	1.2 (4)	F2—C15—C16—F3	−0.3 (4)
C9—C10—C6—C3	−179.3 (2)	C14—C15—C16—F3	179.2 (2)
C10—C6—C7—C8	−0.2 (4)	F2—C15—C16—C17	179.4 (2)
C3—C6—C7—C8	−179.6 (3)	C14—C15—C16—C17	−1.0 (4)
C9—N2—C8—C7	2.3 (5)	F3—C16—C17—C12	−178.7 (2)
C6—C7—C8—N2	−1.7 (5)	C15—C16—C17—C12	1.5 (4)
C10—C6—C3—C4	14.1 (4)	C13—C12—C17—C16	−1.0 (3)
C7—C6—C3—C4	−166.5 (3)	C11—C12—C17—C16	175.2 (2)
C10—C6—C3—C2	−165.7 (2)	F1—C13—C14—O3	−2.3 (4)
C7—C6—C3—C2	13.6 (4)	C12—C13—C14—O3	179.2 (2)
C2—C3—C4—C5	0.5 (4)	F1—C13—C14—C15	179.1 (2)
C6—C3—C4—C5	−179.4 (2)	C12—C13—C14—C15	0.5 (4)
C1—N1—C5—C4	−1.5 (4)	F2—C15—C14—O3	0.7 (4)
Mn1—N1—C5—C4	171.9 (2)	C16—C15—C14—O3	−178.8 (2)
C3—C4—C5—N1	0.6 (4)	F2—C15—C14—C13	179.5 (2)
C5—N1—C1—C2	1.3 (4)	C16—C15—C14—C13	0.0 (4)

Symmetry code: (i) −*x*, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H2*W*···O2	0.85	2.04	2.839 (2)	155
O1*W*—H1*W*···O2^{ii}	0.84	1.97	2.773 (2)	159
O3—H3···N2^{iii}	0.82	1.89	2.641 (3)	152

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