Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Tetraaquabis[4-(4*H*-1,2,4-triazol-4-yl)-benzoato-κN^1]manganese(II) decahydrate

Ying-Ai Piao and Zhen-Yu Xuan*

Department of Laboratory and Equipment Management, Yanbian University, Yanbian 133002, People's Republic of China
Correspondence e-mail: zyxuan2011@163.com

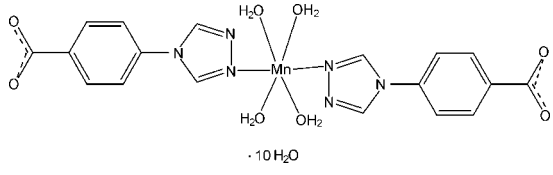
Received 21 June 2011; accepted 28 June 2011

Key indicators: single-crystal X-ray study; T = 76 K; mean σ(C–C) = 0.002 Å; R factor = 0.029; wR factor = 0.073; data-to-parameter ratio = 13.4.

In the title compound, $[Mn(C_9H_6N_3O_2)_2(H_2O)_4]\cdot 10H_2O$, the Mn^{II} ion is coordinated by two N atoms from two 4-(4*H*-1,2,4-triazol-4-yl)benzoate ligands and four water molecules in a distorted octahedral geometry. The Mn^{II} ion and two coordinated water molecules lie on a twofold rotation axis. The water molecules are involved in O—H···N and O—H···O hydrogen bonds with the triazole N atoms and carboxylate O atoms, yielding a three-dimensional supramolecular network. π–π interactions between the benzene rings [centroid–centroid distance = 3.836 (9) Å] are observed.

Related literature

For general background to the applications of coordination polymers, see: Guo *et al.* (2009); Wang *et al.* (2009); Zang *et al.* (2006). For a related structure, see: Wang (2011).



Experimental

Crystal data

$[Mn(C_9H_6N_3O_2)_2(H_2O)_4]\cdot 10H_2O$
M_r = 683.50
Monoclinic, $C2/c$
a = 25.9966 (13) Å
b = 7.9393 (4) Å
c = 16.8495 (9) Å
β = 112.214 (1)°
V = 3219.5 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.49 mm^{-1}
T = 76 K
0.28 × 0.23 × 0.20 mm

Data collection

Bruker APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.85, T_{max} = 0.91
8592 measured reflections
3189 independent reflections
2760 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.073
S = 0.99
3189 reflections
238 parameters
14 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1*W*—H1*A*···O4*W*	0.82 (2)	1.94 (2)	2.7602 (17)	171 (2)
O1*W*—H1*B*···O5*W*	0.85 (2)	1.83 (2)	2.6724 (16)	169 (2)
O2*W*—H2*A*···O1^{i}	0.84 (1)	1.87 (1)	2.6936 (15)	164 (2)
O3*W*—H3*A*···O1^{ii}	0.85 (2)	1.91 (2)	2.7445 (15)	166 (2)
O4*W*—H4*A*···O2^{iii}	0.85 (2)	1.95 (2)	2.7985 (15)	176 (2)
O4*W*—H4*B*···N2^{iv}	0.82 (2)	2.17 (2)	2.9369 (17)	154 (2)
O5*W*—H5*A*···O2^{v}	0.85 (2)	1.83 (2)	2.6765 (16)	171 (2)
O5*W*—H5*B*···O8*W*^{ii}	0.83 (2)	1.90 (2)	2.7299 (18)	172 (2)
O6*W*—H6*A*···O7*W*^{vi}	0.86 (2)	1.89 (2)	2.754 (2)	177 (2)
O6*W*—H6*B*···O5*W*^{ii}	0.83 (2)	1.95 (2)	2.7828 (18)	173 (2)
O7*W*—H7*A*···O6*W*	0.84 (2)	1.89 (2)	2.7256 (19)	171 (2)
O7*W*—H7*B*···O8*W*^{vi}	0.83 (2)	1.94 (2)	2.7605 (18)	171 (2)
O8*W*—H8*A*···O1	0.84 (2)	1.92 (2)	2.7564 (16)	173 (2)
O8*W*—H8*B*···O4*W*^{i}	0.86 (2)	1.91 (2)	2.7616 (17)	172 (2)

Symmetry codes: (i) $-x+\frac{1}{2}, -y+\frac{3}{2}, -z+2$; (ii) $-x+\frac{1}{2}, -y+\frac{1}{2}, -z+2$; (iii) $x-\frac{1}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$; (iv) $x, -y+1, z-\frac{1}{2}$; (v) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$; (vi) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{5}{2}$.

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; 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*.

The authors thank Yanbian University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2445).

References

Bruker (2001). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2007). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Guo, H.-D., Guo, X.-M., Batten, S. R., Song, J.-F., Song, S.-Y., Dang, S., Zheng, G.-L., Tang, J.-K. & Zhang, H.-J. (2009). *Cryst. Growth Des.* **9**, 2098–2109.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Wang, X.-H. (2011). *Acta Cryst.* E**67**, m423–m424.
Wang, G.-H., Li, Z.-G., Jia, H.-Q., Hu, N.-H. & Xu, J.-W. (2009). *Acta Cryst.* E**65**, m1568–m1569.
Zang, S.-Q., Su, Y., Li, Y.-Z., Ni, Z.-P. & Meng, Q.-J. (2006). *Inorg. Chem.* **44**, 7122–7129.

supplementary materials

Acta Cryst. (2011). E**67**, m1072 [**doi:10.1107/S1600536811025335**]

Tetraaquabis[4-(4*H*-1,2,4-triazol-4-yl)benzoato-κN^1]manganese(II) decahydrate

Y.-A. Piao and Z.-Y. Xuan

Comment

The construction of novel coordination polymers is the current interest in the field of supramolecular chemistry and crystal engineering, not only for their interesting topologies and crystal packing motifs but also for their potential applications as functional materials (Wang *et al.*, 2009; Zang *et al.*, 2006). As an important family of multidentate O-donor ligands, organic aromatic carboxylate ligands have been extensively employed in the preparation of metal-organic complexes (Guo *et al.*, 2009). In this paper, we selected 4-(1,2,4-triazol-4-yl)benzoic acid as an organic carboxylate ligand, generating the title compound, which is reported here.

In the title compound, the Mn^{II} ions lies on a twofold rotation axis and is approximately octahedrally coordinated by two N atoms from two 4-(1,2,4-triazol-4-yl)benzoate ligands and four water molecules, two of which lie on the twofold rotation axis (Fig. 1). The Mn—N and Mn—O bond lengths and the O—Mn—O and N—Mn—O bond angles are comparable to those found in the other crystallographically characterized Mn(II) complexes (Wang, 2011). The water molecules are involved in O—H···N and O—H···O hydrogen bonds with the triazole N atoms and carboxylate O atoms (Table 1), yielding a three-dimensional supramolecular network (Fig. 2). π–π interactions between the benzene rings [centroid–centroid distance = 3.836 (9) Å] are observed.

Experimental

The synthesis was performed under hydrothermal conditions. A mixture of $Mn(CH_3COO)_2.4H_2O$ (0.2 mmol, 0.049 g), 4-(1,2,4-triazol-4-yl)benzoic acid (0.4 mmol, 0.075 g), NaOH (0.4 mmol, 0.016 g) and H_2O (15 ml) in a 25 ml stainless steel reactor with a Teflon liner was heated from 293 to 443 K in 2 h and a constant temperature was maintained at 443 K for 72 h. After the mixture was cooled to 298 K, purple crystals of the title compound were obtained from the reaction.

Refinement

H atoms on C atoms were positioned geometrically and refined as riding atoms, with C—H = 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C). H atoms of water molecules were located in a difference Fourier map and refined with an O—H distance restraint of 0.85 (2) Å and with U_{iso}(H) = 1.5U_{eq}(O).

Figures

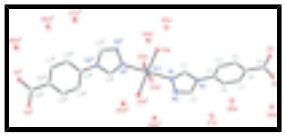


Fig. 1. The molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (i) -*x*, *y*, 3/2-*z*.]

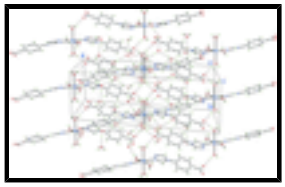


Fig. 2. View of the three-dimensional network of the title compound, built by hydrogen bonds (dashed lines).

Tetraaquabis[4-(4*H*-1,2,4-triazol-4-yl)benzoato- κN^1]manganese(II) decahydrate

Crystal data

$[Mn(C_9H_6N_3O_2)_2(H_2O)_4]\cdot 10H_2O$	$F(000) = 1436$
$M_r = 683.50$	$D_x = 1.410$ Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation, λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 3198 reflections
a = 25.9966 (13) Å	θ = 1.0–26.1°
b = 7.9393 (4) Å	μ = 0.49 mm^{-1}
c = 16.8495 (9) Å	*T* = 76 K
β = 112.214 (1)°	Block, purple
V = 3219.5 (3) Å^3	0.28 × 0.23 × 0.20 mm
Z = 4	

Data collection

Bruker APEX CCD diffractometer	3189 independent reflections
Radiation source: fine-focus sealed tube	2760 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.023$
φ and ω scans	$\theta_{max} = 26.1°$, $\theta_{min} = 1.7°$
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)	$h = -19\rightarrow32$
$T_{min} = 0.85$, $T_{max} = 0.91$	$k = -8\rightarrow9$
8592 measured reflections	$l = -20\rightarrow20$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.029$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.073$	H atoms treated by a mixture of independent and constrained refinement
$S = 0.99$	$w = 1/[\sigma^2(F_o^2) + (0.036P)^2 + 1.9266P]$ where $P = (F_o^2 + 2F_c^2)/3$
3189 reflections	$(\Delta/\sigma)_{max} = 0.008$
238 parameters	$\Delta\rho_{max} = 0.27$ e Å^{-3}
14 restraints	$\Delta\rho_{min} = -0.22$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.12836 (6)	0.4382 (2)	0.87216 (9)	0.0226 (3)
H1	0.1368	0.4674	0.8237	0.027*
C2	0.13557 (6)	0.3880 (2)	1.00119 (10)	0.0263 (4)
H2	0.1504	0.3752	1.0617	0.032*
C3	0.22362 (6)	0.48018 (19)	0.98458 (9)	0.0195 (3)
C4	0.24336 (6)	0.5736 (2)	0.93267 (9)	0.0229 (3)
H4	0.2190	0.6071	0.8770	0.027*
C5	0.29901 (6)	0.6175 (2)	0.96291 (10)	0.0232 (3)
H5	0.3129	0.6801	0.9272	0.028*
C6	0.33496 (6)	0.57157 (18)	1.04481 (9)	0.0200 (3)
C7	0.31413 (6)	0.47742 (19)	1.09554 (9)	0.0229 (3)
H7	0.3383	0.4451	1.1515	0.027*
C8	0.25869 (6)	0.42984 (19)	1.06575 (10)	0.0231 (3)
H8	0.2450	0.3638	1.1005	0.028*
C9	0.39483 (6)	0.62809 (19)	1.07889 (10)	0.0210 (3)
N1	0.07926 (5)	0.39357 (16)	0.86873 (8)	0.0218 (3)
N2	0.08381 (5)	0.36106 (18)	0.95205 (8)	0.0266 (3)
N3	0.16569 (5)	0.43720 (16)	0.95412 (8)	0.0203 (3)
O1	0.42246 (4)	0.60776 (13)	1.15861 (7)	0.0245 (2)
O2	0.41384 (4)	0.69525 (16)	1.02887 (7)	0.0324 (3)
Mn1	0.0000	0.39602 (4)	0.7500	0.01689 (10)
O1W	0.05118 (5)	0.41965 (15)	0.67562 (7)	0.0284 (3)
H1A	0.0417 (8)	0.493 (2)	0.6382 (11)	0.043*
H1B	0.0664 (8)	0.341 (2)	0.6578 (12)	0.043*
O2W	0.0000	0.6681 (2)	0.7500	0.0256 (3)
H2A	0.0229 (7)	0.732 (2)	0.7865 (11)	0.038*
O3W	0.0000	0.1260 (2)	0.7500	0.0381 (4)
H3A	0.0248 (8)	0.065 (3)	0.7856 (12)	0.057*
O4W	0.02208 (5)	0.69006 (15)	0.56446 (7)	0.0278 (3)
H4A	−0.0110 (6)	0.724 (2)	0.5514 (12)	0.042*
H4B	0.0298 (8)	0.688 (3)	0.5212 (11)	0.042*
O5W	0.10937 (5)	0.17426 (16)	0.63970 (8)	0.0301 (3)
H5A	0.1048 (8)	0.174 (3)	0.5870 (10)	0.045*
H5B	0.1054 (9)	0.075 (2)	0.6528 (13)	0.045*
O6W	0.29468 (5)	0.16683 (18)	1.25059 (9)	0.0427 (3)
H6A	0.2976 (10)	0.062 (2)	1.2643 (15)	0.064*
H6B	0.3218 (8)	0.217 (3)	1.2862 (13)	0.064*
O7W	0.19555 (5)	0.32849 (17)	1.21048 (8)	0.0363 (3)
H7A	0.2252 (7)	0.272 (3)	1.2263 (14)	0.054*
H7B	0.1697 (8)	0.268 (3)	1.2113 (14)	0.054*
O8W	0.39715 (5)	0.64318 (16)	1.30252 (8)	0.0318 (3)
H8A	0.4037 (8)	0.640 (3)	1.2571 (11)	0.048*
H8B	0.4240 (7)	0.696 (3)	1.3407 (12)	0.048*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0166 (7)	0.0320 (8)	0.0177 (7)	−0.0016 (6)	0.0046 (6)	0.0000 (6)
C2	0.0190 (8)	0.0397 (9)	0.0194 (8)	−0.0045 (7)	0.0061 (6)	0.0039 (7)
C3	0.0131 (7)	0.0232 (8)	0.0205 (7)	−0.0022 (6)	0.0043 (6)	−0.0030 (6)
C4	0.0179 (7)	0.0326 (9)	0.0153 (7)	−0.0009 (6)	0.0030 (6)	0.0011 (6)
C5	0.0192 (8)	0.0307 (9)	0.0202 (8)	−0.0038 (6)	0.0081 (6)	0.0007 (6)
C6	0.0163 (7)	0.0214 (8)	0.0213 (7)	−0.0010 (6)	0.0059 (6)	−0.0036 (6)
C7	0.0181 (7)	0.0271 (8)	0.0187 (7)	−0.0005 (6)	0.0015 (6)	0.0020 (6)
C8	0.0197 (8)	0.0272 (8)	0.0208 (8)	−0.0035 (6)	0.0059 (6)	0.0049 (6)
C9	0.0171 (7)	0.0219 (8)	0.0232 (8)	−0.0008 (6)	0.0065 (6)	−0.0032 (6)
N1	0.0169 (6)	0.0286 (7)	0.0188 (6)	−0.0017 (5)	0.0055 (5)	0.0004 (5)
N2	0.0180 (6)	0.0403 (8)	0.0199 (7)	−0.0037 (6)	0.0054 (5)	0.0032 (6)
N3	0.0145 (6)	0.0272 (7)	0.0174 (6)	−0.0024 (5)	0.0040 (5)	0.0001 (5)
O1	0.0164 (5)	0.0294 (6)	0.0218 (6)	−0.0021 (4)	0.0005 (4)	−0.0002 (5)
O2	0.0201 (6)	0.0497 (8)	0.0257 (6)	−0.0113 (5)	0.0070 (5)	−0.0001 (5)
Mn1	0.01246 (16)	0.01903 (17)	0.01757 (17)	0.000	0.00386 (12)	0.000
O1W	0.0300 (6)	0.0310 (7)	0.0296 (6)	0.0080 (5)	0.0173 (5)	0.0054 (5)
O2W	0.0204 (8)	0.0201 (8)	0.0269 (9)	0.000	−0.0017 (7)	0.000
O3W	0.0310 (10)	0.0205 (9)	0.0420 (11)	0.000	−0.0100 (8)	0.000
O4W	0.0209 (6)	0.0408 (7)	0.0226 (6)	0.0057 (5)	0.0092 (5)	0.0024 (5)
O5W	0.0345 (7)	0.0308 (6)	0.0286 (6)	0.0019 (5)	0.0161 (5)	−0.0011 (5)
O6W	0.0335 (7)	0.0381 (8)	0.0489 (9)	−0.0018 (6)	0.0070 (6)	−0.0009 (7)
O7W	0.0291 (7)	0.0362 (7)	0.0402 (7)	−0.0020 (6)	0.0092 (6)	0.0045 (6)
O8W	0.0277 (7)	0.0374 (7)	0.0319 (7)	−0.0053 (5)	0.0131 (5)	−0.0047 (6)

Geometric parameters (Å, °)

C1—N1	1.3049 (19)	N1—N2	1.3877 (17)
C1—N3	1.3549 (19)	Mn1—N1	2.2652 (12)
C1—H1	0.9500	Mn1—O3W	2.1438 (17)
C2—N2	1.304 (2)	Mn1—O1W	2.1534 (11)
C2—N3	1.365 (2)	Mn1—O2W	2.1598 (16)
C2—H2	0.9500	O1W—H1A	0.82 (2)
C3—C4	1.385 (2)	O1W—H1B	0.85 (2)
C3—C8	1.385 (2)	O2W—H2A	0.84 (1)
C3—N3	1.4363 (18)	O3W—H3A	0.85 (2)
C4—C5	1.384 (2)	O4W—H4A	0.85 (2)
C4—H4	0.9500	O4W—H4B	0.82 (2)
C5—C6	1.391 (2)	O5W—H5A	0.85 (2)
C5—H5	0.9500	O5W—H5B	0.83 (2)
C6—C7	1.390 (2)	O6W—H6A	0.86 (2)
C6—C9	1.509 (2)	O6W—H6B	0.83 (2)
C7—C8	1.387 (2)	O7W—H7A	0.84 (2)
C7—H7	0.9500	O7W—H7B	0.83 (2)
C8—H8	0.9500	O8W—H8A	0.84 (2)
C9—O2	1.2466 (18)	O8W—H8B	0.86 (2)

C9—O1	1.2715 (18)		
N1—C1—N3	110.81 (13)	C2—N2—N1	106.54 (12)
N1—C1—H1	124.6	C1—N3—C2	104.28 (12)
N3—C1—H1	124.6	C1—N3—C3	127.81 (12)
N2—C2—N3	111.04 (14)	C2—N3—C3	127.91 (13)
N2—C2—H2	124.5	O3W—Mn1—O1W	95.00 (3)
N3—C2—H2	124.5	O3W—Mn1—O1W^{i}	95.00 (3)
C4—C3—C8	121.02 (13)	O1W—Mn1—O1W^{i}	170.01 (7)
C4—C3—N3	119.36 (13)	O3W—Mn1—O2W	180.000 (1)
C8—C3—N3	119.61 (13)	O1W—Mn1—O2W	85.00 (3)
C5—C4—C3	119.19 (14)	O1W^{i}—Mn1—O2W	85.00 (3)
C5—C4—H4	120.4	O3W—Mn1—N1	89.51 (3)
C3—C4—H4	120.4	O1W—Mn1—N1	87.64 (4)
C4—C5—C6	121.04 (14)	O1W^{i}—Mn1—N1	92.44 (4)
C4—C5—H5	119.5	O2W—Mn1—N1	90.49 (3)
C6—C5—H5	119.5	O3W—Mn1—N1^{i}	89.51 (3)
C7—C6—C5	118.62 (13)	O1W—Mn1—N1^{i}	92.44 (4)
C7—C6—C9	120.75 (13)	O1W^{i}—Mn1—N1^{i}	87.64 (4)
C5—C6—C9	120.59 (13)	O2W—Mn1—N1^{i}	90.49 (3)
C8—C7—C6	121.12 (14)	N1—Mn1—N1^{i}	179.02 (7)
C8—C7—H7	119.4	Mn1—O1W—H1A	115.8 (14)
C6—C7—H7	119.4	Mn1—O1W—H1B	127.7 (14)
C3—C8—C7	118.98 (14)	H1A—O1W—H1B	107.0 (19)
C3—C8—H8	120.5	Mn1—O2W—H2A	127.0 (13)
C7—C8—H8	120.5	Mn1—O3W—H3A	125.0 (15)
O2—C9—O1	123.96 (14)	H4A—O4W—H4B	109.8 (19)
O2—C9—C6	119.03 (13)	H5A—O5W—H5B	107 (2)
O1—C9—C6	116.98 (13)	H6A—O6W—H6B	108 (2)
C1—N1—N2	107.33 (12)	H7A—O7W—H7B	110 (2)
C1—N1—Mn1	125.78 (10)	H8A—O8W—H8B	108 (2)
N2—N1—Mn1	126.61 (9)		
C8—C3—C4—C5	−0.3 (2)	Mn1—N1—N2—C2	−174.12 (11)
N3—C3—C4—C5	178.76 (14)	N1—C1—N3—C2	0.07 (18)
C3—C4—C5—C6	−1.0 (2)	N1—C1—N3—C3	−179.24 (14)
C4—C5—C6—C7	1.2 (2)	N2—C2—N3—C1	−0.05 (18)
C4—C5—C6—C9	−176.69 (14)	N2—C2—N3—C3	179.26 (14)
C5—C6—C7—C8	−0.1 (2)	C4—C3—N3—C1	18.3 (2)
C9—C6—C7—C8	177.78 (14)	C8—C3—N3—C1	−162.65 (15)
C4—C3—C8—C7	1.3 (2)	C4—C3—N3—C2	−160.86 (16)
N3—C3—C8—C7	−177.70 (14)	C8—C3—N3—C2	18.2 (2)
C6—C7—C8—C3	−1.2 (2)	C1—N1—Mn1—O3W	109.92 (13)
C7—C6—C9—O2	171.81 (15)	N2—N1—Mn1—O3W	−76.98 (12)
C5—C6—C9—O2	−10.4 (2)	C1—N1—Mn1—O1W	14.90 (13)
C7—C6—C9—O1	−10.1 (2)	N2—N1—Mn1—O1W	−172.00 (12)
C5—C6—C9—O1	167.71 (14)	C1—N1—Mn1—O1W^{i}	−155.10 (13)
N3—C1—N1—N2	−0.06 (18)	N2—N1—Mn1—O1W^{i}	18.00 (12)

N3—C1—N1—Mn1	174.15 (10)	C1—N1—Mn1—O2W	−70.08 (13)
N3—C2—N2—N1	0.02 (19)	N2—N1—Mn1—O2W	103.02 (12)
C1—N1—N2—C2	0.02 (17)		

Symmetry codes: (i) −*x*, *y*, −*z*+3/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1A···O4W	0.82 (2)	1.94 (2)	2.7602 (17)	171 (2)
O1W—H1B···O5W	0.85 (2)	1.83 (2)	2.6724 (16)	169 (2)
O2W—H2A···O1^{ii}	0.84 (1)	1.87 (1)	2.6936 (15)	164 (2)
O3W—H3A···O1^{iii}	0.85 (2)	1.91 (2)	2.7445 (15)	166 (2)
O4W—H4A···O2^{iv}	0.85 (2)	1.95 (2)	2.7985 (15)	176 (2)
O4W—H4B···N2^{v}	0.82 (2)	2.17 (2)	2.9369 (17)	154 (2)
O5W—H5A···O2^{vi}	0.85 (2)	1.83 (2)	2.6765 (16)	171 (2)
O5W—H5B···O8W^{iii}	0.83 (2)	1.90 (2)	2.7299 (18)	172 (2)
O6W—H6A···O7W^{vii}	0.86 (2)	1.89 (2)	2.754 (2)	177 (2)
O6W—H6B···O5W^{iii}	0.83 (2)	1.95 (2)	2.7828 (18)	173 (2)
O7W—H7A···O6W	0.84 (2)	1.89 (2)	2.7256 (19)	171 (2)
O7W—H7B···O8W^{vii}	0.83 (2)	1.94 (2)	2.7605 (18)	171 (2)
O8W—H8A···O1	0.84 (2)	1.92 (2)	2.7564 (16)	173 (2)
O8W—H8B···O4W^{ii}	0.86 (2)	1.91 (2)	2.7616 (17)	172 (2)

Symmetry codes: (ii) −*x*+1/2, −*y*+3/2, −*z*+2; (iii) −*x*+1/2, −*y*+1/2, −*z*+2; (iv) *x*−1/2, −*y*+3/2, *z*−1/2; (v) *x*, −*y*+1, *z*−1/2; (vi) −*x*+1/2, *y*−1/2, −*z*+3/2; (vii) −*x*+1/2, *y*−1/2, −*z*+5/2.

Fig. 1

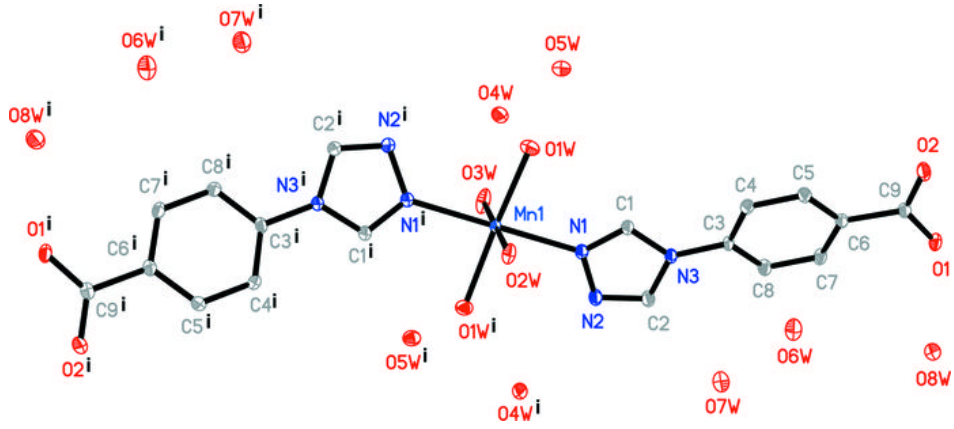

O7W^{i}
O6W^{i}
O5W
O8W^{i}
O4W
C2^{i}
N2^{i}
O1W
O2
C8^{i}
C7^{i}
N3^{i}
O3W
C4
C5
C9
C1
Mn1
N1
C3
O1^{i}
C6^{i}
C3^{i}
N1^{i}
C1^{i}
O2W
N3
O1
C6
C8
C7
C9^{i}
C5^{i}
C4^{i}
O1W^{i}
N2
C2
O5W^{i}
O6W
O8W
O2^{i}
O4W^{i}
O7W

Fig. 2