Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Triaqua[2-(4-carboxylatophenoxy)propionato-κO](1,10-phenanthroline-$\kappa^2 N,N'$)manganese(II) monohydrate

Ying-Hui Xiao,[a,b] Li-Li Kong[a] and Shan Gao[a]*

[a]School of Chemistry and Materials Science, Heilongjiang University, Harbin 150080, People's Republic of China, and [b]School of Chemistry and Chemical Engineering, Qiqihar University, QiQihar 161006, People's Republic of China
Correspondence e-mail: shangao67@yahoo.com

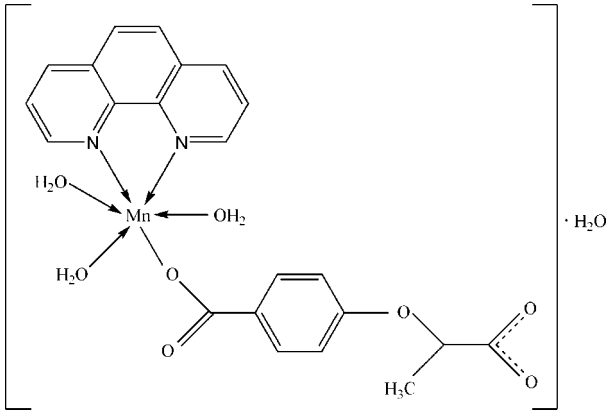
Received 26 April 2007; accepted 27 April 2007

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.005 Å; R factor = 0.038; wR factor = 0.100; data-to-parameter ratio = 15.9.

The zwitterionic title compound, $[Mn(C_{10}H_8O_5)(C_{12}H_8N_2)(H_2O)_3]\cdot H_2O$, has the Mn atom in an octahedral geometry that comprises the O atom of the 2-(4-carboxylatophenoxy)propionate group, two N atoms of the 1,10-phenanthroline ligand and three water molecules. Extensive hydrogen-bonding and π–π stacking interactions lead to a three-dimensional supramolecular network.

Related literature

For the cobalt(II) and nickel(II) complexes of the same carboxylic acid, see: Deng *et al.* (2007*a*,*b*).



Experimental

Crystal data

$[Mn(C_{10}H_8O_5)(C_{12}H_8N_2)(H_2O)_3]\cdot H_2O$
M_r = 515.37
Triclinic, $P\overline{1}$
a = 7.5457 (15) Å
b = 11.073 (2) Å
c = 15.372 (3) Å
α = 106.16 (3)°
β = 99.53 (3)°
γ = 103.14 (3)°
V = 1164.8 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.62 mm^{-1}
T = 295 (2) K
0.38 × 0.25 × 0.17 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.826, T_{max} = 0.893
11565 measured reflections
5280 independent reflections
3105 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.100
S = 1.12
5280 reflections
332 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.73 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Mn1—O1	2.1318 (19)	Mn1—O3*W*	2.204 (2)
Mn1—O2*W*	2.156 (2)	Mn1—N1	2.290 (2)
Mn1—O1*W*	2.174 (2)	Mn1—N2	2.292 (2)
O1—Mn1—O2*W*	108.33 (8)	O1*W*—Mn1—N1	90.74 (10)
O1—Mn1—O1*W*	83.81 (9)	O3*W*—Mn1—N1	98.24 (9)
O2*W*—Mn1—O1*W*	85.84 (9)	O1—Mn1—N2	88.65 (9)
O1—Mn1—O3*W*	90.70 (8)	O2*W*—Mn1—N2	162.90 (8)
O2*W*—Mn1—O3*W*	85.06 (9)	O1*W*—Mn1—N2	98.30 (9)
O1*W*—Mn1—O3*W*	167.32 (8)	O3*W*—Mn1—N2	92.97 (9)
O1—Mn1—N1	159.22 (8)	N1—Mn1—N2	72.27 (9)
O2*W*—Mn1—N1	91.18 (8)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*1···O5^{i}	0.84 (4)	1.92 (4)	2.754 (3)	170 (3)
O1*W*—H1*W*2···O4*W*^{ii}	0.83 (4)	1.96 (4)	2.774 (4)	168 (4)
O2*W*—H2*W*1···O3^{i}	0.83 (4)	2.03 (4)	2.847 (3)	167 (3)
O2*W*—H2*W*2···O4^{iii}	0.90 (4)	1.73 (4)	2.634 (3)	173 (3)
O3*W*—H3*W*1···O5^{iii}	0.90 (3)	1.87 (3)	2.759 (3)	170 (3)
O3*W*—H3*W*2···O2	0.85 (3)	1.82 (3)	2.647 (3)	163 (3)
O4*W*—H4*W*1···O2	0.91 (4)	1.85 (4)	2.744 (3)	168 (4)
O4*W*—H4*W*2···O4^{iv}	0.85 (4)	2.08 (4)	2.925 (3)	171 (4)

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

The authors thank the Heilongjiang Province Natural Science Foundation (grant No. B200501), the Scientific Fund of Remarkable Teachers of Heilongjiang Province (1054 G036), and Heilongjiang University for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2262).

 doi:10.1107/S1600536807021101

References

Deng, Z.-P., Gao, S. & Chen, P.-G. (2007*a*). *Acta Cryst.* E**63**, m296–m298.
Deng, Z.-P., Gao, S. & Chen, P.-G. (2007*b*). *Acta Cryst.* E**63**, m553–m554.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Johnson, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
Rigaku (1998). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
Rigaku/MSC (2002). *CrystalStructure*. Rigaku/MSC, The Woodlands, Texas, USA.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

supplementary materials

Acta Cryst. (2007). E**63**, m1587-m1588 [**doi:10.1107/S1600536807021101**]

Triaqua[2-(4-carboxylatophenoxy)propionato-κO](1,10-phenanthroline-$\kappa^2 N,N'$)manganese(II) monohydrate

Y.-H. Xiao, L.-L. Kong and S. Gao

Comment

Our studies have addressed the metal derivatives of carboxyphenoxypropionic acids for the construction of supramolecular architectures. ecently, we have reported the structures of cobalt(II) and nickel(II) derivatives of 2-(4-carboxylatophenoxy)propionic acid (Deng *et al.*, 2007*a*,b). In the title Mn complex (I) (Fig. 1), the 2-(*p*-CPOP)$^{2-}$ anion coordinates in a monodentate fashion to the Mn atom through the carboxylate group. The Mn atom is chelated by the phenanthroline and is also linked to three water molecules. A three-dimensional supramolecular network is constructed from π-π stacking between the 1,10-phenanthroline rings (centroid-centroid distance being 3.689 (5) and 3.869 (5) Å) and hydrogen-bonding interactions (Table 2).

Experimental

The title complex was prepared by the addition of $MnCl_2{\cdot}4H_2O$ (10 mmol) and 1,10-phenanthroline (10 mmol) to a solution of 2-(*p*-$CPOPH_2$) (15 mmol) in H_2O/MeOH (V/V = 1:1) solution. The pH value was adjusted to 5 with NaOH (0.2 *M*) solution. Colorless crystals were obtained from the filtered solution at room temperature over several days. CH&N analysis. Calc. for $C_{22}H_{24}N_2O_9Mn$: C 51.27, H 4.69, N 5.43. Found: C 51.26, H 4.67, N 5.46%.

Refinement

The H atoms were placed in calculated positions with C—H = 0.93 or 0.97 Å and U_{iso}(H) = 1.2U_{eq} (C) and were included in the refinement in the riding model approximation. The H atoms of water molecules and hydroxyl groups were located in difference Fourier maps and refined with the O—H distance restrained to 0.85 (1) Å and U_{iso}(H) = 1.5U_{eq}(O).

Figures

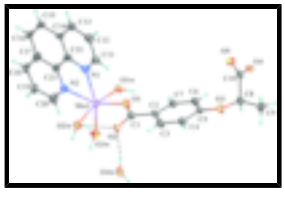


Fig. 1. Molecular structure of the title compound with 30% probability ellipsoid for the non-H atoms. Dashed lines indicate O—H···O hydrogen bonds.

Triaqua[2-(4-carboxylatophenoxy)propionato-κ*O*](1,10-phenanthroline- $\kappa^2 N,N'$)manganese(II) monohydrate

Crystal data

$[Mn(C_{10}H_8O_5)(C_{12}H_8N_2)(H_2O)_3]{\cdot}H_2O$ $Z = 2$

M_r = 515.37	F_{000} = 534
Triclinic, $P\bar{1}$	D_x = 1.469 Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 7.5457 (15) Å	Cell parameters from 7678 reflections
b = 11.073 (2) Å	θ = 3.3–27.5º
c = 15.372 (3) Å	μ = 0.62 mm^{-1}
α = 106.16 (3)º	T = 295 (2) K
β = 99.53 (3)º	Prism, colourless
γ = 103.14 (3)º	0.38 × 0.25 × 0.17 mm
V = 1164.8 (5) Å^3	

Data collection

Rigaku R-AXIS RAPID diffractometer	5280 independent reflections
Radiation source: fine-focus sealed tube	3105 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.036
Detector resolution: 10.000 pixels mm^{-1}	θ_{max} = 27.5º
T = 295(2) K	θ_{min} = 3.3º
ω scans	h = −9→9
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	k = −14→14
T_{min} = 0.826, T_{max} = 0.893	l = −19→19
11565 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.038	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.100	$w = 1/[\sigma^2(F_o^2) + (0.0275P)^2 + 0.6167P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.12	$(\Delta/\sigma)_{max}$ = 0.001
5280 reflections	$\Delta\rho_{max}$ = 0.56 e Å^{-3}
332 parameters	$\Delta\rho_{min}$ = −0.73 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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

	x	y	z	U_{iso}*/U_{eq}
Mn1	0.27669 (6)	0.37228 (4)	0.71204 (3)	0.03294 (13)
O1W	0.5797 (3)	0.4182 (2)	0.75865 (16)	0.0471 (5)
H1W1	0.624 (5)	0.362 (3)	0.774 (2)	0.071*
H1W2	0.633 (5)	0.493 (4)	0.796 (3)	0.071*

O2W	0.2654 (3)	0.3051 (2)	0.83041 (14)	0.0432 (5)
H2W1	0.353 (5)	0.286 (3)	0.859 (2)	0.065*
H2W2	0.170 (5)	0.286 (3)	0.857 (2)	0.065*
O3W	−0.0264 (3)	0.34586 (19)	0.69778 (14)	0.0385 (5)
H3W1	−0.086 (4)	0.309 (3)	0.734 (2)	0.058*
H3W2	−0.026 (5)	0.426 (3)	0.717 (2)	0.058*
O4W	−0.1908 (3)	0.6600 (2)	0.88034 (17)	0.0560 (6)
H4W1	−0.098 (6)	0.649 (4)	0.851 (3)	0.084*
H4W2	−0.146 (6)	0.686 (4)	0.939 (3)	0.084*
O1	0.3311 (3)	0.58037 (17)	0.75925 (14)	0.0424 (5)
O2	0.0499 (3)	0.60400 (18)	0.76959 (15)	0.0479 (5)
O3	0.5231 (3)	1.20164 (16)	0.92263 (13)	0.0364 (4)
O4	1.0045 (3)	1.2598 (2)	0.92143 (14)	0.0485 (5)
O5	0.7683 (3)	1.25399 (18)	0.81085 (13)	0.0425 (5)
N1	0.2598 (3)	0.1668 (2)	0.61862 (15)	0.0386 (6)
N2	0.2602 (3)	0.3778 (2)	0.56302 (16)	0.0424 (6)
C1	0.2238 (4)	0.6494 (2)	0.78069 (18)	0.0343 (6)
C2	0.3088 (4)	0.7955 (2)	0.82068 (18)	0.0334 (6)
C3	0.5007 (4)	0.8509 (2)	0.84896 (18)	0.0355 (6)
H3	0.5789	0.7967	0.8443	0.043*
C4	0.5795 (4)	0.9867 (3)	0.88444 (19)	0.0366 (6)
H4	0.7091	1.0229	0.9028	0.044*
C5	0.4628 (4)	1.0666 (2)	0.89205 (17)	0.0306 (6)
C6	0.2693 (4)	1.0124 (3)	0.8677 (2)	0.0382 (7)
H6	0.1911	1.0665	0.8754	0.046*
C7	0.1938 (4)	0.8781 (3)	0.8321 (2)	0.0382 (7)
H7	0.0641	0.8420	0.8153	0.046*
C8	0.7194 (4)	1.2660 (2)	0.96311 (18)	0.0332 (6)
H8	0.7654	1.2279	1.0096	0.040*
C9	0.7334 (4)	1.4088 (3)	1.0117 (2)	0.0434 (7)
H9A	0.6928	1.4472	0.9661	0.065*
H9B	0.8612	1.4559	1.0448	0.065*
H9C	0.6549	1.4135	1.0550	0.065*
C10	0.8382 (4)	1.2573 (2)	0.89161 (19)	0.0332 (6)
C11	0.2577 (5)	0.4808 (3)	0.5357 (2)	0.0569 (9)
H11	0.2552	0.5577	0.5790	0.068*
C12	0.2588 (5)	0.4788 (4)	0.4442 (3)	0.0722 (11)
H12	0.2587	0.5533	0.4275	0.087*
C13	0.2601 (5)	0.3666 (4)	0.3804 (2)	0.0705 (11)
H13	0.2611	0.3640	0.3195	0.085*
C14	0.2599 (5)	0.2548 (4)	0.4058 (2)	0.0551 (9)
C15	0.2562 (5)	0.1317 (5)	0.3425 (2)	0.0727 (11)
H15	0.2568	0.1249	0.2809	0.087*
C16	0.2517 (6)	0.0256 (4)	0.3689 (2)	0.0722 (11)
H16	0.2492	−0.0529	0.3256	0.087*
C17	0.2506 (5)	0.0323 (3)	0.4632 (2)	0.0529 (8)
C18	0.2449 (5)	−0.0746 (3)	0.4952 (3)	0.0653 (10)
H18	0.2390	−0.1559	0.4543	0.078*
C19	0.2480 (5)	−0.0595 (3)	0.5858 (3)	0.0641 (10)

H19	0.2452	−0.1298	0.6079	0.077*
C20	0.2553 (5)	0.0628 (3)	0.6457 (2)	0.0523 (8)
H20	0.2572	0.0720	0.7079	0.063*
C21	0.2571 (4)	0.1526 (3)	0.52810 (18)	0.0395 (7)
C22	0.2592 (4)	0.2654 (3)	0.49881 (19)	0.0407 (7)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0368 (3)	0.0277 (2)	0.0340 (2)	0.00985 (18)	0.00952 (18)	0.00888 (18)
O1W	0.0373 (13)	0.0414 (12)	0.0608 (14)	0.0123 (10)	0.0063 (11)	0.0165 (11)
O2W	0.0430 (14)	0.0543 (13)	0.0474 (12)	0.0224 (11)	0.0180 (10)	0.0291 (11)
O3W	0.0381 (12)	0.0318 (10)	0.0457 (12)	0.0092 (9)	0.0120 (9)	0.0123 (10)
O4W	0.0417 (15)	0.0607 (15)	0.0568 (14)	0.0119 (12)	0.0060 (12)	0.0115 (13)
O1	0.0402 (12)	0.0265 (10)	0.0585 (13)	0.0100 (9)	0.0148 (10)	0.0090 (9)
O2	0.0359 (13)	0.0308 (10)	0.0685 (14)	0.0059 (9)	0.0089 (11)	0.0086 (10)
O3	0.0350 (11)	0.0247 (9)	0.0492 (11)	0.0085 (8)	0.0103 (9)	0.0118 (9)
O4	0.0355 (13)	0.0656 (14)	0.0499 (12)	0.0150 (11)	0.0133 (10)	0.0253 (11)
O5	0.0472 (13)	0.0460 (11)	0.0385 (11)	0.0160 (10)	0.0134 (10)	0.0166 (10)
N1	0.0442 (15)	0.0344 (13)	0.0342 (12)	0.0113 (11)	0.0091 (11)	0.0070 (11)
N2	0.0449 (16)	0.0479 (15)	0.0378 (13)	0.0128 (12)	0.0085 (11)	0.0207 (13)
C1	0.0390 (17)	0.0281 (14)	0.0371 (15)	0.0102 (13)	0.0097 (13)	0.0123 (12)
C2	0.0384 (17)	0.0299 (14)	0.0348 (14)	0.0086 (12)	0.0111 (13)	0.0149 (12)
C3	0.0361 (17)	0.0294 (14)	0.0440 (16)	0.0115 (12)	0.0142 (13)	0.0127 (13)
C4	0.0306 (16)	0.0316 (14)	0.0488 (16)	0.0079 (12)	0.0121 (13)	0.0145 (13)
C5	0.0367 (16)	0.0245 (13)	0.0331 (14)	0.0088 (12)	0.0126 (12)	0.0112 (12)
C6	0.0366 (17)	0.0301 (14)	0.0541 (17)	0.0143 (13)	0.0159 (14)	0.0166 (14)
C7	0.0299 (16)	0.0311 (14)	0.0542 (18)	0.0077 (12)	0.0072 (13)	0.0180 (14)
C8	0.0320 (16)	0.0276 (13)	0.0355 (14)	0.0048 (12)	0.0055 (12)	0.0080 (12)
C9	0.050 (2)	0.0333 (15)	0.0421 (16)	0.0116 (14)	0.0123 (14)	0.0056 (13)
C10	0.0365 (17)	0.0235 (13)	0.0372 (15)	0.0057 (12)	0.0081 (13)	0.0091 (12)
C11	0.065 (2)	0.059 (2)	0.0528 (19)	0.0197 (18)	0.0097 (17)	0.0297 (18)
C12	0.076 (3)	0.084 (3)	0.068 (2)	0.019 (2)	0.006 (2)	0.052 (2)
C13	0.062 (3)	0.107 (3)	0.044 (2)	0.015 (2)	0.0071 (18)	0.036 (2)
C14	0.046 (2)	0.082 (2)	0.0347 (16)	0.0144 (18)	0.0073 (15)	0.0201 (18)
C15	0.065 (3)	0.108 (3)	0.0323 (18)	0.022 (2)	0.0141 (17)	0.006 (2)
C16	0.074 (3)	0.081 (3)	0.044 (2)	0.028 (2)	0.0130 (19)	−0.010 (2)
C17	0.044 (2)	0.058 (2)	0.0418 (17)	0.0126 (16)	0.0072 (15)	−0.0031 (16)
C18	0.066 (3)	0.045 (2)	0.069 (2)	0.0215 (18)	0.009 (2)	−0.0064 (19)
C19	0.075 (3)	0.0363 (18)	0.075 (2)	0.0192 (17)	0.010 (2)	0.0101 (18)
C20	0.071 (2)	0.0362 (17)	0.0478 (18)	0.0167 (16)	0.0122 (17)	0.0106 (15)
C21	0.0330 (17)	0.0440 (16)	0.0319 (15)	0.0068 (13)	0.0059 (12)	0.0024 (14)
C22	0.0306 (16)	0.0554 (19)	0.0320 (14)	0.0091 (14)	0.0082 (12)	0.0105 (14)

Geometric parameters (Å, °)

Mn1—O1	2.1318 (19)	C5—C6	1.389 (4)
Mn1—O2W	2.156 (2)	C6—C7	1.376 (4)
Mn1—O1W	2.174 (2)	C6—H6	0.9300

Mn1—O3W	2.204 (2)	C7—H7	0.9300
Mn1—N1	2.290 (2)	C8—C9	1.521 (4)
Mn1—N2	2.292 (2)	C8—C10	1.526 (4)
O1W—H1W1	0.84 (4)	C8—H8	0.9800
O1W—H1W2	0.83 (4)	C9—H9A	0.9600
O2W—H2W1	0.83 (4)	C9—H9B	0.9600
O2W—H2W2	0.90 (4)	C9—H9C	0.9600
O3W—H3W1	0.90 (3)	C11—C12	1.402 (5)
O3W—H3W2	0.85 (3)	C11—H11	0.9300
O4W—H4W1	0.91 (4)	C12—C13	1.354 (5)
O4W—H4W2	0.85 (4)	C12—H12	0.9300
O1—C1	1.256 (3)	C13—C14	1.398 (5)
O2—C1	1.257 (3)	C13—H13	0.9300
O3—C5	1.375 (3)	C14—C22	1.403 (4)
O3—C8	1.435 (3)	C14—C15	1.429 (5)
O4—C10	1.253 (3)	C15—C16	1.340 (5)
O5—C10	1.253 (3)	C15—H15	0.9300
N1—C20	1.324 (3)	C16—C17	1.432 (5)
N1—C21	1.352 (3)	C16—H16	0.9300
N2—C11	1.322 (4)	C17—C18	1.397 (5)
N2—C22	1.354 (4)	C17—C21	1.410 (4)
C1—C2	1.501 (4)	C18—C19	1.352 (5)
C2—C3	1.379 (4)	C18—H18	0.9300
C2—C7	1.393 (4)	C19—C20	1.393 (4)
C3—C4	1.393 (4)	C19—H19	0.9300
C3—H3	0.9300	C20—H20	0.9300
C4—C5	1.380 (4)	C21—C22	1.439 (4)
C4—H4	0.9300		
O1—Mn1—O2W	108.33 (8)	C2—C7—H7	119.5
O1—Mn1—O1W	83.81 (9)	O3—C8—C9	105.4 (2)
O2W—Mn1—O1W	85.84 (9)	O3—C8—C10	113.6 (2)
O1—Mn1—O3W	90.70 (8)	C9—C8—C10	109.8 (2)
O2W—Mn1—O3W	85.06 (9)	O3—C8—H8	109.3
O1W—Mn1—O3W	167.32 (8)	C9—C8—H8	109.3
O1—Mn1—N1	159.22 (8)	C10—C8—H8	109.3
O2W—Mn1—N1	91.18 (8)	C8—C9—H9A	109.5
O1W—Mn1—N1	90.74 (10)	C8—C9—H9B	109.5
O3W—Mn1—N1	98.24 (9)	H9A—C9—H9B	109.5
O1—Mn1—N2	88.65 (9)	C8—C9—H9C	109.5
O2W—Mn1—N2	162.90 (8)	H9A—C9—H9C	109.5
O1W—Mn1—N2	98.30 (9)	H9B—C9—H9C	109.5
O3W—Mn1—N2	92.97 (9)	O5—C10—O4	125.3 (3)
N1—Mn1—N2	72.27 (9)	O5—C10—C8	119.3 (3)
Mn1—O1W—H1W1	118 (2)	O4—C10—C8	115.4 (2)
Mn1—O1W—H1W2	115 (3)	N2—C11—C12	122.7 (3)
H1W1—O1W—H1W2	111 (4)	N2—C11—H11	118.6
Mn1—O2W—H2W1	124 (2)	C12—C11—H11	118.6
Mn1—O2W—H2W2	130 (2)	C13—C12—C11	119.0 (3)
H2W1—O2W—H2W2	105 (3)	C13—C12—H12	120.5

Mn1—O3W—H3W1	120 (2)	C11—C12—H12	120.5
Mn1—O3W—H3W2	100 (2)	C12—C13—C14	120.3 (3)
H3W1—O3W—H3W2	105 (3)	C12—C13—H13	119.9
H4W1—O4W—H4W2	110 (4)	C14—C13—H13	119.9
C1—O1—Mn1	130.21 (18)	C13—C14—C22	117.0 (3)
C5—O3—C8	118.4 (2)	C13—C14—C15	124.0 (3)
C20—N1—C21	117.9 (2)	C22—C14—C15	119.0 (3)
C20—N1—Mn1	125.92 (19)	C16—C15—C14	122.3 (3)
C21—N1—Mn1	116.17 (18)	C16—C15—H15	118.9
C11—N2—C22	118.1 (3)	C14—C15—H15	118.9
C11—N2—Mn1	126.1 (2)	C15—C16—C17	120.5 (3)
C22—N2—Mn1	115.78 (17)	C15—C16—H16	119.8
O1—C1—O2	124.3 (2)	C17—C16—H16	119.8
O1—C1—C2	117.6 (3)	C18—C17—C21	117.6 (3)
O2—C1—C2	118.1 (2)	C18—C17—C16	123.5 (3)
C3—C2—C7	118.6 (2)	C21—C17—C16	119.0 (3)
C3—C2—C1	121.2 (3)	C19—C18—C17	119.8 (3)
C7—C2—C1	120.2 (3)	C19—C18—H18	120.1
C2—C3—C4	121.1 (3)	C17—C18—H18	120.1
C2—C3—H3	119.4	C18—C19—C20	119.1 (3)
C4—C3—H3	119.4	C18—C19—H19	120.4
C5—C4—C3	119.2 (3)	C20—C19—H19	120.4
C5—C4—H4	120.4	N1—C20—C19	123.4 (3)
C3—C4—H4	120.4	N1—C20—H20	118.3
O3—C5—C4	124.8 (2)	C19—C20—H20	118.3
O3—C5—C6	114.9 (2)	N1—C21—C17	122.3 (3)
C4—C5—C6	120.4 (2)	N1—C21—C22	117.6 (2)
C7—C6—C5	119.6 (3)	C17—C21—C22	120.1 (3)
C7—C6—H6	120.2	N2—C22—C14	122.8 (3)
C5—C6—H6	120.2	N2—C22—C21	118.0 (2)
C6—C7—C2	121.0 (3)	C14—C22—C21	119.2 (3)
C6—C7—H7	119.5		
O2W—Mn1—O1—C1	−76.5 (2)	C5—O3—C8—C9	−165.6 (2)
O1W—Mn1—O1—C1	−160.0 (2)	C5—O3—C8—C10	74.1 (3)
O3W—Mn1—O1—C1	8.5 (2)	O3—C8—C10—O5	31.7 (3)
N1—Mn1—O1—C1	124.4 (3)	C9—C8—C10—O5	−86.1 (3)
N2—Mn1—O1—C1	101.5 (2)	O3—C8—C10—O4	−151.2 (2)
O1—Mn1—N1—C20	157.5 (3)	C9—C8—C10—O4	91.0 (3)
O2W—Mn1—N1—C20	−2.7 (3)	C22—N2—C11—C12	−1.6 (5)
O1W—Mn1—N1—C20	83.2 (3)	Mn1—N2—C11—C12	176.0 (3)
O3W—Mn1—N1—C20	−87.9 (3)	N2—C11—C12—C13	0.8 (6)
N2—Mn1—N1—C20	−178.4 (3)	C11—C12—C13—C14	0.1 (6)
O1—Mn1—N1—C21	−21.4 (4)	C12—C13—C14—C22	−0.3 (5)
O2W—Mn1—N1—C21	178.4 (2)	C12—C13—C14—C15	178.3 (4)
O1W—Mn1—N1—C21	−95.8 (2)	C13—C14—C15—C16	−178.4 (4)
O3W—Mn1—N1—C21	93.2 (2)	C22—C14—C15—C16	0.1 (6)
N2—Mn1—N1—C21	2.71 (19)	C14—C15—C16—C17	0.0 (6)
O1—Mn1—N2—C11	−9.4 (3)	C15—C16—C17—C18	179.6 (4)
O2W—Mn1—N2—C11	164.1 (3)	C15—C16—C17—C21	−0.9 (5)

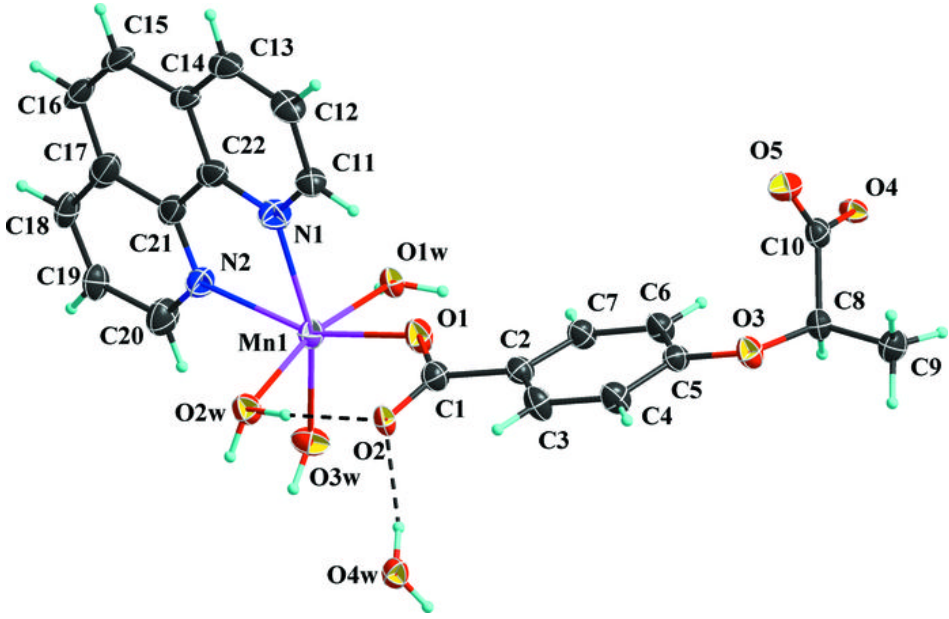
O1W—Mn1—N2—C11	−92.9 (3)	C21—C17—C18—C19	−0.8 (5)
O3W—Mn1—N2—C11	81.3 (3)	C16—C17—C18—C19	178.7 (4)
N1—Mn1—N2—C11	179.0 (3)	C17—C18—C19—C20	0.5 (6)
O1—Mn1—N2—C22	168.3 (2)	C21—N1—C20—C19	0.0 (5)
O2W—Mn1—N2—C22	−18.2 (4)	Mn1—N1—C20—C19	−178.9 (3)
O1W—Mn1—N2—C22	84.8 (2)	C18—C19—C20—N1	−0.1 (6)
O3W—Mn1—N2—C22	−101.0 (2)	C20—N1—C21—C17	−0.3 (4)
N1—Mn1—N2—C22	−3.33 (19)	Mn1—N1—C21—C17	178.7 (2)
Mn1—O1—C1—O2	−6.8 (4)	C20—N1—C21—C22	179.1 (3)
Mn1—O1—C1—C2	174.23 (16)	Mn1—N1—C21—C22	−1.9 (3)
O1—C1—C2—C3	−11.7 (4)	C18—C17—C21—N1	0.7 (5)
O2—C1—C2—C3	169.3 (2)	C16—C17—C21—N1	−178.8 (3)
O1—C1—C2—C7	169.9 (2)	C18—C17—C21—C22	−178.7 (3)
O2—C1—C2—C7	−9.1 (4)	C16—C17—C21—C22	1.8 (5)
C7—C2—C3—C4	−2.8 (4)	C11—N2—C22—C14	1.4 (4)
C1—C2—C3—C4	178.8 (2)	Mn1—N2—C22—C14	−176.4 (2)
C2—C3—C4—C5	0.6 (4)	C11—N2—C22—C21	−178.5 (3)
C8—O3—C5—C4	−10.1 (4)	Mn1—N2—C22—C21	3.7 (3)
C8—O3—C5—C6	170.2 (2)	C13—C14—C22—N2	−0.5 (5)
C3—C4—C5—O3	−177.5 (2)	C15—C14—C22—N2	−179.1 (3)
C3—C4—C5—C6	2.2 (4)	C13—C14—C22—C21	179.4 (3)
O3—C5—C6—C7	177.0 (2)	C15—C14—C22—C21	0.8 (5)
C4—C5—C6—C7	−2.8 (4)	N1—C21—C22—N2	−1.2 (4)
C5—C6—C7—C2	0.5 (4)	C17—C21—C22—N2	178.2 (3)
C3—C2—C7—C6	2.3 (4)	N1—C21—C22—C14	178.9 (3)
C1—C2—C7—C6	−179.3 (2)	C17—C21—C22—C14	−1.7 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1W1···O5^{i}	0.84 (4)	1.92 (4)	2.754 (3)	170 (3)
O1W—H1W2···O4W^{ii}	0.83 (4)	1.96 (4)	2.774 (4)	168 (4)
O2W—H2W1···O3^{i}	0.83 (4)	2.03 (4)	2.847 (3)	167 (3)
O2W—H2W2···O4^{iii}	0.90 (4)	1.73 (4)	2.634 (3)	173 (3)
O3W—H3W1···O5^{iii}	0.90 (3)	1.87 (3)	2.759 (3)	170 (3)
O3W—H3W2···O2	0.85 (3)	1.82 (3)	2.647 (3)	163 (3)
O4W—H4W1···O2	0.91 (4)	1.85 (4)	2.744 (3)	168 (4)
O4W—H4W2···O4^{iv}	0.85 (4)	2.08 (4)	2.925 (3)	171 (4)

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

Fig. 1


C15
C14
C13
C16
C12
C17
C22
C11
C18
C21
N1
N2
C19
O1w
C20
Mn1
O1
C7
C6
O5
O4
C10
C2
O3
C8
C9
C5
C1
C4
C3
O2w
O2
O3w
O4w