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(2,9-Dimethyl-1,10-phenanthroline-κ^2N,N')bis(3-hydroxybenzoato-κ^2O,O')-manganese(II) 2,9-dimethyl-1,10-phenanthroline dihydrate

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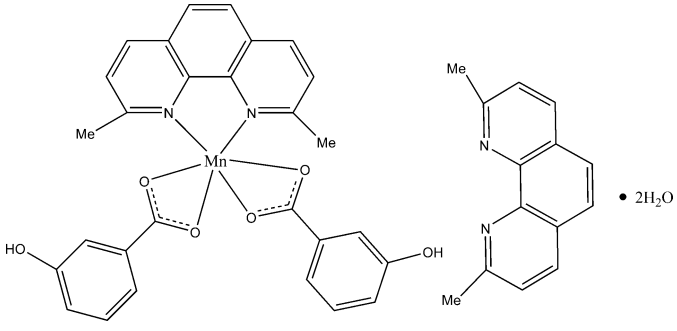
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.006 Å; R factor = 0.053; wR factor = 0.170; data-to-parameter ratio = 14.3.

In the title compound, $[Mn(C_7H_5O_3)_2(C_{14}H_{12}N_2)]\cdot C_{14}H_{12}N_2\cdot 2H_2O$, the Mn^{II} ion is coordinated by a bidentate 2,9-dimethyl-1,10-phenanthroline (dmphen) ligand and two bidentate 3-hydroxybenzoate anions in a distorted octahedral environment. The structure is stabilized by O—H···O and O—H···N hydrogen bonds involving water molecules, the 3-hydroxybenzoate ligands and the uncoordinated dmphen molecules to form a three-dimensional network.

Related literature

The closely related complex bis(benzoato-κ^2O,O')-(2,9-dimethyl-1,10-phenanthroline-κ^2N,N')manganese(II) was reported by Zhao, Xuan *et al.* (2007). For other related structures, see: Fu *et al.* (2006); Liu & Ng (2007); Niu *et al.* (2002); Pan, Liu *et al.* (2006); Pan, Su *et al.* (2006*a*,*b*); Shi *et al.* (2001); Su, Gu *et al.* (2005*a*,*b*); Su & Xu (2005); Su, Zhang & Xu (2005); Xu *et al.* (2004); Xuan, Zhao & Tang (2007); Xuan, Zhao & Zhang (2007); Zhao, Yan *et al.* (2007); Zhao, Xuan *et al.* (2007).



Experimental

Crystal data

$[Mn(C_7H_5O_3)_2(C_{14}H_{12}N_2)]\cdot C_{14}H_{12}N_2\cdot 2H_2O$
M_r = 781.70
Monoclinic, $P2_1/n$
a = 10.7010 (9) Å
b = 24.865 (2) Å
c = 14.5083 (12) Å
β = 94.514 (1)°
V = 3848.5 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.40 mm^{-1}
T = 291 (2) K
0.34 × 0.25 × 0.24 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.876, T_{max} = 0.910
26490 measured reflections
7162 independent reflections
5040 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.170
S = 1.03
7162 reflections
502 parameters
18 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.87 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

Table 1
Selected bond lengths (Å).

Mn1—O5	2.157 (2)	Mn1—N2	2.261 (2)
Mn1—O1	2.210 (2)	Mn1—O2	2.284 (2)
Mn1—N1	2.214 (2)	Mn1—O4	2.329 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
O6—H6···O7	0.82	1.89	2.709 (5)	179
O7—H1*W*···O8	0.85	2.20	2.891 (6)	139
O8—H4*W*···O4	0.85	2.17	3.020 (4)	179
O7—H2*W*···O1^{i}	0.83	1.96	2.774 (4)	165
O8—H3*W*···O3^{ii}	0.85	2.16	2.943 (5)	153
O3—H3···N4^{iii}	0.82	2.15	2.964 (5)	175

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 1990); 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: BG2114).

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supplementary materials

Acta Cryst. (2007). E**63**, m2813-m2814 [**doi:10.1107/S1600536807051628**]

(2,9-Dimethyl-1,10-phenanthroline-κ^2N,N')bis(3-hydroxybenzoato-κ^2O,O')manganese(II) 2,9-dimethyl-1,10-phenanthroline dihydrate

X. Xuan, P. Zhao and S. Zhang

Comment

Crystal structures of metal complexes of 1,10-phenanthroline or its derivatives combinated with benzoic anions have been reported (Fu *et al.*, 2006; Liu & Ng, 2007; Niu *et al.*, 2002; Pan, Liu *et al.*, 2006; Pan, Su *et al.*, 2006*a*,b; Shi *et al.*, 2001; Su, Gu *et al.*, 2005*a*,b; Su & Xu, 2005; Su, Zhang & Xu,2005; Xu *et al.*, 2004). Recently, as part of our ongoing studies (Xuan, Zhao & Tang, 2007; Xuan, Zhao & Zhang, 2007); Zhao, Xuan & Wang, 2007; Zhao, Yan *et al.*, 2007) of mixed-ligand complexes, we have reported the structure of bis(benzoato-κ^2O,O')(2,9-dimethyl-1,10-phenanthroline-κ^2N,N') manganese(II) (Zhao, Xuan *et al.*, 2007). In this paper, we present the crystal structure of the manganese complex of dmphen and 3-hydroxy-benzoate anion, $[Mn(C_7H_5O_3)_2(C_{14}H_{12}N_2)]$. $(C_{14}H_{12}N_2)\cdot 2H_2O$, (I) which was obtained by reaction of dmphen, sodium 3-hydroxy-benzoate and $Mn(NO_3)_2$ aqueous solutions.

As shown in Fig. 1, the structure unit of (I) is composed of a Mn^{II} complex, $[Mn(C_7H_5O_3)_2(C_{14}H_{12}N_2)]$, one non-coordinated dmphen molecule and two crystal water molecules. Two N atoms of one dmphen ligand and four O atoms of two 3-hydroxy-benzoate anions are coordinated to the Mn^{II} ion in a strongly distorted octahedral arrangement. The corresponding bond lengths are listed in Table 1.

The crystal structure of (I) is stabilized by a profuse network of O—H···O and O—H···N hydrogen bonds having water molecules and the 3-hydroxy-benzoate anion as donors and the same groups plus the non-coordinated dmphen molecule as acceptors (Table 2 and Fig. 2).

Experimental

To a solution of 2,9-dimethyl-1,10-phenanthroline ($C_{14}H_{12}N_2\cdot 0.5H_2O$, 0.1089 g, 0.5 mmol), 3-hydroxy-benzoate (0.0693 g, 0.5 mmol) and sodium hydroxide (0.01979 g,0.5 mmol) in ethanol/water (v:v=1:1, 5 ml) was added a solution of 50% $Mn(NO_3)_2$(0.2016 g, 0.5 mmol) in distilled water (5 ml). The resulting solution was stirred for 3 h at 323 K and filtered. Yellow single crystals of (I) were obtained by slow evaporation of the filtrate over 30 days.

Refinement

The H atoms bound to O were found *via* Fourier difference map,and refined as riding in their as-found relative positions with $U_{iso}(H) = 1.5U_{eq}(O)$. Other H atoms were positioned geometrically and refined using a riding model, with fixed C—H distances of 0.93 Å (C—H) [$U_{iso}(H) = 1.2U_{eq}(C)$] and 0.96 Å ($CH_3$) [$U_{iso}(H) = 1.5U_{eq}(C)$].

Figures

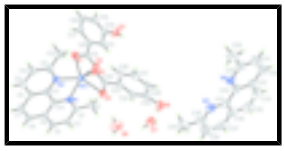


Fig. 1. The molecular structure of (I), with atom labels and 30% probability displacement ellipsoids for Non-H atoms.

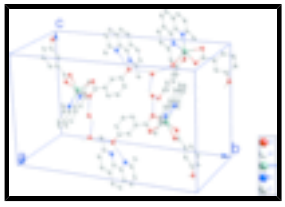


Fig. 2. Packing diagram of (I), showing the formation of hydrogen-bonded(dashed lines) interactions. H atoms not intervening in H bonding not shown, for clarity.

(2,9-Dimethyl-1,10-phenanthroline-κ^2*N*,*N*')bis(3-hydroxybenzoato- κ^2*O*,*O*')manganese(II) 2,9-dimethyl-1,10-phenanthroline solvate dihydrate

Crystal data

$[Mn(C_7H_5O_3)_2(C_{14}H_{12}N_2)]\cdot C_{14}H_{12}N_2\cdot 2H_2O$	F_{000} = 1628
M_r = 781.70	D_x = 1.349 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 5503 reflections
a = 10.7010 (9) Å	θ = 2.4–22.2º
b = 24.865 (2) Å	μ = 0.40 mm^{-1}
c = 14.5083 (12) Å	T = 291 (2) K
β = 94.5140 (10)º	Block, yellow
V = 3848.5 (5) Å^3	0.34 × 0.25 × 0.24 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	7162 independent reflections
Radiation source: fine-focus sealed tube	5040 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.031
T = 291(2) K	θ_{max} = 25.5º
φ and ω scans	θ_{min} = 2.4º
Absorption correction: multi-scan (SADABS in SAINT; Bruker, 1997)	h = −12→12
T_{min} = 0.876, T_{max} = 0.910	k = −30→30
26490 measured reflections	l = −17→17

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.053$	H-atom parameters constrained
$wR(F^2) = 0.170$	$w = 1/[\sigma^2(F_o^2) + (0.0901P)^2 + 1.8289P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} = 0.001$
7162 reflections	$\Delta\rho_{max} = 0.87$ e Å^{-3}
502 parameters	$\Delta\rho_{min} = -0.37$ e Å^{-3}
18 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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	0.00824 (4)	0.244319 (18)	0.09991 (3)	0.04685 (17)
O1	0.0685 (2)	0.16091 (9)	0.07514 (16)	0.0633 (6)
O2	−0.0670 (2)	0.17259 (9)	0.17687 (16)	0.0612 (6)
O3	−0.1536 (4)	−0.01844 (12)	0.2890 (3)	0.1281 (14)
H3	−0.1653	0.0020	0.3318	0.192*
O4	−0.0488 (2)	0.30156 (10)	0.21655 (15)	0.0644 (6)
O5	0.1445 (2)	0.27461 (10)	0.20459 (15)	0.0639 (6)
O6	−0.0292 (3)	0.39008 (14)	0.53298 (18)	0.0950 (9)
H6	−0.1002	0.3850	0.5091	0.143*
N1	−0.1434 (2)	0.27463 (9)	0.00078 (16)	0.0431 (5)
N2	0.1071 (2)	0.27329 (10)	−0.02296 (16)	0.0471 (6)
N3	0.1062 (3)	0.46939 (12)	0.8100 (3)	0.0790 (9)
N4	0.2962 (3)	0.43994 (12)	0.9354 (2)	0.0705 (8)
C1	−0.3072 (3)	0.25456 (15)	0.1030 (3)	0.0633 (9)
H1A	−0.3388	0.2187	0.0932	0.095*
H1B	−0.3721	0.2771	0.1239	0.095*
H1C	−0.2375	0.2539	0.1489	0.095*
C2	−0.2657 (3)	0.27613 (12)	0.0151 (2)	0.0494 (7)
C3	−0.3528 (3)	0.29696 (14)	−0.0524 (2)	0.0616 (9)
H3A	−0.4371	0.2984	−0.0410	0.074*
C4	−0.3167 (3)	0.31506 (14)	−0.1338 (3)	0.0634 (9)

H4	−0.3760	0.3282	−0.1785	0.076*
C5	−0.1884 (3)	0.31413 (12)	−0.1510 (2)	0.0535 (8)
C6	−0.1424 (4)	0.33335 (14)	−0.2343 (2)	0.0651 (9)
H6A	−0.1987	0.3461	−0.2814	0.078*
C7	−0.0209 (4)	0.33350 (14)	−0.2459 (2)	0.0672 (10)
H7	0.0067	0.3467	−0.3008	0.081*
C8	0.0693 (3)	0.31352 (13)	−0.1751 (2)	0.0561 (8)
C9	0.1994 (4)	0.31283 (15)	−0.1838 (2)	0.0655 (9)
H9	0.2317	0.3269	−0.2363	0.079*
C10	0.2770 (3)	0.29172 (16)	−0.1155 (3)	0.0684 (10)
H10	0.3626	0.2900	−0.1223	0.082*
C11	0.2295 (3)	0.27208 (14)	−0.0335 (2)	0.0551 (8)
C12	0.3154 (3)	0.25003 (16)	0.0437 (3)	0.0698 (10)
H12A	0.3482	0.2790	0.0820	0.105*
H12B	0.3833	0.2312	0.0186	0.105*
H12C	0.2698	0.2257	0.0801	0.105*
C13	0.0274 (3)	0.29343 (11)	−0.09279 (19)	0.0456 (7)
C14	−0.1051 (3)	0.29368 (11)	−0.08021 (19)	0.0442 (7)
C15	−0.0003 (3)	0.14134 (13)	0.1343 (2)	0.0496 (7)
C16	0.0001 (3)	0.08214 (12)	0.1523 (2)	0.0521 (7)
C17	0.0791 (4)	0.04892 (15)	0.1076 (3)	0.0736 (10)
H17	0.1321	0.0633	0.0662	0.088*
C18	0.0792 (4)	−0.00595 (16)	0.1247 (3)	0.0868 (12)
H18	0.1325	−0.0283	0.0946	0.104*
C19	0.0016 (4)	−0.02744 (15)	0.1854 (3)	0.0847 (12)
H19	0.0021	−0.0643	0.1961	0.102*
C20	−0.0777 (4)	0.00548 (15)	0.2310 (3)	0.0832 (12)
C21	−0.0775 (4)	0.06064 (14)	0.2143 (2)	0.0679 (10)
H21	−0.1299	0.0831	0.2451	0.081*
C22	0.0647 (3)	0.29992 (12)	0.2478 (2)	0.0533 (8)
C23	0.1069 (3)	0.32856 (12)	0.3350 (2)	0.0518 (7)
C24	0.0192 (3)	0.34615 (13)	0.3921 (2)	0.0588 (8)
H24	−0.0655	0.3405	0.3757	0.071*
C25	0.0564 (4)	0.37238 (14)	0.4747 (2)	0.0696 (10)
C26	0.1824 (5)	0.38026 (16)	0.4978 (3)	0.0802 (12)
H26	0.2085	0.3978	0.5526	0.096*
C27	0.2688 (4)	0.36263 (16)	0.4411 (3)	0.0767 (11)
H27	0.3535	0.3684	0.4577	0.092*
C28	0.2336 (3)	0.33635 (14)	0.3596 (2)	0.0650 (9)
H28	0.2937	0.3240	0.3217	0.078*
C29	0.5222 (5)	0.4329 (2)	0.9678 (4)	0.1206 (19)
H29A	0.5484	0.4009	0.9376	0.181*
H29B	0.5781	0.4398	1.0215	0.181*
H29C	0.5236	0.4628	0.9260	0.181*
C30	0.3907 (5)	0.42520 (16)	0.9965 (3)	0.0848 (12)
C31	0.3687 (6)	0.40379 (19)	1.0822 (4)	0.1083 (17)
H31	0.4355	0.3935	1.1233	0.130*
C32	0.2499 (7)	0.39805 (19)	1.1056 (3)	0.1040 (17)
H32	0.2357	0.3842	1.1633	0.125*

C33	0.1481 (5)	0.41253 (16)	1.0448 (3)	0.0836 (12)
C34	0.0234 (7)	0.4081 (2)	1.0641 (4)	0.1109 (19)
H34	0.0054	0.3936	1.1207	0.133*
C35	−0.0717 (6)	0.4236 (2)	1.0052 (5)	0.1099 (19)
H35	−0.1536	0.4205	1.0216	0.132*
C36	−0.0483 (5)	0.44495 (17)	0.9178 (4)	0.0929 (14)
C37	−0.1403 (6)	0.4617 (2)	0.8523 (7)	0.133 (3)
H37	−0.2237	0.4594	0.8656	0.159*
C38	−0.1130 (8)	0.4816 (2)	0.7681 (6)	0.141 (3)
H38	−0.1764	0.4926	0.7247	0.170*
C39	0.0158 (7)	0.48497 (18)	0.7488 (4)	0.1102 (18)
C40	0.0548 (8)	0.5065 (2)	0.6580 (4)	0.162 (3)
H40A	0.0907	0.5416	0.6675	0.243*
H40B	−0.0173	0.5087	0.6144	0.243*
H40C	0.1156	0.4828	0.6346	0.243*
C41	0.0765 (4)	0.44945 (14)	0.8927 (3)	0.0722 (10)
C42	0.1765 (4)	0.43374 (13)	0.9578 (3)	0.0670 (10)
O7	−0.2628 (3)	0.37352 (15)	0.4519 (2)	0.1150 (11)
H2W	−0.3165	0.3589	0.4818	0.172*
H1W	−0.2969	0.3827	0.3996	0.172*
O8	−0.2740 (4)	0.36941 (17)	0.2523 (3)	0.1431 (14)
H4W	−0.2110	0.3501	0.2421	0.215*
H3W	−0.2710	0.4016	0.2325	0.215*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0433 (3)	0.0551 (3)	0.0423 (3)	0.00193 (19)	0.00362 (19)	0.00095 (19)
O1	0.0647 (15)	0.0598 (13)	0.0681 (14)	0.0006 (11)	0.0217 (12)	0.0033 (11)
O2	0.0637 (14)	0.0533 (13)	0.0692 (14)	0.0057 (11)	0.0214 (12)	0.0033 (11)
O3	0.198 (4)	0.0631 (18)	0.137 (3)	0.015 (2)	0.100 (3)	0.0235 (18)
O4	0.0550 (15)	0.0795 (16)	0.0576 (14)	−0.0023 (11)	−0.0028 (11)	−0.0154 (11)
O5	0.0606 (14)	0.0775 (16)	0.0531 (13)	0.0039 (12)	0.0014 (11)	−0.0087 (12)
O6	0.130 (3)	0.102 (2)	0.0547 (16)	−0.004 (2)	0.0184 (17)	−0.0175 (15)
N1	0.0409 (14)	0.0437 (13)	0.0441 (13)	0.0009 (10)	0.0001 (10)	−0.0021 (10)
N2	0.0435 (14)	0.0546 (14)	0.0438 (13)	−0.0009 (11)	0.0076 (11)	−0.0026 (11)
N3	0.100 (3)	0.0529 (18)	0.083 (2)	0.0053 (16)	−0.005 (2)	−0.0104 (16)
N4	0.082 (2)	0.0534 (17)	0.076 (2)	0.0055 (15)	0.0108 (18)	−0.0059 (15)
C1	0.0452 (19)	0.075 (2)	0.070 (2)	−0.0018 (16)	0.0109 (16)	0.0020 (18)
C2	0.0419 (17)	0.0480 (16)	0.0577 (18)	−0.0005 (13)	−0.0007 (14)	−0.0080 (14)
C3	0.0451 (19)	0.068 (2)	0.071 (2)	0.0040 (15)	−0.0031 (17)	−0.0063 (17)
C4	0.058 (2)	0.067 (2)	0.062 (2)	0.0121 (16)	−0.0182 (17)	−0.0043 (17)
C5	0.063 (2)	0.0486 (17)	0.0466 (17)	0.0026 (14)	−0.0091 (15)	−0.0056 (13)
C6	0.085 (3)	0.063 (2)	0.0452 (18)	0.0078 (18)	−0.0082 (18)	0.0017 (15)
C7	0.101 (3)	0.063 (2)	0.0372 (17)	−0.004 (2)	0.0049 (18)	0.0013 (15)
C8	0.072 (2)	0.0553 (18)	0.0418 (16)	−0.0081 (16)	0.0127 (15)	−0.0069 (14)
C9	0.075 (3)	0.077 (2)	0.0475 (19)	−0.0164 (19)	0.0202 (18)	−0.0080 (17)
C10	0.050 (2)	0.091 (3)	0.067 (2)	−0.0146 (18)	0.0223 (18)	−0.012 (2)

C11	0.0431 (18)	0.067 (2)	0.0555 (19)	−0.0043 (14)	0.0078 (14)	−0.0079 (15)
C12	0.0391 (18)	0.099 (3)	0.072 (2)	0.0020 (17)	0.0072 (16)	−0.006 (2)
C13	0.0538 (18)	0.0453 (16)	0.0378 (15)	−0.0030 (13)	0.0035 (13)	−0.0055 (12)
C14	0.0492 (17)	0.0402 (15)	0.0428 (16)	−0.0003 (12)	0.0010 (13)	−0.0071 (12)
C15	0.0434 (17)	0.0613 (19)	0.0435 (16)	0.0012 (14)	0.0002 (13)	0.0007 (14)
C16	0.0556 (19)	0.0512 (17)	0.0491 (18)	0.0031 (14)	0.0019 (14)	−0.0009 (14)
C17	0.077 (3)	0.065 (2)	0.081 (3)	0.0072 (19)	0.020 (2)	−0.0006 (19)
C18	0.096 (3)	0.065 (2)	0.103 (3)	0.018 (2)	0.030 (3)	−0.008 (2)
C19	0.117 (4)	0.052 (2)	0.087 (3)	0.017 (2)	0.022 (3)	0.0040 (19)
C20	0.119 (4)	0.057 (2)	0.078 (3)	0.007 (2)	0.035 (3)	0.0093 (19)
C21	0.089 (3)	0.0513 (19)	0.066 (2)	0.0122 (18)	0.023 (2)	0.0055 (16)
C22	0.061 (2)	0.0515 (18)	0.0473 (17)	−0.0044 (15)	0.0028 (16)	0.0039 (14)
C23	0.061 (2)	0.0486 (17)	0.0444 (16)	−0.0067 (14)	−0.0036 (15)	0.0059 (13)
C24	0.074 (2)	0.0529 (18)	0.0491 (18)	−0.0082 (16)	−0.0004 (16)	0.0030 (14)
C25	0.104 (3)	0.056 (2)	0.0477 (19)	−0.0047 (19)	0.002 (2)	0.0032 (15)
C26	0.114 (4)	0.068 (2)	0.054 (2)	−0.014 (2)	−0.024 (2)	0.0009 (18)
C27	0.079 (3)	0.080 (3)	0.066 (2)	−0.015 (2)	−0.023 (2)	0.009 (2)
C28	0.068 (2)	0.064 (2)	0.061 (2)	−0.0062 (17)	−0.0070 (17)	0.0090 (17)
C29	0.087 (4)	0.099 (4)	0.174 (6)	0.014 (3)	0.001 (4)	−0.024 (4)
C30	0.102 (3)	0.052 (2)	0.098 (3)	0.003 (2)	−0.003 (3)	−0.012 (2)
C31	0.141 (5)	0.075 (3)	0.105 (4)	−0.003 (3)	−0.023 (4)	0.003 (3)
C32	0.164 (6)	0.074 (3)	0.073 (3)	−0.017 (3)	0.006 (4)	0.007 (2)
C33	0.119 (4)	0.055 (2)	0.079 (3)	−0.015 (2)	0.025 (3)	−0.008 (2)
C34	0.148 (5)	0.075 (3)	0.118 (4)	−0.032 (3)	0.065 (4)	−0.018 (3)
C35	0.106 (4)	0.075 (3)	0.156 (6)	−0.025 (3)	0.060 (4)	−0.031 (3)
C36	0.079 (3)	0.061 (2)	0.139 (5)	−0.005 (2)	0.013 (3)	−0.032 (3)
C37	0.087 (4)	0.083 (4)	0.226 (8)	0.006 (3)	−0.009 (5)	−0.053 (5)
C38	0.137 (6)	0.077 (4)	0.196 (8)	0.021 (4)	−0.072 (6)	−0.031 (4)
C39	0.147 (5)	0.058 (3)	0.118 (4)	0.011 (3)	−0.042 (4)	−0.016 (3)
C40	0.289 (9)	0.084 (4)	0.101 (4)	0.003 (5)	−0.064 (5)	0.004 (3)
C41	0.083 (3)	0.0473 (19)	0.088 (3)	−0.0022 (17)	0.013 (2)	−0.0178 (19)
C42	0.089 (3)	0.0451 (18)	0.068 (2)	−0.0070 (17)	0.015 (2)	−0.0111 (16)
O7	0.102 (2)	0.146 (3)	0.103 (2)	0.002 (2)	0.0468 (19)	0.014 (2)
O8	0.133 (3)	0.114 (3)	0.184 (4)	0.020 (2)	0.024 (3)	−0.014 (3)

Geometric parameters (Å, °)

Mn1—O5	2.157 (2)	C16—C21	1.378 (5)
Mn1—O1	2.210 (2)	C16—C17	1.380 (5)
Mn1—N1	2.214 (2)	C17—C18	1.386 (6)
Mn1—N2	2.261 (2)	C17—H17	0.9300
Mn1—O2	2.284 (2)	C18—C19	1.366 (6)
Mn1—O4	2.329 (2)	C18—H18	0.9300
Mn1—C22	2.584 (3)	C19—C20	1.384 (5)
Mn1—C15	2.612 (3)	C19—H19	0.9300
O1—C15	1.270 (4)	C20—C21	1.393 (5)
O2—C15	1.251 (4)	C21—H21	0.9300
O3—C20	1.353 (5)	C22—C23	1.490 (4)
O3—H3	0.8200	C23—C24	1.372 (5)

O4—C22	1.263 (4)	C23—C28	1.388 (5)
O5—C22	1.266 (4)	C24—C25	1.395 (5)
O6—C25	1.367 (5)	C24—H24	0.9300
O6—H6	0.8200	C25—C26	1.378 (6)
N1—C2	1.342 (4)	C26—C27	1.358 (6)
N1—C14	1.360 (4)	C26—H26	0.9300
N2—C11	1.332 (4)	C27—C28	1.378 (5)
N2—C13	1.367 (4)	C27—H27	0.9300
N3—C39	1.318 (6)	C28—H28	0.9300
N3—C41	1.360 (5)	C29—C30	1.511 (6)
N4—C30	1.342 (5)	C29—H29A	0.9600
N4—C42	1.354 (5)	C29—H29B	0.9600
C1—C2	1.483 (5)	C29—H29C	0.9600
C1—H1A	0.9600	C30—C31	1.390 (7)
C1—H1B	0.9600	C31—C32	1.348 (7)
C1—H1C	0.9600	C31—H31	0.9300
C2—C3	1.398 (4)	C32—C33	1.395 (7)
C3—C4	1.348 (5)	C32—H32	0.9300
C3—H3A	0.9300	C33—C34	1.389 (7)
C4—C5	1.415 (5)	C33—C42	1.423 (6)
C4—H4	0.9300	C34—C35	1.334 (8)
C5—C14	1.402 (4)	C34—H34	0.9300
C5—C6	1.422 (5)	C35—C36	1.414 (8)
C6—C7	1.324 (5)	C35—H35	0.9300
C6—H6A	0.9300	C36—C37	1.378 (9)
C7—C8	1.441 (5)	C36—C41	1.416 (6)
C7—H7	0.9300	C37—C38	1.371 (9)
C8—C13	1.401 (4)	C37—H37	0.9300
C8—C9	1.408 (5)	C38—C39	1.430 (9)
C9—C10	1.348 (5)	C38—H38	0.9300
C9—H9	0.9300	C39—C40	1.511 (8)
C10—C11	1.417 (5)	C40—H40A	0.9600
C10—H10	0.9300	C40—H40B	0.9600
C11—C12	1.496 (5)	C40—H40C	0.9600
C12—H12A	0.9600	C41—C42	1.424 (6)
C12—H12B	0.9600	O7—H2W	0.8299
C12—H12C	0.9600	O7—H1W	0.8468
C13—C14	1.443 (4)	O8—H4W	0.8502
C15—C16	1.495 (4)	O8—H3W	0.8517
O5—Mn1—O1	104.63 (9)	O1—C15—Mn1	57.64 (16)
O5—Mn1—N1	139.36 (9)	C16—C15—Mn1	177.6 (2)
O1—Mn1—N1	114.97 (9)	C21—C16—C17	119.8 (3)
O5—Mn1—N2	96.42 (9)	C21—C16—C15	120.2 (3)
O1—Mn1—N2	90.59 (9)	C17—C16—C15	120.0 (3)
N1—Mn1—N2	75.15 (9)	C16—C17—C18	119.8 (4)
O5—Mn1—O2	99.97 (9)	C16—C17—H17	120.1
O1—Mn1—O2	57.67 (8)	C18—C17—H17	120.1
N1—Mn1—O2	108.35 (9)	C19—C18—C17	120.5 (4)
N2—Mn1—O2	147.03 (9)	C19—C18—H18	119.7

O5—Mn1—O4	58.41 (8)	C17—C18—H18	119.7
O1—Mn1—O4	142.02 (9)	C18—C19—C20	120.2 (4)
N1—Mn1—O4	92.49 (8)	C18—C19—H19	119.9
N2—Mn1—O4	122.94 (9)	C20—C19—H19	119.9
O2—Mn1—O4	89.96 (8)	O3—C20—C19	117.3 (4)
O5—Mn1—C22	29.24 (9)	O3—C20—C21	123.4 (4)
O1—Mn1—C22	125.81 (10)	C19—C20—C21	119.3 (4)
N1—Mn1—C22	117.96 (10)	C16—C21—C20	120.3 (3)
N2—Mn1—C22	113.02 (9)	C16—C21—H21	119.8
O2—Mn1—C22	94.59 (9)	C20—C21—H21	119.8
O4—Mn1—C22	29.20 (9)	O4—C22—O5	120.3 (3)
O5—Mn1—C15	103.86 (9)	O4—C22—C23	120.6 (3)
O1—Mn1—C15	29.05 (8)	O5—C22—C23	119.1 (3)
N1—Mn1—C15	115.03 (9)	O4—C22—Mn1	64.12 (17)
N2—Mn1—C15	119.24 (9)	O5—C22—Mn1	56.31 (16)
O2—Mn1—C15	28.62 (8)	C23—C22—Mn1	174.8 (2)
O4—Mn1—C15	116.44 (9)	C24—C23—C28	120.1 (3)
C22—Mn1—C15	112.04 (9)	C24—C23—C22	119.3 (3)
C15—O1—Mn1	93.31 (18)	C28—C23—C22	120.6 (3)
C15—O2—Mn1	90.38 (18)	C23—C24—C25	120.4 (3)
C20—O3—H3	109.5	C23—C24—H24	119.8
C22—O4—Mn1	86.67 (19)	C25—C24—H24	119.8
C22—O5—Mn1	94.5 (2)	O6—C25—C26	119.6 (4)
C25—O6—H6	109.5	O6—C25—C24	121.5 (4)
C2—N1—C14	119.2 (2)	C26—C25—C24	118.9 (4)
C2—N1—Mn1	125.6 (2)	C27—C26—C25	120.4 (4)
C14—N1—Mn1	115.12 (18)	C27—C26—H26	119.8
C11—N2—C13	119.0 (3)	C25—C26—H26	119.8
C11—N2—Mn1	127.5 (2)	C26—C27—C28	121.4 (4)
C13—N2—Mn1	113.44 (18)	C26—C27—H27	119.3
C39—N3—C41	119.4 (5)	C28—C27—H27	119.3
C30—N4—C42	119.2 (4)	C27—C28—C23	118.8 (4)
C2—C1—H1A	109.5	C27—C28—H28	120.6
C2—C1—H1B	109.5	C23—C28—H28	120.6
H1A—C1—H1B	109.5	C30—C29—H29A	109.5
C2—C1—H1C	109.5	C30—C29—H29B	109.5
H1A—C1—H1C	109.5	H29A—C29—H29B	109.5
H1B—C1—H1C	109.5	C30—C29—H29C	109.5
N1—C2—C3	120.4 (3)	H29A—C29—H29C	109.5
N1—C2—C1	119.0 (3)	H29B—C29—H29C	109.5
C3—C2—C1	120.5 (3)	N4—C30—C31	121.6 (5)
C4—C3—C2	121.0 (3)	N4—C30—C29	116.9 (5)
C4—C3—H3A	119.5	C31—C30—C29	121.5 (5)
C2—C3—H3A	119.5	C32—C31—C30	119.7 (5)
C3—C4—C5	119.9 (3)	C32—C31—H31	120.2
C3—C4—H4	120.0	C30—C31—H31	120.2
C5—C4—H4	120.0	C31—C32—C33	121.3 (5)
C14—C5—C4	116.5 (3)	C31—C32—H32	119.4
C14—C5—C6	120.1 (3)	C33—C32—H32	119.4

C4—C5—C6	123.4 (3)	C34—C33—C32	124.5 (5)
C7—C6—C5	121.2 (3)	C34—C33—C42	119.0 (5)
C7—C6—H6A	119.4	C32—C33—C42	116.5 (4)
C5—C6—H6A	119.4	C35—C34—C33	122.9 (6)
C6—C7—C8	121.1 (3)	C35—C34—H34	118.5
C6—C7—H7	119.4	C33—C34—H34	118.5
C8—C7—H7	119.4	C34—C35—C36	120.2 (5)
C13—C8—C9	117.2 (3)	C34—C35—H35	119.9
C13—C8—C7	119.3 (3)	C36—C35—H35	119.9
C9—C8—C7	123.5 (3)	C37—C36—C35	124.3 (6)
C10—C9—C8	119.8 (3)	C37—C36—C41	115.9 (6)
C10—C9—H9	120.1	C35—C36—C41	119.8 (5)
C8—C9—H9	120.1	C38—C37—C36	122.2 (7)
C9—C10—C11	120.7 (3)	C38—C37—H37	118.9
C9—C10—H10	119.7	C36—C37—H37	118.9
C11—C10—H10	119.7	C37—C38—C39	118.2 (6)
N2—C11—C10	120.7 (3)	C37—C38—H38	120.9
N2—C11—C12	118.3 (3)	C39—C38—H38	120.9
C10—C11—C12	121.0 (3)	N3—C39—C38	121.2 (6)
C11—C12—H12A	109.5	N3—C39—C40	116.9 (6)
C11—C12—H12B	109.5	C38—C39—C40	121.8 (6)
H12A—C12—H12B	109.5	C39—C40—H40A	109.5
C11—C12—H12C	109.5	C39—C40—H40B	109.5
H12A—C12—H12C	109.5	H40A—C40—H40B	109.5
H12B—C12—H12C	109.5	C39—C40—H40C	109.5
N2—C13—C8	122.7 (3)	H40A—C40—H40C	109.5
N2—C13—C14	118.0 (2)	H40B—C40—H40C	109.5
C8—C13—C14	119.3 (3)	N3—C41—C36	123.1 (5)
N1—C14—C5	122.8 (3)	N3—C41—C42	118.0 (4)
N1—C14—C13	118.3 (3)	C36—C41—C42	118.9 (4)
C5—C14—C13	118.9 (3)	N4—C42—C33	121.8 (4)
O2—C15—O1	118.6 (3)	N4—C42—C41	119.0 (4)
O2—C15—C16	121.2 (3)	C33—C42—C41	119.2 (4)
O1—C15—C16	120.1 (3)	H2W—O7—H1W	108.5
O2—C15—Mn1	61.00 (16)	H4W—O8—H3W	114.8
O5—Mn1—O1—C15	92.30 (19)	Mn1—O2—C15—O1	−0.6 (3)
N1—Mn1—O1—C15	−97.05 (19)	Mn1—O2—C15—C16	179.0 (3)
N2—Mn1—O1—C15	−170.92 (19)	Mn1—O1—C15—O2	0.7 (3)
O2—Mn1—O1—C15	−0.37 (17)	Mn1—O1—C15—C16	−179.0 (2)
O4—Mn1—O1—C15	35.4 (3)	O5—Mn1—C15—O2	85.42 (19)
C22—Mn1—O1—C15	69.8 (2)	O1—Mn1—C15—O2	−179.3 (3)
O5—Mn1—O2—C15	−100.70 (19)	N1—Mn1—C15—O2	−82.51 (19)
O1—Mn1—O2—C15	0.38 (17)	N2—Mn1—C15—O2	−168.92 (17)
N1—Mn1—O2—C15	108.83 (18)	O4—Mn1—C15—O2	24.1 (2)
N2—Mn1—O2—C15	18.0 (3)	C22—Mn1—C15—O2	55.8 (2)
O4—Mn1—O2—C15	−158.56 (19)	O5—Mn1—C15—O1	−95.24 (19)
C22—Mn1—O2—C15	−129.69 (19)	N1—Mn1—C15—O1	96.83 (19)
O5—Mn1—O4—C22	−2.24 (17)	N2—Mn1—C15—O1	10.4 (2)
O1—Mn1—O4—C22	69.9 (2)	O2—Mn1—C15—O1	179.3 (3)

N1—Mn1—O4—C22	−152.12 (18)	O4—Mn1—C15—O1	−156.56 (17)
N2—Mn1—O4—C22	−78.2 (2)	C22—Mn1—C15—O1	−124.82 (19)
O2—Mn1—O4—C22	99.51 (19)	O2—C15—C16—C21	2.4 (5)
C15—Mn1—O4—C22	88.24 (19)	O1—C15—C16—C21	−177.9 (3)
O1—Mn1—O5—C22	−140.49 (18)	O2—C15—C16—C17	−176.9 (3)
N1—Mn1—O5—C22	52.6 (2)	O1—C15—C16—C17	2.8 (5)
N2—Mn1—O5—C22	127.21 (19)	C21—C16—C17—C18	0.6 (6)
O2—Mn1—O5—C22	−81.51 (19)	C15—C16—C17—C18	179.9 (4)
O4—Mn1—O5—C22	2.24 (17)	C16—C17—C18—C19	0.0 (7)
C15—Mn1—O5—C22	−110.51 (19)	C17—C18—C19—C20	−0.3 (7)
O5—Mn1—N1—C2	−95.7 (2)	C18—C19—C20—O3	178.9 (5)
O1—Mn1—N1—C2	98.3 (2)	C18—C19—C20—C21	0.0 (7)
N2—Mn1—N1—C2	−178.1 (2)	C17—C16—C21—C20	−0.9 (6)
O2—Mn1—N1—C2	36.1 (2)	C15—C16—C21—C20	179.8 (4)
O4—Mn1—N1—C2	−54.7 (2)	O3—C20—C21—C16	−178.2 (4)
C22—Mn1—N1—C2	−69.6 (2)	C19—C20—C21—C16	0.6 (7)
C15—Mn1—N1—C2	66.1 (2)	Mn1—O4—C22—O5	3.8 (3)
O5—Mn1—N1—C14	83.3 (2)	Mn1—O4—C22—C23	−177.4 (3)
O1—Mn1—N1—C14	−82.7 (2)	Mn1—O5—C22—O4	−4.1 (3)
N2—Mn1—N1—C14	0.88 (18)	Mn1—O5—C22—C23	177.1 (2)
O2—Mn1—N1—C14	−144.85 (18)	O5—Mn1—C22—O4	176.1 (3)
O4—Mn1—N1—C14	124.36 (19)	O1—Mn1—C22—O4	−134.53 (17)
C22—Mn1—N1—C14	109.39 (19)	N1—Mn1—C22—O4	31.9 (2)
C15—Mn1—N1—C14	−114.83 (19)	N2—Mn1—C22—O4	116.79 (18)
O5—Mn1—N2—C11	40.9 (3)	O2—Mn1—C22—O4	−81.66 (18)
O1—Mn1—N2—C11	−63.9 (3)	C15—Mn1—C22—O4	−105.09 (19)
N1—Mn1—N2—C11	−179.7 (3)	O1—Mn1—C22—O5	49.4 (2)
O2—Mn1—N2—C11	−78.7 (3)	N1—Mn1—C22—O5	−144.16 (18)
O4—Mn1—N2—C11	97.1 (3)	N2—Mn1—C22—O5	−59.3 (2)
C22—Mn1—N2—C11	65.9 (3)	O2—Mn1—C22—O5	102.25 (19)
C15—Mn1—N2—C11	−69.0 (3)	O4—Mn1—C22—O5	−176.1 (3)
O5—Mn1—N2—C13	−139.89 (19)	C15—Mn1—C22—O5	78.8 (2)
O1—Mn1—N2—C13	115.3 (2)	O4—C22—C23—C24	15.0 (4)
N1—Mn1—N2—C13	−0.41 (18)	O5—C22—C23—C24	−166.2 (3)
O2—Mn1—N2—C13	100.5 (2)	O4—C22—C23—C28	−166.6 (3)
O4—Mn1—N2—C13	−83.6 (2)	O5—C22—C23—C28	12.2 (4)
C22—Mn1—N2—C13	−114.9 (2)	C28—C23—C24—C25	0.6 (5)
C15—Mn1—N2—C13	110.3 (2)	C22—C23—C24—C25	179.1 (3)
C14—N1—C2—C3	0.1 (4)	C23—C24—C25—O6	−179.7 (3)
Mn1—N1—C2—C3	179.1 (2)	C23—C24—C25—C26	0.0 (5)
C14—N1—C2—C1	179.1 (3)	O6—C25—C26—C27	179.6 (4)
Mn1—N1—C2—C1	−1.9 (4)	C24—C25—C26—C27	−0.2 (6)
N1—C2—C3—C4	1.2 (5)	C25—C26—C27—C28	−0.3 (6)
C1—C2—C3—C4	−177.8 (3)	C26—C27—C28—C23	0.8 (6)
C2—C3—C4—C5	−1.3 (5)	C24—C23—C28—C27	−1.0 (5)
C3—C4—C5—C14	0.1 (5)	C22—C23—C28—C27	−179.5 (3)
C3—C4—C5—C6	−178.8 (3)	C42—N4—C30—C31	−0.1 (6)
C14—C5—C6—C7	−1.5 (5)	C42—N4—C30—C29	179.8 (3)
C4—C5—C6—C7	177.5 (3)	N4—C30—C31—C32	−0.7 (7)

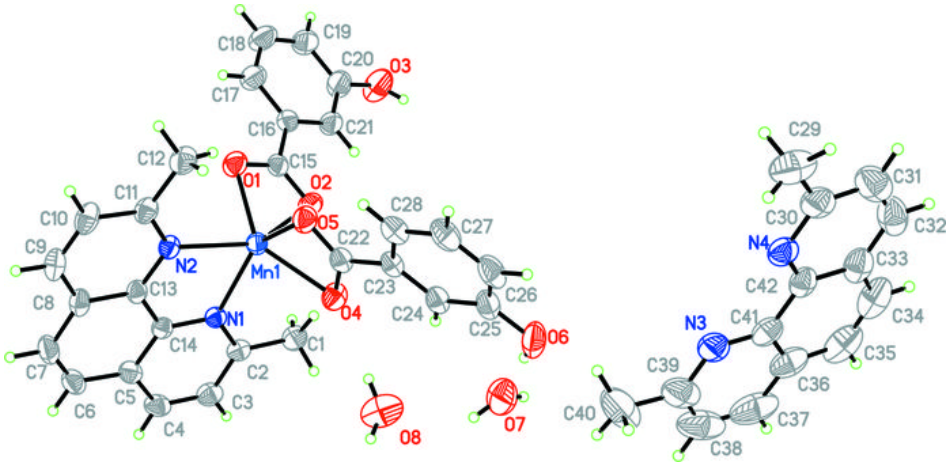
C5—C6—C7—C8	0.8 (5)	C29—C30—C31—C32	179.4 (4)
C6—C7—C8—C13	0.2 (5)	C30—C31—C32—C33	0.9 (7)
C6—C7—C8—C9	−179.8 (3)	C31—C32—C33—C34	−179.6 (5)
C13—C8—C9—C10	2.2 (5)	C31—C32—C33—C42	−0.3 (7)
C7—C8—C9—C10	−177.7 (3)	C32—C33—C34—C35	178.2 (5)
C8—C9—C10—C11	−2.5 (5)	C42—C33—C34—C35	−1.1 (7)
C13—N2—C11—C10	0.5 (5)	C33—C34—C35—C36	1.2 (8)
Mn1—N2—C11—C10	179.7 (2)	C34—C35—C36—C37	179.5 (5)
C13—N2—C11—C12	179.8 (3)	C34—C35—C36—C41	0.3 (7)
Mn1—N2—C11—C12	−0.9 (4)	C35—C36—C37—C38	−179.4 (5)
C9—C10—C11—N2	1.1 (5)	C41—C36—C37—C38	−0.2 (8)
C9—C10—C11—C12	−178.2 (3)	C36—C37—C38—C39	−0.1 (9)
C11—N2—C13—C8	−0.7 (4)	C41—N3—C39—C38	0.4 (6)
Mn1—N2—C13—C8	180.0 (2)	C41—N3—C39—C40	−179.7 (4)
C11—N2—C13—C14	179.2 (3)	C37—C38—C39—N3	0.0 (8)
Mn1—N2—C13—C14	−0.1 (3)	C37—C38—C39—C40	−179.9 (5)
C9—C8—C13—N2	−0.6 (4)	C39—N3—C41—C36	−0.7 (5)
C7—C8—C13—N2	179.3 (3)	C39—N3—C41—C42	−179.1 (3)
C9—C8—C13—C14	179.5 (3)	C37—C36—C41—N3	0.6 (6)
C7—C8—C13—C14	−0.6 (4)	C35—C36—C41—N3	179.8 (4)
C2—N1—C14—C5	−1.3 (4)	C37—C36—C41—C42	178.9 (4)
Mn1—N1—C14—C5	179.6 (2)	C35—C36—C41—C42	−1.8 (5)
C2—N1—C14—C13	177.8 (2)	C30—N4—C42—C33	0.7 (5)
Mn1—N1—C14—C13	−1.3 (3)	C30—N4—C42—C41	180.0 (3)
C4—C5—C14—N1	1.1 (4)	C34—C33—C42—N4	178.9 (4)
C6—C5—C14—N1	−179.8 (3)	C32—C33—C42—N4	−0.5 (5)
C4—C5—C14—C13	−178.0 (3)	C34—C33—C42—C41	−0.4 (5)
C6—C5—C14—C13	1.1 (4)	C32—C33—C42—C41	−179.8 (3)
N2—C13—C14—N1	0.9 (4)	N3—C41—C42—N4	0.9 (5)
C8—C13—C14—N1	−179.2 (3)	C36—C41—C42—N4	−177.5 (3)
N2—C13—C14—C5	−179.9 (3)	N3—C41—C42—C33	−179.7 (3)
C8—C13—C14—C5	0.0 (4)	C36—C41—C42—C33	1.8 (5)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O6—H6···O7	0.82	1.89	2.709 (5)	179
O7—H1W···O8	0.85	2.20	2.891 (6)	139
O8—H4W···O4	0.85	2.17	3.020 (4)	179
O7—H2W···O1^{i}	0.83	1.96	2.774 (4)	165
O8—H3W···O3^{ii}	0.85	2.16	2.943 (5)	153
O3—H3···N4^{iii}	0.82	2.15	2.964 (5)	175

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

Fig. 1


C18
C19
C20
O3
C17
C16
C21
C12
C15
O1
O2
C11
O5
C28
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C10
C22
C9
N2
Mn1
C23
C26
C8
C13
O4
C24
C25
O6
N1
C1
C7
C14
C2
C5
C3
C6
C4
O8
O7
C29
C31
C30
C32
N4
C33
C42
C34
N3
C41
C35
C39
C36
C40
C37
C38

Fig. 2