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Diacetato(1,4,8,11-tetraazacyclotetradecane)manganese(III) perchlorate monohydrate

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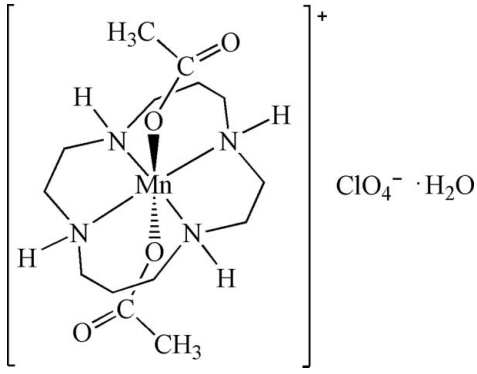
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.007 Å; R factor = 0.058; wR factor = 0.172; data-to-parameter ratio = 16.6.

The title compound, $[Mn(CH_3COO)_2(C_{10}H_{24}N_4)]ClO_4\cdot H_2O$, contains two crystallographically independent cationic complexes, each located with their central Mn^{III} atom on a centre of inversion. Each Mn^{III} atom is six-coordinated in a distorted octahedral geometry by two O atoms from acetate anions occupying axial positions and four N atoms from 1,4,8,11-tetraazacyclotetradecane (cyclam) occupying equatorial positions. The compound displays intra- and intermolecular N—H···O and O—H···O hydrogen bonding.

Related literature

For some related Mn^{III} cyclam complexes, see: Mossin *et al.* (2005).



Experimental

Crystal data

$[Mn(C_2H_3O_2)_2(C_{10}H_{24}N_4)]ClO_4\cdot H_2O$
M_r = 490.83
Monoclinic, $P2_1/c$
a = 16.0734 (17) Å
b = 8.5147 (9) Å
c = 17.3393 (18) Å
β = 113.446 (2)°
V = 2177.1 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.78 mm^{-1}
T = 293 (2) K
0.26 × 0.25 × 0.15 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.747, T_{max} = 0.889
12476 measured reflections
4452 independent reflections
3154 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.172
S = 1.06
4452 reflections
269 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.66 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O9^{i}	0.91	2.04	2.916 (4)	163
N2—H2···O2	0.91	2.03	2.865 (4)	153
N3—H3···O4	0.91	1.98	2.831 (4)	155
N4—H4···O5^{ii}	0.91	2.46	3.283 (7)	151
N4—H4···O8^{ii}	0.91	2.43	3.171 (6)	139
O9—H9*WA*···O2	0.89	1.92	2.794 (4)	171
O9—H9*WB*···O4^{iii}	0.90	2.07	2.954 (4)	170

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BI2218).

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supplementary materials

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Diacetato(1,4,8,11-tetraazacyclotetradecane)manganese(III) perchlorate monohydrate

I.-C. Hwang and K. Ha

Comment

The structure of the title compound contains two chemically equivalent, but crystallographically independent, cationic complexes, both located with their central Mn^{III} atom on a centre of inversion (Fig. 1). In both cations, the Mn^{III} atom is six-coordinated in a distorted octahedral geometry by two O atoms from acetato anions occupying axial positions and four N atoms from 1,4,8,11-tetraazacyclotetradecane (cyclam) occupying equatorial positions (mean lengths: Mn—N 2.036 Å, Mn—O 2.123 Å). The compound displays intra- and intermolecular hydrogen bonding (Fig. 2 & Table 1).

Experimental

To a solution of $Mn(CH_3COO)_3{\cdot}2H_2O$ (0.55 g, 2.05 mmol) and 1,4,8,11-tetraazacyclotetradecane (0.40 g, 2.00 mmol) in EtOH (30 ml) were added 20 drops of perchloric acid (60%) and the mixture was stirred for 8 h at room temparature. The resulting precipitate was separated by filtration, washed with EtOH and diethyl ether, then dried to give a yellow powder (0.72 g). Crystals suitable for X-ray analysis were obtained by slow evaporation from a MeOH solution.

Refinement

H atoms on N and C atoms were positioned geometrically and allowed to ride on their respective carrier atoms [N—H = 0.91 Å, C—H = 0.97 or 0.96 Å and U_{iso}(H) = 1.2U_{eq}(N or C) or 1.5U_{eq}(methyl C)]. The H atoms of the water were located from difference maps then allowed to ride on their parent O atom in the final cycles of refinement.

Figures

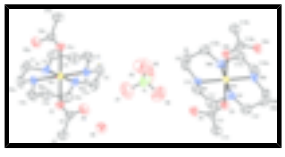


Fig. 1. The structure of the title compound with two crystallographically independent cations [Symmetry codes: (*a*) −*x*, 2 − *y*, −*z*; (*b*) 1 − *x*, −*y*, −*z*]. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity.

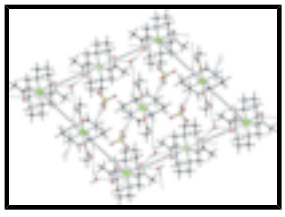


Fig. 2. View of the unit-cell contents of the title compound. Hydrogen-bond interactions are drawn with dashed lines.

Diacetato(1,4,8,11-tetraazacyclotetradecane)manganese(III) perchlorate monohydrate

Crystal data

$[Mn(C_2H_3O_2)_2(C_{10}H_{24}N_4)]ClO_4·H_2O$	F_{000} = 1032
M_r = 490.83	D_x = 1.497 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 2981 reflections
a = 16.0734 (17) Å	θ = 2.4–24.9º
b = 8.5147 (9) Å	μ = 0.78 mm^{-1}
c = 17.3393 (18) Å	T = 293 (2) K
β = 113.446 (2)º	Prism, yellow
V = 2177.1 (4) Å^3	0.26 × 0.25 × 0.15 mm
Z = 4	

Data collection

Bruker SMART 1000 CCD diffractometer	4452 independent reflections
Radiation source: fine-focus sealed tube	3154 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.029
T = 293(2) K	θ_{max} = 26.4º
φ and ω scans	θ_{min} = 1.4º
Absorption correction: multi-scan (SADABS; Bruker, 2000)	h = −20→19
T_{min} = 0.747, T_{max} = 0.889	k = −7→10
12476 measured reflections	l = −15→21

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.058	H-atom parameters constrained
$wR(F^2)$ = 0.172	$w = 1/[\sigma^2(F_o^2) + (0.082P)^2 + 1.5997P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.06	$(\Delta/\sigma)_{max} < 0.001$
4452 reflections	$\Delta\rho_{max}$ = 1.20 e Å^{-3}
269 parameters	$\Delta\rho_{min}$ = −0.66 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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	0.0000	1.0000	0.0000	0.0269 (2)
O1	−0.07775 (17)	0.8393 (3)	0.03744 (17)	0.0394 (6)
O2	0.0207 (2)	0.6979 (4)	0.1400 (2)	0.0601 (9)
N1	0.0091 (2)	1.1441 (3)	0.09685 (19)	0.0374 (7)
H1	−0.0110	1.0882	0.1308	0.045*
N2	0.11842 (19)	0.8864 (4)	0.06720 (19)	0.0356 (7)
H2	0.1057	0.8123	0.0987	0.043*
C1	−0.0573 (3)	1.2712 (5)	0.0589 (3)	0.0525 (12)
H1A	−0.0330	1.3467	0.0315	0.063*
H1B	−0.0702	1.3254	0.1021	0.063*
C2	0.1008 (3)	1.2034 (5)	0.1507 (3)	0.0510 (11)
H2A	0.0970	1.2659	0.1960	0.061*
H2B	0.1225	1.2709	0.1176	0.061*
C3	0.1673 (3)	1.0717 (6)	0.1874 (3)	0.0556 (12)
H3A	0.1418	0.9987	0.2150	0.067*
H3B	0.2222	1.1149	0.2301	0.067*
C4	0.1927 (3)	0.9818 (5)	0.1251 (3)	0.0533 (12)
H4A	0.2120	1.0556	0.0928	0.064*
H4B	0.2438	0.9139	0.1555	0.064*
C5	0.1431 (3)	0.8011 (5)	0.0045 (3)	0.0499 (11)
H5A	0.1874	0.7199	0.0320	0.060*
H5B	0.1691	0.8731	−0.0232	0.060*
C6	−0.0578 (3)	0.7385 (4)	0.0952 (3)	0.0364 (9)
C7	−0.1366 (3)	0.6656 (5)	0.1080 (3)	0.0509 (11)
H7A	−0.1144	0.5987	0.1566	0.076*
H7B	−0.1719	0.6046	0.0594	0.076*
H7C	−0.1737	0.7468	0.1162	0.076*
Mn2	0.5000	0.0000	0.0000	0.0314 (2)
O3	0.39455 (17)	−0.1607 (3)	−0.06614 (18)	0.0443 (7)
O4	0.26686 (18)	−0.0244 (3)	−0.1028 (2)	0.0506 (8)
N3	0.4109 (2)	0.1552 (4)	0.0126 (2)	0.0403 (8)
H3	0.3546	0.1194	−0.0207	0.048*
N4	0.5073 (2)	−0.0929 (4)	0.1113 (2)	0.0420 (8)

H4	0.5579	−0.0522	0.1523	0.050*
C8	0.4055 (3)	0.3291 (5)	−0.1034 (3)	0.0600 (13)
H8A	0.3962	0.4382	−0.1210	0.072*
H8B	0.3516	0.2714	−0.1382	0.072*
C9	0.4157 (3)	0.3193 (5)	−0.0138 (3)	0.0526 (12)
H9A	0.4735	0.3645	0.0223	0.063*
H9B	0.3682	0.3806	−0.0071	0.063*
C10	0.4189 (3)	0.1401 (6)	0.1013 (3)	0.0557 (12)
H10A	0.4714	0.1980	0.1387	0.067*
H10B	0.3654	0.1834	0.1062	0.067*
C11	0.4283 (3)	−0.0287 (6)	0.1249 (3)	0.0565 (12)
H11A	0.4377	−0.0403	0.1834	0.068*
H11B	0.3737	−0.0852	0.0906	0.068*
C12	0.5150 (3)	−0.2662 (5)	0.1197 (3)	0.0545 (12)
H12A	0.4595	−0.3137	0.0802	0.065*
H12B	0.5219	−0.2958	0.1759	0.065*
C13	0.3090 (2)	−0.1448 (4)	−0.1038 (2)	0.0366 (9)
C14	0.2588 (3)	−0.2852 (5)	−0.1506 (3)	0.0576 (13)
H14A	0.1997	−0.2540	−0.1899	0.086*
H14B	0.2527	−0.3599	−0.1117	0.086*
H14C	0.2916	−0.3321	−0.1804	0.086*
Cl	0.31158 (9)	0.51504 (14)	0.17560 (8)	0.0584 (3)
O5	0.3699 (4)	0.6269 (7)	0.2282 (4)	0.135 (2)
O6	0.3098 (4)	0.5158 (6)	0.0945 (3)	0.1171 (18)
O7	0.2216 (3)	0.5651 (6)	0.1679 (3)	0.1184 (17)
O8	0.3259 (3)	0.3683 (5)	0.2134 (3)	0.1128 (16)
O9	0.0709 (2)	0.5285 (3)	0.28972 (19)	0.0508 (8)
H9WA	0.0613	0.5829	0.2434	0.073 (16)*
H9WB	0.1307	0.5167	0.3184	0.10 (2)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0259 (4)	0.0280 (4)	0.0273 (4)	0.0048 (3)	0.0111 (3)	0.0044 (3)
O1	0.0397 (15)	0.0389 (15)	0.0398 (15)	−0.0022 (12)	0.0162 (13)	0.0127 (12)
O2	0.0449 (18)	0.074 (2)	0.067 (2)	0.0167 (15)	0.0273 (16)	0.0418 (17)
N1	0.049 (2)	0.0316 (17)	0.0346 (18)	0.0024 (14)	0.0195 (15)	0.0019 (13)
N2	0.0284 (16)	0.0414 (18)	0.0381 (18)	0.0093 (13)	0.0143 (14)	0.0161 (14)
C1	0.077 (3)	0.039 (2)	0.053 (3)	0.020 (2)	0.038 (3)	0.004 (2)
C2	0.059 (3)	0.047 (3)	0.042 (2)	−0.015 (2)	0.016 (2)	−0.009 (2)
C3	0.043 (3)	0.071 (3)	0.037 (2)	−0.012 (2)	−0.002 (2)	0.002 (2)
C4	0.031 (2)	0.073 (3)	0.050 (3)	0.002 (2)	0.010 (2)	0.019 (2)
C5	0.048 (3)	0.059 (3)	0.051 (3)	0.030 (2)	0.029 (2)	0.020 (2)
C6	0.046 (2)	0.030 (2)	0.041 (2)	−0.0015 (17)	0.0254 (19)	0.0028 (17)
C7	0.054 (3)	0.048 (3)	0.060 (3)	−0.006 (2)	0.032 (2)	0.008 (2)
Mn2	0.0239 (4)	0.0317 (4)	0.0368 (5)	0.0003 (3)	0.0103 (3)	−0.0059 (3)
O3	0.0288 (14)	0.0404 (16)	0.0572 (19)	−0.0048 (11)	0.0104 (13)	−0.0111 (13)
O4	0.0306 (15)	0.0455 (18)	0.068 (2)	−0.0027 (12)	0.0112 (14)	−0.0175 (14)

N3	0.0263 (16)	0.0394 (19)	0.051 (2)	0.0003 (14)	0.0104 (15)	−0.0141 (15)
N4	0.0379 (18)	0.046 (2)	0.0399 (19)	−0.0079 (15)	0.0129 (15)	−0.0059 (15)
C8	0.053 (3)	0.038 (2)	0.072 (3)	0.007 (2)	0.007 (2)	0.009 (2)
C9	0.036 (2)	0.035 (2)	0.078 (3)	0.0042 (18)	0.014 (2)	−0.012 (2)
C10	0.047 (3)	0.064 (3)	0.064 (3)	0.001 (2)	0.031 (2)	−0.022 (2)
C11	0.054 (3)	0.074 (3)	0.053 (3)	−0.007 (2)	0.034 (2)	−0.008 (2)
C12	0.052 (3)	0.048 (3)	0.056 (3)	−0.004 (2)	0.013 (2)	0.010 (2)
C13	0.031 (2)	0.037 (2)	0.043 (2)	−0.0075 (17)	0.0159 (18)	−0.0045 (17)
C14	0.035 (2)	0.045 (3)	0.082 (4)	−0.0107 (19)	0.013 (2)	−0.016 (2)
Cl	0.0691 (8)	0.0525 (7)	0.0457 (6)	0.0054 (6)	0.0145 (6)	0.0030 (5)
O5	0.131 (4)	0.141 (5)	0.128 (5)	−0.054 (4)	0.047 (4)	−0.053 (4)
O6	0.146 (4)	0.147 (4)	0.059 (3)	0.073 (3)	0.042 (3)	0.010 (3)
O7	0.092 (3)	0.142 (4)	0.137 (4)	0.043 (3)	0.062 (3)	0.036 (4)
O8	0.128 (4)	0.089 (3)	0.113 (4)	0.017 (3)	0.038 (3)	0.035 (3)
O9	0.0491 (19)	0.062 (2)	0.0436 (17)	0.0016 (14)	0.0206 (15)	0.0116 (15)

Geometric parameters (Å, °)

Mn1—N1^{i}	2.037 (3)	Mn2—N4	2.045 (3)
Mn1—N1	2.037 (3)	Mn2—O3^{ii}	2.124 (2)
Mn1—N2	2.038 (3)	Mn2—O3	2.124 (2)
Mn1—N2^{i}	2.038 (3)	O3—C13	1.274 (4)
Mn1—O1^{i}	2.122 (2)	O4—C13	1.232 (4)
Mn1—O1	2.122 (2)	N3—C9	1.482 (5)
O1—C6	1.260 (4)	N3—C10	1.497 (6)
O2—C6	1.239 (5)	N3—H3	0.910
N1—C1	1.478 (5)	N4—C12	1.483 (5)
N1—C2	1.485 (5)	N4—C11	1.485 (5)
N1—H1	0.910	N4—H4	0.910
N2—C4	1.463 (5)	C8—C9	1.498 (7)
N2—C5	1.487 (5)	C8—C12^{ii}	1.511 (6)
N2—H2	0.910	C8—H8A	0.970
C1—C5^{i}	1.511 (6)	C8—H8B	0.970
C1—H1A	0.970	C9—H9A	0.970
C1—H1B	0.970	C9—H9B	0.970
C2—C3	1.505 (6)	C10—C11	1.486 (6)
C2—H2A	0.970	C10—H10A	0.970
C2—H2B	0.970	C10—H10B	0.970
C3—C4	1.507 (7)	C11—H11A	0.970
C3—H3A	0.970	C11—H11B	0.970
C3—H3B	0.970	C12—C8^{ii}	1.511 (6)
C4—H4A	0.970	C12—H12A	0.970
C4—H4B	0.970	C12—H12B	0.970
C5—C1^{i}	1.511 (6)	C13—C14	1.490 (5)
C5—H5A	0.970	C14—H14A	0.960
C5—H5B	0.970	C14—H14B	0.960
C6—C7	1.503 (5)	C14—H14C	0.960

C7—H7A	0.960	Cl—O8	1.386 (4)
C7—H7B	0.960	Cl—O5	1.391 (5)
C7—H7C	0.960	Cl—O6	1.395 (5)
Mn2—N3^{ii}	2.023 (3)	Cl—O7	1.462 (4)
Mn2—N3	2.023 (3)	O9—H9WA	0.89
Mn2—N4^{ii}	2.045 (3)	O9—H9WB	0.90
N1^{i}—Mn1—N1	180.00 (18)	N3—Mn2—N4	85.90 (14)
N1^{i}—Mn1—N2	85.98 (13)	N4^{ii}—Mn2—N4	180.0 (2)
N1—Mn1—N2	94.02 (13)	N3^{ii}—Mn2—O3^{ii}	91.82 (11)
N1^{i}—Mn1—N2^{i}	94.02 (13)	N3—Mn2—O3^{ii}	88.18 (11)
N1—Mn1—N2^{i}	85.98 (13)	N4^{ii}—Mn2—O3^{ii}	89.66 (12)
N2—Mn1—N2^{i}	180.00 (12)	N4—Mn2—O3^{ii}	90.34 (12)
N1^{i}—Mn1—O1^{i}	89.66 (12)	N3^{ii}—Mn2—O3	88.18 (11)
N1—Mn1—O1^{i}	90.34 (12)	N3—Mn2—O3	91.82 (11)
N2—Mn1—O1^{i}	87.21 (11)	N4^{ii}—Mn2—O3	90.34 (12)
N2^{i}—Mn1—O1^{i}	92.79 (11)	N4—Mn2—O3	89.66 (12)
N1^{i}—Mn1—O1	90.34 (12)	O3^{ii}—Mn2—O3	180.0
N1—Mn1—O1	89.66 (12)	C13—O3—Mn2	132.5 (2)
N2—Mn1—O1	92.79 (11)	C9—N3—C10	113.8 (3)
N2^{i}—Mn1—O1	87.21 (11)	C9—N3—Mn2	117.2 (3)
O1^{i}—Mn1—O1	180.00 (13)	C10—N3—Mn2	106.2 (2)
C6—O1—Mn1	133.5 (3)	C9—N3—H3	106.3
C1—N1—C2	113.0 (3)	C10—N3—H3	106.3
C1—N1—Mn1	105.8 (2)	Mn2—N3—H3	106.3
C2—N1—Mn1	116.8 (2)	C12—N4—C11	113.2 (3)
C1—N1—H1	106.9	C12—N4—Mn2	116.7 (3)
C2—N1—H1	106.9	C11—N4—Mn2	106.0 (3)
Mn1—N1—H1	106.9	C12—N4—H4	106.8
C4—N2—C5	113.0 (3)	C11—N4—H4	106.8
C4—N2—Mn1	116.8 (2)	Mn2—N4—H4	106.8
C5—N2—Mn1	105.9 (2)	C9—C8—C12^{ii}	114.9 (4)
C4—N2—H2	106.9	C9—C8—H8A	108.5
C5—N2—H2	106.9	C12^{ii}—C8—H8A	108.5
Mn1—N2—H2	106.9	C9—C8—H8B	108.5
N1—C1—C5^{i}	108.3 (3)	C12^{ii}—C8—H8B	108.5
N1—C1—H1A	110.0	H8A—C8—H8B	107.5
C5^{i}—C1—H1A	110.0	N3—C9—C8	112.0 (3)
N1—C1—H1B	110.0	N3—C9—H9A	109.2
C5^{i}—C1—H1B	110.0	C8—C9—H9A	109.2
H1A—C1—H1B	108.4	N3—C9—H9B	109.2
N1—C2—C3	111.9 (3)	C8—C9—H9B	109.2
N1—C2—H2A	109.2	H9A—C9—H9B	107.9
C3—C2—H2A	109.2	C11—C10—N3	108.9 (3)
N1—C2—H2B	109.2	C11—C10—H10A	109.9
C3—C2—H2B	109.2	N3—C10—H10A	109.9

H2A—C2—H2B	107.9	C11—C10—H10B	109.9
C2—C3—C4	115.2 (4)	N3—C10—H10B	109.9
C2—C3—H3A	108.5	H10A—C10—H10B	108.3
C4—C3—H3A	108.5	N4—C11—C10	108.2 (4)
C2—C3—H3B	108.5	N4—C11—H11A	110.1
C4—C3—H3B	108.5	C10—C11—H11A	110.1
H3A—C3—H3B	107.5	N4—C11—H11B	110.1
N2—C4—C3	113.2 (3)	C10—C11—H11B	110.1
N2—C4—H4A	108.9	H11A—C11—H11B	108.4
C3—C4—H4A	108.9	N4—C12—C8^{ii}	112.2 (4)
N2—C4—H4B	108.9	N4—C12—H12A	109.2
C3—C4—H4B	108.9	C8^{ii}—C12—H12A	109.2
H4A—C4—H4B	107.8	N4—C12—H12B	109.2
N2—C5—C1^{i}	107.4 (3)	C8^{ii}—C12—H12B	109.2
N2—C5—H5A	110.2	H12A—C12—H12B	107.9
C1^{i}—C5—H5A	110.2	O4—C13—O3	124.7 (3)
N2—C5—H5B	110.2	O4—C13—C14	119.6 (3)
C1^{i}—C5—H5B	110.2	O3—C13—C14	115.7 (3)
H5A—C5—H5B	108.5	C13—C14—H14A	109.5
O2—C6—O1	124.1 (3)	C13—C14—H14B	109.5
O2—C6—C7	120.0 (3)	H14A—C14—H14B	109.5
O1—C6—C7	115.9 (4)	C13—C14—H14C	109.5
C6—C7—H7A	109.5	H14A—C14—H14C	109.5
C6—C7—H7B	109.5	H14B—C14—H14C	109.5
H7A—C7—H7B	109.5	O8—Cl—O5	111.4 (4)
C6—C7—H7C	109.5	O8—Cl—O6	114.4 (3)
H7A—C7—H7C	109.5	O5—Cl—O6	113.3 (4)
H7B—C7—H7C	109.5	O8—Cl—O7	106.1 (3)
N3^{ii}—Mn2—N3	180.00 (19)	O5—Cl—O7	104.2 (4)
N3^{ii}—Mn2—N4^{ii}	85.90 (14)	O6—Cl—O7	106.5 (3)
N3—Mn2—N4^{ii}	94.10 (14)	H9WA—O9—H9WB	108.9
N3^{ii}—Mn2—N4	94.10 (14)		
N1^{i}—Mn1—O1—C6	102.2 (4)	N3^{ii}—Mn2—O3—C13	−162.3 (4)
N1—Mn1—O1—C6	−77.8 (4)	N3—Mn2—O3—C13	17.7 (4)
N2—Mn1—O1—C6	16.2 (4)	N4^{ii}—Mn2—O3—C13	−76.4 (4)
N2^{i}—Mn1—O1—C6	−163.8 (4)	N4—Mn2—O3—C13	103.6 (4)
N2—Mn1—N1—C1	165.2 (3)	N4^{ii}—Mn2—N3—C9	−38.1 (3)
N2^{i}—Mn1—N1—C1	−14.8 (3)	N4—Mn2—N3—C9	141.9 (3)
O1^{i}—Mn1—N1—C1	77.9 (3)	O3^{ii}—Mn2—N3—C9	51.4 (3)
O1—Mn1—N1—C1	−102.1 (3)	O3—Mn2—N3—C9	−128.6 (3)
N2—Mn1—N1—C2	38.4 (3)	N4^{ii}—Mn2—N3—C10	−166.6 (3)
N2^{i}—Mn1—N1—C2	−141.6 (3)	N4—Mn2—N3—C10	13.4 (3)
O1^{i}—Mn1—N1—C2	−48.8 (3)	O3^{ii}—Mn2—N3—C10	−77.1 (3)
O1—Mn1—N1—C2	131.2 (3)	O3—Mn2—N3—C10	102.9 (3)
N1^{i}—Mn1—N2—C4	142.1 (3)	N3^{ii}—Mn2—N4—C12	−37.6 (3)

N1—Mn1—N2—C4	−37.9 (3)	N3—Mn2—N4—C12	142.4 (3)
O1^{i}—Mn1—N2—C4	52.2 (3)	O3^{ii}—Mn2—N4—C12	−129.4 (3)
O1—Mn1—N2—C4	−127.8 (3)	O3—Mn2—N4—C12	50.6 (3)
N1^{i}—Mn1—N2—C5	15.3 (3)	N3^{ii}—Mn2—N4—C11	−164.7 (3)
N1—Mn1—N2—C5	−164.7 (3)	N3—Mn2—N4—C11	15.3 (3)
O1^{i}—Mn1—N2—C5	−74.5 (3)	O3^{ii}—Mn2—N4—C11	103.5 (3)
O1—Mn1—N2—C5	105.5 (3)	O3—Mn2—N4—C11	−76.5 (3)
C2—N1—C1—C5^{i}	171.3 (3)	C10—N3—C9—C8	−178.8 (3)
Mn1—N1—C1—C5^{i}	42.3 (4)	Mn2—N3—C9—C8	56.4 (4)
C1—N1—C2—C3	−179.1 (4)	C12^{ii}—C8—C9—N3	−70.3 (5)
Mn1—N1—C2—C3	−56.0 (4)	C9—N3—C10—C11	−170.8 (3)
N1—C2—C3—C4	69.2 (5)	Mn2—N3—C10—C11	−40.4 (4)
C5—N2—C4—C3	178.6 (3)	C12—N4—C11—C10	−170.8 (4)
Mn1—N2—C4—C3	55.4 (4)	Mn2—N4—C11—C10	−41.7 (4)
C2—C3—C4—N2	−69.4 (5)	N3—C10—C11—N4	55.9 (5)
C4—N2—C5—C1^{i}	−171.3 (3)	C11—N4—C12—C8^{ii}	178.6 (4)
Mn1—N2—C5—C1^{i}	−42.3 (3)	Mn2—N4—C12—C8^{ii}	55.2 (4)
Mn1—O1—C6—O2	−9.6 (6)	Mn2—O3—C13—O4	−6.9 (6)
Mn1—O1—C6—C7	170.8 (3)	Mn2—O3—C13—C14	174.0 (3)

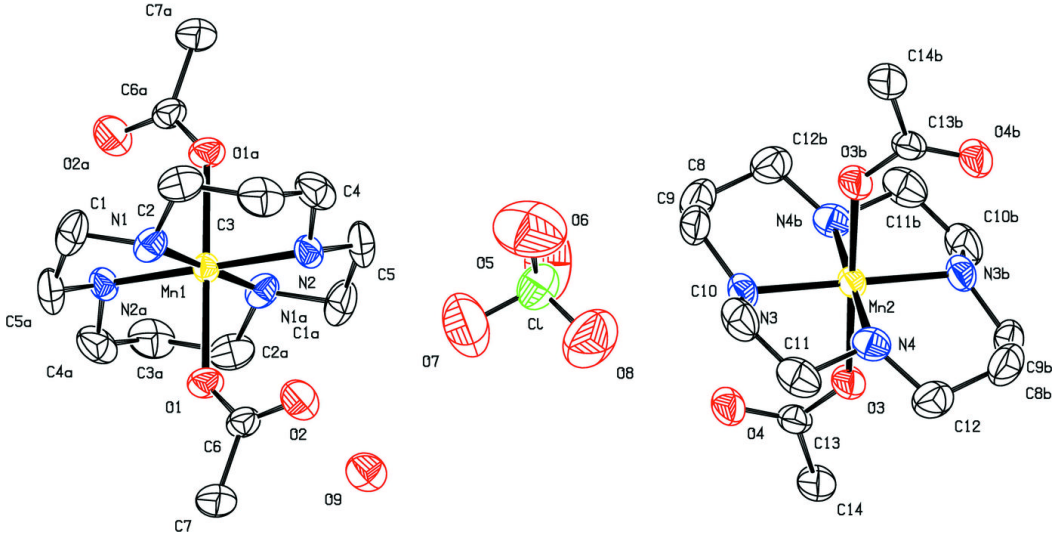
Symmetry codes: (i) −*x*, −*y*+2, −*z*; (ii) −*x*+1, −*y*, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O9^{iii}	0.91	2.04	2.916 (4)	163
N2—H2···O2	0.91	2.03	2.865 (4)	153
N3—H3···O4	0.91	1.98	2.831 (4)	155
N4—H4···O5^{iv}	0.91	2.46	3.283 (7)	151
N4—H4···O8^{iv}	0.91	2.43	3.171 (6)	139
O9—H9WA···O2	0.89	1.92	2.794 (4)	171
O9—H9WB···O4^{v}	0.90	2.07	2.954 (4)	170

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

Fig. 1


C7a
C6a
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O1a
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N1
C2
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C4
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N2
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C2a
C5a
C4a
C3a
O1
C6
O2
C7
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O6
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O3b
C8
C9
N4b
C11b
C10b
N3b
C10
Mn2
N3
C11
N4
C9b
C8b
O3
O4
C12
C13
C14

Fig. 2