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A tetranuclear chlorido-bridged manganese(II) cluster with imidazole ligands

Mukhtar A. Kurawa, Christopher J. Adams* and A. Guy. Orpen

School of Chemistry, University of Bristol, Bristol, BS8 1TS, UK
Correspondence e-mail: C.J.Adams@bris.ac.uk

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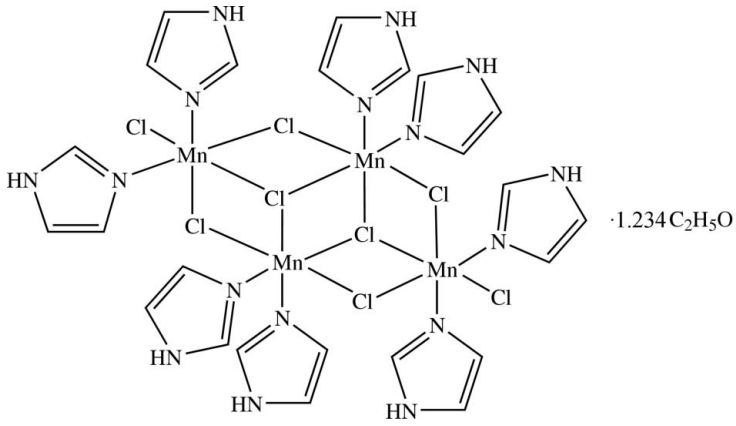
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.009 Å; disorder in main residue; R factor = 0.058; wR factor = 0.143; data-to-parameter ratio = 18.6.

The crystal structure of di-μ_3-chlorido-tetra-μ_2-chlorido-dichloridooctа(imidazole-κN)tetramanganese(II) ethanol 1.234 solvate, $[Mn_4Cl_8(C_3H_4N_2)_8]\cdot1.234C_2H_5O$ or $[Mn_4Cl_8(Him)_8]\cdot1.234$EtOH, where Him is imidazole ($C_3H_4N_2$), is based upon two Mn_4Cl_4 cubes which share one face, and which each lack one manganese vertex, giving a Mn_4Cl_6 unit. This contains two different octahedral coordination environments for the Mn atoms. Mn1 is coordinated by four bridging chlorido ligands and two imidazole N atoms, whereas Mn2 is coordinated by three bridging and one terminal Cl and two imidazole N atoms. The remaining two Mn centres are generated by inversion symmetry. A partial occupancy solvent molecule (ethanol) is present. The crystal structure displays several N—H···Cl and N—H···O hydrogen bonds.

Related literature

Lee *et al.* (2000) reported the structure and magnetic properties of a similar chlorido-bridged tetranuclear cluster of cadmium(II) with 2(2-pyridyl)-4,4′,5,5′-tetramethyl-4,5-dihydro-1*H*-imidazol-1-oxy-3-*N*-oxide (NIToPY). For the structure of $[\{CdCl_2(Him)_2\}_n]$, see: Flook *et al.* (1973).



Experimental

Crystal data

$[Mn_4Cl_8(C_3H_4N_2)_8]\cdot1.234C_2H_5O$
M_r = 1103.45
Triclinic, $P\overline{1}$
a = 8.4763 (16) Å
b = 10.696 (2) Å
c = 12.764 (2) Å
α = 99.206 (3)°
β = 105.706 (4)°
γ = 96.187 (3)°
V = 1085.7 (3) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 1.68 mm^{-1}
T = 173 (2) K
0.35 × 0.10 × 0.10 mm

Data collection

Bruker APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2008*a*)
T_{min} = 0.815, T_{max} = 0.850
11294 measured reflections
4920 independent reflections
3315 reflections with $I > 2\sigma(I)$
R_{int} = 0.048

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.142
S = 1.04
4920 reflections
265 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.77 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N8—H8···O1^{i}	0.88	2.09	2.865 (15)	147
N4—H6A···Cl3^{ii}	0.88	2.49	3.289 (4)	152
N6—H10A···Cl4^{ii}	0.88	2.48	3.247 (4)	146
N2—H2A···Cl4^{iii}	0.88	2.55	3.292 (4)	143

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008*b*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008*b*); molecular graphics: *SHELXTL* (Sheldrick, 2008*b*); 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: SG2263).

References

Bruker (2001). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Flook, R. J., Freeman, H. C., Huq, F. & Rosalky, J. M. (1973). *Acta Cryst.* B**29**, 903–906.
Lee, C.-J., Wei, H.-H., Lee, G.-H. & Wang, Y. (2000). *Inorg. Chem. Commun.* **3**, 690–693.
Sheldrick, G. M. (2008*a*). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008*b*). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2008). E**64**, m1276–m1277 [doi:10.1107/S1600536808029139]

A tetranuclear chlorido-bridged manganese(II) cluster with imidazole ligands

Mukhtar A. Kurawa, Christopher J. Adams and A. Guy. Orpen

S1. Comment

During our exploration of solid state routes for accessing coordination compounds, we ground $CdCl_2$ with imidazole to form polymeric [$\{CdCl_2(Him)_2\}_n$], whose structure was reported by Flook *et al.* (1973). We sought to synthesize the manganese analogue in a similar fashion by grinding $MnCl_2.4H_2O$ with an equimolar amount of imidazole. The resulting polycrystalline powder (of unknown structure) was recrystallized from absolute ethanol to afford a single-crystal. The title compound **I** was obtained, which crystallizes in the triclinic crystal system in the $P\overline{1}$ space group. The molecule is centrosymmetric, containing four manganese atoms in two different coordination environments and crystallizes across an inversion centre so there is a half a molecule in the asymmetric unit. One type of manganese atom is bonded to four bridging (two μ_2-Cl and two μ_3-Cl) chlorine atoms, and two imidazole N atoms, completing an octahedral coordination sphere. The second is type is bonded to three bridging (two μ_2-Cl and one μ_3-Cl) and one terminal chlorine atoms, again with two imidazole N atoms completing octahedral coordination. One of the imidazole ligands shows a carbon-nitrogen disorder, and a partial occupancy solvent molecule (ethanol) is present in the crystal structure, giving rise to N—H···O hydrogen bonds in addition to the N—H···Cl bonds between the chlorine atoms and the imidazole NH donors. The calculated powder pattern of **I** does not match that obtained from the crude material.

S2. Experimental

1 mmol of $MnCl_2.4H_2O$ was ground with 2 mmol of imidazole resulting in the formation of an off-white polycrystalline powder. This was dissolved in absolute alcohol and the resulting solution allowed to evaporate slowly at room temperature, leading to the formation of colourless needle-like crystals.

S3. Refinement

H atoms were positioned geometrically and refined using a riding model, with C—H = 0.95 (2) Å and N—H = 0.88 (2) Å and U_{iso}(H) = 1.2 times U_{eq}(C, N) for the imidazole rings and C—H = 0.99 (2) Å and U_{iso}(H) = 1.5 times U_{eq}(C) for the ethanol molecule.

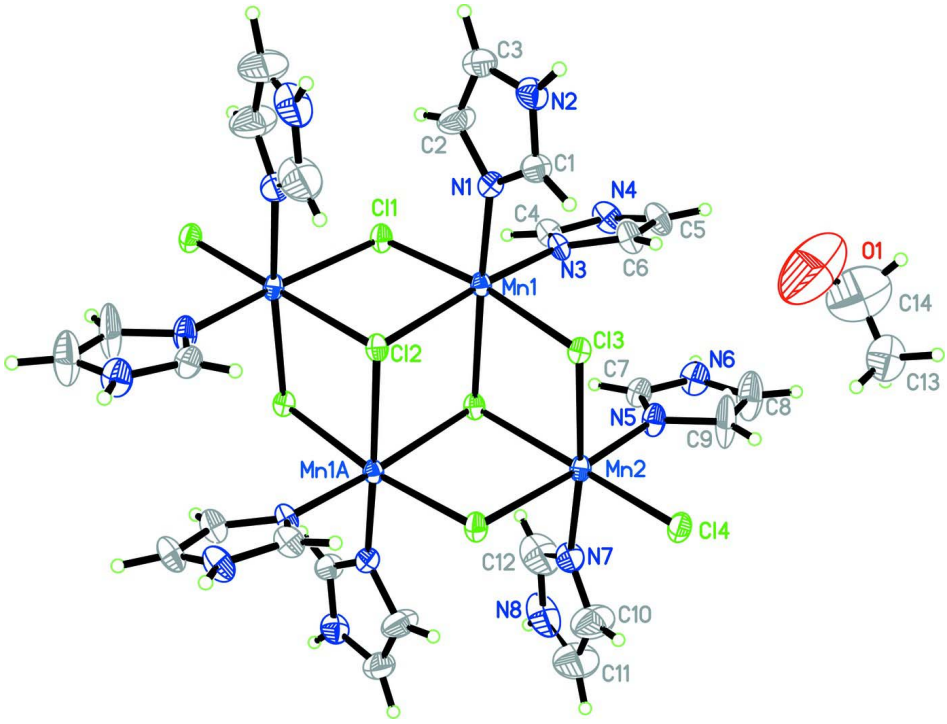

Figure 1

The molecular structure of **I** with atom labels and 50% probability displacement ellipsoids for non-H atoms. [Symmetry code (A):-*x*, -*y*, -*z* + 1]

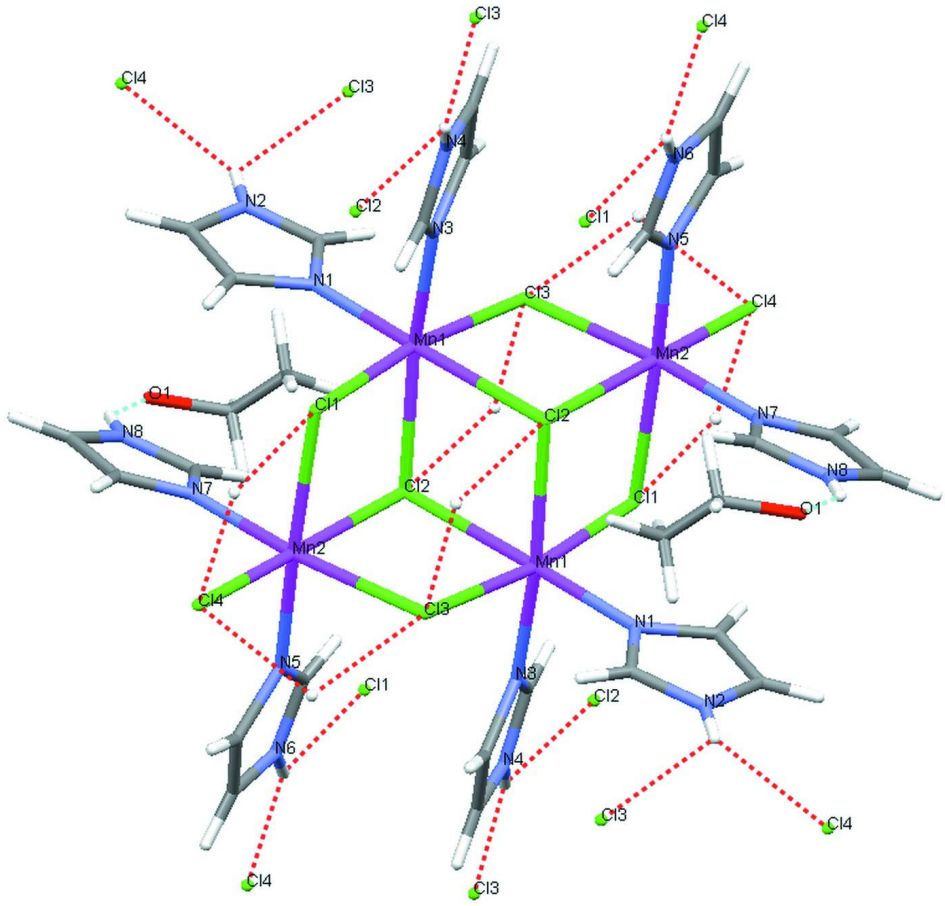

Figure 2

Hydrogen bond environment for **I**, showing only chlorine atoms of the neighbouring cluster.

di-μ_3-chlorido-tetra-μ_2-chlorido-dichloridoocta(imidazole- κN)tetramanganese(II) ethanol 1.234-solvate

Crystal data

$[Mn_4Cl_8(C_3H_4N_2)_8]\cdot 1.234C_2H_5O$
$M_r = 1103.45$
Triclinic, $P\overline{1}$
$a = 8.4763\ (16)$ Å
$b = 10.696\ (2)$ Å
$c = 12.764\ (2)$ Å
$\alpha = 99.206\ (3)°$
$\beta = 105.706\ (4)°$
$\gamma = 96.187\ (3)°$
$V = 1085.7\ (3)$ Å^3
$Z = 1$
$F(000) = 554.8$
$D_x = 1.688$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3784 reflections
$\theta = 2.3–27.5°$
$\mu = 1.68$ mm^{-1}
$T = 173$ K
Needle, colourless
0.35 × 0.10 × 0.10 mm

Data collection

Bruker APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2008a)
$T_{min} = 0.815$, $T_{max} = 0.850$
11294 measured reflections
4920 independent reflections
3315 reflections with $I > 2\sigma(I)$

R_{int} = 0.048
θ_{max} = 27.5°, θ_{min} = 1.7°
h = −11→10
k = −13→13
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.142
S = 1.04
4920 reflections
265 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
$w = 1/[\sigma^2(F_o^2) + (0.055P)^2 + 2.417P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.77 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}	Occ. (<1)
Mn1	0.11612 (8)	0.13627 (6)	0.44334 (5)	0.01743 (18)	
Mn2	0.14342 (8)	0.17089 (6)	0.75623 (5)	0.01930 (19)	
Cl1	0.15783 (14)	−0.04351 (11)	0.30310 (9)	0.0227 (3)	
Cl2	−0.18410 (13)	0.00684 (10)	0.40027 (9)	0.0191 (2)	
Cl3	0.05611 (13)	0.29485 (10)	0.59545 (9)	0.0194 (2)	
Cl4	0.07690 (15)	0.33793 (11)	0.88887 (9)	0.0258 (3)	
N1	0.0440 (5)	0.2621 (4)	0.3243 (3)	0.0242 (9)	
N2	−0.0167 (5)	0.4279 (4)	0.2492 (3)	0.0319 (10)	
H2A	−0.0456	0.5033	0.2418	0.038*	
N3	0.3775 (5)	0.2228 (3)	0.4924 (3)	0.0208 (8)	
N4	0.6483 (5)	0.2509 (4)	0.5285 (4)	0.0313 (10)	
H6A	0.7486	0.2343	0.5312	0.038*	
N5	0.4062 (5)	0.2587 (4)	0.7973 (3)	0.0273 (9)	
N6	0.6744 (5)	0.2843 (4)	0.8230 (4)	0.0339 (10)	
H10A	0.7720	0.2686	0.8176	0.041*	
N7	0.2169 (5)	0.0477 (4)	0.8769 (3)	0.0305 (10)	
C11	0.2455 (11)	−0.0398 (8)	1.0273 (6)	0.093 (4)	0.14 (9)
H11	0.2351	−0.0564	1.0963	0.111*	
N8′	0.2455 (11)	−0.0398 (8)	1.0273 (6)	0.093 (4)	0.86 (9)
C1	−0.0020 (6)	0.3753 (5)	0.3382 (4)	0.0276 (11)	
H1A	−0.0224	0.4151	0.4043	0.033*	
C2	0.0570 (9)	0.2431 (6)	0.2190 (4)	0.0452 (16)	

H4B	0.0877	0.1684	0.1835	0.054*	
C3	0.0209 (8)	0.3439 (5)	0.1723 (5)	0.0419 (15)	
H3B	0.0216	0.3543	0.0999	0.050*	
C4	0.5062 (6)	0.1690 (5)	0.4816 (4)	0.0274 (11)	
H5A	0.4992	0.0830	0.4451	0.033*	
C5	0.6102 (6)	0.3629 (5)	0.5705 (5)	0.0346 (13)	
H7B	0.6861	0.4390	0.6082	0.042*	
C6	0.4431 (6)	0.3469 (5)	0.5491 (4)	0.0280 (11)	
H8A	0.3811	0.4105	0.5697	0.034*	
C7	0.5294 (6)	0.2089 (5)	0.7709 (4)	0.0266 (11)	
H9A	0.5164	0.1296	0.7212	0.032*	
C8	0.6458 (8)	0.3888 (6)	0.8853 (6)	0.0563 (19)	
H11A	0.7259	0.4591	0.9312	0.068*	
C9	0.4800 (8)	0.3732 (6)	0.8693 (6)	0.060 (2)	
H12B	0.4230	0.4321	0.9026	0.072*	
C10	0.1834 (11)	0.0537 (8)	0.9716 (6)	0.071 (2)	
H13A	0.1235	0.1149	0.9989	0.085*	
N8	0.3293 (11)	−0.1058 (8)	0.9569 (8)	0.079 (4)	0.14 (9)
H8	0.3828	−0.1704	0.9700	0.095*	
C11′	0.3293 (11)	−0.1058 (8)	0.9569 (8)	0.079 (4)	0.86 (9)
C12	0.3115 (11)	−0.0513 (9)	0.8673 (8)	0.090 (3)	
H16A	0.3556	−0.0757	0.8075	0.108*	
O1	0.5305 (15)	0.7035 (11)	0.9177 (10)	0.111 (4)	0.617 (10)
C13	0.443 (2)	0.6632 (16)	0.7342 (11)	0.097 (6)	0.617 (10)
H17A	0.3723	0.7299	0.7260	0.145*	0.617 (10)
H18B	0.3765	0.5830	0.7359	0.145*	0.617 (10)
H19C	0.4887	0.6497	0.6713	0.145*	0.617 (10)
C14	0.548 (3)	0.694 (2)	0.8143 (16)	0.128 (8)	0.617 (10)
H20A	0.6028	0.7797	0.8117	0.154*	0.617 (10)
H21B	0.6291	0.6350	0.8098	0.154*	0.617 (10)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0148 (4)	0.0163 (4)	0.0199 (4)	0.0015 (3)	0.0049 (3)	0.0011 (3)
Mn2	0.0151 (4)	0.0200 (4)	0.0188 (4)	0.0021 (3)	0.0003 (3)	0.0009 (3)
Cl1	0.0185 (6)	0.0204 (6)	0.0263 (6)	0.0020 (5)	0.0062 (5)	−0.0021 (4)
Cl2	0.0148 (6)	0.0177 (5)	0.0223 (5)	0.0032 (4)	0.0025 (4)	0.0014 (4)
Cl3	0.0173 (6)	0.0194 (6)	0.0200 (5)	0.0041 (4)	0.0040 (4)	0.0013 (4)
Cl4	0.0244 (6)	0.0255 (6)	0.0237 (6)	0.0007 (5)	0.0069 (5)	−0.0036 (5)
N1	0.026 (2)	0.025 (2)	0.0202 (19)	0.0022 (18)	0.0055 (17)	0.0034 (16)
N2	0.036 (3)	0.024 (2)	0.035 (2)	0.008 (2)	0.006 (2)	0.0108 (19)
N3	0.017 (2)	0.016 (2)	0.030 (2)	0.0015 (16)	0.0058 (17)	0.0050 (16)
N4	0.011 (2)	0.036 (3)	0.046 (3)	0.0024 (18)	0.0052 (19)	0.012 (2)
N5	0.016 (2)	0.028 (2)	0.030 (2)	0.0015 (18)	0.0011 (17)	−0.0047 (18)
N6	0.016 (2)	0.042 (3)	0.038 (2)	0.006 (2)	0.0026 (19)	0.003 (2)
N7	0.031 (3)	0.030 (2)	0.027 (2)	0.006 (2)	−0.0024 (19)	0.0121 (18)
C11	0.119 (7)	0.097 (7)	0.067 (5)	0.025 (6)	0.014 (5)	0.049 (5)

N8′	0.119 (7)	0.097 (7)	0.067 (5)	0.025 (6)	0.014 (5)	0.049 (5)
C1	0.037 (3)	0.021 (3)	0.028 (3)	0.012 (2)	0.013 (2)	0.007 (2)
C2	0.081 (5)	0.034 (3)	0.030 (3)	0.019 (3)	0.028 (3)	0.008 (2)
C3	0.065 (4)	0.035 (3)	0.029 (3)	0.004 (3)	0.019 (3)	0.010 (2)
C4	0.020 (3)	0.027 (3)	0.036 (3)	0.006 (2)	0.007 (2)	0.009 (2)
C5	0.021 (3)	0.031 (3)	0.048 (3)	−0.005 (2)	0.008 (2)	0.008 (2)
C6	0.020 (3)	0.022 (3)	0.040 (3)	0.004 (2)	0.008 (2)	0.004 (2)
C7	0.020 (3)	0.030 (3)	0.026 (2)	0.007 (2)	0.003 (2)	0.002 (2)
C8	0.026 (3)	0.052 (4)	0.069 (4)	−0.004 (3)	0.004 (3)	−0.025 (3)
C9	0.033 (4)	0.045 (4)	0.081 (5)	−0.009 (3)	0.017 (3)	−0.038 (3)
C10	0.103 (7)	0.069 (5)	0.053 (4)	0.032 (5)	0.025 (4)	0.031 (4)
N8	0.076 (6)	0.059 (5)	0.087 (7)	0.011 (4)	−0.011 (5)	0.033 (5)
C11′	0.076 (6)	0.059 (5)	0.087 (7)	0.011 (4)	−0.011 (5)	0.033 (5)
C12	0.075 (6)	0.087 (7)	0.091 (6)	−0.005 (5)	−0.014 (5)	0.050 (6)
O1	0.111 (10)	0.106 (9)	0.117 (9)	0.045 (7)	0.025 (8)	0.015 (7)
C13	0.145 (17)	0.109 (13)	0.043 (8)	0.071 (12)	0.023 (9)	0.009 (8)
C14	0.15 (2)	0.18 (2)	0.097 (14)	0.066 (17)	0.072 (15)	0.041 (15)

Geometric parameters (Å, º)

Mn1—N3	2.186 (4)	N6—H10A	0.8800
Mn1—N1	2.196 (4)	N7—C10	1.308 (8)
Mn1—Cl1	2.5328 (13)	N7—C12	1.405 (10)
Mn1—Cl3	2.5636 (13)	C11—C10	1.387 (10)
Mn1—Cl2	2.6332 (13)	C11—N8	1.436 (11)
Mn1—Cl2^{i}	2.6841 (13)	C11—H11	0.9500
Mn2—N7	2.192 (4)	C1—H1A	0.9500
Mn2—N5	2.208 (4)	C2—C3	1.338 (8)
Mn2—Cl4	2.4784 (14)	C2—H4B	0.9500
Mn2—Cl3	2.6033 (13)	C3—H3B	0.9500
Mn2—Cl1^{i}	2.6121 (14)	C4—H5A	0.9500
Mn2—Cl2^{i}	2.6498 (13)	C5—C6	1.355 (7)
Cl1—Mn2^{i}	2.6121 (14)	C5—H7B	0.9500
Cl2—Mn2^{i}	2.6498 (13)	C6—H8A	0.9500
Cl2—Mn1^{i}	2.6841 (13)	C7—H9A	0.9500
N1—C1	1.311 (6)	C8—C9	1.353 (8)
N1—C2	1.364 (6)	C8—H11A	0.9500
N2—C1	1.329 (6)	C9—H12B	0.9500
N2—C3	1.349 (7)	C10—H13A	0.9500
N2—H2A	0.8800	N8—C12	1.345 (10)
N3—C4	1.316 (6)	N8—H8	0.8800
N3—C6	1.382 (6)	C12—H16A	0.9500
N4—C4	1.338 (6)	O1—C14	1.356 (18)
N4—C5	1.341 (7)	C13—C14	1.13 (2)
N4—H6A	0.8800	C13—H17A	0.9800
N5—C7	1.319 (6)	C13—H18B	0.9800
N5—C9	1.378 (7)	C13—H19C	0.9800
N6—C7	1.332 (6)	C14—H20A	0.9900

N6—C8	1.349 (7)	C14—H21B	0.9900
N3—Mn1—N1	92.56 (14)	C7—N6—H10A	125.9
N3—Mn1—Cl1	92.29 (10)	C8—N6—H10A	125.9
N1—Mn1—Cl1	95.12 (11)	C10—N7—C12	107.3 (6)
N3—Mn1—Cl3	92.37 (10)	C10—N7—Mn2	126.6 (5)
N1—Mn1—Cl3	90.64 (11)	C12—N7—Mn2	126.1 (5)
Cl1—Mn1—Cl3	172.42 (5)	C10—C11—N8	104.1 (7)
N3—Mn1—Cl2	171.84 (10)	C10—C11—H11	128.0
N1—Mn1—Cl2	95.45 (11)	N8—C11—H11	128.0
Cl1—Mn1—Cl2	85.48 (4)	N1—C1—N2	112.2 (4)
Cl3—Mn1—Cl2	89.08 (4)	N1—C1—H1A	123.9
N3—Mn1—Cl2^{i}	90.21 (10)	N2—C1—H1A	123.9
N1—Mn1—Cl2^{i}	174.19 (11)	C3—C2—N1	110.8 (5)
Cl1—Mn1—Cl2^{i}	89.87 (4)	C3—C2—H4B	124.6
Cl3—Mn1—Cl2^{i}	84.14 (4)	N1—C2—H4B	124.6
Cl2—Mn1—Cl2^{i}	81.95 (4)	C2—C3—N2	105.9 (5)
N7—Mn2—N5	89.13 (16)	C2—C3—H3B	127.0
N7—Mn2—Cl4	94.57 (12)	N2—C3—H3B	127.0
N5—Mn2—Cl4	94.27 (11)	N3—C4—N4	111.4 (4)
N7—Mn2—Cl3	173.40 (12)	N3—C4—H5A	124.3
N5—Mn2—Cl3	91.82 (11)	N4—C4—H5A	124.3
Cl4—Mn2—Cl3	91.88 (4)	N4—C5—C6	107.0 (5)
N7—Mn2—Cl1^{i}	88.65 (12)	N4—C5—H7B	126.5
N5—Mn2—Cl1^{i}	173.48 (11)	C6—C5—H7B	126.5
Cl4—Mn2—Cl1^{i}	92.01 (4)	C5—C6—N3	108.8 (5)
Cl3—Mn2—Cl1^{i}	89.69 (4)	C5—C6—H8A	125.6
N7—Mn2—Cl2^{i}	89.40 (12)	N3—C6—H8A	125.6
N5—Mn2—Cl2^{i}	90.27 (11)	N5—C7—N6	111.2 (4)
Cl4—Mn2—Cl2^{i}	174.01 (5)	N5—C7—H9A	124.4
Cl3—Mn2—Cl2^{i}	84.06 (4)	N6—C7—H9A	124.4
Cl1^{i}—Mn2—Cl2^{i}	83.58 (4)	N6—C8—C9	106.0 (5)
Mn1—Cl1—Mn2^{i}	97.01 (4)	N6—C8—H11A	127.0
Mn1—Cl2—Mn2^{i}	93.69 (4)	C9—C8—H11A	127.0
Mn1—Cl2—Mn1^{i}	98.05 (4)	C8—C9—N5	109.6 (5)
Mn2^{i}—Cl2—Mn1^{i}	93.71 (4)	C8—C9—H12B	125.2
Mn1—Cl3—Mn2	97.74 (4)	N5—C9—H12B	125.2
C1—N1—C2	104.0 (4)	N7—C10—C11	112.0 (8)
C1—N1—Mn1	130.2 (3)	N7—C10—H13A	124.0
C2—N1—Mn1	125.4 (4)	C11—C10—H13A	124.0
C1—N2—C3	107.1 (4)	C12—N8—C11	107.9 (8)
C1—N2—H2A	126.4	C12—N8—H8	126.1
C3—N2—H2A	126.4	C11—N8—H8	126.1
C4—N3—C6	105.2 (4)	N8—C12—N7	108.7 (9)
C4—N3—Mn1	128.8 (3)	N8—C12—H16A	125.7
C6—N3—Mn1	125.9 (3)	N7—C12—H16A	125.7
C4—N4—C5	107.7 (4)	C13—C14—O1	125 (2)
C4—N4—H6A	126.2	C13—C14—H20A	106.1

C5—N4—H6A	126.2	O1—C14—H20A	106.1
C7—N5—C9	105.0 (4)	C13—C14—H21B	106.1
C7—N5—Mn2	128.7 (3)	O1—C14—H21B	106.1
C9—N5—Mn2	125.9 (4)	H20A—C14—H21B	106.3
C7—N6—C8	108.2 (5)		

N3—Mn1—Cl1—Mn2^{i}	175.98 (10)	N7—Mn2—N5—C9	−98.3 (5)
N1—Mn1—Cl1—Mn2^{i}	−91.24 (11)	Cl4—Mn2—N5—C9	−3.8 (5)
Cl2—Mn1—Cl1—Mn2^{i}	3.85 (4)	Cl3—Mn2—N5—C9	88.3 (5)
Cl2^{i}—Mn1—Cl1—Mn2^{i}	85.78 (4)	Cl2^{i}—Mn2—N5—C9	172.3 (5)
N1—Mn1—Cl2—Mn2^{i}	90.95 (11)	N5—Mn2—N7—C10	110.9 (6)
Cl1—Mn1—Cl2—Mn2^{i}	−3.77 (4)	Cl4—Mn2—N7—C10	16.7 (6)
Cl3—Mn1—Cl2—Mn2^{i}	−178.49 (4)	Cl1^{i}—Mn2—N7—C10	−75.2 (6)
Cl2^{i}—Mn1—Cl2—Mn2^{i}	−94.28 (4)	Cl2^{i}—Mn2—N7—C10	−158.8 (6)
N1—Mn1—Cl2—Mn1^{i}	−174.77 (11)	N5—Mn2—N7—C12	−68.0 (5)
Cl1—Mn1—Cl2—Mn1^{i}	90.51 (4)	Cl4—Mn2—N7—C12	−162.2 (5)
Cl3—Mn1—Cl2—Mn1^{i}	−84.21 (4)	Cl1^{i}—Mn2—N7—C12	105.9 (5)
Cl2^{i}—Mn1—Cl2—Mn1^{i}	0.0	Cl2^{i}—Mn2—N7—C12	22.3 (5)
N3—Mn1—Cl3—Mn2	−85.49 (10)	C2—N1—C1—N2	−0.6 (6)
N1—Mn1—Cl3—Mn2	−178.08 (11)	Mn1—N1—C1—N2	172.4 (3)
Cl2—Mn1—Cl3—Mn2	86.47 (4)	C3—N2—C1—N1	0.4 (6)
Cl2^{i}—Mn1—Cl3—Mn2	4.47 (4)	C1—N1—C2—C3	0.6 (7)
N5—Mn2—Cl3—Mn1	85.55 (11)	Mn1—N1—C2—C3	−172.9 (4)
Cl4—Mn2—Cl3—Mn1	179.89 (5)	N1—C2—C3—N2	−0.4 (8)
Cl1^{i}—Mn2—Cl3—Mn1	−88.11 (4)	C1—N2—C3—C2	0.0 (7)
Cl2^{i}—Mn2—Cl3—Mn1	−4.53 (4)	C6—N3—C4—N4	0.4 (5)
N3—Mn1—N1—C1	−89.6 (5)	Mn1—N3—C4—N4	−175.7 (3)
Cl1—Mn1—N1—C1	177.8 (4)	C5—N4—C4—N3	−0.6 (6)
Cl3—Mn1—N1—C1	2.8 (4)	C4—N4—C5—C6	0.5 (6)
Cl2—Mn1—N1—C1	91.9 (4)	N4—C5—C6—N3	−0.2 (6)
N3—Mn1—N1—C2	82.0 (5)	C4—N3—C6—C5	−0.1 (5)
Cl1—Mn1—N1—C2	−10.5 (5)	Mn1—N3—C6—C5	176.2 (3)
Cl3—Mn1—N1—C2	174.4 (5)	C9—N5—C7—N6	0.8 (6)
Cl2—Mn1—N1—C2	−96.5 (5)	Mn2—N5—C7—N6	−171.6 (3)
N1—Mn1—N3—C4	−117.3 (4)	C8—N6—C7—N5	−0.7 (6)
Cl1—Mn1—N3—C4	−22.1 (4)	C7—N6—C8—C9	0.3 (8)
Cl3—Mn1—N3—C4	151.9 (4)	N6—C8—C9—N5	0.2 (9)
Cl2^{i}—Mn1—N3—C4	67.8 (4)	C7—N5—C9—C8	−0.6 (8)
N1—Mn1—N3—C6	67.3 (4)	Mn2—N5—C9—C8	172.1 (5)
Cl1—Mn1—N3—C6	162.5 (4)	C12—N7—C10—C11	−2.1 (9)
Cl3—Mn1—N3—C6	−23.4 (4)	Mn2—N7—C10—C11	178.9 (5)
Cl2^{i}—Mn1—N3—C6	−107.6 (4)	N8—C11—C10—N7	1.7 (10)
N7—Mn2—N5—C7	72.7 (4)	C10—C11—N8—C12	−0.6 (10)
Cl4—Mn2—N5—C7	167.2 (4)	C11—N8—C12—N7	−0.6 (9)
Cl3—Mn2—N5—C7	−100.8 (4)	C10—N7—C12—N8	1.6 (9)
Cl2^{i}—Mn2—N5—C7	−16.7 (4)	Mn2—N7—C12—N8	−179.3 (5)

Symmetry code: (i) $-x, -y, -z+1$.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N8—H8···O1^{ii}	0.88	2.09	2.865 (15)	147
N4—H6*A*···Cl3^{iii}	0.88	2.49	3.289 (4)	152
N6—H10*A*···Cl4^{iii}	0.88	2.48	3.247 (4)	146
N2—H2*A*···Cl4^{iv}	0.88	2.55	3.292 (4)	143

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