

Dichlorido(methanol- κ O)[2-(2-pyridyl-methoxy)-1,10-phenanthroline- κ^3 N,N',N'']manganese(II)

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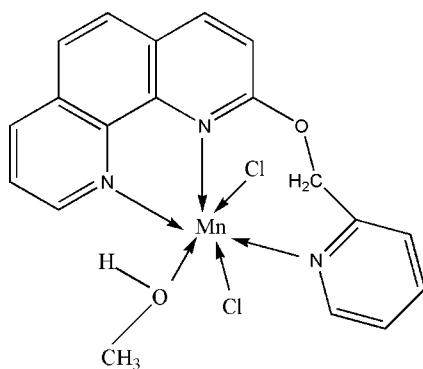
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(C-C) = 0.003$ Å; R factor = 0.037; wR factor = 0.090; data-to-parameter ratio = 16.5.

In the title mononuclear complex, $[MnCl_2(C_{18}H_{13}N_3O)(CH_4O)]$, the Mn^{II} ion assumes a distorted octahedral geometry. There is a $\pi-\pi$ stacking interaction between the phenanthroline ligand and the pyridine ring of a neighboring complex [centroid-to-centroid distance 3.5518 (13) Å]. The crystal structure also contains weak intermolecular O—H···Cl hydrogen bonds that link neighboring complex molecules into a one-dimensional chain along the b axis.

Related literature

For related structures, see: Liu *et al.* (2008); Li *et al.* (2008).



Experimental

Crystal data

| | |
|-------------------------------------|-----------------------------------|
| $[MnCl_2(C_{18}H_{13}N_3O)(CH_4O)]$ | $V = 1861.2$ (5) Å ³ |
| $M_r = 445.20$ | $Z = 4$ |
| Monoclinic, $P2_1/n$ | Mo $K\alpha$ radiation |
| $a = 10.0390$ (16) Å | $\mu = 1.02$ mm ⁻¹ |
| $b = 13.667$ (2) Å | $T = 298$ (2) K |
| $c = 13.583$ (2) Å | $0.38 \times 0.18 \times 0.13$ mm |
| $\beta = 92.874$ (2)° | |

Data collection

| | |
|--|--|
| Bruker SMART APEX CCD diffractometer | 10717 measured reflections |
| Absorption correction: multi-scan (<i>SADABS</i> ; Sheldrick, 2008) | 4048 independent reflections |
| $T_{min} = 0.699$, $T_{max} = 0.879$ | 3278 reflections with $I > 2\sigma(I)$ |
| | $R_{int} = 0.033$ |

Refinement

| | |
|---------------------------------|---|
| $R[F^2 > 2\sigma(F^2)] = 0.036$ | 1 restraint |
| $wR(F^2) = 0.090$ | H-atom parameters constrained |
| $S = 1.01$ | $\Delta\rho_{\text{max}} = 0.28$ e Å ⁻³ |
| 4048 reflections | $\Delta\rho_{\text{min}} = -0.26$ e Å ⁻³ |
| 245 parameters | |

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

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|---------------------------|-------|-------------|-------------|---------------|
| O2—H10···Cl1 ⁱ | 0.80 | 2.39 | 3.1581 (16) | 161 |

Symmetry code: (i) $-x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and local programs.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2150).

References

- Bruker (1997). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Li, H. L. & Liu, Q. S. (2008). *Acta Cryst. E* **64**, m847.
- Liu, Q. S., Liu, L. D. & Shi, J. M. (2008). *Acta Cryst. C* **64**, m58–m60.
- Sheldrick, G. M. (2008). *Acta Cryst. A* **64**, 112–122.

supporting information

Acta Cryst. (2008). E64, m962 [doi:10.1107/S1600536808018631]

Dichlorido(methanol- κO)[2-(2-pyridylmethoxy)-1,10-phenanthroline- $\kappa^3 N,N',N''$]manganese(II)

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S1. Comment

Derivatives of 1,10-phenanthroline play an important role in modern coordination chemistry and many complexes have been reported with different substituent groups (Li *et al.* 2008; Liu *et al.* 2008), but no complex with (pyridyl-2-yl)methoxy as substituent has been published. We report here the crystal structure of the title complex, Fig1.

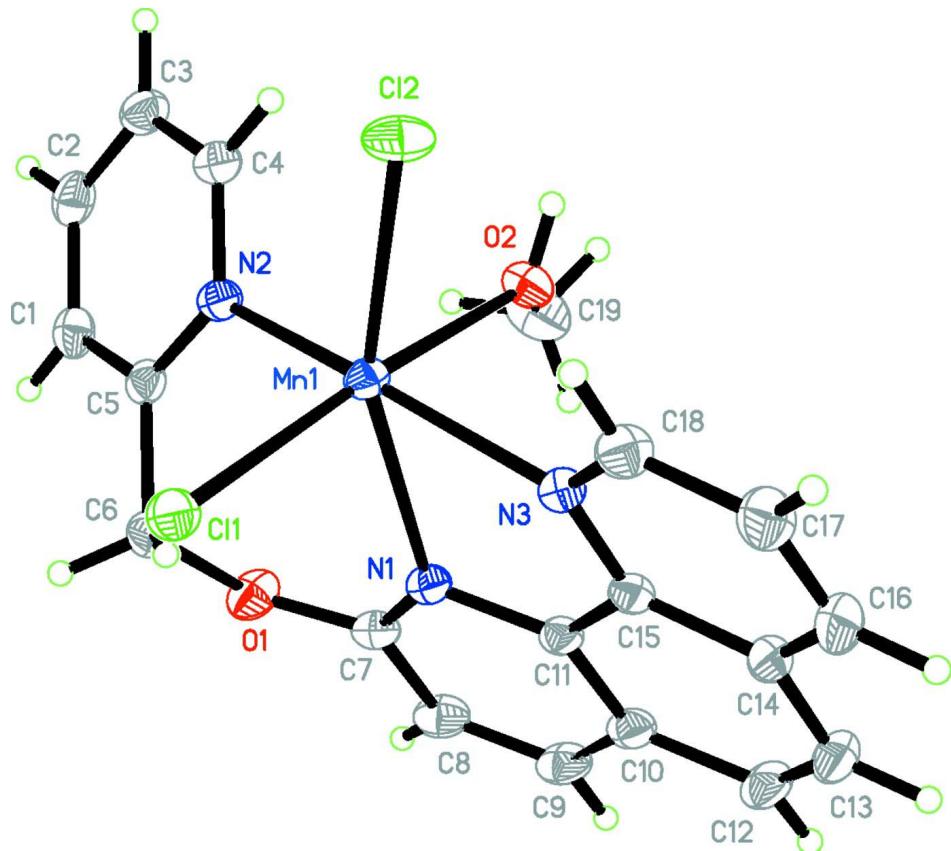
Compound (I) is a monomer, in which the Mn atom adopts a distorted octahedral geometry completed by two N-atom donors from 1,10-phenanthroline, one N atom from pyridine ring, two Cl atom and one O atom from methanol molecule. In neighboring monomers, there is a strong π - π interaction between 1,10-phenanthroline ligand and pyridine ring with a centroid-to-centroid distance of 3.5518 (13) Å. In addition, the crystal structure contains O—H \cdots Cl hydrogen bonds that made the neighboring complexes connect into a one-dimensional chain along *b* axis as shown in Fig. 2.

S2. Experimental

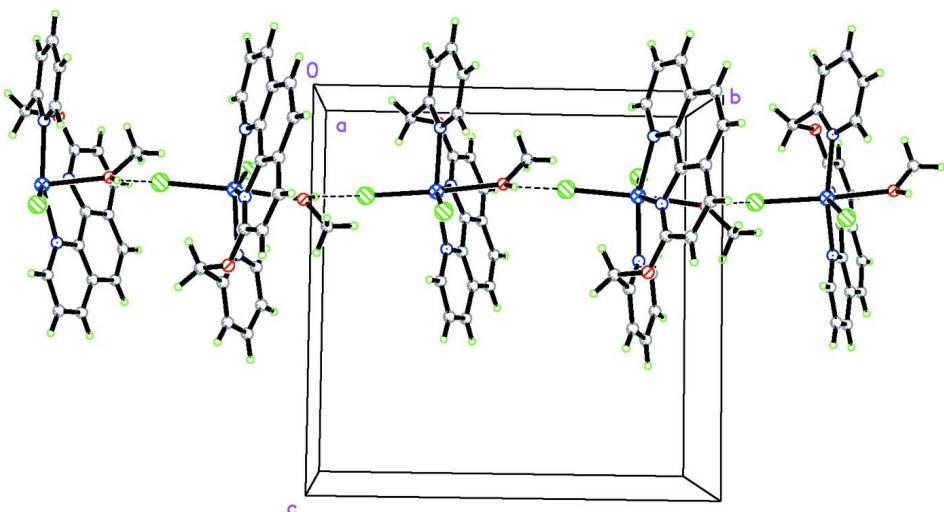
10 ml methanol solution of (2-((pyridin-2-yl)methoxy)-1,10-phenanthroline (0.1200 g, 0.418 mmol) was added into 15 ml methanol solution of MnCl₂.4H₂O (0.0827 g, 0.418 mmol) and the mixture was stirred for a few minutes. The colorless single crystals were obtained after the filtrate had been allowed to stand at room temperature for a week.

S3. Refinement

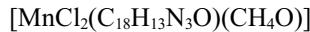
H atoms from the hydroxyl group of methanol was located in a difference Fourier map with O—H = 0.80 Å and refined as riding with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$; Other H atoms were placed in calculated positions with C—H = 0.96 Å for methyl group, C—H = 0.97 Å for methylene group and C—H = 0.93 Å for other H atoms, and refined as riding with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl group and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for other H atoms.

**Figure 1**

Structure of the title complex with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

**Figure 2**

A view of the packing in the crystal structure. Intermolecular Hydrogen bonds as dashed lines.

Dichlorido(methanol- κ O)[2-(2-pyridylmethoxy)-1,10-phenanthroline- κ^3 N,N',N'']manganese(II)*Crystal data*

$M_r = 445.20$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 10.0390 (16) \text{ \AA}$

$b = 13.667 (2) \text{ \AA}$

$c = 13.583 (2) \text{ \AA}$

$\beta = 92.874 (2)^\circ$

$V = 1861.2 (5) \text{ \AA}^3$

$Z = 4$

$F(000) = 908$

$D_x = 1.589 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 3203 reflections

$\theta = 2.5\text{--}25.7^\circ$

$\mu = 1.02 \text{ mm}^{-1}$

$T = 298 \text{ K}$

Block, colorless

$0.38 \times 0.18 \times 0.13 \text{ mm}$

Data collection

Bruker SMART APEX CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan
(SADABS; Sheldrick, 2008)

$T_{\min} = 0.699$, $T_{\max} = 0.879$

10717 measured reflections

4048 independent reflections

3278 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.033$

$\theta_{\max} = 27.0^\circ$, $\theta_{\min} = 2.1^\circ$

$h = -12 \rightarrow 12$

$k = -13 \rightarrow 17$

$l = -15 \rightarrow 17$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.036$

$wR(F^2) = 0.090$

$S = 1.01$

4048 reflections

245 parameters

1 restraint

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

$w = 1/[\sigma^2(F_o^2) + (0.0466P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.29 \text{ e \AA}^{-3}$

$\Delta\rho_{\min} = -0.26 \text{ e \AA}^{-3}$

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 (\AA^2)

| | x | y | z | $U_{\text{iso}}^* / U_{\text{eq}}$ |
|----|------------|--------------|--------------|------------------------------------|
| C1 | 0.1526 (2) | 0.79472 (15) | 0.58696 (17) | 0.0372 (5) |
| H1 | 0.0945 | 0.7746 | 0.6342 | 0.045* |
| C2 | 0.2736 (2) | 0.83666 (16) | 0.61481 (17) | 0.0409 (6) |
| H2 | 0.2988 | 0.8449 | 0.6811 | 0.049* |

| | | | | |
|------|---------------|--------------|---------------|--------------|
| C3 | 0.3567 (2) | 0.86618 (16) | 0.54275 (17) | 0.0399 (5) |
| H3 | 0.4390 | 0.8944 | 0.5596 | 0.048* |
| C4 | 0.3163 (2) | 0.85338 (16) | 0.44621 (17) | 0.0373 (5) |
| H4 | 0.3726 | 0.8743 | 0.3981 | 0.045* |
| C5 | 0.1191 (2) | 0.78311 (14) | 0.48767 (16) | 0.0308 (5) |
| C6 | -0.01179 (19) | 0.73705 (16) | 0.45422 (16) | 0.0355 (5) |
| H6A | -0.0034 | 0.7067 | 0.3903 | 0.043* |
| H6B | -0.0349 | 0.6865 | 0.5005 | 0.043* |
| C7 | -0.1580 (2) | 0.84967 (15) | 0.36073 (17) | 0.0331 (5) |
| C8 | -0.2826 (2) | 0.89726 (17) | 0.36516 (18) | 0.0409 (6) |
| H8 | -0.3257 | 0.9010 | 0.4241 | 0.049* |
| C9 | -0.3375 (2) | 0.93711 (16) | 0.28180 (19) | 0.0420 (6) |
| H9 | -0.4195 | 0.9687 | 0.2829 | 0.050* |
| C10 | -0.2712 (2) | 0.93111 (14) | 0.19319 (18) | 0.0361 (5) |
| C11 | -0.14608 (19) | 0.88455 (14) | 0.19628 (16) | 0.0293 (5) |
| C12 | -0.3287 (2) | 0.96695 (16) | 0.1018 (2) | 0.0461 (6) |
| H12 | -0.4100 | 0.9996 | 0.1010 | 0.055* |
| C13 | -0.2673 (2) | 0.95437 (17) | 0.0167 (2) | 0.0476 (6) |
| H13 | -0.3079 | 0.9764 | -0.0422 | 0.057* |
| C14 | -0.1406 (2) | 0.90753 (15) | 0.01644 (17) | 0.0375 (5) |
| C15 | -0.0780 (2) | 0.87583 (14) | 0.10597 (16) | 0.0309 (5) |
| C16 | -0.0753 (3) | 0.88884 (18) | -0.07041 (18) | 0.0499 (7) |
| H16 | -0.1147 | 0.9070 | -0.1311 | 0.060* |
| C17 | 0.0457 (3) | 0.84415 (18) | -0.06574 (18) | 0.0474 (6) |
| H17 | 0.0891 | 0.8303 | -0.1230 | 0.057* |
| C18 | 0.1037 (2) | 0.81939 (16) | 0.02599 (17) | 0.0395 (5) |
| H18 | 0.1878 | 0.7907 | 0.0286 | 0.047* |
| C19 | 0.0884 (3) | 1.03698 (18) | 0.3451 (2) | 0.0593 (7) |
| H19A | -0.0056 | 1.0389 | 0.3283 | 0.089* |
| H19B | 0.1245 | 1.1019 | 0.3419 | 0.089* |
| H19C | 0.1031 | 1.0117 | 0.4106 | 0.089* |
| C11 | 0.10996 (5) | 0.62442 (4) | 0.24263 (4) | 0.03925 (15) |
| C12 | 0.36834 (5) | 0.82286 (5) | 0.19848 (5) | 0.04570 (17) |
| Mn1 | 0.14453 (3) | 0.80494 (2) | 0.25537 (2) | 0.02795 (11) |
| N1 | -0.08860 (16) | 0.84415 (12) | 0.28120 (13) | 0.0288 (4) |
| N2 | 0.19883 (16) | 0.81198 (12) | 0.41697 (13) | 0.0314 (4) |
| N3 | 0.04509 (16) | 0.83459 (12) | 0.10973 (13) | 0.0304 (4) |
| O1 | -0.11631 (14) | 0.81011 (12) | 0.44771 (12) | 0.0424 (4) |
| O2 | 0.15254 (14) | 0.97535 (10) | 0.27729 (11) | 0.0372 (4) |
| H10 | 0.2227 | 1.0012 | 0.2676 | 0.056* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|----|-------------|-------------|-------------|--------------|--------------|--------------|
| C1 | 0.0430 (13) | 0.0372 (13) | 0.0317 (12) | 0.0068 (10) | 0.0055 (10) | 0.0042 (9) |
| C2 | 0.0529 (15) | 0.0374 (13) | 0.0315 (13) | 0.0060 (11) | -0.0074 (11) | -0.0010 (10) |
| C3 | 0.0361 (12) | 0.0417 (14) | 0.0408 (14) | -0.0015 (10) | -0.0076 (10) | -0.0019 (10) |
| C4 | 0.0295 (11) | 0.0426 (13) | 0.0397 (14) | -0.0022 (9) | -0.0004 (10) | 0.0040 (10) |

| | | | | | | |
|-----|--------------|--------------|--------------|--------------|--------------|---------------|
| C5 | 0.0294 (11) | 0.0290 (11) | 0.0340 (12) | 0.0056 (8) | 0.0021 (9) | 0.0025 (9) |
| C6 | 0.0322 (11) | 0.0375 (12) | 0.0372 (13) | 0.0016 (9) | 0.0063 (9) | 0.0059 (10) |
| C7 | 0.0260 (10) | 0.0348 (12) | 0.0386 (13) | -0.0033 (9) | 0.0006 (9) | -0.0047 (9) |
| C8 | 0.0259 (11) | 0.0466 (14) | 0.0508 (15) | 0.0023 (10) | 0.0083 (10) | -0.0090 (11) |
| C9 | 0.0253 (11) | 0.0357 (13) | 0.0647 (17) | 0.0054 (9) | -0.0015 (11) | -0.0082 (11) |
| C10 | 0.0283 (11) | 0.0253 (11) | 0.0539 (15) | 0.0003 (9) | -0.0058 (10) | -0.0022 (10) |
| C11 | 0.0261 (10) | 0.0225 (10) | 0.0389 (13) | -0.0022 (8) | -0.0037 (9) | -0.0016 (8) |
| C12 | 0.0345 (12) | 0.0364 (13) | 0.0657 (18) | 0.0071 (10) | -0.0153 (12) | 0.0040 (12) |
| C13 | 0.0455 (14) | 0.0414 (14) | 0.0538 (17) | 0.0008 (11) | -0.0184 (12) | 0.0109 (11) |
| C14 | 0.0389 (12) | 0.0306 (11) | 0.0420 (14) | -0.0058 (10) | -0.0092 (10) | 0.0066 (10) |
| C15 | 0.0290 (11) | 0.0253 (11) | 0.0376 (13) | -0.0056 (8) | -0.0043 (9) | 0.0005 (9) |
| C16 | 0.0564 (16) | 0.0565 (16) | 0.0355 (15) | -0.0093 (13) | -0.0107 (12) | 0.0141 (11) |
| C17 | 0.0545 (16) | 0.0569 (16) | 0.0309 (13) | -0.0074 (13) | 0.0024 (11) | 0.0023 (11) |
| C18 | 0.0364 (12) | 0.0465 (14) | 0.0356 (13) | -0.0016 (10) | 0.0030 (10) | -0.0020 (10) |
| C19 | 0.0622 (17) | 0.0401 (15) | 0.078 (2) | -0.0018 (12) | 0.0270 (15) | -0.0142 (13) |
| C11 | 0.0355 (3) | 0.0310 (3) | 0.0508 (4) | 0.0014 (2) | -0.0029 (2) | -0.0018 (2) |
| C12 | 0.0283 (3) | 0.0637 (4) | 0.0460 (4) | -0.0058 (3) | 0.0106 (2) | -0.0148 (3) |
| Mn1 | 0.02338 (17) | 0.03248 (19) | 0.02796 (19) | 0.00096 (12) | 0.00103 (13) | -0.00058 (13) |
| N1 | 0.0243 (9) | 0.0298 (9) | 0.0322 (10) | 0.0001 (7) | -0.0003 (7) | -0.0021 (7) |
| N2 | 0.0266 (9) | 0.0361 (10) | 0.0313 (10) | -0.0010 (7) | 0.0000 (8) | 0.0022 (7) |
| N3 | 0.0273 (9) | 0.0324 (10) | 0.0312 (10) | -0.0013 (7) | -0.0004 (7) | 0.0011 (7) |
| O1 | 0.0303 (8) | 0.0628 (11) | 0.0345 (9) | 0.0104 (7) | 0.0074 (7) | 0.0018 (7) |
| O2 | 0.0357 (8) | 0.0323 (8) | 0.0443 (9) | -0.0042 (6) | 0.0076 (7) | -0.0018 (7) |

Geometric parameters (\AA , $^\circ$)

| | | | |
|---------|-----------|----------|-------------|
| C1—C2 | 1.379 (3) | C12—C13 | 1.347 (3) |
| C1—C5 | 1.382 (3) | C12—H12 | 0.9300 |
| C1—H1 | 0.9300 | C13—C14 | 1.424 (3) |
| C2—C3 | 1.377 (3) | C13—H13 | 0.9300 |
| C2—H2 | 0.9300 | C14—C16 | 1.402 (3) |
| C3—C4 | 1.364 (3) | C14—C15 | 1.409 (3) |
| C3—H3 | 0.9300 | C15—N3 | 1.357 (3) |
| C4—N2 | 1.350 (3) | C16—C17 | 1.358 (3) |
| C4—H4 | 0.9300 | C16—H16 | 0.9300 |
| C5—N2 | 1.340 (3) | C17—C18 | 1.390 (3) |
| C5—C6 | 1.507 (3) | C17—H17 | 0.9300 |
| C6—O1 | 1.448 (2) | C18—N3 | 1.323 (3) |
| C6—H6A | 0.9700 | C18—H18 | 0.9300 |
| C6—H6B | 0.9700 | C19—O2 | 1.425 (3) |
| C7—N1 | 1.316 (3) | C19—H19A | 0.9600 |
| C7—O1 | 1.347 (3) | C19—H19B | 0.9600 |
| C7—C8 | 1.414 (3) | C19—H19C | 0.9600 |
| C8—C9 | 1.349 (3) | C11—Mn1 | 2.4961 (7) |
| C8—H8 | 0.9300 | C12—Mn1 | 2.4248 (7) |
| C9—C10 | 1.407 (3) | Mn1—N3 | 2.2082 (18) |
| C9—H9 | 0.9300 | Mn1—N2 | 2.2370 (18) |
| C10—C11 | 1.407 (3) | Mn1—O2 | 2.3487 (14) |

| | | | |
|-------------|-------------|---------------|-------------|
| C10—C12 | 1.430 (3) | Mn1—N1 | 2.4434 (17) |
| C11—N1 | 1.379 (3) | O2—H10 | 0.8048 |
| C11—C15 | 1.439 (3) | | |
| | | | |
| C2—C1—C5 | 118.9 (2) | N3—C15—C11 | 118.23 (18) |
| C2—C1—H1 | 120.6 | C14—C15—C11 | 119.99 (19) |
| C5—C1—H1 | 120.6 | C17—C16—C14 | 119.8 (2) |
| C3—C2—C1 | 118.9 (2) | C17—C16—H16 | 120.1 |
| C3—C2—H2 | 120.6 | C14—C16—H16 | 120.1 |
| C1—C2—H2 | 120.6 | C16—C17—C18 | 119.0 (2) |
| C4—C3—C2 | 119.0 (2) | C16—C17—H17 | 120.5 |
| C4—C3—H3 | 120.5 | C18—C17—H17 | 120.5 |
| C2—C3—H3 | 120.5 | N3—C18—C17 | 123.2 (2) |
| N2—C4—C3 | 123.3 (2) | N3—C18—H18 | 118.4 |
| N2—C4—H4 | 118.3 | C17—C18—H18 | 118.4 |
| C3—C4—H4 | 118.3 | O2—C19—H19A | 109.5 |
| N2—C5—C1 | 122.74 (19) | O2—C19—H19B | 109.5 |
| N2—C5—C6 | 116.75 (19) | H19A—C19—H19B | 109.5 |
| C1—C5—C6 | 120.5 (2) | O2—C19—H19C | 109.5 |
| O1—C6—C5 | 110.41 (17) | H19A—C19—H19C | 109.5 |
| O1—C6—H6A | 109.6 | H19B—C19—H19C | 109.5 |
| C5—C6—H6A | 109.6 | N3—Mn1—N2 | 161.46 (6) |
| O1—C6—H6B | 109.6 | N3—Mn1—O2 | 86.71 (6) |
| C5—C6—H6B | 109.6 | N2—Mn1—O2 | 80.09 (6) |
| H6A—C6—H6B | 108.1 | N3—Mn1—Cl2 | 94.62 (5) |
| N1—C7—O1 | 122.89 (18) | N2—Mn1—Cl2 | 97.14 (5) |
| N1—C7—C8 | 124.5 (2) | O2—Mn1—Cl2 | 85.06 (4) |
| O1—C7—C8 | 112.6 (2) | N3—Mn1—N1 | 72.25 (6) |
| C9—C8—C7 | 118.4 (2) | N2—Mn1—N1 | 92.16 (6) |
| C9—C8—H8 | 120.8 | O2—Mn1—N1 | 77.95 (5) |
| C7—C8—H8 | 120.8 | Cl2—Mn1—N1 | 158.93 (5) |
| C8—C9—C10 | 120.2 (2) | N3—Mn1—Cl1 | 93.68 (5) |
| C8—C9—H9 | 119.9 | N2—Mn1—Cl1 | 97.86 (5) |
| C10—C9—H9 | 119.9 | O2—Mn1—Cl1 | 173.00 (4) |
| C11—C10—C9 | 117.5 (2) | Cl2—Mn1—Cl1 | 101.86 (2) |
| C11—C10—C12 | 120.1 (2) | N1—Mn1—Cl1 | 95.50 (4) |
| C9—C10—C12 | 122.4 (2) | C7—N1—Cl1 | 116.55 (17) |
| N1—C11—C10 | 122.8 (2) | C7—N1—Mn1 | 132.87 (14) |
| N1—C11—C15 | 118.89 (17) | C11—N1—Mn1 | 109.35 (13) |
| C10—C11—C15 | 118.28 (19) | C5—N2—C4 | 117.19 (19) |
| C13—C12—C10 | 121.3 (2) | C5—N2—Mn1 | 124.45 (13) |
| C13—C12—H12 | 119.4 | C4—N2—Mn1 | 118.23 (14) |
| C10—C12—H12 | 119.4 | C18—N3—C15 | 118.45 (19) |
| C12—C13—C14 | 120.5 (2) | C18—N3—Mn1 | 122.74 (14) |
| C12—C13—H13 | 119.8 | C15—N3—Mn1 | 118.68 (14) |
| C14—C13—H13 | 119.8 | C7—O1—C6 | 121.52 (17) |
| C16—C14—C15 | 117.6 (2) | C19—O2—Mn1 | 130.86 (14) |
| C16—C14—C13 | 122.7 (2) | C19—O2—H10 | 105.9 |

| | | | |
|-----------------|--------------|----------------|--------------|
| C15—C14—C13 | 119.7 (2) | Mn1—O2—H10 | 116.0 |
| N3—C15—C14 | 121.8 (2) | | |
| C5—C1—C2—C3 | 0.5 (3) | C11—Mn1—N1—C7 | 87.71 (18) |
| C1—C2—C3—C4 | 0.3 (3) | N3—Mn1—N1—C11 | -13.64 (12) |
| C2—C3—C4—N2 | -0.8 (3) | N2—Mn1—N1—C11 | 156.13 (12) |
| C2—C1—C5—N2 | -0.8 (3) | O2—Mn1—N1—C11 | 76.75 (12) |
| C2—C1—C5—C6 | 179.61 (19) | Cl2—Mn1—N1—C11 | 39.8 (2) |
| N2—C5—C6—O1 | -93.6 (2) | Cl1—Mn1—N1—C11 | -105.76 (12) |
| C1—C5—C6—O1 | 86.0 (2) | C1—C5—N2—C4 | 0.4 (3) |
| N1—C7—C8—C9 | 2.4 (3) | C6—C5—N2—C4 | 179.96 (18) |
| O1—C7—C8—C9 | -177.8 (2) | C1—C5—N2—Mn1 | -175.49 (14) |
| C7—C8—C9—C10 | -0.1 (3) | C6—C5—N2—Mn1 | 4.1 (2) |
| C8—C9—C10—C11 | -1.4 (3) | C3—C4—N2—C5 | 0.4 (3) |
| C8—C9—C10—C12 | 176.2 (2) | C3—C4—N2—Mn1 | 176.55 (17) |
| C9—C10—C11—N1 | 1.0 (3) | N3—Mn1—N2—C5 | 67.7 (3) |
| C12—C10—C11—N1 | -176.65 (18) | O2—Mn1—N2—C5 | 112.92 (16) |
| C9—C10—C11—C15 | 178.68 (18) | Cl2—Mn1—N2—C5 | -163.39 (15) |
| C12—C10—C11—C15 | 1.0 (3) | N1—Mn1—N2—C5 | 35.55 (16) |
| C11—C10—C12—C13 | 2.2 (3) | Cl1—Mn1—N2—C5 | -60.30 (16) |
| C9—C10—C12—C13 | -175.4 (2) | N3—Mn1—N2—C4 | -108.1 (2) |
| C10—C12—C13—C14 | -2.1 (3) | O2—Mn1—N2—C4 | -62.89 (15) |
| C12—C13—C14—C16 | 177.1 (2) | Cl2—Mn1—N2—C4 | 20.79 (15) |
| C12—C13—C14—C15 | -1.2 (3) | N1—Mn1—N2—C4 | -140.26 (15) |
| C16—C14—C15—N3 | 4.4 (3) | Cl1—Mn1—N2—C4 | 123.88 (15) |
| C13—C14—C15—N3 | -177.20 (19) | C17—C18—N3—C15 | 0.4 (3) |
| C16—C14—C15—C11 | -174.03 (19) | C17—C18—N3—Mn1 | -175.35 (17) |
| C13—C14—C15—C11 | 4.4 (3) | C14—C15—N3—C18 | -3.7 (3) |
| N1—C11—C15—N3 | -4.9 (3) | C11—C15—N3—C18 | 174.77 (18) |
| C10—C11—C15—N3 | 177.29 (17) | C14—C15—N3—Mn1 | 172.26 (14) |
| N1—C11—C15—C14 | 173.53 (17) | C11—C15—N3—Mn1 | -9.3 (2) |
| C10—C11—C15—C14 | -4.2 (3) | N2—Mn1—N3—C18 | 154.10 (19) |
| C15—C14—C16—C17 | -1.8 (3) | O2—Mn1—N3—C18 | 109.61 (17) |
| C13—C14—C16—C17 | 179.8 (2) | Cl2—Mn1—N3—C18 | 24.84 (16) |
| C14—C16—C17—C18 | -1.2 (4) | N1—Mn1—N3—C18 | -172.00 (18) |
| C16—C17—C18—N3 | 2.0 (4) | Cl1—Mn1—N3—C18 | -77.39 (16) |
| O1—C7—N1—C11 | 177.43 (18) | N2—Mn1—N3—C15 | -21.6 (3) |
| C8—C7—N1—C11 | -2.8 (3) | O2—Mn1—N3—C15 | -66.13 (14) |
| O1—C7—N1—Mn1 | -16.8 (3) | Cl2—Mn1—N3—C15 | -150.90 (14) |
| C8—C7—N1—Mn1 | 162.96 (16) | N1—Mn1—N3—C15 | 12.26 (13) |
| C10—C11—N1—C7 | 1.1 (3) | Cl1—Mn1—N3—C15 | 106.87 (14) |
| C15—C11—N1—C7 | -176.61 (17) | N1—C7—O1—C6 | -16.9 (3) |
| C10—C11—N1—Mn1 | -167.94 (15) | C8—C7—O1—C6 | 163.28 (18) |
| C15—C11—N1—Mn1 | 14.4 (2) | C5—C6—O1—C7 | 100.3 (2) |
| N3—Mn1—N1—C7 | 179.82 (19) | N3—Mn1—O2—C19 | 114.2 (2) |
| N2—Mn1—N1—C7 | -10.41 (18) | N2—Mn1—O2—C19 | -52.8 (2) |
| O2—Mn1—N1—C7 | -89.79 (18) | Cl2—Mn1—O2—C19 | -150.9 (2) |
| Cl2—Mn1—N1—C7 | -126.75 (17) | N1—Mn1—O2—C19 | 41.6 (2) |

Hydrogen-bond geometry (Å, °)

| <i>D—H···A</i> | <i>D—H</i> | <i>H···A</i> | <i>D···A</i> | <i>D—H···A</i> |
|---------------------------|------------|--------------|--------------|----------------|
| O2—H10···Cl1 ⁱ | 0.80 | 2.39 | 3.1581 (16) | 161 |

Symmetry code: (i) $-x+1/2, y+1/2, -z+1/2$.