Acta Crystallographica Section E
**Structure Reports**
**Online**
ISSN 1600-5368

# *cis*-Dichloridobis(5,5′-dimethyl-2,2′-bipyridine)manganese(II) 2.5-hydrate

**Lívia Batista Lopes, Charlane Cimini Corrêa and Renata Diniz***

Núcleo de Espectroscopia e Estrutura Molecular (NEEM), Department of Chemistry - Federal University of Juiz de Fora - Minas Gerais, 36036-900, Brazil
Correspondence e-mail: renata.diniz@ufjf.edu.br

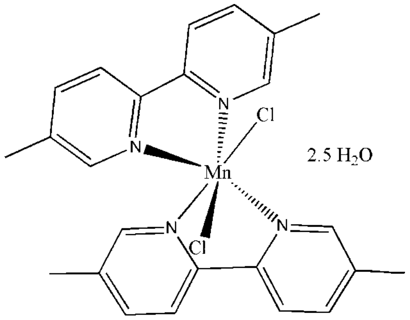
Received 4 May 2011; accepted 6 June 2011

Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.004 Å; disorder in solvent or counterion; $R$ factor = 0.043; $wR$ factor = 0.150; data-to-parameter ratio = 21.4.

The metal site in the title compound $[MnCl_2(C_{12}H_{12}N_2)_2]\cdot 2.5H_2O$ has a distorted octahedral geometry, coordinated by four N atoms of two 5,5′-dimethyl-2,2′-dipyridine ligands and two Cl atoms. Two and a half water molecules of hydration per complex unit are observed in the crystal structure. The compounds extend along the $c$ axis with O—H···Cl, O—H···O, C—H···Cl and C—H···O hydrogen bonds and $\pi$–$\pi$ interactions [centroid-centroid distance = 3.70 (2) Å] contributing substantially to the crystal packing. The Mn and one of the water O atoms, the latter being half-occupied, are located on special positions, in this case a rotation axis of order 2.

## Related literature

For the structures and applications of bipyridine and analogous ligands, see: Hazell (2004); Bakir *et al.* (1992); Cordes *et al.* (1982); Hung-Low *et al.* (2009). For the structure and applications of 5,5′-dimethyl-2,2′-dipyridine, see: Marandi *et al.* (2009); van Albada *et al.* (2005). For weak intermolecular interactions, see: Calhorda (2000); Desiraju (1996); Janiak (2000).



## Experimental

### *Crystal data*

| | |
|---|---|
| $[MnCl_2(C_{12}H_{12}N_2)_2]\cdot 2.5H_2O$ | $V$ = 2670.6 (2) Å$^3$ |
| $M_r$ = 539.35 | $Z$ = 4 |
| Monoclinic, $C2/c$ | Mo $K\alpha$ radiation |
| $a$ = 18.6703 (9) Å | $\mu$ = 0.72 mm$^{-1}$ |
| $b$ = 14.0598 (4) Å | $T$ = 293 K |
| $c$ = 12.0536 (7) Å | 0.47 × 0.35 × 0.34 mm |
| $\beta$ = 122.430 (7)° | |

### *Data collection*

| | |
|---|---|
| Oxford Diffraction Xcalibur Atlas Gemini ultra diffractometer | 11860 measured reflections |
| Absorption correction: analytical [*CrysAlis PRO* (Oxford Diffraction, 2008) based on expressions derived by Clark & Reid (1995)] | 3317 independent reflections |
| $T_{min}$ = 0.470, $T_{max}$ = 0.697 | 2499 reflections with $I > 2\sigma(I)$ |
| | $R_{int}$ = 0.025 |

### *Refinement*

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)]$ = 0.043 | 155 parameters |
| $wR(F^2)$ = 0.150 | H-atom parameters constrained |
| $S$ = 1.09 | $\Delta\rho_{max}$ = 0.72 e Å$^{-3}$ |
| 3317 reflections | $\Delta\rho_{min}$ = −0.31 e Å$^{-3}$ |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1$A$···Cl1 | 0.84 | 2.42 | 3.243 (3) | 168 |
| O1—H1$B$···Cl1$^i$ | 0.81 | 2.73 | 3.358 (4) | 136 |
| O2—H2$A$···O1 | 0.86 | 2.16 | 2.951 (6) | 153 |
| C3—H3···O1$^{ii}$ | 0.93 | 2.49 | 3.257 (5) | 140 |
| C6—H6$A$···Cl1$^i$ | 0.96 | 2.79 | 3.717 (4) | 162 |

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

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2008); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *PLATON* (Spek, 2009).

The authors thank CNPq, CAPES and FAPEMIG (Brazilian agencies) for financial support, and LabCri (Federal University of Minas Gerais) for measuring the X-ray diffraction data.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IM2285).

## References

Albada, G. A. van, Mutikainen, I., Turpeinen, U. & Reedijk, J. (2005). *Acta Cryst.* E**61**, m1411–m1412.
Bakir, M., Paulson, S., Goodson, P. & Sullivan, B. P. (1992). *Inorg. Chem.* **31**, 1127–1129.
Calhorda, M. J. (2000). *Chem. Commun.* pp. 801–809.
Clark, R. C. & Reid, J. S. (1995). *Acta Cryst.* A**51**, 887–897.
Cordes, A. W., Durham, B., Swepston, P. N., Pennington, W. T., Condren, S. M., Jensen, R. & Walsh, J. L. (1982). *J. Coord. Chem.* **11**, 251–260.
Desiraju, G. R. (1996). *Acc. Chem. Res.* **29**, 441–449.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.

Hazell, A. (2004). *Polyhedron*, **23**, 2081–2083.

Hung-Low, F., Renz, A. & Klausmeyer, K. K. (2009). *Polyhedron*, **28**, 407–415.

Janiak, C. (2000). *J. Chem. Soc. Dalton Trans.* pp. 3885–3896.

Macrae, C. F., Edgington, P. R., McCabe, P., Pidcock, E., Shields, G. P., Taylor, R., Towler, M. & van de Streek, J. (2006). *J. Appl. Cryst.* **39**, 453–457.

Marandi, F., Pantenburg, I. & Meyer, G. (2009). *Z. Anorg. Allg. Chem.* **635**, 2558–2562.

Oxford Diffraction (2008). *CrysAlis PRO*. Oxford Diffraction Ltd, Yarnton, England.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

*Acta Cryst.* (2011). E**67**, m906–m907 Lopes *et al.* • $[MnCl_2(C_{12}H_{12}N_2)_2]_2\cdot 5H_2O$ **m907**

# supporting information

*Acta Cryst.* (2011). E**67**, m906–m907    [doi:10.1107/S1600536811021805]

## *cis*-Dichloridobis(5,5′-dimethyl-2,2′-bipyridine)manganese(II) 2.5-hydrate

**Lívia Batista Lopes, Charlane Cimini Corrêa and Renata Diniz**

### S1. Comment

Bipyridine and analogous ligands are commonly used in the formation of different complexes with a general variety of transition metals (Hazell, 2004; Bakir *et al.*, 1992; Cordes *et al.*,1982; Hung-Low *et al.*,2009;). The ligand 5,5′-Dimethyl-2,2′-dipyridine (abbreviated as dmdpy) acts as a chelator and usually gives rise to monomeric compounds (Marandi *et al.*, 2009). Only a limited number of X-ray crystal structures with the ligand dmdpy has been published (van Albada *et al.*, 2005). In this study we used the ligand 5,5′-dimethyl-2,2′-dipyridine and manganese chloride tetrahydrate. This mixture resulted in the compound $[Mn(C_{12}H_{12}N_2)_2Cl_2] \times 2.5\ H_2O$ (Scheme 1).

The molecular structure of the complex unit of the titlecompound $[Mn(C_{12}H_{12}N_2)_2Cl_2] \times 2.5\ H_2O$ is shown in Figure 1. The metal site is coordinated by four nitrogen atoms N1, N2, $N1^i$ and $N2^i$ of the ligand dmdpy and two chlorides Cl1 and $Cl1^i$ adopting a distorted octahedral geometry as evidenced by the Mn—N1 distances (2.3111 (19) Å), Mn—N2 (2.245 (2) Å) and Mn—Cl1 (2.4702 (6) Å). The Mn atom is located in a special position, which in this case is a rotation axis of order 2.

The compound crystallizes in the monoclinic system and its unit cell is shown in Figure 2. The compound $[Mn(C_{12}H_{12}N_2)_2Cl_2] \times 2.5\ H_2O$ is a complex that stretches along the crystallographic *c* axis with the molecular entities being interconnected by weak hydrogen bonds (Desiraju, 1996; Calhorda, 2000) shown in Figure 2. These hydrogen bonds are formed by the interaction between oxygen atoms of water molecules O1 and O2 and the chlorine atom Cl1 which is coordinated to the metal. The distances O1—O2 and O1—Cl1 charge 2.951 (6) Å and 3.243 (3) Å, respectively. $\pi$-$\pi$ interactions between aromatic rings of the nitrogen ligand dmdpy are also shown in Figure 2. These interactions contribute substantially to the crystal packing (Janiak, 2000). In this compound the centroid-centroid distance is 3.70 (2) Å, and there was a substantial overlap between the aromatic rings of the ligand dmdpy, being centroid-plane distance of 3.45 (1)Å and the horizontal displacement of 1.37 (2) Å.

### S2. Experimental

All chemicals were obtained commercially and used without further purification. The complex was synthesized by mixing of 0.38 mmol of dmdpy dissolved in ethanol and 0.38 mmol of $MnCl_2 \times 4\ H_2O$ dissolved in water. The mixture was placed under agitation for 40 h. After a few weeks, yellow single crystals suitable for the analysis of X-ray diffraction were obtained (yield: 39%).

### S3. Refinement

H atoms were positioned geometrically and refined using the riding model approximation with C—H = 0.95 Å, and $U_{iso}(H)$ was refined in group. H atoms of water molecule were located from electron density map, fixed in these positions and assigned the same isotropic displacement parameters for all H atoms.

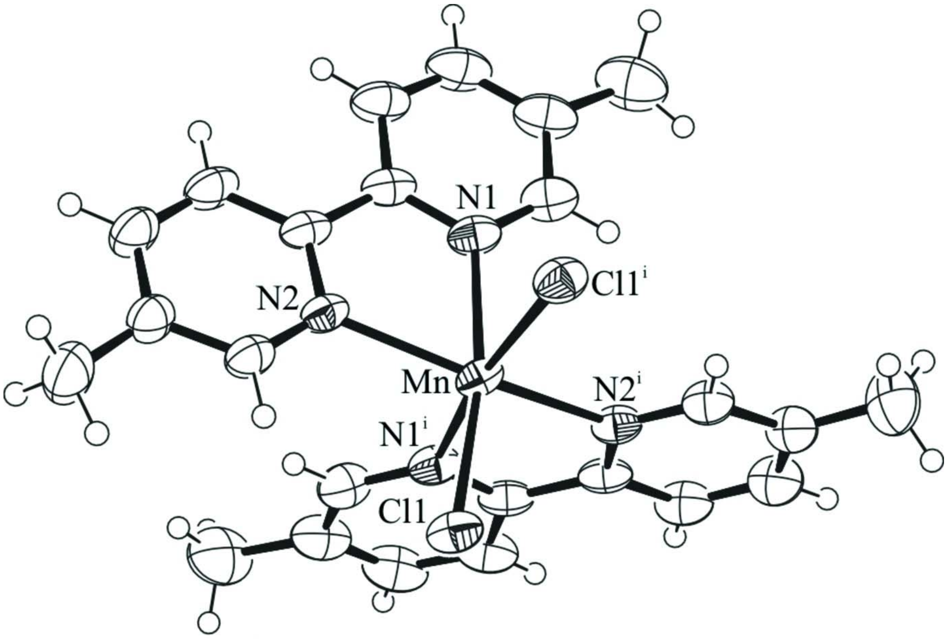


**Figure 1**

Molecular structure of the complex unit of the title compound [$Mn(C_{12}H_{12}N_2)_2Cl_2$] × 2.5 $H_2O$. Water molecules were omitted for better visualization. Symmetry code: i (1 - *x*, *y*, 1/2 - *z*).

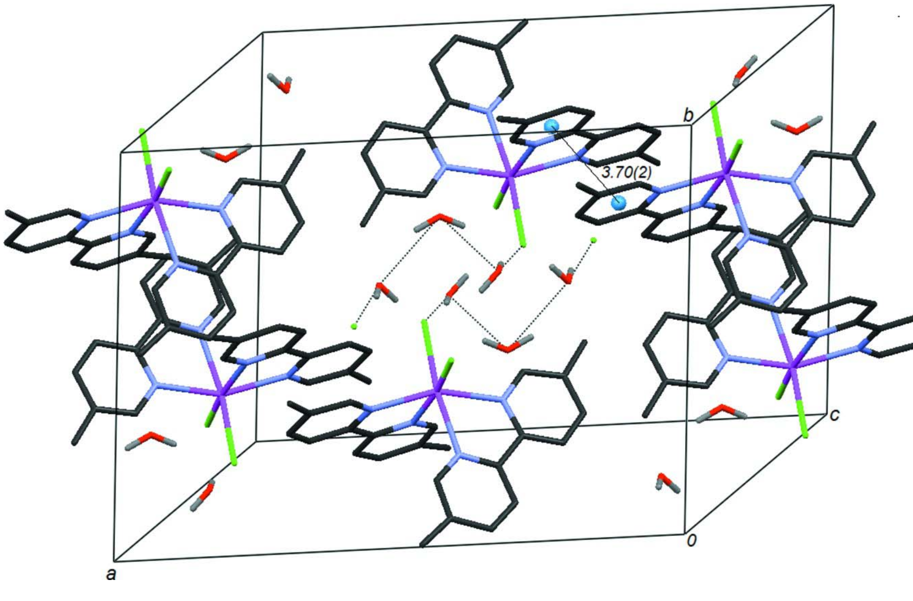


**Figure 2**

Unit cell of the compound [$Mn(C_{12}H_{12}N_2)_2Cl_2$] × 2.5 $H_2O$ ($z = 4$), hydrogen bonds chain extending along the *c* axis and *π*-*π* interactions between the rings aromatic ligand dmdpy are depicted as dashed lines.

## *cis*-Dichloridobis(5,5′-dimethyl-2,2′-bipyridine)manganese(II) 2.5-hydrate

### *Crystal data*

$[MnCl_2(C_{12}H_{12}N_2)_2]\cdot 2.5H_2O$
$M_r = 539.35$
Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a = 18.6703 (9)$ Å
$b = 14.0598 (4)$ Å
$c = 12.0536 (7)$ Å
$\beta = 122.430 (7)°$
$V = 2670.6 (2)$ Å$^3$
$Z = 4$

$F(000) = 1120$
$D_x = 1.341$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6304 reflections
$\theta = 2.9–29.4°$
$\mu = 0.72$ mm$^{-1}$
$T = 293$ K
Prismatic, yellow
0.47 × 0.35 × 0.34 mm

### *Data collection*

Oxford Diffraction Xcalibur Atlas Gemini ultra diffractometer
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 10.4186 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: analytical [*CrysAlis PRO* (Oxford Diffraction, 2008) based on expressions derived by Clark & Reid (1995)]

$T_{min} = 0.470$, $T_{max} = 0.697$
11860 measured reflections
3317 independent reflections
2499 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 29.4°$, $\theta_{min} = 2.9°$
$h = -25 \rightarrow 23$
$k = -14 \rightarrow 18$
$l = -16 \rightarrow 16$

### *Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.150$
$S = 1.09$
3317 reflections
155 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.094P)^2 + 0.4813P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.72$ e Å$^{-3}$
$\Delta\rho_{min} = -0.31$ e Å$^{-3}$
Extinction correction: *SHELXL*
Absolute structure: no

### *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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Mn | 0.5000 | 0.31073 (3) | 0.2500 | 0.03326 (18) | |
| Cl1 | 0.56731 (3) | 0.43196 (4) | 0.42532 (6) | 0.0429 (2) | |

| | | | | | |
|---|---|---|---|---|---|
| N1 | 0.42155 (12) | 0.19415 (12) | 0.0968 (2) | 0.0391 (4) | |
| N2 | 0.38759 (11) | 0.27687 (13) | 0.26398 (18) | 0.0359 (4) | |
| C1 | 0.37348 (15) | 0.32044 (16) | 0.3488 (2) | 0.0407 (5) | |
| H1 | 0.4120 | 0.3667 | 0.4034 | 0.049* | |
| C5 | 0.33239 (14) | 0.20969 (15) | 0.1835 (2) | 0.0368 (5) | |
| C4 | 0.26252 (15) | 0.18577 (17) | 0.1891 (3) | 0.0466 (6) | |
| H4 | 0.2249 | 0.1393 | 0.1334 | 0.056* | |
| C2 | 0.30477 (16) | 0.30103 (17) | 0.3606 (3) | 0.0447 (6) | |
| C3 | 0.24897 (16) | 0.2312 (2) | 0.2779 (3) | 0.0523 (7) | |
| H3 | 0.2023 | 0.2150 | 0.2824 | 0.063* | |
| C7 | 0.35069 (14) | 0.16493 (14) | 0.0903 (2) | 0.0386 (5) | |
| C8 | 0.29693 (17) | 0.09802 (17) | −0.0022 (2) | 0.0511 (6) | |
| H8 | 0.2475 | 0.0794 | −0.0072 | 0.061* | |
| C11 | 0.43965 (16) | 0.15765 (17) | 0.0132 (2) | 0.0477 (6) | |
| H11 | 0.4884 | 0.1792 | 0.0182 | 0.057* | |
| C10 | 0.39085 (19) | 0.08913 (18) | −0.0818 (3) | 0.0552 (7) | |
| C9 | 0.3180 (2) | 0.05955 (18) | −0.0865 (3) | 0.0580 (7) | |
| H9 | 0.2833 | 0.0135 | −0.1470 | 0.070* | |
| C6 | 0.2939 (2) | 0.3543 (2) | 0.4579 (3) | 0.0689 (9) | |
| H6A | 0.3391 | 0.3995 | 0.5036 | 0.103* | |
| H6B | 0.2950 | 0.3105 | 0.5199 | 0.103* | |
| H6C | 0.2405 | 0.3872 | 0.4128 | 0.103* | |
| C12 | 0.4172 (2) | 0.0531 (2) | −0.1719 (3) | 0.0782 (10) | |
| H12A | 0.4692 | 0.0834 | −0.1506 | 0.117* | |
| H12B | 0.3737 | 0.0673 | −0.2613 | 0.117* | |
| H12C | 0.4257 | −0.0145 | −0.1614 | 0.117* | |
| O1 | 0.5956 (2) | 0.4141 (2) | 0.7145 (3) | 0.1311 (14) | |
| H1A | 0.5803 | 0.4187 | 0.6356 | 0.197* | |
| H1B | 0.5699 | 0.4548 | 0.7272 | 0.197* | |
| O2 | 0.5000 | 0.2629 (5) | 0.7500 | 0.112 (3) | 0.50 |
| H2A | 0.5382 | 0.2904 | 0.7422 | 0.168* | 0.50 |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Mn | 0.0241 (3) | 0.0282 (3) | 0.0388 (3) | 0.000 | 0.0111 (2) | 0.000 |
| Cl1 | 0.0341 (3) | 0.0394 (3) | 0.0431 (3) | −0.0026 (2) | 0.0127 (3) | −0.0082 (2) |
| N1 | 0.0330 (10) | 0.0304 (9) | 0.0398 (10) | 0.0005 (7) | 0.0101 (8) | −0.0025 (7) |
| N2 | 0.0286 (9) | 0.0321 (9) | 0.0364 (9) | −0.0054 (7) | 0.0105 (8) | 0.0017 (7) |
| C1 | 0.0339 (11) | 0.0390 (12) | 0.0416 (12) | −0.0089 (9) | 0.0153 (10) | −0.0011 (9) |
| C5 | 0.0307 (11) | 0.0281 (10) | 0.0350 (11) | −0.0042 (8) | 0.0067 (9) | 0.0071 (8) |
| C4 | 0.0370 (12) | 0.0404 (13) | 0.0477 (14) | −0.0143 (10) | 0.0130 (11) | 0.0020 (10) |
| C2 | 0.0415 (13) | 0.0437 (13) | 0.0475 (14) | −0.0073 (10) | 0.0230 (11) | 0.0053 (10) |
| C3 | 0.0403 (13) | 0.0560 (16) | 0.0563 (15) | −0.0153 (12) | 0.0231 (12) | 0.0050 (12) |
| C7 | 0.0364 (11) | 0.0249 (9) | 0.0354 (11) | −0.0015 (9) | 0.0065 (9) | 0.0046 (8) |
| C8 | 0.0501 (14) | 0.0383 (12) | 0.0428 (13) | −0.0147 (11) | 0.0102 (12) | −0.0001 (10) |
| C11 | 0.0422 (13) | 0.0402 (12) | 0.0487 (14) | 0.0020 (10) | 0.0163 (11) | −0.0068 (11) |
| C10 | 0.0615 (17) | 0.0373 (13) | 0.0454 (14) | 0.0039 (12) | 0.0146 (13) | −0.0061 (10) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C9 | 0.0666 (18) | 0.0354 (13) | 0.0454 (15) | −0.0120 (12) | 0.0125 (13) | −0.0077 (10) |
| C6 | 0.0645 (18) | 0.080 (2) | 0.079 (2) | −0.0247 (17) | 0.0493 (17) | −0.0175 (17) |
| C12 | 0.092 (3) | 0.068 (2) | 0.060 (2) | 0.0055 (18) | 0.0315 (19) | −0.0192 (15) |
| O1 | 0.166 (3) | 0.157 (3) | 0.110 (2) | 0.121 (3) | 0.101 (2) | 0.068 (2) |
| O2 | 0.092 (5) | 0.047 (4) | 0.135 (7) | 0.000 | 0.020 (5) | 0.000 |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Mn—Cl1 | 2.4702 (6) | C7—C8 | 1.391 (3) |
| Mn—N1 | 2.3111 (19) | C8—C9 | 1.382 (5) |
| Mn—N2 | 2.245 (2) | C9—C10 | 1.394 (6) |
| O1—H1B | 0.8100 | C10—C12 | 1.502 (6) |
| O1—H1A | 0.8400 | C10—C11 | 1.397 (4) |
| O2—H2A | 0.8600 | C1—H1 | 0.9300 |
| O2—H2A$^{i}$ | 0.8600 | C3—H3 | 0.9300 |
| N1—C11 | 1.326 (4) | C4—H4 | 0.9300 |
| N1—C7 | 1.347 (3) | C6—H6A | 0.9600 |
| N2—C5 | 1.350 (2) | C6—H6B | 0.9600 |
| N2—C1 | 1.334 (3) | C6—H6C | 0.9600 |
| C1—C2 | 1.391 (5) | C8—H8 | 0.9300 |
| C2—C3 | 1.389 (4) | C9—H9 | 0.9300 |
| C2—C6 | 1.494 (5) | C11—H11 | 0.9300 |
| C3—C4 | 1.381 (4) | C12—H12B | 0.9600 |
| C4—C5 | 1.383 (4) | C12—H12C | 0.9600 |
| C5—C7 | 1.480 (3) | C12—H12A | 0.9600 |
| | | | |
| Cl1···C1 | 3.581 (3) | O1$^{iv}$···C3$^{ii}$ | 3.257 (5) |
| Cl1···O1 | 3.243 (3) | N1···N1$^{ii}$ | 3.259 (3) |
| Cl1···Cl1$^{ii}$ | 3.5759 (9) | N1···N2$^{ii}$ | 3.233 (3) |
| Cl1···N1$^{ii}$ | 3.3695 (18) | N1···N2 | 2.681 (3) |
| Cl1···O1$^{iii}$ | 3.358 (4) | N2···C11$^{ii}$ | 3.337 (4) |
| O1···O2 | 2.951 (6) | C3···O1$^{v}$ | 3.257 (5) |
| O1···Cl1$^{iii}$ | 3.358 (4) | | |
| | | | |
| Cl1—Mn—N1 | 170.62 (6) | N1—C7—C5 | 116.49 (19) |
| Cl1—Mn—N2 | 98.59 (5) | C5—C7—C8 | 122.4 (3) |
| Cl1—Mn—Cl1$^{ii}$ | 92.74 (2) | C7—C8—C9 | 119.1 (3) |
| Cl1—Mn—N1$^{ii}$ | 89.55 (5) | C8—C9—C10 | 120.7 (3) |
| Cl1—Mn—N2$^{ii}$ | 98.24 (5) | C9—C10—C12 | 124.2 (3) |
| N1—Mn—N2 | 72.07 (8) | C11—C10—C12 | 120.2 (4) |
| Cl1$^{ii}$—Mn—N1 | 89.55 (5) | C9—C10—C11 | 115.6 (3) |
| N1—Mn—N1$^{ii}$ | 89.65 (7) | N1—C11—C10 | 124.8 (3) |
| N1—Mn—N2$^{ii}$ | 90.40 (8) | C2—C1—H1 | 118.00 |
| Cl1$^{ii}$—Mn—N2 | 98.24 (5) | N2—C1—H1 | 118.00 |
| N1$^{ii}$—Mn—N2 | 90.40 (8) | C4—C3—H3 | 120.00 |
| N2—Mn—N2$^{ii}$ | 155.51 (7) | C2—C3—H3 | 120.00 |
| Cl1$^{ii}$—Mn—N1$^{ii}$ | 170.62 (6) | C5—C4—H4 | 120.00 |
| Cl1$^{ii}$—Mn—N2$^{ii}$ | 98.59 (5) | C3—C4—H4 | 120.00 |

| | | | |
|---|---|---|---|
| N1$^{ii}$—Mn—N2$^{ii}$ | 72.07 (8) | C2—C6—H6C | 109.00 |
| H1A—O1—H1B | 107.00 | C2—C6—H6A | 110.00 |
| H2A—O2—H2A$^{i}$ | 127.00 | C2—C6—H6B | 110.00 |
| Mn—N1—C11 | 124.8 (2) | H6B—C6—H6C | 109.00 |
| Mn—N1—C7 | 116.40 (15) | H6A—C6—H6C | 109.00 |
| C7—N1—C11 | 118.7 (2) | H6A—C6—H6B | 110.00 |
| C1—N2—C5 | 118.9 (2) | C9—C8—H8 | 120.00 |
| Mn—N2—C5 | 118.63 (17) | C7—C8—H8 | 120.00 |
| Mn—N2—C1 | 122.49 (17) | C8—C9—H9 | 120.00 |
| N2—C1—C2 | 124.1 (2) | C10—C9—H9 | 120.00 |
| C3—C2—C6 | 123.5 (3) | N1—C11—H11 | 118.00 |
| C1—C2—C3 | 116.3 (3) | C10—C11—H11 | 118.00 |
| C1—C2—C6 | 120.2 (3) | C10—C12—H12B | 109.00 |
| C2—C3—C4 | 120.3 (3) | C10—C12—H12C | 109.00 |
| C3—C4—C5 | 119.6 (3) | H12A—C12—H12C | 110.00 |
| N2—C5—C7 | 116.4 (2) | H12B—C12—H12C | 109.00 |
| N2—C5—C4 | 120.8 (2) | H12A—C12—H12B | 110.00 |
| C4—C5—C7 | 122.8 (2) | C10—C12—H12A | 109.00 |
| N1—C7—C8 | 121.1 (2) | | |

| | | | |
|---|---|---|---|
| N2—Mn—N1—C7 | 0.40 (15) | Mn—N2—C1—C2 | −179.72 (19) |
| N2—Mn—N1—C11 | 177.7 (2) | C5—N2—C1—C2 | 0.1 (3) |
| Cl1$^{ii}$—Mn—N1—C7 | −98.41 (15) | Mn—N2—C5—C4 | 179.52 (18) |
| Cl1$^{ii}$—Mn—N1—C11 | 78.9 (2) | Mn—N2—C5—C7 | −1.1 (2) |
| N1$^{ii}$—Mn—N1—C7 | 90.94 (16) | C1—N2—C5—C4 | −0.3 (3) |
| N1$^{ii}$—Mn—N1—C11 | −91.8 (2) | C1—N2—C5—C7 | 179.10 (19) |
| N2$^{ii}$—Mn—N1—C7 | 163.01 (16) | N2—C1—C2—C3 | 0.4 (4) |
| N2$^{ii}$—Mn—N1—C11 | −19.7 (2) | N2—C1—C2—C6 | −179.4 (3) |
| Cl1—Mn—N2—C1 | 1.11 (17) | C1—C2—C3—C4 | −0.7 (4) |
| Cl1—Mn—N2—C5 | −178.73 (15) | C6—C2—C3—C4 | 179.1 (3) |
| N1—Mn—N2—C1 | −179.78 (19) | C2—C3—C4—C5 | 0.5 (4) |
| N1—Mn—N2—C5 | 0.38 (15) | C3—C4—C5—N2 | 0.0 (4) |
| Cl1$^{ii}$—Mn—N2—C1 | −92.95 (17) | C3—C4—C5—C7 | −179.4 (2) |
| Cl1$^{ii}$—Mn—N2—C5 | 87.21 (16) | N2—C5—C7—N1 | 1.4 (3) |
| N1$^{ii}$—Mn—N2—C1 | 90.71 (17) | N2—C5—C7—C8 | −176.9 (2) |
| N1$^{ii}$—Mn—N2—C5 | −89.13 (16) | C4—C5—C7—N1 | −179.2 (2) |
| N2$^{ii}$—Mn—N2—C1 | 134.05 (18) | C4—C5—C7—C8 | 2.5 (3) |
| N2$^{ii}$—Mn—N2—C5 | −45.8 (3) | N1—C7—C8—C9 | 1.5 (3) |
| Mn—N1—C7—C5 | −1.1 (2) | C5—C7—C8—C9 | 179.7 (2) |
| Mn—N1—C7—C8 | 177.24 (16) | C7—C8—C9—C10 | −1.8 (4) |
| C11—N1—C7—C5 | −178.5 (2) | C8—C9—C10—C11 | 0.8 (4) |
| C11—N1—C7—C8 | −0.2 (3) | C8—C9—C10—C12 | −178.3 (3) |
| Mn—N1—C11—C10 | −178.1 (2) | C9—C10—C11—N1 | 0.6 (4) |
| C7—N1—C11—C10 | −0.9 (4) | C12—C10—C11—N1 | 179.7 (3) |

Symmetry codes: (i) −*x*+1, *y*, −*z*+3/2; (ii) −*x*+1, *y*, −*z*+1/2; (iii) −*x*+1, −*y*+1, −*z*+1; (iv) −*x*+3/2, −*y*+1/2, −*z*+1; (v) *x*−1/2, −*y*+1/2, *z*−1/2.

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1*A*···Cl1 | 0.84 | 2.42 | 3.243 (3) | 168 |
| O1—H1*B*···Cl1$^{iii}$ | 0.81 | 2.73 | 3.358 (4) | 136 |
| O2—H2*A*···O1 | 0.86 | 2.16 | 2.951 (6) | 153 |
| C3—H3···O1$^{v}$ | 0.93 | 2.49 | 3.257 (5) | 140 |
| C6—H6*A*···Cl1$^{iii}$ | 0.96 | 2.79 | 3.717 (4) | 162 |

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