

catena-Poly[[2-[[2-(dimethylammonio)ethyl]iminomethyl]pyridine- κ^2N,N']bis-(thiocyanato- κN)manganese(II)]- μ -thiocyanato- $\kappa^2N:S$]

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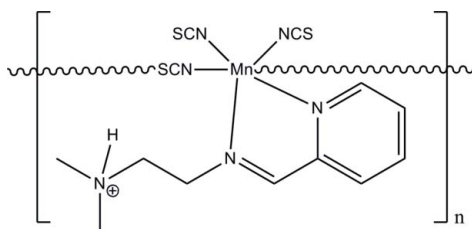
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 Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(C-C) = 0.005$ Å; R factor = 0.043; wR factor = 0.098; data-to-parameter ratio = 17.4.

In the title one-dimensional coordination polymer, $[Mn(NCS)_3(C_{10}H_{16}N_3)]_n$, the Mn^{II} atom is coordinated by an N,N' -bidentate Schiff base and four thiocyanate ligands in a distorted octahedral N_5S geometry. Bridging thiocyanate ligands interconnect adjacent $[Mn(NCS)_2(C_{10}H_{16}N_3)]$ units, giving rise to helical chains extending along the b axis. The chains are further linked through $N-H \cdots S$ hydrogen bonds, leading to a three-dimensional supramolecular network.

Related literature

For the structure of Cu^{II} and Pt^I complexes of the same Schiff base, see: Hinman *et al.* (2000); Mukherjee *et al.* (2002).



Experimental

Crystal data

$[Mn(NCS)_3(C_{10}H_{16}N_3)]$
 $M_r = 407.44$
 Orthorhombic, $Pbca$
 $a = 8.5603$ (12) Å
 $b = 11.0699$ (15) Å
 $c = 37.346$ (5) Å

$V = 3539.0$ (8) Å³
 $Z = 8$
 Mo $K\alpha$ radiation
 $\mu = 1.11$ mm⁻¹
 $T = 296$ K
 $0.25 \times 0.19 \times 0.11$ mm

Data collection

Bruker APEXII area-detector diffractometer
 Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
 $T_{min} = 0.770$, $T_{max} = 0.888$

18847 measured reflections
 3660 independent reflections
 2397 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.076$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.043$
 $wR(F^2) = 0.098$
 $S = 1.04$
 3660 reflections

210 parameters
 H-atom parameters constrained
 $\Delta\rho_{max} = 0.29$ e Å⁻³
 $\Delta\rho_{min} = -0.35$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| $D-H \cdots A$ | $D-H$ | $H \cdots A$ | $D \cdots A$ | $D-H \cdots A$ |
|---------------------|-------|--------------|--------------|----------------|
| $N3-H3 \cdots S1^i$ | 0.87 | 2.47 | 3.294 (3) | 159 |

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: RZ2792).

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supporting information

Acta Cryst. (2012). E68, m1131 [https://doi.org/10.1107/S1600536812032874]

***catena*-Poly[[2-[[2-(dimethylammonio)ethyl]iminomethyl]pyridine- κ^2 N,N']bis-(thiocyanato- κ N)manganese(II)]- μ -thiocyanato- κ^2 N:S]**

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S1. Comment

The title compound (Fig. 1) was obtained upon complexation of the Schiff base *N,N*-dimethyl-*N'*-[(pyridin-2-yl)methylene]ethane-1,2-diamine with Mn(ClO₄)₂ and KNCS. Similarly to what observed in a related platinum(II) complex (Hinman *et al.*, 2000), due to the protonation of the amine nitrogen atom the Schiff base acts as a bidentate ligand instead as tridentate (Mukherjee *et al.*, 2002). The Mn(II) ion is in a distorted octahedral coordination environment, provided by an *N,N'*-bidentate Schiff base and four NCS ligands. The μ_2 -isothiocyanato ligands interconnect the [Mn(NCS)₂(C₁₀H₁₆N₃)] units, giving rise to one-dimensional helical chains along the *b* axis. Adjacent helical chains are further connected *via* N—H \cdots S hydrogen bonds (Table 1) into a three-dimensional supramolecular structure.

S2. Experimental

A mixture of 2-pyridinecarboxaldehyde (0.107 g, 1 mmol) and *N,N*-dimethylethyldiamine (0.088 g, 1 mmol) in ethanol (5 ml) was refluxed for 2 h followed by addition of a solution of Mn(ClO₄)₂·6H₂O (0.362 g, 1 mmol) and KNCS (0.291, 3 mmol) in a minimum amount of water. The resulting solution was refluxed for 30 min, then set aside at room temperature. Crystals of the title compound suitable for X-ray analysis were obtained after few days on slow evaporation of the solvent.

S3. Refinement

Hydrogen atoms were located in a difference Fourier map or placed at calculated positions (C—H = 0.95–0.99 Å; N—H = 0.87 Å), and were treated as riding on their parent atoms, with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$ or $1.5 U_{\text{eq}}(\text{C}, \text{N})$ for amine and methyl H atoms.

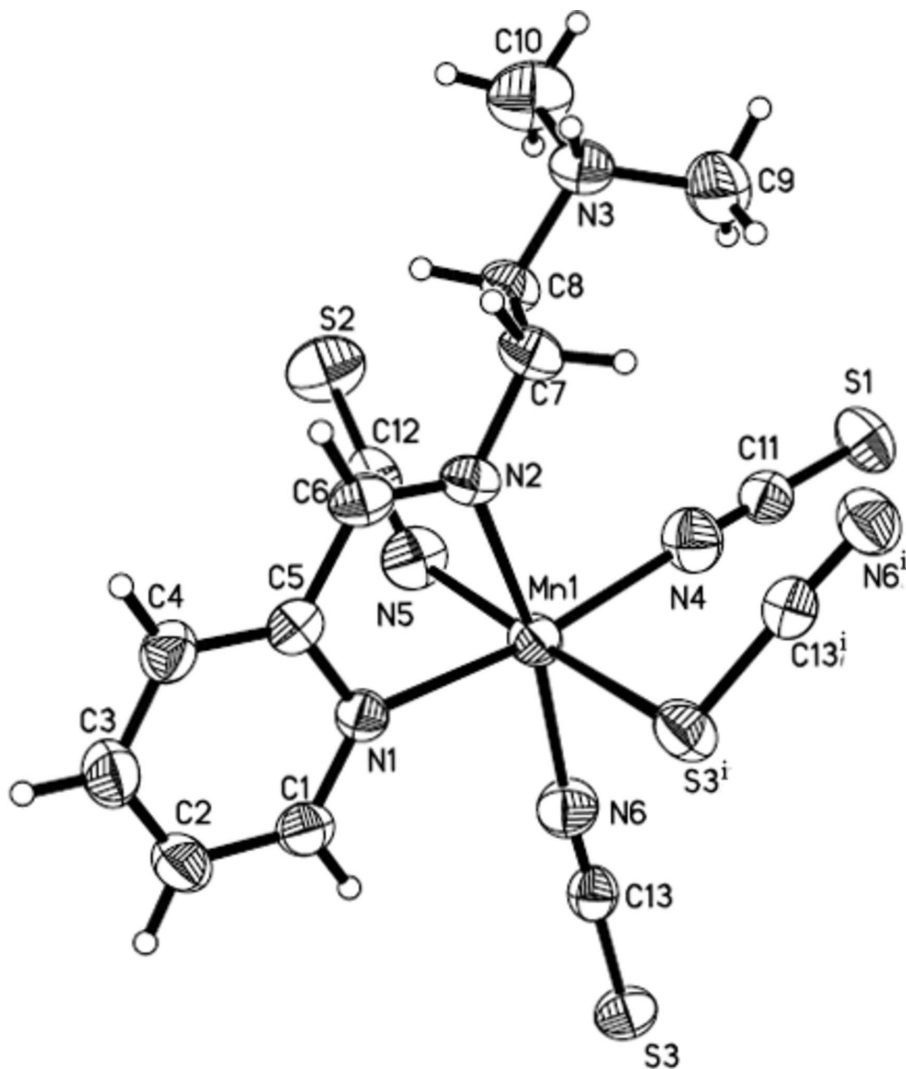


Figure 1

The asymmetric unit of the title compound with displacement ellipsoids drawn at the 50% probability level. Symmetry code: (i) $2.5-x, 0.5+y, z$.

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Crystal data

$[\text{Mn}(\text{NCS})_3(\text{C}_{10}\text{H}_{16}\text{N}_3)]$

$M_r = 407.44$

Orthorhombic, *Pbca*

Hall symbol: $-P\ 2ac\ 2ab$

$a = 8.5603\ (12)\ \text{\AA}$

$b = 11.0699\ (15)\ \text{\AA}$

$c = 37.346\ (5)\ \text{\AA}$

$V = 3539.0\ (8)\ \text{\AA}^3$

$Z = 8$

$F(000) = 1672$

$D_x = 1.529\ \text{Mg m}^{-3}$

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

Cell parameters from 3600 reflections

$\theta = 1.2\text{--}28.0^\circ$

$\mu = 1.11\ \text{mm}^{-1}$

$T = 296\ \text{K}$

Block, yellow

$0.25 \times 0.19 \times 0.11\ \text{mm}$

Data collection

| | |
|---|--|
| Bruker APEXII area-detector diffractometer | 18847 measured reflections |
| Radiation source: fine-focus sealed tube | 3660 independent reflections |
| Graphite monochromator | 2397 reflections with $I > 2\sigma(I)$ |
| φ and ω scan | $R_{\text{int}} = 0.076$ |
| Absorption correction: multi-scan (SADABS; Sheldrick, 1996) | $\theta_{\text{max}} = 26.5^\circ$, $\theta_{\text{min}} = 2.2^\circ$ |
| $T_{\text{min}} = 0.770$, $T_{\text{max}} = 0.888$ | $h = -10 \rightarrow 10$ |
| | $k = -13 \rightarrow 12$ |
| | $l = -46 \rightarrow 44$ |

Refinement

| | |
|--|--|
| Refinement on F^2 | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.043$ | H-atom parameters constrained |
| $wR(F^2) = 0.098$ | $w = 1/[\sigma^2(F_o^2) + (0.0371P)^2 + 0.1816P]$ |
| $S = 1.04$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| 3660 reflections | $(\Delta/\sigma)_{\text{max}} = 0.001$ |
| 210 parameters | $\Delta\rho_{\text{max}} = 0.29 \text{ e } \text{\AA}^{-3}$ |
| 0 restraints | $\Delta\rho_{\text{min}} = -0.35 \text{ e } \text{\AA}^{-3}$ |
| 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 (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|------------|------------|-------------|----------------------------------|
| C1 | 0.8026 (4) | 1.0515 (3) | 0.29186 (7) | 0.0365 (7) |
| H1 | 0.8775 | 1.1075 | 0.2848 | 0.044* |
| C2 | 0.6523 (4) | 1.0652 (3) | 0.27924 (8) | 0.0427 (8) |
| H2 | 0.6263 | 1.1293 | 0.2643 | 0.051* |
| C3 | 0.5419 (4) | 0.9820 (3) | 0.28924 (8) | 0.0470 (9) |
| H3A | 0.4396 | 0.9885 | 0.2811 | 0.056* |
| C4 | 0.5847 (4) | 0.8885 (3) | 0.31150 (8) | 0.0390 (8) |
| H4 | 0.5115 | 0.8311 | 0.3185 | 0.047* |
| C5 | 0.7368 (4) | 0.8806 (3) | 0.32342 (7) | 0.0328 (7) |
| C6 | 0.7882 (4) | 0.7845 (3) | 0.34732 (8) | 0.0365 (8) |
| H6 | 0.7188 | 0.7237 | 0.3539 | 0.044* |
| C7 | 0.9714 (4) | 0.6847 (3) | 0.38312 (8) | 0.0400 (8) |
| H7A | 1.0726 | 0.6528 | 0.3762 | 0.048* |
| H7B | 0.8954 | 0.6198 | 0.3818 | 0.048* |
| C8 | 0.9784 (4) | 0.7345 (3) | 0.42070 (8) | 0.0381 (8) |
| H8A | 1.0409 | 0.8076 | 0.4207 | 0.046* |

| | | | | |
|------|--------------|--------------|---------------|--------------|
| H8B | 0.8736 | 0.7561 | 0.4283 | 0.046* |
| C9 | 1.2174 (4) | 0.6312 (3) | 0.44276 (10) | 0.0601 (11) |
| H9A | 1.2693 | 0.7068 | 0.4469 | 0.090* |
| H9B | 1.2399 | 0.6036 | 0.4189 | 0.090* |
| H9C | 1.2538 | 0.5726 | 0.4598 | 0.090* |
| C10 | 1.0076 (5) | 0.6853 (4) | 0.48428 (8) | 0.0679 (12) |
| H10A | 1.0542 | 0.6297 | 0.5009 | 0.102* |
| H10B | 0.8963 | 0.6854 | 0.4874 | 0.102* |
| H10C | 1.0477 | 0.7650 | 0.4885 | 0.102* |
| C11 | 1.3790 (4) | 0.8798 (3) | 0.39279 (8) | 0.0358 (7) |
| C12 | 0.9167 (4) | 1.0407 (3) | 0.41865 (10) | 0.0411 (8) |
| C13 | 1.2401 (4) | 1.1848 (3) | 0.30617 (8) | 0.0351 (7) |
| Mn1 | 1.07355 (5) | 0.94723 (4) | 0.344285 (12) | 0.03482 (15) |
| N1 | 0.8468 (3) | 0.9621 (2) | 0.31373 (6) | 0.0312 (6) |
| N2 | 0.9266 (3) | 0.7830 (2) | 0.35923 (6) | 0.0335 (6) |
| N3 | 1.0459 (3) | 0.6475 (2) | 0.44693 (7) | 0.0398 (7) |
| N4 | 1.2709 (3) | 0.8875 (2) | 0.37436 (7) | 0.0469 (7) |
| N5 | 0.9625 (4) | 1.0375 (2) | 0.38952 (8) | 0.0500 (8) |
| N6 | 1.1752 (3) | 1.1042 (2) | 0.31952 (7) | 0.0447 (7) |
| H3 | 0.9996 | 0.5806 | 0.4412 | 0.067* |
| S1 | 1.53139 (11) | 0.87179 (8) | 0.41894 (2) | 0.0482 (3) |
| S2 | 0.85784 (14) | 1.04061 (10) | 0.46007 (2) | 0.0646 (3) |
| S3 | 1.32720 (10) | 1.29615 (7) | 0.28601 (2) | 0.0427 (2) |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| C1 | 0.040 (2) | 0.0343 (18) | 0.0352 (17) | 0.0006 (15) | 0.0050 (15) | 0.0024 (15) |
| C2 | 0.045 (2) | 0.042 (2) | 0.0411 (19) | 0.0111 (17) | -0.0011 (17) | 0.0056 (16) |
| C3 | 0.037 (2) | 0.060 (2) | 0.044 (2) | 0.0059 (18) | -0.0041 (17) | 0.0013 (18) |
| C4 | 0.0304 (19) | 0.044 (2) | 0.0424 (19) | -0.0054 (15) | 0.0004 (15) | 0.0008 (16) |
| C5 | 0.0332 (19) | 0.0328 (18) | 0.0325 (17) | -0.0029 (14) | 0.0030 (14) | -0.0017 (14) |
| C6 | 0.044 (2) | 0.0306 (18) | 0.0350 (17) | -0.0069 (14) | 0.0037 (16) | 0.0018 (14) |
| C7 | 0.050 (2) | 0.0276 (17) | 0.0426 (19) | 0.0029 (15) | -0.0033 (16) | 0.0048 (15) |
| C8 | 0.047 (2) | 0.0307 (18) | 0.0366 (18) | 0.0059 (15) | -0.0006 (16) | 0.0037 (14) |
| C9 | 0.048 (2) | 0.067 (3) | 0.065 (3) | 0.003 (2) | -0.009 (2) | 0.005 (2) |
| C10 | 0.094 (3) | 0.078 (3) | 0.032 (2) | -0.003 (2) | 0.002 (2) | -0.006 (2) |
| C11 | 0.0377 (19) | 0.0300 (18) | 0.0398 (19) | -0.0024 (14) | 0.0013 (16) | -0.0002 (15) |
| C12 | 0.038 (2) | 0.0301 (18) | 0.055 (2) | -0.0001 (15) | -0.0126 (18) | -0.0077 (17) |
| C13 | 0.0318 (19) | 0.0372 (19) | 0.0362 (17) | -0.0002 (14) | -0.0020 (15) | -0.0036 (15) |
| Mn1 | 0.0324 (3) | 0.0317 (3) | 0.0404 (3) | -0.0035 (2) | -0.0037 (2) | 0.0040 (2) |
| N1 | 0.0315 (15) | 0.0291 (14) | 0.0328 (14) | 0.0003 (11) | 0.0012 (11) | 0.0017 (12) |
| N2 | 0.0421 (17) | 0.0280 (14) | 0.0304 (14) | 0.0007 (12) | -0.0001 (12) | 0.0023 (11) |
| N3 | 0.0482 (19) | 0.0363 (15) | 0.0349 (14) | -0.0042 (13) | -0.0040 (13) | 0.0010 (12) |
| N4 | 0.0424 (18) | 0.0521 (18) | 0.0463 (17) | -0.0019 (14) | -0.0078 (15) | -0.0031 (14) |
| N5 | 0.058 (2) | 0.0441 (18) | 0.0483 (18) | -0.0010 (14) | 0.0039 (16) | -0.0054 (15) |
| N6 | 0.0447 (18) | 0.0370 (16) | 0.0525 (18) | -0.0050 (14) | 0.0026 (14) | 0.0029 (14) |
| S1 | 0.0476 (6) | 0.0432 (5) | 0.0538 (5) | 0.0057 (4) | -0.0176 (4) | -0.0027 (4) |

| | | | | | | |
|----|------------|------------|------------|-------------|------------|-------------|
| S2 | 0.0818 (8) | 0.0664 (7) | 0.0455 (6) | -0.0123 (6) | 0.0038 (5) | -0.0092 (5) |
| S3 | 0.0478 (6) | 0.0360 (5) | 0.0442 (5) | -0.0086 (4) | 0.0037 (4) | 0.0034 (4) |

Geometric parameters (Å, °)

| | | | |
|-----------|-----------|------------------------|-------------|
| C1—N1 | 1.337 (3) | C9—H9A | 0.9600 |
| C1—C2 | 1.379 (4) | C9—H9B | 0.9600 |
| C1—H1 | 0.9300 | C9—H9C | 0.9600 |
| C2—C3 | 1.371 (5) | C10—N3 | 1.492 (4) |
| C2—H2 | 0.9300 | C10—H10A | 0.9600 |
| C3—C4 | 1.377 (4) | C10—H10B | 0.9600 |
| C3—H3A | 0.9300 | C10—H10C | 0.9600 |
| C4—C5 | 1.379 (4) | C11—N4 | 1.157 (4) |
| C4—H4 | 0.9300 | C11—S1 | 1.632 (3) |
| C5—N1 | 1.354 (4) | C12—N5 | 1.157 (4) |
| C5—C6 | 1.457 (4) | C12—S2 | 1.627 (4) |
| C6—N2 | 1.266 (4) | C13—N6 | 1.162 (4) |
| C6—H6 | 0.9300 | C13—S3 | 1.626 (3) |
| C7—N2 | 1.459 (3) | Mn1—N4 | 2.133 (3) |
| C7—C8 | 1.509 (4) | Mn1—N6 | 2.153 (3) |
| C7—H7A | 0.9700 | Mn1—N5 | 2.181 (3) |
| C7—H7B | 0.9700 | Mn1—N1 | 2.257 (2) |
| C8—N3 | 1.490 (4) | Mn1—N2 | 2.280 (2) |
| C8—H8A | 0.9700 | Mn1—S3 ⁱ | 2.8731 (10) |
| C8—H8B | 0.9700 | N3—H3 | 0.8675 |
| C9—N3 | 1.487 (4) | S3—Mn1 ⁱⁱ | 2.8732 (10) |
| | | | |
| N1—C1—C2 | 123.6 (3) | H10A—C10—H10B | 109.5 |
| N1—C1—H1 | 118.2 | N3—C10—H10C | 109.5 |
| C2—C1—H1 | 118.2 | H10A—C10—H10C | 109.5 |
| C3—C2—C1 | 118.4 (3) | H10B—C10—H10C | 109.5 |
| C3—C2—H2 | 120.8 | N4—C11—S1 | 178.9 (3) |
| C1—C2—H2 | 120.8 | N5—C12—S2 | 177.5 (3) |
| C2—C3—C4 | 119.0 (3) | N6—C13—S3 | 177.7 (3) |
| C2—C3—H3A | 120.5 | N4—Mn1—N6 | 98.99 (11) |
| C4—C3—H3A | 120.5 | N4—Mn1—N5 | 94.55 (11) |
| C3—C4—C5 | 119.6 (3) | N6—Mn1—N5 | 98.00 (10) |
| C3—C4—H4 | 120.2 | N4—Mn1—N1 | 165.80 (10) |
| C5—C4—H4 | 120.2 | N6—Mn1—N1 | 94.10 (9) |
| N1—C5—C4 | 121.9 (3) | N5—Mn1—N1 | 89.04 (10) |
| N1—C5—C6 | 116.1 (3) | N4—Mn1—N2 | 93.50 (10) |
| C4—C5—C6 | 122.0 (3) | N6—Mn1—N2 | 166.41 (10) |
| N2—C6—C5 | 120.5 (3) | N5—Mn1—N2 | 86.27 (10) |
| N2—C6—H6 | 119.8 | N1—Mn1—N2 | 72.99 (9) |
| C5—C6—H6 | 119.8 | N4—Mn1—S3 ⁱ | 89.10 (8) |
| N2—C7—C8 | 107.8 (2) | N6—Mn1—S3 ⁱ | 91.43 (7) |
| N2—C7—H7A | 110.1 | N5—Mn1—S3 ⁱ | 169.22 (8) |
| C8—C7—H7A | 110.1 | N1—Mn1—S3 ⁱ | 85.06 (6) |

| | | | |
|----------------------------|------------|-----------------------------|-------------|
| N2—C7—H7B | 110.1 | N2—Mn1—S3 ⁱ | 83.38 (6) |
| C8—C7—H7B | 110.1 | C1—N1—C5 | 117.3 (3) |
| H7A—C7—H7B | 108.5 | C1—N1—Mn1 | 127.3 (2) |
| N3—C8—C7 | 113.0 (2) | C5—N1—Mn1 | 114.49 (19) |
| N3—C8—H8A | 109.0 | C6—N2—C7 | 118.1 (3) |
| C7—C8—H8A | 109.0 | C6—N2—Mn1 | 114.85 (19) |
| N3—C8—H8B | 109.0 | C7—N2—Mn1 | 126.8 (2) |
| C7—C8—H8B | 109.0 | C9—N3—C10 | 110.4 (3) |
| H8A—C8—H8B | 107.8 | C9—N3—C8 | 113.1 (3) |
| N3—C9—H9A | 109.5 | C10—N3—C8 | 110.4 (3) |
| N3—C9—H9B | 109.5 | C9—N3—H3 | 108.7 |
| H9A—C9—H9B | 109.5 | C10—N3—H3 | 111.8 |
| N3—C9—H9C | 109.5 | C8—N3—H3 | 102.2 |
| H9A—C9—H9C | 109.5 | C11—N4—Mn1 | 165.9 (3) |
| H9B—C9—H9C | 109.5 | C12—N5—Mn1 | 152.9 (3) |
| N3—C10—H10A | 109.5 | C13—N6—Mn1 | 175.2 (3) |
| N3—C10—H10B | 109.5 | C13—S3—Mn1 ⁱⁱ | 103.08 (11) |
| | | | |
| N1—C1—C2—C3 | -0.8 (5) | C5—C6—N2—Mn1 | 5.0 (4) |
| C1—C2—C3—C4 | 0.3 (5) | C8—C7—N2—C6 | -104.8 (3) |
| C2—C3—C4—C5 | 0.3 (5) | C8—C7—N2—Mn1 | 69.3 (3) |
| C3—C4—C5—N1 | -0.3 (5) | N4—Mn1—N2—C6 | 177.1 (2) |
| C3—C4—C5—C6 | 179.3 (3) | N6—Mn1—N2—C6 | -26.1 (5) |
| N1—C5—C6—N2 | 3.2 (4) | N5—Mn1—N2—C6 | 82.8 (2) |
| C4—C5—C6—N2 | -176.4 (3) | N1—Mn1—N2—C6 | -7.4 (2) |
| N2—C7—C8—N3 | -171.4 (3) | S3 ⁱ —Mn1—N2—C6 | -94.2 (2) |
| C2—C1—N1—C5 | 0.8 (4) | N4—Mn1—N2—C7 | 2.8 (2) |
| C2—C1—N1—Mn1 | -167.9 (2) | N6—Mn1—N2—C7 | 159.5 (4) |
| C4—C5—N1—C1 | -0.2 (4) | N5—Mn1—N2—C7 | -91.6 (2) |
| C6—C5—N1—C1 | -179.9 (2) | N1—Mn1—N2—C7 | 178.3 (2) |
| C4—C5—N1—Mn1 | 169.9 (2) | S3 ⁱ —Mn1—N2—C7 | 91.4 (2) |
| C6—C5—N1—Mn1 | -9.8 (3) | C7—C8—N3—C9 | 72.4 (4) |
| N4—Mn1—N1—C1 | -163.6 (4) | C7—C8—N3—C10 | -163.3 (3) |
| N6—Mn1—N1—C1 | -6.4 (2) | N6—Mn1—N4—C11 | 48.5 (11) |
| N5—Mn1—N1—C1 | 91.5 (2) | N5—Mn1—N4—C11 | -50.4 (11) |
| N2—Mn1—N1—C1 | 177.9 (2) | N1—Mn1—N4—C11 | -154.6 (9) |
| S3 ⁱ —Mn1—N1—C1 | -97.5 (2) | N2—Mn1—N4—C11 | -136.9 (11) |
| N4—Mn1—N1—C5 | 27.5 (5) | S3 ⁱ —Mn1—N4—C11 | 139.8 (11) |
| N6—Mn1—N1—C5 | -175.4 (2) | N4—Mn1—N5—C12 | -50.7 (6) |
| N5—Mn1—N1—C5 | -77.4 (2) | N6—Mn1—N5—C12 | -150.4 (6) |
| N2—Mn1—N1—C5 | 8.97 (19) | N1—Mn1—N5—C12 | 115.6 (6) |
| S3 ⁱ —Mn1—N1—C5 | 93.54 (19) | N2—Mn1—N5—C12 | 42.5 (6) |
| C5—C6—N2—C7 | 179.9 (2) | S3 ⁱ —Mn1—N5—C12 | 58.8 (9) |

Symmetry codes: (i) $-x+5/2, y-1/2, z$; (ii) $-x+5/2, y+1/2, z$.

Hydrogen-bond geometry (Å, °)

| <i>D</i> —H \cdots <i>A</i> | <i>D</i> —H | H \cdots <i>A</i> | <i>D</i> \cdots <i>A</i> | <i>D</i> —H \cdots <i>A</i> |
|--------------------------------|-------------|---------------------|----------------------------|-------------------------------|
| N3—H3 \cdots S1 ⁱ | 0.87 | 2.47 | 3.294 (3) | 159 |

Symmetry code: (i) $-x+5/2, y-1/2, z$.