

catena-Poly[[diazidomanganese(II)]bis[μ -1-(4-pyridylmethyl)-1*H*-benzimidazole]]

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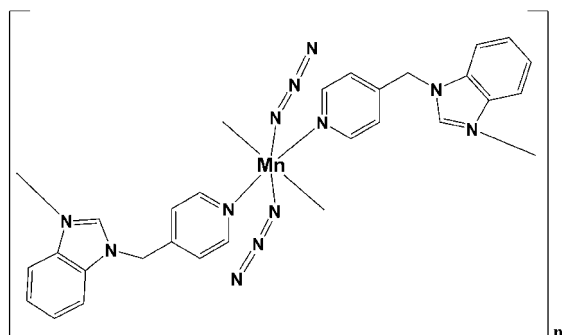
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 Key indicators: single-crystal X-ray study; $T = 294$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.029; wR factor = 0.081; data-to-parameter ratio = 16.5.

In the title polymeric compound, $[\text{Mn}(\text{N}_3)_2(\text{C}_{13}\text{H}_{11}\text{N}_3)_2]_n$, each Mn^{II} centre is six-coordinated in an octahedral geometry by six N atoms from four 1-(4-pyridylmethyl)-1*H*-benzimidazole (*L*) ligands and two azide anions (N_3^-). Each of the Mn^{II} ions lies on an inversion centre. The *L* ligands and N_3^- anions bridge adjacent Mn^{II} centres, generating a polymeric chain running along the [110] direction. Adjacent polymeric chains are arranged in a two-dimensional network parallel to the (001) plane, linked by $\text{C}-\text{H}\cdots\text{N}$ hydrogen bonds.

Related literature

For related literature, see: Chang *et al.* (2005); Desiraju & Steiner (1999); Fan *et al.* (2006); Huang *et al.* (2006); Kitagawa *et al.* (2004); Li *et al.* (2007); Meng *et al.* (2004); Steel (2005); Su *et al.* (2001); Xiao *et al.* (2004).



Experimental

Crystal data

 $[\text{Mn}(\text{N}_3)_2(\text{C}_{13}\text{H}_{11}\text{N}_3)_2]$
 $M_r = 557.50$

 Triclinic, $P\bar{1}$
 $a = 8.4135$ (17) Å

 $b = 8.5823$ (17) Å

 $c = 10.399$ (2) Å

 $\alpha = 67.86$ (3)°

 $\beta = 86.03$ (3)°

 $\gamma = 69.80$ (3)°

 $V = 651.1$ (3) Å³
 $Z = 1$

 Mo $K\alpha$ radiation

 $\mu = 0.55$ mm⁻¹
 $T = 294$ (2) K

 $0.36 \times 0.32 \times 0.30$ mm

Data collection

Bruker SMART CCD area-detector diffractometer

Absorption correction: multi-scan

 (*SADABS*; Bruker, 1998)

 $T_{\text{min}} = 0.827$, $T_{\text{max}} = 0.853$

6780 measured reflections

2954 independent reflections

 2828 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.019$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.029$
 $wR(F^2) = 0.081$
 $S = 1.03$

2954 reflections

179 parameters

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 0.31$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.23$ e Å⁻³
Table 1

Selected geometric parameters (Å, °).

| | | | |
|---------------------------------------|-------------|---|-------------|
| Mn1—N4 | 2.2049 (13) | Mn1—N1 ⁱⁱ | 2.2869 (12) |
| Mn1—N1 ⁱ | 2.2869 (12) | Mn1—N3 | 2.3358 (16) |
| N4—Mn1—N4 ⁱⁱⁱ | 180 | N4—Mn1—N3 ⁱⁱⁱ | 92.39 (5) |
| N4—Mn1—N1 ⁱ | 88.32 (5) | N1 ⁱⁱ —Mn1—N3 ⁱⁱⁱ | 90.37 (5) |
| N4—Mn1—N1 ⁱⁱ | 91.68 (5) | N1 ⁱ —Mn1—N3 | 90.37 (5) |
| N1 ⁱ —Mn1—N1 ⁱⁱ | 180 | N3 ⁱⁱⁱ —Mn1—N3 | 180 |

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

Table 2

Hydrogen-bond geometry (Å, °).

| $D-\text{H}\cdots A$ | $D-\text{H}$ | $\text{H}\cdots A$ | $D\cdots A$ | $D-\text{H}\cdots A$ |
|----------------------------------|--------------|--------------------|-------------|----------------------|
| C1—H1 \cdots N6 ^v | 0.93 | 2.48 | 3.319 (1) | 150 |
| C11—H11 \cdots N6 ^v | 0.93 | 2.58 | 3.305 (2) | 135 |

 Symmetry codes: (iv) $x - 1, y, z$; (v) $-x + 2, -y + 1, -z + 2$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2519).

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supporting information

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catena-Poly[[diazidomanganese(II)]bis[μ -1-(4-pyridylmethyl)-1H-benzimidazole]]**Chun-Sen Liu, Jun-Jie Wang and Li-Fen Yan****S1. Comment**

N-containing heterocyclic aromatic compounds are extensively used as bridging ligands in coordination and metallocsupramolecular chemistry (Steel, 2005). The most frequently used neutral bridging ligands are 4,4'-bipyridine and its derivatives (Kitagawa *et al.*, 2004). In recent years, however, the benzimidazole groups also were used to link different alkyl or aromatic groups to form a series of bi- and multi-dentate flexible ligands, which can adopt different conformations according to the different geometric requirements of metal centers when forming metal complexes (Li *et al.*, 2007). Many complexes with these ligands show unique structural topologies and interesting properties (Meng *et al.*, 2004), such as three-dimensional and two-dimensional networks (Chang *et al.*, 2005; Fan *et al.*, 2006; Su *et al.*, 2001) and one-dimensional helical chains (Xiao *et al.*, 2004). Recently, we found that Liu and co-workers synthesized a flexible bridging ligand 1-(pyridin-4-ylmethyl)-1H-benzo[*d*]imidazole (*L*) as well as its chiral one-dimensional double helix polymer, [Ag(*L*)(NO₃)_n]_n (Huang *et al.*, 2006). As such, we also used *L* as a μ_2 -bridging ligand to react with Mn^{II} salt, meanwhile together with azido anion as a co-ligand, to obtain a one-dimensional manganese coordination polymer [Mn(C₁₃H₁₁N₃)₂(N₃)₂]_n (I). We report here the crystal structure of (I).

The title compound (I) consists of linear polymeric coordination chains containing only one kind of Mn^{II} coordination environment (Fig. 1). The asymmetric unit of (I) is composed of one Mn^{II} ion which lies on an inversion centre, one *L* ligand and one N₃⁻ anion (*L* is 1-(pyridin-4-ylmethyl)-1H-benzo[*d*]imidazole). The geometry around each Mn^{II} ion can be best described as a ideal octahedron (Fig. 1). The Mn^{II} center is six-coordinated by six N atoms from four different *L* ligands and two N₃⁻ anions, respectively (Table 1). In the crystal structure of (I), *L* adopts μ_2 -bridging 4,4'-bipyridine-like coordination mode and N₃⁻ serves as a mono-terminal coordination mode [Mn1—N4: 2.2049 (13) Å], which together link the adjacent Mn^{II} ions into a linear chain along the [1 1 0] direction, with the shortest intrachain non-bonding Mn...Mn separation being 9.725 (2) Å (Fig. 2).

In the crystal structure of (I), the adjacent one-dimensional chains [Mn(C₁₃H₁₁N₃)₂(N₃)₂]_n are arranged into a two-dimensional network parallel to the (0 0 1) plane by interchain C—H...N hydrogen bonding interactions between the coordinated *L* ligands and N atoms of azido anions (see Fig. 3 and Table 2) (Desiraju *et al.*, 1999).

S2. Experimental

The ligand 1-(pyridin-4-ylmethyl)-1H-benzo[*d*]imidazole (*L*) was synthesized according to a method reported in the literature (Li *et al.*, 2007). The reaction of *L* (58 mg, 0.2 mmol), NaN₃ (13 mg, 0.2 mmol) with Mn(ClO₄)₂ (25 mg, 0.1 mmol) in a mixed solution of methanol and aqua (*v/v* = 1:1, 10 ml) for a few minutes afforded a yellow solid, which was then filtered. The resulting solution was kept at room temperature. Yellow single crystals of compound (I) suitable for X-ray analysis were obtained by slow evaporation of the solvent after several days (yield: 40%). Analysis calculated for C₂₆H₂₂MnN₁₂: C 56.02, H 3.98, N 30.15%; found: C 55.88, H 3.79, N 30.37%.

S3. Refinement

H atoms were included in calculated positions and treated in the subsequent refinement as riding atoms, with C—H = 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

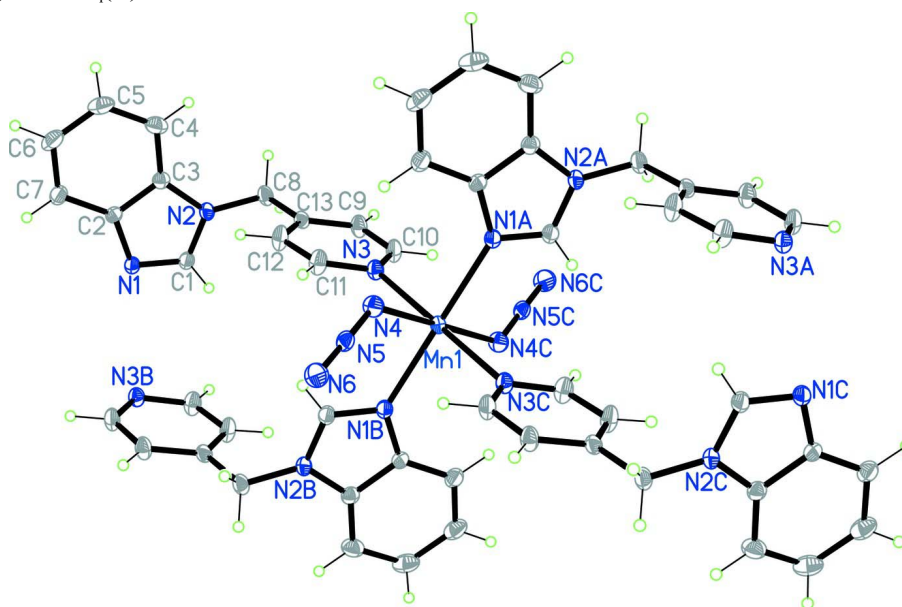


Figure 1

The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. The atoms labelled with the suffixes A, B and C are generated by the symmetry operations $(1 + x, -1 + y, z)$, $(1 - x, 1 - y, 2 - z)$ and $(2 - x, -y, 2 - z)$, respectively.

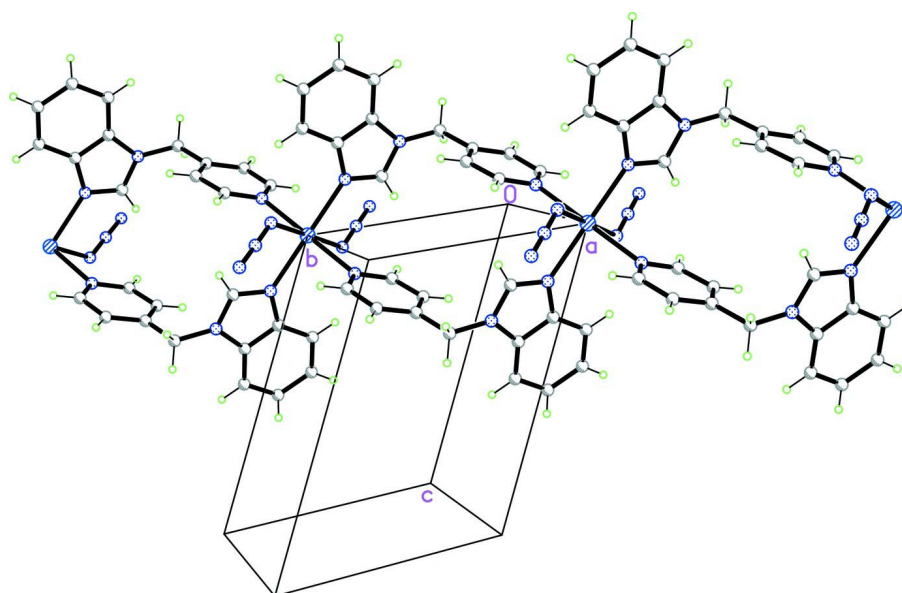


Figure 2

View of a polymeric chain running along the $[1\ 1\ 0]$.

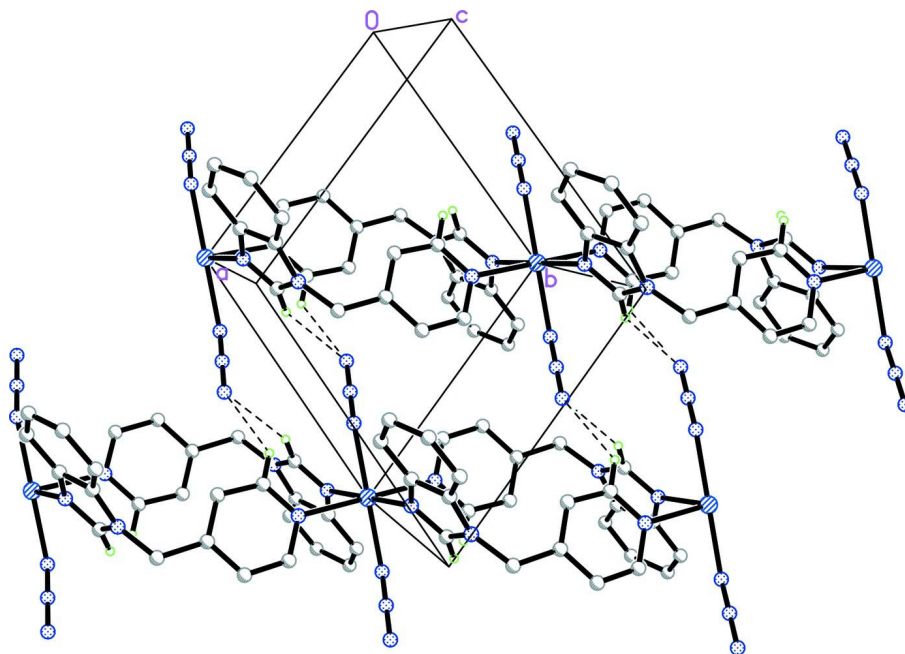


Figure 3

Part of the crystal packing showing the two-dimensional network in the title compound formed by interchain C—H...N hydrogen-bonded interactions (fine dashed lines). For the sake of clarity, only H atoms involved in the interactions are shown.

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Crystal data

[Mn(N₃)₂(C₁₃H₁₁N₃)₂]

$M_r = 557.50$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 8.4135$ (17) Å

$b = 8.5823$ (17) Å

$c = 10.399$ (2) Å

$\alpha = 67.86$ (3)°

$\beta = 86.03$ (3)°

$\gamma = 69.80$ (3)°

$V = 651.1$ (3) Å³

$Z = 1$

$F(000) = 287$

$D_x = 1.422$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 6008 reflections

$\theta = 3.2$ – 27.5 °

$\mu = 0.55$ mm⁻¹

$T = 294$ K

Block, yellow

$0.36 \times 0.32 \times 0.30$ mm

Data collection

Bruker SMART CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 1998)

$T_{\min} = 0.827$, $T_{\max} = 0.853$

6780 measured reflections

2954 independent reflections

2828 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.019$

$\theta_{\text{max}} = 27.5$ °, $\theta_{\text{min}} = 3.2$ °

$h = -10 \rightarrow 10$

$k = -11 \rightarrow 11$

$l = -13 \rightarrow 13$

*Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.029$ $wR(F^2) = 0.081$ $S = 1.03$

2954 reflections

179 parameters

0 restraints

Primary atom site location: structure-invariant
direct methodsSecondary atom site location: difference Fourier
mapHydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0415P)^2 + 0.2403P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} = 0.003$ $\Delta\rho_{\max} = 0.31 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{\min} = -0.23 \text{ e } \text{\AA}^{-3}$ Extinction correction: *SHELXL97*, $F_c^* = kF_c[1 + 0.001 \times F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.188 (10)

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> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|--------------|--------------|----------------------------------|
| Mn1 | 1.0000 | 0.0000 | 1.0000 | 0.02268 (12) |
| C1 | 0.13527 (18) | 0.75738 (18) | 0.81818 (14) | 0.0299 (3) |
| H1 | 0.1225 | 0.6635 | 0.8954 | 0.036* |
| C2 | 0.13205 (16) | 1.01940 (17) | 0.68138 (13) | 0.0259 (3) |
| C3 | 0.19824 (16) | 0.90468 (18) | 0.60918 (14) | 0.0281 (3) |
| C4 | 0.2474 (2) | 0.9643 (2) | 0.47385 (16) | 0.0421 (4) |
| H4 | 0.2914 | 0.8870 | 0.4269 | 0.050* |
| C5 | 0.2277 (3) | 1.1436 (3) | 0.41276 (17) | 0.0511 (4) |
| H5 | 0.2594 | 1.1883 | 0.3224 | 0.061* |
| C6 | 0.1610 (2) | 1.2603 (2) | 0.48348 (17) | 0.0463 (4) |
| H6 | 0.1498 | 1.3804 | 0.4390 | 0.056* |
| C7 | 0.1116 (2) | 1.20089 (19) | 0.61774 (16) | 0.0351 (3) |
| H7 | 0.0665 | 1.2789 | 0.6639 | 0.042* |
| C8 | 0.25306 (18) | 0.57026 (19) | 0.67617 (16) | 0.0332 (3) |
| H8A | 0.2516 | 0.5976 | 0.5768 | 0.040* |
| H8B | 0.1726 | 0.5091 | 0.7140 | 0.040* |
| C9 | 0.47260 (18) | 0.26337 (19) | 0.77339 (17) | 0.0351 (3) |
| H9 | 0.3960 | 0.2185 | 0.7525 | 0.042* |
| C10 | 0.63090 (19) | 0.14894 (19) | 0.83664 (17) | 0.0365 (3) |
| H10 | 0.6578 | 0.0269 | 0.8580 | 0.044* |
| C11 | 0.70528 (19) | 0.3804 (2) | 0.83490 (19) | 0.0392 (4) |
| H11 | 0.7856 | 0.4224 | 0.8536 | 0.047* |
| C12 | 0.5485 (2) | 0.5042 (2) | 0.77332 (19) | 0.0401 (4) |

| | | | | |
|-----|--------------|--------------|--------------|------------|
| H12 | 0.5243 | 0.6254 | 0.7538 | 0.048* |
| C13 | 0.42862 (16) | 0.44572 (18) | 0.74119 (14) | 0.0265 (3) |
| N1 | 0.09396 (15) | 0.92194 (15) | 0.81364 (12) | 0.0285 (2) |
| N2 | 0.19812 (14) | 0.73794 (15) | 0.69955 (12) | 0.0278 (2) |
| N3 | 0.74795 (14) | 0.20399 (15) | 0.86900 (12) | 0.0297 (3) |
| N4 | 1.10239 (16) | 0.22079 (17) | 0.92696 (13) | 0.0341 (3) |
| N5 | 1.16197 (15) | 0.28050 (15) | 0.98900 (12) | 0.0298 (3) |
| N6 | 1.2213 (2) | 0.3409 (2) | 1.04762 (16) | 0.0492 (4) |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|--------------|--------------|--------------|---------------|--------------|---------------|
| Mn1 | 0.02229 (16) | 0.02034 (16) | 0.02660 (17) | -0.00730 (11) | 0.00254 (10) | -0.01032 (11) |
| C1 | 0.0331 (7) | 0.0231 (6) | 0.0295 (6) | -0.0071 (5) | 0.0051 (5) | -0.0086 (5) |
| C2 | 0.0241 (6) | 0.0249 (6) | 0.0252 (6) | -0.0061 (5) | -0.0014 (5) | -0.0072 (5) |
| C3 | 0.0234 (6) | 0.0291 (6) | 0.0277 (6) | -0.0055 (5) | -0.0001 (5) | -0.0092 (5) |
| C4 | 0.0469 (9) | 0.0503 (9) | 0.0304 (7) | -0.0167 (7) | 0.0093 (6) | -0.0178 (7) |
| C5 | 0.0629 (11) | 0.0599 (11) | 0.0269 (7) | -0.0293 (9) | 0.0070 (7) | -0.0057 (7) |
| C6 | 0.0581 (10) | 0.0373 (8) | 0.0355 (8) | -0.0227 (8) | -0.0042 (7) | 0.0016 (7) |
| C7 | 0.0401 (8) | 0.0274 (7) | 0.0345 (7) | -0.0111 (6) | -0.0048 (6) | -0.0072 (6) |
| C8 | 0.0279 (7) | 0.0288 (7) | 0.0421 (8) | -0.0001 (5) | -0.0058 (6) | -0.0201 (6) |
| C9 | 0.0287 (7) | 0.0283 (7) | 0.0514 (9) | -0.0073 (6) | -0.0056 (6) | -0.0194 (6) |
| C10 | 0.0334 (7) | 0.0244 (7) | 0.0511 (9) | -0.0042 (6) | -0.0073 (6) | -0.0170 (6) |
| C11 | 0.0303 (7) | 0.0292 (7) | 0.0585 (10) | -0.0097 (6) | -0.0075 (6) | -0.0157 (7) |
| C12 | 0.0338 (7) | 0.0234 (7) | 0.0604 (10) | -0.0065 (6) | -0.0077 (7) | -0.0141 (7) |
| C13 | 0.0236 (6) | 0.0257 (6) | 0.0293 (6) | -0.0038 (5) | 0.0018 (5) | -0.0137 (5) |
| N1 | 0.0325 (6) | 0.0226 (5) | 0.0280 (6) | -0.0073 (4) | 0.0047 (4) | -0.0094 (4) |
| N2 | 0.0262 (5) | 0.0230 (5) | 0.0309 (6) | -0.0025 (4) | 0.0012 (4) | -0.0118 (4) |
| N3 | 0.0261 (5) | 0.0259 (6) | 0.0364 (6) | -0.0055 (4) | -0.0008 (4) | -0.0137 (5) |
| N4 | 0.0392 (7) | 0.0336 (6) | 0.0365 (6) | -0.0207 (5) | 0.0047 (5) | -0.0135 (5) |
| N5 | 0.0356 (6) | 0.0219 (5) | 0.0304 (6) | -0.0125 (5) | 0.0040 (5) | -0.0062 (5) |
| N6 | 0.0717 (10) | 0.0397 (7) | 0.0456 (8) | -0.0301 (7) | -0.0050 (7) | -0.0148 (6) |

Geometric parameters (Å, °)

| | | | |
|-----------------------|-------------|---------|-------------|
| Mn1—N4 | 2.2049 (13) | C6—H6 | 0.93 |
| Mn1—N4 ⁱ | 2.2049 (13) | C7—H7 | 0.93 |
| Mn1—N1 ⁱⁱ | 2.2869 (12) | C8—N2 | 1.4603 (17) |
| Mn1—N1 ⁱⁱⁱ | 2.2869 (12) | C8—C13 | 1.5115 (19) |
| Mn1—N3 ⁱ | 2.3358 (16) | C8—H8A | 0.97 |
| Mn1—N3 | 2.3358 (16) | C8—H8B | 0.97 |
| C1—N1 | 1.3156 (18) | C9—C10 | 1.379 (2) |
| C1—N2 | 1.3540 (18) | C9—C13 | 1.3858 (19) |
| C1—H1 | 0.93 | C9—H9 | 0.93 |
| C2—C7 | 1.395 (2) | C10—N3 | 1.3392 (19) |
| C2—N1 | 1.3968 (18) | C10—H10 | 0.93 |
| C2—C3 | 1.4014 (19) | C11—N3 | 1.3354 (19) |
| C3—N2 | 1.3849 (19) | C11—C12 | 1.384 (2) |

| | | | |
|---|--------------|-------------------------|--------------|
| C3—C4 | 1.391 (2) | C11—H11 | 0.93 |
| C4—C5 | 1.379 (3) | C12—C13 | 1.380 (2) |
| C4—H4 | 0.93 | C12—H12 | 0.93 |
| C5—C6 | 1.403 (3) | N1—Mn1 ^{iv} | 2.2869 (12) |
| C5—H5 | 0.93 | N4—N5 | 1.1838 (17) |
| C6—C7 | 1.383 (2) | N5—N6 | 1.1612 (18) |
| | | | |
| N4—Mn1—N4 ⁱ | 180 | C6—C7—H7 | 121.3 |
| N4—Mn1—N1 ⁱⁱ | 88.32 (5) | C2—C7—H7 | 121.3 |
| N4 ⁱ —Mn1—N1 ⁱⁱ | 91.68 (5) | N2—C8—C13 | 113.50 (11) |
| N4—Mn1—N1 ⁱⁱⁱ | 91.68 (5) | N2—C8—H8A | 108.9 |
| N4 ⁱ —Mn1—N1 ⁱⁱⁱ | 88.32 (5) | C13—C8—H8A | 108.9 |
| N1 ⁱⁱ —Mn1—N1 ⁱⁱⁱ | 180 | N2—C8—H8B | 108.9 |
| N4—Mn1—N3 ⁱ | 92.39 (5) | C13—C8—H8B | 108.9 |
| N4 ⁱ —Mn1—N3 ⁱ | 87.61 (5) | H8A—C8—H8B | 107.7 |
| N1 ⁱⁱ —Mn1—N3 ⁱ | 89.63 (5) | C10—C9—C13 | 119.48 (13) |
| N1 ⁱⁱⁱ —Mn1—N3 ⁱ | 90.37 (5) | C10—C9—H9 | 120.3 |
| N4—Mn1—N3 | 87.61 (5) | C13—C9—H9 | 120.3 |
| N4 ⁱ —Mn1—N3 | 92.39 (5) | N3—C10—C9 | 123.55 (13) |
| N1 ⁱⁱ —Mn1—N3 | 90.37 (5) | N3—C10—H10 | 118.2 |
| N1 ⁱⁱⁱ —Mn1—N3 | 89.63 (5) | C9—C10—H10 | 118.2 |
| N3 ⁱ —Mn1—N3 | 180 | N3—C11—C12 | 123.86 (14) |
| N1—C1—N2 | 113.45 (12) | N3—C11—H11 | 118.1 |
| N1—C1—H1 | 123.3 | C12—C11—H11 | 118.1 |
| N2—C1—H1 | 123.3 | C13—C12—C11 | 119.19 (14) |
| C7—C2—N1 | 130.51 (13) | C13—C12—H12 | 120.4 |
| C7—C2—C3 | 120.29 (13) | C11—C12—H12 | 120.4 |
| N1—C2—C3 | 109.19 (12) | C12—C13—C9 | 117.52 (13) |
| N2—C3—C4 | 132.11 (14) | C12—C13—C8 | 123.05 (12) |
| N2—C3—C2 | 105.56 (11) | C9—C13—C8 | 119.42 (13) |
| C4—C3—C2 | 122.33 (14) | C1—N1—C2 | 105.01 (11) |
| C5—C4—C3 | 116.72 (15) | C1—N1—Mn1 ^{iv} | 123.01 (10) |
| C5—C4—H4 | 121.6 | C2—N1—Mn1 ^{iv} | 131.84 (9) |
| C3—C4—H4 | 121.6 | C1—N2—C3 | 106.79 (11) |
| C4—C5—C6 | 121.63 (15) | C1—N2—C8 | 124.89 (12) |
| C4—C5—H5 | 119.2 | C3—N2—C8 | 128.32 (12) |
| C6—C5—H5 | 119.2 | C11—N3—C10 | 116.38 (12) |
| C7—C6—C5 | 121.56 (16) | C11—N3—Mn1 | 121.80 (10) |
| C7—C6—H6 | 119.2 | C10—N3—Mn1 | 121.47 (9) |
| C5—C6—H6 | 119.2 | N5—N4—Mn1 | 131.21 (10) |
| C6—C7—C2 | 117.48 (15) | N6—N5—N4 | 178.77 (15) |
| | | | |
| C7—C2—C3—N2 | -178.72 (12) | N1—C1—N2—C3 | 0.08 (16) |
| N1—C2—C3—N2 | 0.39 (15) | N1—C1—N2—C8 | -179.71 (12) |
| C7—C2—C3—C4 | 0.6 (2) | C4—C3—N2—C1 | -179.55 (16) |
| N1—C2—C3—C4 | 179.75 (13) | C2—C3—N2—C1 | -0.29 (14) |
| N2—C3—C4—C5 | 179.05 (15) | C4—C3—N2—C8 | 0.2 (2) |
| C2—C3—C4—C5 | -0.1 (2) | C2—C3—N2—C8 | 179.50 (12) |

| | | | |
|----------------------------|--------------|-------------------------------|--------------|
| C3—C4—C5—C6 | -0.1 (3) | C13—C8—N2—C1 | -79.95 (18) |
| C4—C5—C6—C7 | -0.1 (3) | C13—C8—N2—C3 | 100.30 (16) |
| C5—C6—C7—C2 | 0.6 (3) | C12—C11—N3—C10 | 2.0 (2) |
| N1—C2—C7—C6 | -179.76 (15) | C12—C11—N3—Mn1 | -171.37 (14) |
| C3—C2—C7—C6 | -0.9 (2) | C9—C10—N3—C11 | -0.9 (2) |
| C13—C9—C10—N3 | -0.4 (3) | C9—C10—N3—Mn1 | 172.44 (12) |
| N3—C11—C12—C13 | -1.7 (3) | N4—Mn1—N3—C11 | -23.66 (13) |
| C11—C12—C13—C9 | 0.2 (2) | N4 ⁱ —Mn1—N3—C11 | 156.34 (13) |
| C11—C12—C13—C8 | 178.92 (15) | N1 ⁱⁱ —Mn1—N3—C11 | 64.64 (13) |
| C10—C9—C13—C12 | 0.7 (2) | N1 ⁱⁱⁱ —Mn1—N3—C11 | -115.36 (13) |
| C10—C9—C13—C8 | -178.01 (14) | N4—Mn1—N3—C10 | 163.34 (12) |
| N2—C8—C13—C12 | -22.6 (2) | N4 ⁱ —Mn1—N3—C10 | -16.66 (12) |
| N2—C8—C13—C9 | 156.11 (14) | N1 ⁱⁱ —Mn1—N3—C10 | -108.36 (12) |
| N2—C1—N1—C2 | 0.17 (16) | N1 ⁱⁱⁱ —Mn1—N3—C10 | 71.64 (12) |
| N2—C1—N1—Mn1 ^{iv} | -175.95 (9) | N1 ⁱⁱ —Mn1—N4—N5 | 33.89 (14) |
| C7—C2—N1—C1 | 178.65 (14) | N1 ⁱⁱⁱ —Mn1—N4—N5 | -146.11 (14) |
| C3—C2—N1—C1 | -0.35 (15) | N3 ⁱ —Mn1—N4—N5 | -55.67 (14) |
| C7—C2—N1—Mn1 ^{iv} | -5.7 (2) | N3—Mn1—N4—N5 | 124.33 (14) |
| C3—C2—N1—Mn1 ^{iv} | 175.28 (9) | | |

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

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> |
|-----------------------------------|-------------|---------------------|----------------------------|-------------------------------|
| C1—H1 \cdots N6 ^v | 0.93 | 2.48 | 3.319 (1) | 150 |
| C11—H11 \cdots N6 ^{vi} | 0.93 | 2.58 | 3.305 (2) | 135 |

Symmetry codes: (v) $x-1, y, z$; (vi) $-x+2, -y+1, -z+2$.