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

Chun-Sen Liu,[a,b]* Jun-Jie Wang[b] and Li-Fen Yan[b]

[a]Zhengzhou University of Light Industry, Henan Provincial Key Laboratory of Surface and Interface Science, Henan, Zhengzhou 450002, People's Republic of China, and [b]Department of Chemistry, Nankai University, Tianjin 300071, People's Republic of China

Correspondence e-mail: chunsenliu@mail.nankai.edu.cn

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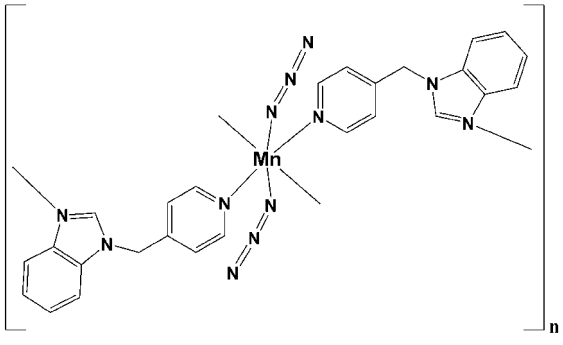
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.002 Å; R factor = 0.029; wR factor = 0.081; data-to-parameter ratio = 16.5.

In the title polymeric compound, $[Mn(N_3)_2(C_{13}H_{11}N_3)_2]_n$, 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 C—H···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

$[Mn(N_3)_2(C_{13}H_{11}N_3)_2]$
M_r = 557.50
Triclinic, $P\overline{1}$
a = 8.4135 (17) Å
b = 8.5823 (17) Å
c = 10.399 (2) Å
α = 67.86 (3)°
β = 86.03 (3)°
γ = 69.80 (3)°
V = 651.1 (3) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.55 mm^{-1}
T = 294 (2) K
0.36 × 0.32 × 0.30 mm

Data collection

Bruker SMART CCD area-detector diffractometer
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_{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
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −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—H···A	D—H	H···A	D···A	D—H···A
C1—H1···N6^{iv}	0.93	2.48	3.319 (1)	150
C11—H11···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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supplementary materials

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

C.-S. Liu, J.-J. Wang and L.-F. Yan

Comment

N-containing heterocyclic aromatic compounds are extensively used as bridging ligands in coordination and metallosupramolecular 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)-1*H*-benzo[*d*]imidazole (*L*) as well as its chiral one-dimensional double helix polymer, $[Ag(L)(NO_3)]_n$ (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 $[Mn(C_{13}H_{11}N_3)_2(N_3)_2]_n$ (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 N_3^- anion (*L* is 1-(pyridin-4-ylmethyl)-1*H*-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 N_3^- anions, respectively (Table 1). In the crystal structure of (I), *L* adopts μ_2-bridging 4,4'-bipyridine-like coordination mode and N_3^- 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 $[Mn(C_{13}H_{11}N_3)_2(N_3)_2]_n$ 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).

Experimental

The ligand 1-(pyridin-4-ylmethyl)-1*H*-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), NaN_3 (13 mg, 0.2 mmol) with $Mn(ClO_4)_2$ (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 $C_{26}H_{22}MnN_{12}$: C 56.02, H 3.98, N 30.15%; found: C 55.88, H 3.79, N 30.37%.

Refinement

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

Figures

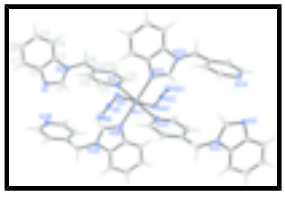

Fig. 1. The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. The atoms labelled with the suffixes A, B and C are generated by the symmetry operations (1 + *x*, -1 + *y*, *z*), (1 - *x*, 1 - *y*, 2 - *z*) and (2 - *x*, -*y*,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

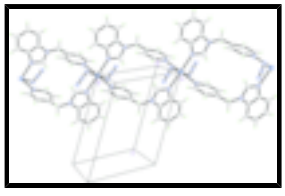

Fig. 2. View of a polymeric chain running along the [1 1 0].

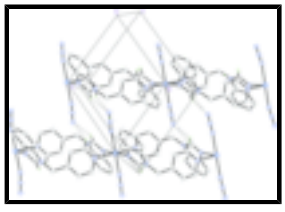

Fig. 3. Part of the crystal packing showing the two-dimensional network in the title compound formed by interchain C—H···N hydrogen-bonded interactions (fine dashed lines). For the sake of clarity, only H atoms involved in the interactions are shown.

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Crystal data

$[Mn(N_3)_2(C_{13}H_{11}N_3)_2]$	$Z = 1$
$M_r = 557.50$	$F_{000} = 287$
Triclinic, $P\overline{1}$	$D_x = 1.422$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.71073 Å
$a = 8.4135$ (17) Å	Cell parameters from 6008 reflections
$b = 8.5823$ (17) Å	θ = 3.2–27.5º
$c = 10.399$ (2) Å	μ = 0.55 mm^{-1}
α = 67.86 (3)º	$T = 294$ (2) K
β = 86.03 (3)º	Block, yellow
γ = 69.80 (3)º	0.36 × 0.32 × 0.30 mm
$V = 651.1$ (3) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	2954 independent reflections
Radiation source: fine-focus sealed tube	2828 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.019$
$T = 294(2)$ K	$\theta_{max} = 27.5^{o}$
φ and ω scans	$\theta_{min} = 3.2^{o}$
Absorption correction: multi-scan (SADABS; Bruker, 1998)	$h = -10 \rightarrow 10$
$T_{min} = 0.827$, $T_{max} = 0.853$	$k = -11 \rightarrow 11$
6780 measured reflections	$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.029$	$w = 1/[\sigma^2(F_o^2) + (0.0415P)^2 + 0.2403P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.081$	$(\Delta/\sigma)_{max} = 0.003$
$S = 1.03$	$\Delta\rho_{max} = 0.31$ e Å^{-3}
2954 reflections	$\Delta\rho_{min} = -0.23$ e Å^{-3}
179 parameters	Extinction correction: SHELXL97, $Fc^{*}=kFc[1+0.001xFc^{2}\lambda^{3}/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.188 (10)
Secondary atom site location: difference Fourier map	

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}
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 (Å^2)

	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, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···N6^{v}	0.93	2.48	3.319 (1)	150

C11—H11···N6^{vi}	0.93	2.58	3.305 (2)	135

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

Fig. 1

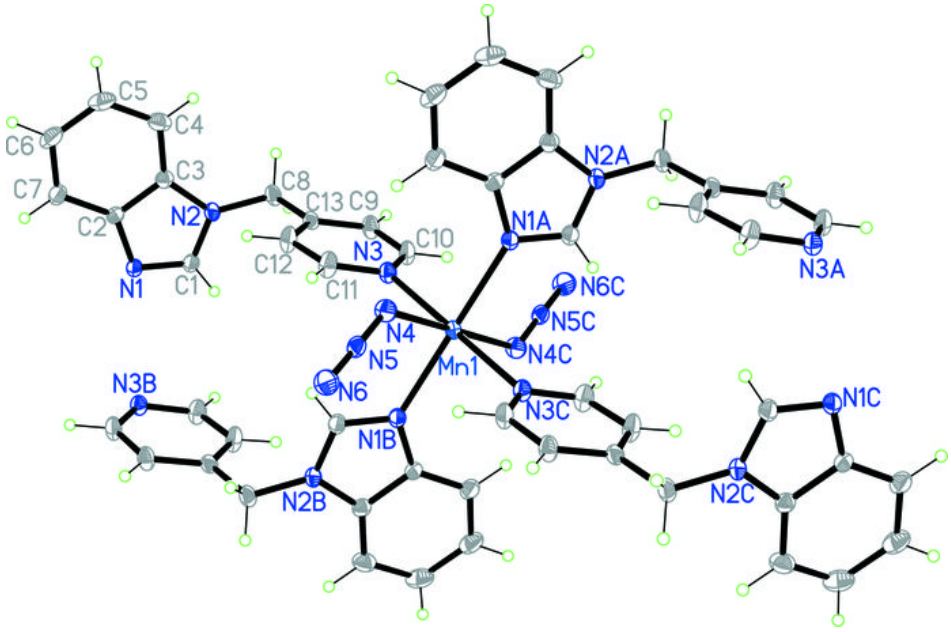

Fig. 2

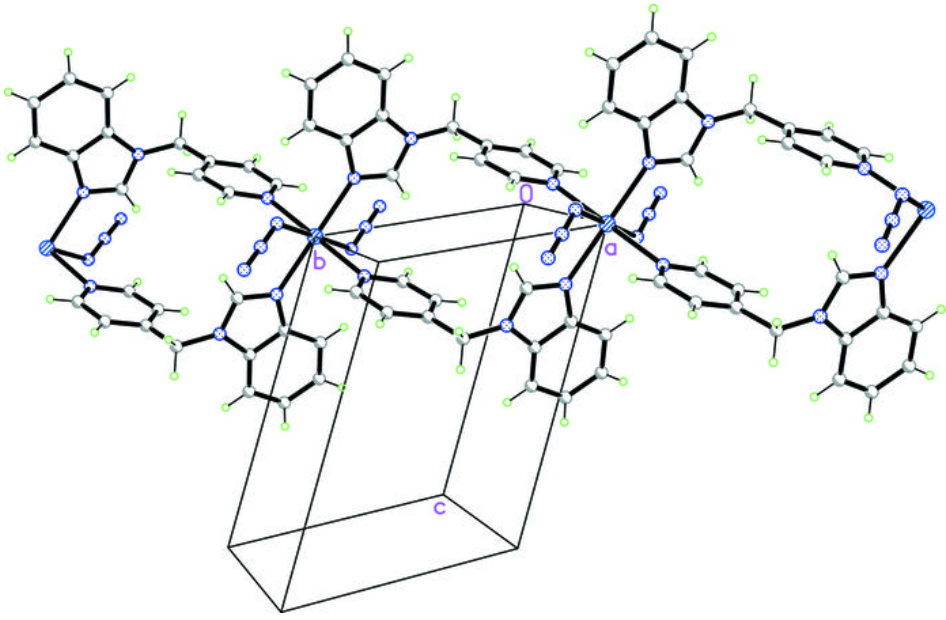

Fig. 3