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A novel two-dimensional Mn^{II} coordination polymer with 1,2-bis(imidazol-1-yl)ethane

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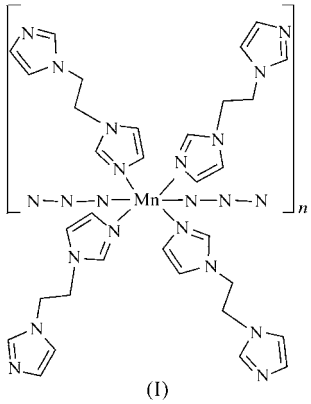
In the crystal structure of the title complex, poly[[diazidomanganese(II)]-di-μ-1,2-bis(imidazol-1-yl)ethane-$\kappa^4N^3:N^{3'}$], $[Mn(N_3)_2(C_8H_{10}N_4)_2]_n$ or $[Mn(N_3)_2(bim)_2]_n$, where bim is 1,2-bis(imidazol-1-yl)ethane, each Mn^{II} atom is six-coordinated in a distorted octahedral coordination environment to four N atoms from four bim ligands and two N atoms from two azide ligands. The Mn^{II} atoms, which lie on inversion centres, are bridged by four bim ligands to form a two-dimensional (4,4)-network. The azide ligands are monodentate (terminal).

Comment

The design of coordination polymers has been developing rapidly because of their fascinating structures and potential applications as functional materials (Batten & Robson, 1998; Blake *et al.*, 1999). A number of infinite one-, two- and three-dimensional frameworks have been synthesized with rigid rod-like organic building blocks, such as 4,4′-bipyridine (Fujita *et al.*, 1994) and 4,4′-azobispyridine (Li *et al.*, 2001). Relatively



(I)

few studies of flexible ligands have been reported to date. Recently, we synthesized several coordination polymers with the flexible ligand 1,2-bis(1,2,4-triazol-1-yl)ethane (bte; Li *et al.*, 1999, 2003; Zhu *et al.*, 2004). In order to extend our research, we have now chosen a similar ligand, namely 1,2-bis(imidazol-1-yl)ethane (bim; Wu *et al.*, 1997). We report here the preparation and crystal structure of the title novel two-dimensional coordination polymer incorporating the bim ligand, *viz*. $[Mn(N_3)_2(bim)_2]_n$, (I).

As shown in Fig. 1, the Mn^{II} atom of (I) occupies an inversion centre. The coordination geometry of the Mn^{II} atom is distorted octahedral; it is coordinated equatorially by four N atoms from the imidazole rings of four symmetry-related

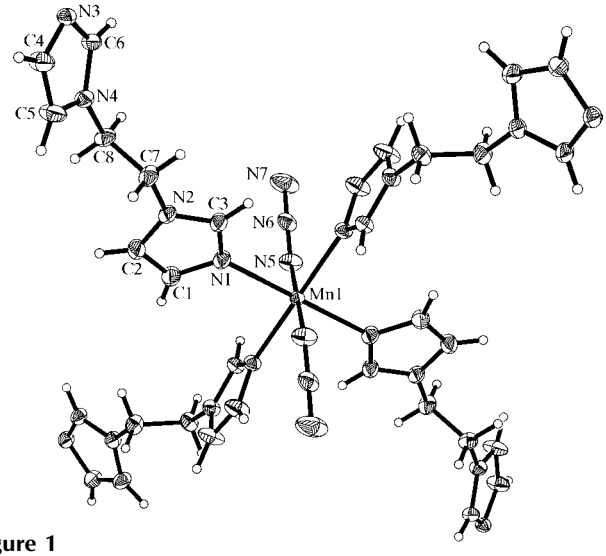


Figure 1
A view of the local coordination of the Mn^{II} atom in (I), with displacement ellipsoids drawn at the 50% probability level. H atoms are shown as small spheres of arbitrary radii.

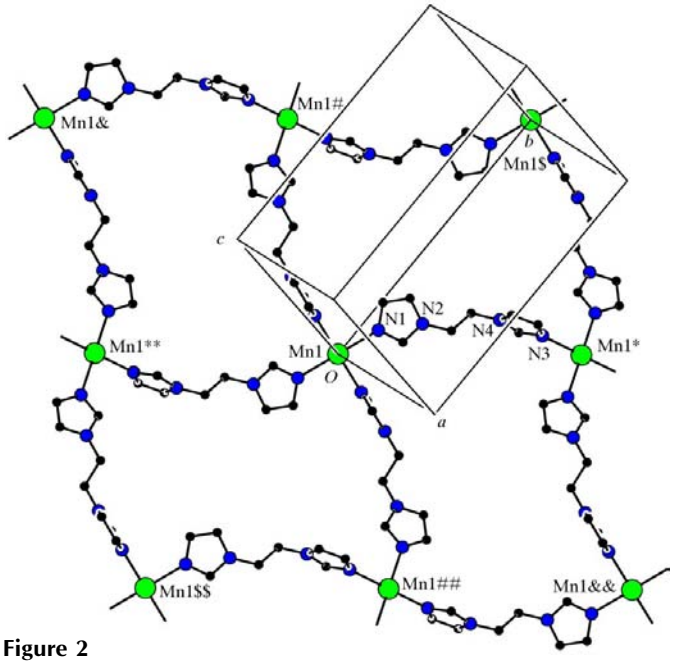


Figure 2
Part of the two-dimensional sheet of the (4,4)-network in (I). The azide groups and H atoms have been omitted for clarity. Atom Mn1 is at the cell origin and the symbols asterisk (*), double asterisk (**), hash (#), double has (##), dollar sign ($), double dollar sign ($$), ampersand (&) and double ampersand (&&) indicate Mn atoms at $(1, \frac{1}{2}, -\frac{1}{2})$, $(-1, -\frac{1}{2}, \frac{1}{2})$, $(-1, \frac{1}{2}, \frac{1}{2})$ $(1, -\frac{1}{2}, -\frac{1}{2})$, $(0, 1, 0)$, $(0, -1, 0)$, $(-2, 0, 1)$ and $(2, 0, -1)$, respectively.

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bim ligands and axially by two N atoms from two symmetry-related azide ligands. The azide anion acts as a monodentate ligand (Ribas *et al.*, 1999). The bim ligands exhibit the *anti* conformation in (I). The two imidazole ring planes, C1–C3/N1/N2 and C4–C6/N3/N4, are planar, with r.m.s. deviations of 0.0015 (12) and 0.0019 (13) Å, respectively. The dihedral angle between these two imidazole ring planes is 177.85 (15)°. The N2—C7—C8—N4 torsion angle is 57.79 (9)°.

As illustrated in Fig. 2, each bim ligand in (I) coordinates two Mn^{II} atoms through its two imidazole N atoms, thus acting as a bridging bidentate ligand. The Mn^{II} atoms are bridged by four bim ligands to form a two-dimensional neutral (4,4)-network. The networks contain square grids (36-membered ring), with an Mn^{II} atom at each corner and a bim ligand at each edge connecting two Mn^{II} atoms. Due to the symmetry of the crystal structure, the edge lengths are equal, and the value of 11.7484 (16) Å is similar to what was observed in the related bte ligand compound $[Cu(TTA)_2]_2$(bte) [TTA is 1,1,1-trifluoro-3-(2-thenoyl)acetone; Li *et al.*, 1999].

The square-grid sheets are stacked in an offset fashion parallel to the *c* direction. The offset superposition of each pair of adjacent networks by half of the edge divides the voids into smaller rectangles. The azide anions of one sheet project into the holes of the next sheet. In the superposition structure, the sheets are arranged in the sequence $\cdots A–B–A–B\cdots$.

Experimental

An aqueous solution (10 ml) of NaN_3 (0.163 g, 2.5 mmol) was mixed with an aqueous solution (10 ml) of $MnSO_4·H_2O$ (0.085 g, 0.5 mmol) and stirred for 20 min. An ethanol solution (10 ml) of 1,2-bis(imidazol-1-yl)ethane (0.081 g, 0.5 mmol) was then added slowly to the above solution. The mixture was stirred at room temperature for 30 min and the resultant solution was filtered. After allowing the filtrate to stand in air at room temperature for two weeks, well formed yellow single crystals of (I) were obtained. The product is stable under ambient conditions and is insoluble in most common inorganic and organic solvents. Analysis found: C 41.43, H 4.37, N 42.36%; calculated for $C_{16}H_{20}MnN_{14}$: C 41.47, H 4.35, N 42.33%.

Crystal data

$[Mn(N_3)_2(C_8H_{10}N_4)_2]$	D_x = 1.464 Mg m^{-3}
M_r = 463.40	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 4684 reflections
a = 6.9636 (16) Å	θ = 3.2–27.5°
b = 14.819 (3) Å	μ = 0.66 mm^{-1}
c = 10.256 (2) Å	T = 193.2 K
β = 96.702 (5)°	Polyhedron, yellow
V = 1051.1 (4) Å^3	0.51 × 0.32 × 0.25 mm
Z = 2	

Table 1
Selected geometric parameters (Å, °).

Mn1—N5	2.2334 (16)	N5—N6	1.170 (2)
Mn1—N3^{i}	2.2400 (15)	N6—N7	1.164 (2)
Mn1—N1	2.2622 (16)		
N5—Mn1—N5^{ii}	180.00 (12)	N3^{i}—Mn1—N1	90.05 (6)
N5—Mn1—N3^{i}	86.80 (6)	N1—Mn1—N1^{ii}	180.00 (3)
N3^{i}—Mn1—N3^{iii}	180.00 (4)	N6—N5—Mn1	135.64 (14)
N5—Mn1—N1	91.86 (6)	N7—N6—N5	177.4 (2)

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

Data collection

Rigaku Mercury CCD area-detector diffractometer	2393 independent reflections
	2287 reflections with $I > 2\sigma(I)$
ω scans	R_{int} = 0.027
Absorption correction: multi-scan (North *et al.*, 1968)	θ_{max} = 27.5°
	$h = -9 \rightarrow 9$
T_{min} = 0.769, T_{max} = 0.851	$k = -19 \rightarrow 19$
11 499 measured reflections	$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0335P)^2 + 1.025P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R(F)$ = 0.040	
$wR(F^2)$ = 0.087	
S = 1.07	$(\Delta/\sigma)_{max} < 0.001$
2393 reflections	$\Delta\rho_{max}$ = 0.34 e Å^{-3}
142 parameters	$\Delta\rho_{min}$ = −0.23 e Å^{-3}
H-atom parameters constrained	

H atoms were placed in idealized positions and refined as riding, with C—H distances of 0.93 (imidazole) and 0.97 Å (CH_2), and with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *CrystalClear* (Rigaku, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: JZ1634). Services for accessing these data are described at the back of the journal.

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