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Poly[[bis(benzimidazole)manganese(II)]-di-μ-1,5-dicyanamido]

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Key indicators

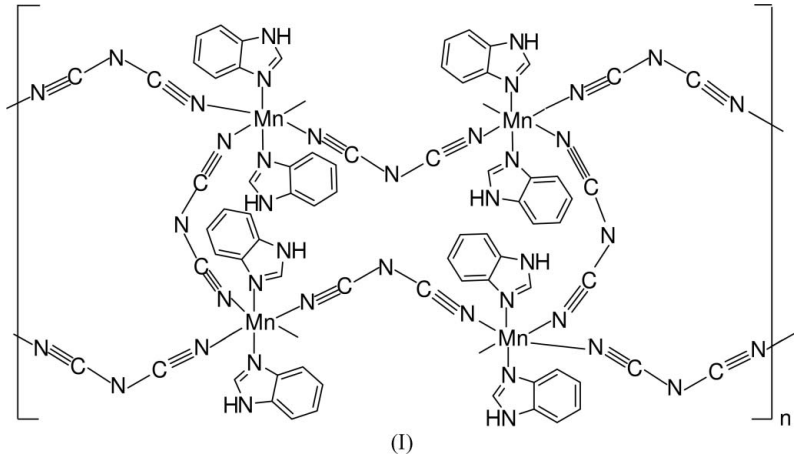
Single-crystal X-ray study
T = 193 K
Mean σ(C–C) = 0.002 Å
R factor = 0.026
wR factor = 0.075
Data-to-parameter ratio = 12.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the crystal structure of the title complex, $[Mn(C_2N_3)_2(C_7H_6N_2)_2]_n$ or $[Mn(dca)_2(bim)_2]_n$, where dca is dicyanamide and bim is benzimidazole, each Mn^{II} atom is located on a center of symmetry and is in a six-coordinated distorted octahedral environment. Four N atoms from four dca ligands fill the equatorial positions, and two N atoms from two bim ligands occupy the axial positions. The dicyanamide ligands adopt an end-to-end coordination mode and link the Mn atoms to form a two-dimensional network.

Comment

Metal coordination polymers with multidimensionality have attracted great interest in coordination chemistry because of their intriguing structural topologies and their interesting applications as functional materials (Batten & Robson, 1998; Blake *et al.*, 1999; Carlucci *et al.*, 2004). The dicyanamide ligand $[N(CN)_2]^-$, (dca), is a remarkably versatile building block for the construction of coordination polymers, since it can act in a mono-, bi- or tridentate coordination manner (Riggio *et al.*, 2001; Li *et al.*, 2003). The introduction of N-based bridging and terminal ligands into the metal–dca system has led to many fascinating structures with interesting magnetic properties (Manson *et al.*, 1998; Manna *et al.*, 2006; Escuer *et al.*, 2000, 2002). In this work, a new Mn^{II} coordination polymer $[Mn(dca)_2(bim)_2]_n$, (I) (bim = benzimidazole), is presented.



(I)

Fig. 1 shows the coordination of the Mn^{II} atom, which is situated on a center of symmetry. The coordination geometry of the Mn^{II} atom is slightly distorted octahedral, coordinated equatorially by four N atoms from four symmetry-related dca ligands and axially by two N atoms from two benzimidazole molecules (Table 1). The Mn—N_{dca} bond lengths are similar to

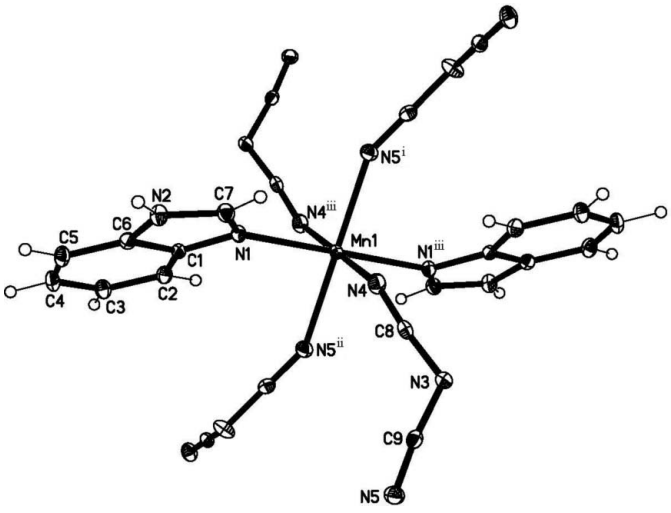


Figure 1
Local coordination of Mn^{II} in (I), with displacement ellipsoids drawn at the 30% probability level. [Symmetry codes: (i) $\frac{1}{2}+x, \frac{1}{2}-y, \frac{1}{2}+z$; (ii) $\frac{3}{2}-x, \frac{1}{2}+y, \frac{1}{2}-z$; (iii) $2-x, 1-y, 1-z$.]

Figure 2
The packing of (I). H atoms have been omitted.

the corresponding values in other Mn–dca complexes (Escuer *et al.*, 2000, 2002; Manson *et al.*, 1999, 2001).

The dicyanamide ligand (dca) adopts an end-to-end coordination mode. Each dca ligand links two Mn^{II} atoms to give a two-dimensional network, resulting in an 'hourglass-shaped' 24-membered $Mn_4(dca)_4$ metallacycle (Manson *et al.*, 2001). The Mn···Mn distance bridged by one dca ligand is 7.6512 (9) Å, which is similar to the corresponding distance (8.405 Å) in $[Mn(dca)_2(H_2O)_2](2,5\text{-bismethylpyrazine})_2$ (Manson *et al.*, 2001). There is a weak N—H···N hydrogen bond (Table 2).

Experimental

A water/methanol (1:1, *v*/*v*) solution (20 ml) of bim (0.117 g, 1.0 mmol) and $MnSO_4\cdot H_2O$ (0.085 g, 0.5 mmol) was added to one leg of an H-shaped tube and a water/methanol (1:1, *v*/*v*) solution (20 ml) of sodium dicyanamide (0.089 g, 1.0 mmol) was added to the other leg of the tube. Colorless crystals suitable for X-ray analysis were obtained after about one month. Elemental analysis found: C 49.95, H 2.81, N 33.04%; calculated for $C_{18}H_{12}MnN_{10}$: C 51.07, H 2.85, N 33.10%.

Crystal data

$[Mn(C_2N_3)_2(C_7H_6N_2)_2]$
M_r = 423.32
Monoclinic, $P2_1/n$
a = 9.2994 (17) Å
b = 9.9531 (18) Å
c = 9.9585 (19) Å
β = 105.839 (4)°
V = 886.7 (3) Å^3
Z = 2
D_x = 1.585 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.77 mm^{-1}
T = 193 (2) K
Block, colorless
0.50 × 0.40 × 0.30 mm

Data collection

Rigaku Mercury CCD diffractometer
ω scans
Absorption correction: multi-scan (Jacobson, 1998)
T_{min} = 0.698, T_{max} = 0.801
8337 measured reflections
1618 independent reflections
1567 reflections with $I > 2\sigma(I)$
R_{int} = 0.020
θ_{max} = 25.3°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.075
S = 1.02
1618 reflections
135 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0487P)^2 + 0.3634P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.032 (3)

Table 1
Selected geometric parameters (Å, °).

Mn1—N5^{i}	2.2199 (15)	N3—C9	1.310 (2)
Mn1—N4	2.2369 (14)	N4—C8	1.157 (2)
Mn1—N1	2.2598 (12)	N5—C9	1.156 (2)
N3—C8	1.307 (2)		
N5^{i}—Mn1—N4	90.28 (5)	C8—N3—C9	119.33 (13)
N5^{i}—Mn1—N1	92.79 (5)	N4—C8—N3	174.47 (15)
N4—Mn1—N1	89.30 (5)	N5—C9—N3	173.85 (16)

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

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2B···N3^{ii}	0.88	2.22	3.043 (2)	155

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

H atoms were placed in idealized positions and refined as riding, with C—H distances of 0.95 Å and N—H distances of 0.88 Å, and with $U_{iso}(H) = 1.2U_{eq}(C,N)$.

Data collection: *CrystalClear* (Rigaku Corporation, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; 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*.

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