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catena-Poly[[diisothiocyanatocadmium(II)]-bis[μ-1,3-bis(1,2,4-triazol-1-ylmethyl)benzene-$\kappa^2N^4:N^{4'}$]]: a double-chain coordination polymer

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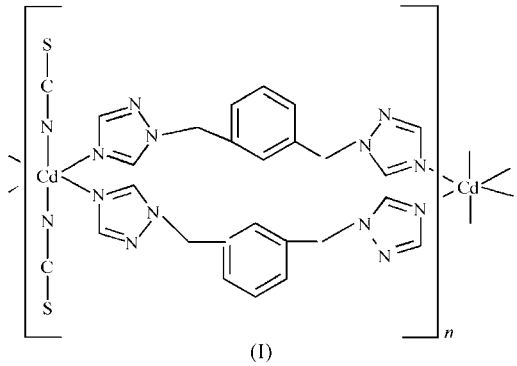
The coordination geometry of the Cd^{II} atom in the title complex, $[Cd(NCS)_2(C_{12}H_{12}N_6)_2]_n$ or $[Cd(NCS)_2(mbtz)_2]_n$, where mbtz is 1,3-bis(1,2,4-triazol-1-ylmethyl)benzene, is a distorted compressed octahedron in which the Cd^{II} atom lies on an inversion centre, coordinated by four N atoms from the triazole rings of four mbtz ligands and two N atoms from two monodentate NCS^- ligands. The structure is polymeric, with 24-membered spiro-fused rings extending along [100] and with the 24-membered ring containing two inversion-related mbtz molecules.

Comment

Recently, considerable attention has been paid to the metal coordination polymers for their intriguing structures and potential application as functional materials (Batten & Robson, 1998; Blake *et al.*, 1999; Kitagawa *et al.*, 2004). The design of coordination polymers is greatly influenced by several factors, such as the metal coordination preference, the structural characteristics of the polydentate organic ligand, the metal–ligand ratio, the solvent system and the counter-ion. The ligand is no doubt the key factor in constructing topological motifs.



(I)

1,2,4-Triazole and its derivatives are very interesting ligands because they combine the coordination geometry of pyrazole and imidazole with regard to the arrangement of the three heteroatoms. Some novel coordination polymers containing flexible bis(triazole) ligands have been reported recently (Haasnoot, 2000; Albada *et al.*, 2000; Zhao *et al.*, 2002; Meng *et al.*, 2004). Our interest is in the study of the coordination chemistry of 1,2,4-triazole and its derivatives, with potential applications in materials science. We have already reported the crystal structures of coordination polymers containing the flexible ligands 1,2-bis(1,2,4-triazol-1-yl)ethane (Li *et al.*, 2004; Wang *et al.*, 2005) and 1,4-bis(1,2,4-triazol-1-ylmethyl)benzene (Li *et al.*, 2005; Peng *et al.*, 2006). We report here the crystal structure of a novel one-dimensional double-stranded chain polymer, $[Cd(NCS)_2(mbtz)_2]_n$, (I), which has been synthesized

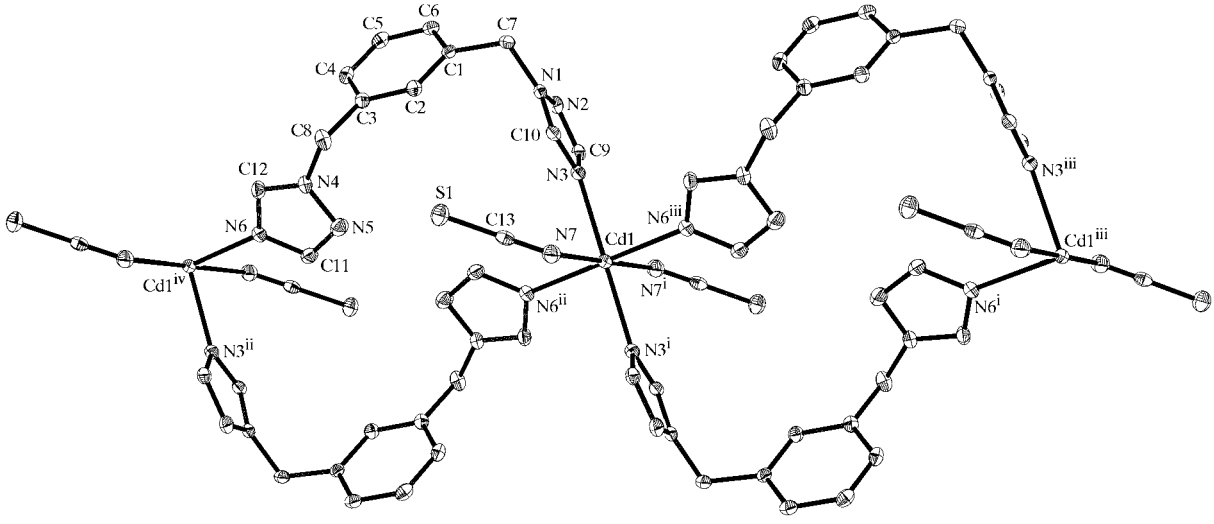


Figure 1
The coordination environment of the Cd atom of (I) at the 30% probability level. For the sake of clarity, H atoms have been omitted. [Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x, -y+1, -z+1$; (iii) $x+1, y, z$; (iv) $x-1, y, z$.]

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using the ligand 1,3-bis(1,2,4-triazol-1-ylmethyl)benzene (mbtz).

In the complex, the Cd atom lies on an inversion centre (Fig. 1). The coordination geometry of the Cd^{II} atom is a distorted compressed octahedron, with four N atoms from the triazole rings of mbtz ligands forming the equatorial plane and two N atoms from two monodentate NCS^- ligands occupying the axial sites. The Cd—N bond lengths (Table 1) are similar to those in Cd–triazole complexes reported previously (Li *et al.*, 2004, 2005; Meng *et al.*, 2004). The r.m.s. deviations of the atoms from the mean planes of the triazole rings N1–N3/C9/C10 and N4–N6/C11/C12 and the benzene ring C1–C6 are 0.0024 (14), 0.0043 (16) and 0.0023 (18) Å, respectively. The dihedral angles between the benzene ring and the N1–N3/C9/C10 and N4–N6/C11/C12 triazole rings are 84.24 (9) and 79.32 (8)°, respectively, and the dihedral angle between the two triazole rings is 70.01 (10)°. The mbtz ligands exhibit the *gauche–gauche* conformation in complex (I). The centroid-to-centroid distance between adjacent triazole rings is 6.921 (2) Å.

Compound (I) has a one-dimensional double-chain structure, with two strands of mbtz ligands held together by Cd^{II} atoms (Li *et al.*, 2004, 2005; Zhao *et al.*, 2002). The chain runs along [100] and consists of 24-membered spiro-fused rings, in which two Cd^{II} atoms are joined *via* two mbtz molecules. The Cd···Cd separation across the bridging mbtz ligand is equal to the *a*-axis translation. The shortest inter-chain Cd···Cd distances are 8.7717 (13) and 8.988 (2) Å, along [010] and [001], respectively (Fig. 2).

The C1–C6 benzene ring plane is parallel to the adjacent C1–C6 benzene ring plane at $(-x, -y, 1 - z)$, with an inter-planar spacing of 3.409 (2) Å and a ring-centroid separation of 3.973 (2) Å, indicating π–π stacking along [010].

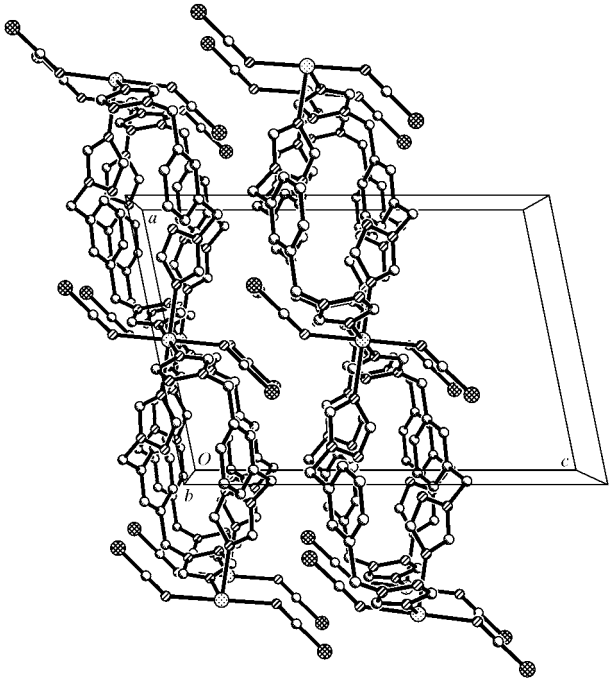

Figure 2
The packing of (I), viewed along [010]. For the sake of clarity, H atoms have been omitted.

Experimental

A water–methanol solution (20 ml, 1:1 *v*/*v*) of $Cd(NO_3)_2{\cdot}4H_2O$ (0.156 g, 0.50 mmol) was added to one leg of a H-shaped tube, and a water–methanol solution (20 ml, 1:1 *v*/*v*) of KNCS (0.097 g, 1.00 mmol) and mbtz (0.240 g, 1.00 mmol) was added to the other leg of the tube. After several weeks, well shaped colourless single crystals were obtained. Analysis found: C 43.95, H 3.3, N 27.6%; $C_{26}H_{24}CdN_{14}S_2$ requires: C 44.0, H 3.4, N 27.7%.

Crystal data

$[Cd(NCS)_2(C_{12}H_{12}N_6)_2]$
M_r = 709.11
Monoclinic, $P2_1/c$
a = 10.9140 (16) Å
b = 8.7717 (13) Å
c = 15.692 (2) Å
β = 101.488 (3)°
V = 1472.1 (4) Å^3
Z = 2
D_x = 1.600 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.93 mm^{-1}
T = 153 (2) K
Block, colourless
0.30 × 0.30 × 0.17 mm

Data collection

Rigaku Mercury CCD diffractometer
ω scans
Absorption correction: multi-scan (Jacobson, 1998)
T_{min} = 0.768, T_{max} = 0.858
13865 measured reflections
2691 independent reflections
2502 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 25.4°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.070
S = 1.08
2691 reflections
197 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0282P)^2 + 1.434P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—N3	2.302 (2)	S1—C13	1.629 (3)
Cd1—N7	2.344 (2)	N7—C13	1.166 (3)
Cd1—N6^{ii}	2.371 (2)		
N3—Cd1—N7	87.95 (8)	N7—Cd1—N6^{ii}	89.71 (8)
N3—Cd1—N6^{ii}	88.48 (7)	N7—C13—S1	179.2 (3)

Symmetry code: (ii) $-x, -y+1, -z+1$.

H atoms were placed in idealized positions and treated as riding atoms, with C—H distances of 0.95 (triazole and benzene) and 0.99 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: *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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Supplementary data for this paper are available from the IUCr electronic archives (Reference: GD3044). Services for accessing these data are described at the back of the journal.

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