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catena-Poly[[bis(*N*,*N*-diethyldithiocarbamato-κ^2S,S')cadmium(II)]-μ-*trans*-1,2-di-4-pyridylethane-κ^2N:N']

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Key indicators

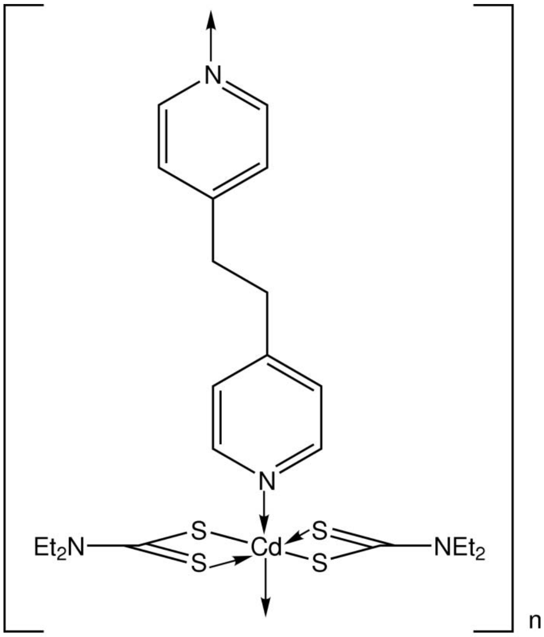
Single-crystal X-ray study
T = 113 K
Mean σ(C–C) = 0.006 Å
R factor = 0.050
wR factor = 0.125
Data-to-parameter ratio = 21.4

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

In the title compound, $[Cd(C_5H_{10}NS_2)_2(C_{12}H_{12}N_2)]_n$, two independent formula units comprise the asymmetic unit in the polymeric structure. Each Cd center exists within a *trans*-N_2S_4 donor set that defines an octahedral geometry. The polymer is approximately linear.

Comment

The title compound was investigated as part of a program designed to control supramolecular aggregation in the zinc-triad 1,1-dithiolates (Lai *et al.*, 2002; Tiekink, 2003) and the polymer topologies of their Lewis base adducts (Chai *et al.*, 2003; Chen *et al.*, 2006; Lai *et al.*, 2004; Lai & Tiekink, 2004, 2006). Briefly, judicious choice of steric profile of the thiolate-bound *R* groups and linkers with specific bridging requirements leads to control over supramolecular aggregation; this concept has applicability beyond the systems mentioned above (Tiekink, 2006*a*,*b*).



(I)

Two independent formula units comprise the asymmetric unit of the title compound, (I) (Figs. 1 and 2), and each features a slightly disorted octahedrally coordinated Cd center within a *trans*-N_2S_4 donor set; each independent formula unit self-associates to form a polymer chain. For each Cd center, the dithiocarbamate ligands are chelating with equivalent Cd—S bond distances; indeed, the eight Cd—S bond distances fall in the narrow range 2.6545 (10)–2.6696 (10) Å, and this

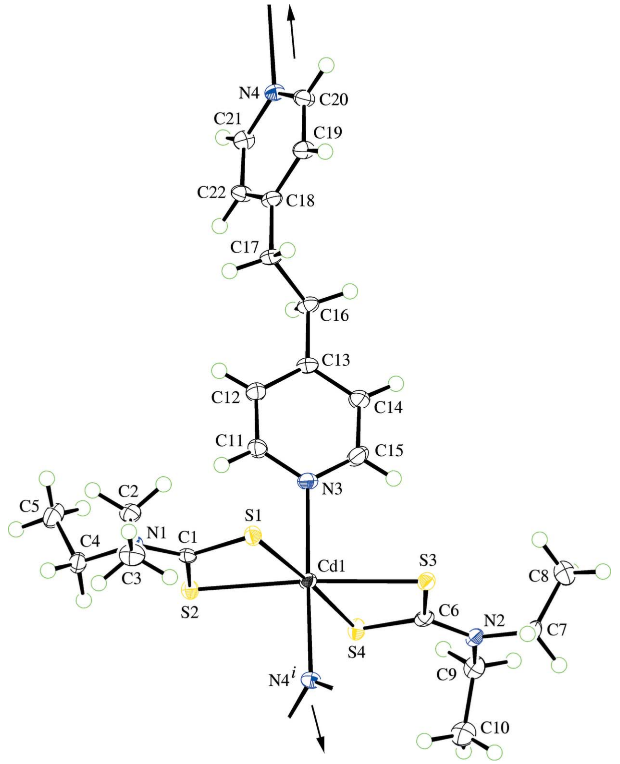


Figure 1
The coordination geometry for one of the two independent formula units in the asymmetric unit in (I), showing the crystallographic numbering scheme. Displacement ellipsoids are shown at the 50% probability level. [Symmetry code: (i) $1 - x, -\frac{1}{2} + y, \frac{3}{2} - z$.]

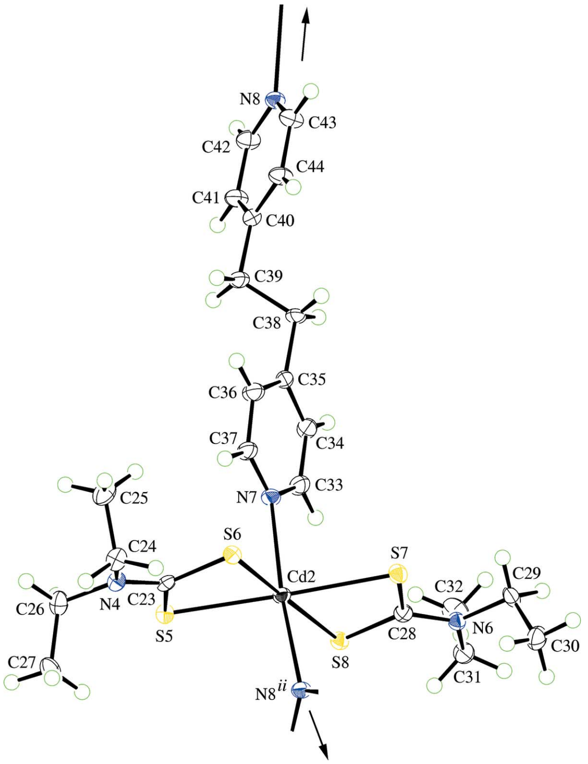


Figure 2
The coordination geometry for the other independent formula unit in the asymmetric unit in (I), showing the crystallographic numbering scheme. Displacement ellipsoids are shown at the 50% probability level. [Symmetry code: (ii) $-x, \frac{1}{2} + y, \frac{1}{2} - z$.]

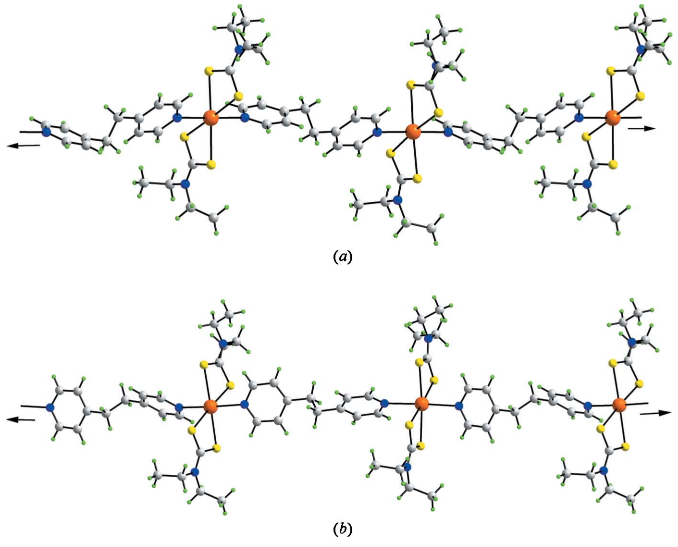


Figure 3
The two independent polymeric chains, (a) and (b), in (I). Color code: Cd orange, O red, N blue, C grey and H green.

equivalence is reflected in the associated C—S bond distances (Table 1). Deviations from the ideal octahedral geometry (Table 1) are directly related to the acute chelate angles subtended by the dithiocarbamate ligands. While there are some minor differences in the chemically equivalent bond distances defining the two monomer units (Table 1), another difference is found in the twist about the central ethyl link in the 1,2-di-4-pyridylethane ligands. This disparity is best illustrated in the dihedral angles formed between the two aromatic rings of each bridging ligand of 65.74 (18) and 56.49 (18)°. This does not result in a significant difference in the polymer topology (Fig. 3). Each polymer is effectively linear, the separations between adjacent Cd centers being 14.2529 (10) and 14.2705 (10) Å, respectively, and the angle subtended at each Cd atom by neigbouring Cd atoms is 173.61 (1) and 172.20 (2)°, respectively. Thus, despite being propagated by 2_1 symmetry, the twist in the bridging ligands masks the inherent helical topology of the polymer. The only other adduct of $Cd[S_2CN(CH_2CH_3)_2]_2$ with a bridging bipyridine-type ligand is that containing the *trans*-1,2-di-4-pyridylethene ligand (Chai *et al.*, 2003). This, too, has a linear topology.

The crystal structure (Fig. 4) comprises layers of alternating Cd1- and Cd2-containing polymeric chains. Layers are separated by hydrophobic interactions between the N-bound ethyl groups.

Experimental

The title compound was prepared by reacting equimolar amounts of $Cd[S_2CN(CH_2CH_3)_2]_2$ (Dee & Tiekink, 2002) with 1,2-di-4-pyridylethane (Aldrich) according to the literature procedure of Chai *et al.* (2003). Crystals were obtained by the slow evaporation of an acetonitrile–chloroform (1:3) solution of the compound (m. p. 440–443 K). IR: S_2CNEt_2 ν(C—N) 1416 (*s*) ν(C—S) 985 cm^{-1}; 1,2-di-4-pyridylethane: ν(C—H) 2966, ν(C=C) 1601, ν(C—N) 1269 cm^{-1}.

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Crystal data

$[Cd(C_5H_{10}NS_2)_2(C_{12}H_{12}N_2)]$
$M_r = 593.16$
Monoclinic, $P2_1/c$
$a = 9.7686$ (8) Å
$b = 28.475$ (2) Å
$c = 18.9966$ (18) Å
$\beta = 96.731$ (4)°
$V = 5247.7$ (8) Å^3

$Z = 8$
$D_x = 1.502$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.17$ mm^{-1}
$T = 113$ (2) K
Plate, colorless
0.50 × 0.47 × 0.17 mm

Data collection

Rigaku SCXmini diffractometer
ω scans
Absorption correction: numerical (*ABSCOR*; Higashi, 1995)
$T_{\min} = 0.593$, $T_{\max} = 0.826$

50346 measured reflections
11980 independent reflections
10413 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.075$
$\theta_{\max} = 27.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.050$
$wR(F^2) = 0.125$
$S = 1.25$
11980 reflections
560 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0273P)^2 + 11.7964P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.82$ e Å^{-3}
$\Delta\rho_{\min} = -0.79$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.00013 (3)

Table 1
Selected geometric parameters (Å, °).

Cd1—S1	2.6546 (10)	S1—C1	1.730 (4)
Cd1—S2	2.6652 (10)	S2—C1	1.737 (4)
Cd1—S3	2.6609 (10)	S3—C6	1.732 (4)
Cd1—S4	2.6696 (10)	S4—C6	1.732 (4)
Cd1—N3	2.464 (3)	S5—C23	1.731 (4)
Cd1—N4^{i}	2.444 (3)	S6—C23	1.731 (4)
Cd2—S5	2.6545 (10)	S7—C28	1.733 (4)
Cd2—S6	2.6621 (10)	S8—C28	1.732 (4)
Cd2—S7	2.6568 (10)	N1—C1	1.335 (5)
Cd2—S8	2.6638 (10)	N2—C6	1.340 (5)
Cd2—N7	2.482 (3)	N5—C23	1.341 (5)
Cd2—N8^{ii}	2.441 (3)	N6—C28	1.340 (5)
S1—Cd1—S2	68.56 (3)	S5—Cd2—S6	68.58 (3)
S1—Cd1—S3	115.12 (3)	S5—Cd2—S7	176.09 (3)
S1—Cd1—S4	176.34 (3)	S5—Cd2—S8	115.27 (3)
S1—Cd1—N3	88.98 (8)	S5—Cd2—N7	92.52 (8)
S1—Cd1—N4^{i}	91.84 (8)	S5—Cd2—N8^{ii}	92.25 (8)
S2—Cd1—S3	175.19 (3)	S6—Cd2—S7	107.50 (3)
S2—Cd1—S4	107.82 (3)	S6—Cd2—S8	174.35 (3)
S2—Cd1—N3	91.56 (8)	S6—Cd2—N7	91.84 (8)
S2—Cd1—N4^{i}	89.82 (8)	S6—Cd2—N8^{ii}	89.33 (8)
S3—Cd1—S4	68.46 (3)	S7—Cd2—S8	68.62 (3)
S3—Cd1—N3	91.61 (8)	S7—Cd2—N7	87.69 (8)
S3—Cd1—N4^{i}	86.99 (8)	S7—Cd2—N8^{ii}	87.51 (8)
S4—Cd1—N3	91.72 (8)	S8—Cd2—N7	92.09 (8)
S4—Cd1—N4^{i}	87.54 (8)	S8—Cd2—N8^{ii}	86.42 (8)
N3—Cd1—N4^{i}	178.58 (10)	N7—Cd2—N8^{ii}	175.19 (11)

Symmetry codes: (i) $-x+1, y-\frac{1}{2}, -z+\frac{3}{2}$; (ii) $-x, y+\frac{1}{2}, -z+\frac{1}{2}$.

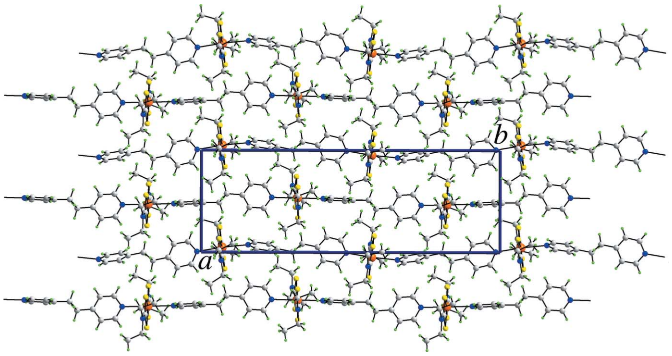

Figure 4
A view, along the *a*-axis direction, of the packing. Color code as for Fig. 3.

H atoms were included in the riding-model approximation, with C—H = 0.95–0.99 Å and $U_{\rm iso}(H) = 1.5U_{\rm eq}(C)$.

Data collection: *SCXmini* (Rigaku, 2006); cell refinement: *PROCESS-AUTO* (Rigaku, 1998); data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976) and *DIAMOND* (Crystal Impact, 2006); software used to prepare material for publication: *SHELXL97*.

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