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catena-Poly[[(10,11,12,13-tetrahydro-4,5,9,14-tetraazabenzo[*b*]triphenylene)cadmium(II)]-di-μ-chlorido]: a stair-like one-dimensional polymer

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Key indicators

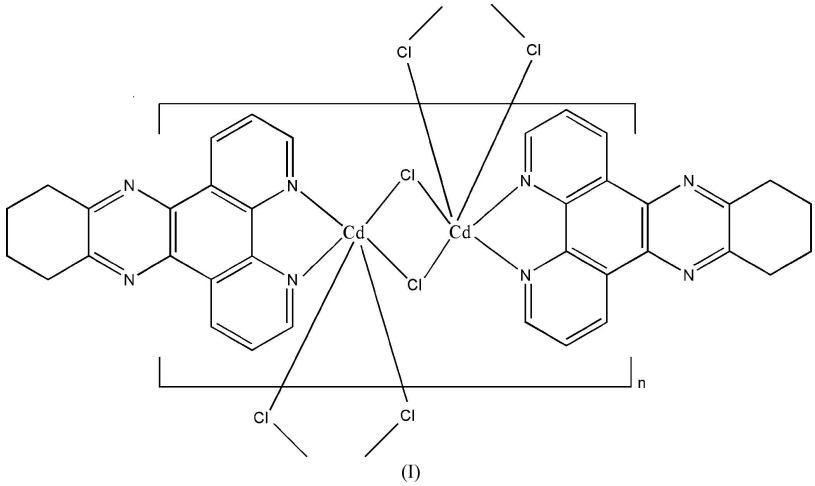
Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.004 Å
R factor = 0.022
wR factor = 0.056
Data-to-parameter ratio = 14.7

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

In the title compound, $[CdCl_2(C_{18}H_{14}N_4)]_n$, the Cd atom displays a distorted octahedral geometry, coordinated by four Cl atoms and two N atoms from a bidentate 10,11,12,13-tetrahydro-4,5,9,14-tetraazabenzo[*b*]triphenylene molecule. Each Cl atom bridges two Cd atoms, forming a stair-like polymer along the *a* axis.

Comment

Coordination polymers based on metals and organic ligands have been extensively studied in recent years owing to their novel topologies and potential applications as functional materials (Eddaoudi *et al.*, 2001). 1,10-Phenanthroline (phen) and its derivatives are important ligands for the formation of metal–organic complexes and polymers (Che, Su *et al.*, 2006; Che, Xu & Liu, 2006). 10,11,12,13-Tetrahydro-4,5,9,14-tetraazabenzo[*b*]triphenylene (*L*), a phen derivative, possesses an extended delocalized aromatic system. As part of our research, we have combined *L* with cadmium(II) halides to synthesize new complexes. We report here the crystal structure of the title compound, $[CdCl_2(L)]_n$, (I) (Fig. 1).



(I)

Selected bond lengths and angles for (I) are given in Table 1. The mean Cd—N and Cd—Cl distances are 2.410 (1) and 2.6016 (6) Å, respectively. Each cadmium(II) cation displays a distorted octahedral coordination provided by four Cl atoms and two N atoms from *L*. Each Cl atom bridges two Cd atoms, forming a zigzag stair-like structure along the *a* axis, as shown in Fig. 2.

The packing in (I) is reinforced by way of π–π stacking interactions with a ring-centroid separation of 3.62 Å between centrosymmetically related *L* ligands [N1–N4/C1–C18 at (x, y, z) and ($3-x$, $1-y$, $-z$)] in adjacent chains (Fig. 3). Such interactions are believed to play an important role in stabilizing network structures (Noveron *et al.*, 2002).

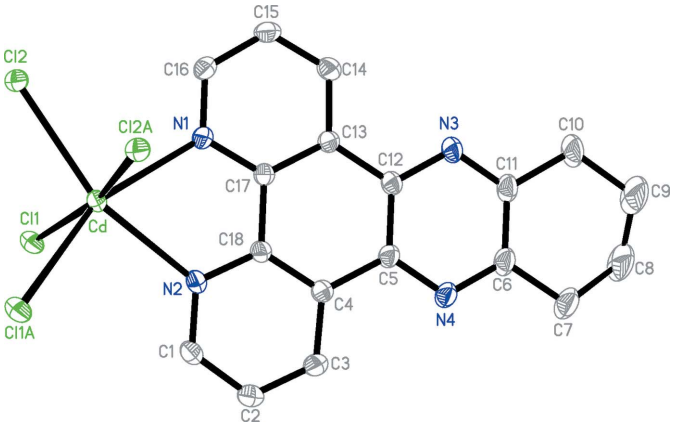


Figure 1
The asymmetric unit of (I), extended to complete the Cd^{II} coordination. Displacement ellipsoids are drawn at the 30% probability level and H atoms are omitted for clarity. Atoms Cl1A and Cl2A are generated by the symmetry operations $(2 - x, -y, -1 - z)$ and $(3 - x, -y, -1 - z)$, respectively.

Experimental

Ligand *L* was synthesized according to the literature method of Che, Li *et al.* (2006). A mixture of *L*, $CdCl_2$ and water in a molar ratio of 2:1:5000 was sealed in a Teflon-lined autoclave and heated to 453 K for 3 d. Brown block-shaped crystals of (I) were obtained upon cooling the autoclave (74% yield, based on Cd).

Crystal data

$[CdCl_2(C_{18}H_{14}N_4)]$
M_r = 469.63
Triclinic, $P\overline{1}$
a = 6.8116 (4) Å
b = 10.0669 (6) Å
c = 12.8482 (8) Å
α = 102.707 (1)°
β = 94.123 (1)°
γ = 97.047 (1)°
V = 848.49 (9) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.61 mm^{-1}
T = 292 (2) K
0.56 × 0.30 × 0.17 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.560, T_{max} = 0.759
7310 measured reflections
3332 independent reflections
3122 reflections with $I > 2\sigma(I)$
R_{int} = 0.015

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.056
S = 1.06
3332 reflections
226 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.57 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd—N1	2.4060 (19)	Cd—Cl2	2.6245 (6)
Cd—N2	2.414 (2)	Cd—Cl2^{i}	2.6271 (6)
Cd—Cl1	2.5787 (6)	Cd—Cl1^{ii}	2.6322 (6)
N1—Cd—N2	68.61 (6)		

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

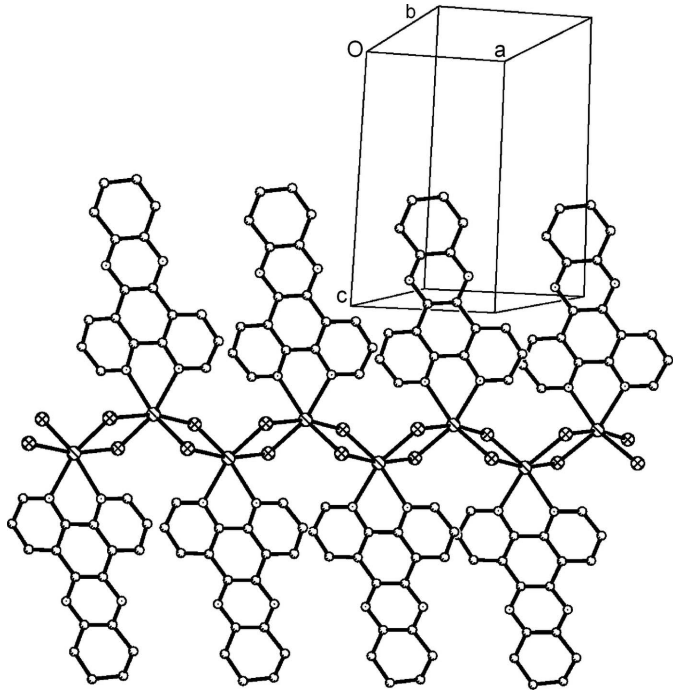


Figure 2
View of the single-chain structure of (I). H atoms have been omitted.

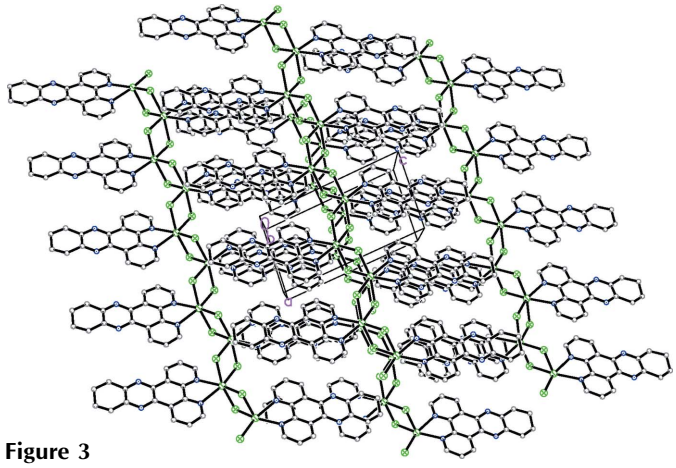


Figure 3
View of the packing of (I). H atoms have been omitted.

All H atoms were positioned geometrically (C—H = 0.93 Å) and refined as riding atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXTL-Plus*.

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