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catena-Poly[[diiodocadmium(II)]-μ-1,4-bis-(1,2,4-triazol-1-ylmethyl)benzene-$\kappa^2N^4:N^{4'}$]

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
R factor = 0.017
wR factor = 0.049
Data-to-parameter ratio = 16.1

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

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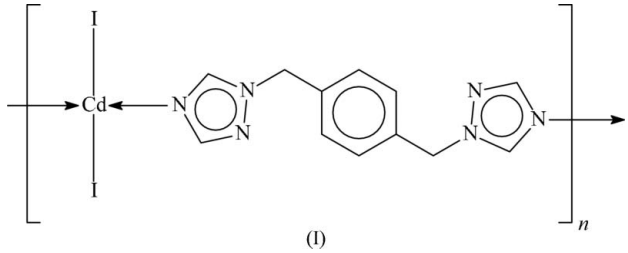
The title compound, $[CdI_2(C_{12}H_{12}N_6)]_n$, is a polymeric 1:1 adduct of cadmium iodide and 1,4-bis(1,2,4-triazol-1-ylmethyl)benzene. The Cd and I atoms lie on special positions of m site symmetry and the complete organic ligand has inversion symmetry. The polymer assumes a zigzag conformation propagating along the c axis. The geometry at Cd is that of a CdI_2N_2 tetrahedron.

Comment

A previous study (Meng *et al.*, 2004) has documented the crystal structures of the compounds isolated from the reaction of cadmium salts and 1,4-bis(1,2,4-triazol-1-ylmethyl)benzene. The cadmium dichloride adduct is a 1:2 adduct, and the Cd atom exists in an all-*trans* octahedral geometry in the resulting layer structure (Meng *et al.*, 2004). The title compound, (I), is, however, a 1:1 adduct (Fig. 1). The metal site is linked to the triazolyl N atoms from two ligands in a tetrahedral environment; the bridging nature of the ligand gives rise to a chain motif that runs along the c-axis direction of the orthorhombic unit cell.



(I)

Cadmium compounds generally show coordination numbers greater than 4 in their complexes with *N*-heterocycles (Cambridge Structural Databse, Version 5.26; Allen, 2002). However, the CdI_2N_2 tetrahedral coordination environment has also been noted in, for example, the pyridine (Hu *et al.*, 2003), di-2-pyridylamine (Pickardt & Staub, 1999), bis(2-pyridylthio)methane (Amoedo-Portela *et al.*, 2003) and bis(3,5-dimethylpyrazol-2-ylethyl)thioether (Ghosh *et al.*, 1999) adducts. The bond dimensions in (I) compare well with values reported in these phases.

Experimental

1,4-Bis(1,2,4-triazol-1-ylmethyl)benzene was synthesized as reported previously by Meng *et al.* (2004). The ligand (0.012 g, 0.1 mmol) was dissolved in a dimethylformamide–methanol solution (1:1 *v*/*v*, 20 ml) along with cadmium iodide (0.037 g, 0.1 mmol). Colourless crystals of (I) separated from the solution after about a month.

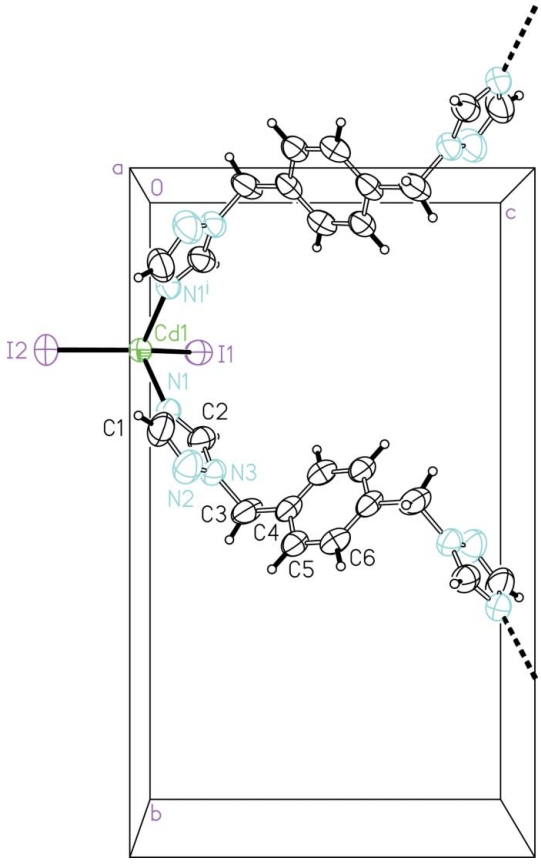


Figure 1
View of a fragment of the polymeric structure of (I). Displacement ellipsoids are drawn at the 70% probability level and H atoms are drawn as spheres of arbitrary radii. The dashed lines indicate the bonds to the next Cd atoms in the polymeric chain. [Symmetry code: (i) $x, -y+\frac{1}{2}, z$.]

Crystal data

$[CdI_2(C_{12}H_{12}N_6)]$
$M_r = 606.48$
Orthorhombic, *Pnma*
$a = 9.3325\ (5)$ Å
$b = 17.6438\ (9)$ Å
$c = 10.3499\ (5)$ Å
$V = 1704.2\ (2)$ Å^3
$Z = 4$
$D_x = 2.364$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5062 reflections
$\theta = 2.4$–$28.2°$
$\mu = 4.91$ mm^{-1}
$T = 295\ (2)$ K
Block, colourless
0.42 × 0.27 × 0.17 mm

Data collection

Bruker APEX-II CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.267$, $T_{max} = 0.434$
14189 measured reflections
2018 independent reflections
1923 reflections with $I > 2\sigma(I)$
$R_{int} = 0.017$
$\theta_{max} = 27.5°$
$h = -12 \rightarrow 11$
$k = -22 \rightarrow 22$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.017$
$wR(F^2) = 0.049$
$S = 0.99$
2018 reflections
125 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0249P)^2 + 1.8633P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.71$ e Å^{-3}
$\Delta\rho_{min} = -0.53$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0032 (1)

Table 1
Selected geometric parameters (Å, °).

Cd1—N1	2.284 (2)	Cd1—I2	2.7066 (3)
Cd1—I1	2.7332 (4)		
N1—Cd1—N1^{i}	102.6 (1)	N1—Cd1—I2	109.61 (5)
N1—Cd1—I1	100.54 (5)	I1—Cd1—I2	130.51 (1)

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

All H atoms were located in difference maps and refined with C—H distance restraints of 0.95 (1) Å. Their isotropic displacement parameters were freely refined.

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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