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catena-Poly[di-μ_2-chloro(1,10-phenanthroline)-cadmium(II)]

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Key indicators

Single-crystal X-ray study
T = 223 K
Mean σ(C–C) = 0.012 Å
R factor = 0.067
wR factor = 0.159
Data-to-parameter ratio = 18.0

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

The crystal structure of the 1/1 adduct of cadmium dichloride with 1,10-phenanthroline, $[CdCl_2(C_{12}H_8N_2)]_n$, is based on an infinite chain of Cd_2Cl_2 parallelograms sharing their Cd corners. The chain propagates in a zigzag manner along the *c* axis of the monoclinic unit cell. The Cd atom and the phenanthroline molecule both lie on special positions of 2 symmetry.

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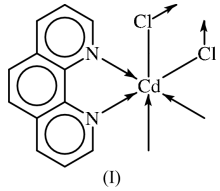
Comment

The 1/1 adduct of cadium dichloride with 1,10-phenanthroline, (I), features corner-sharing Cd_2Cl_2 parallelograms, which are connected through the Cd atoms, leading to a zigzag chain that runs along the *c* axis of the unit cell [Cd—Cl 2.552 (2) and 2.753 (2) Å]. Both the Cd atom and the phenanthroline molecule lie on a twofold axis.



(I)

The title compound was the unexpected product of an attempt to synthesize the 1,10-phenanthroline adduct of

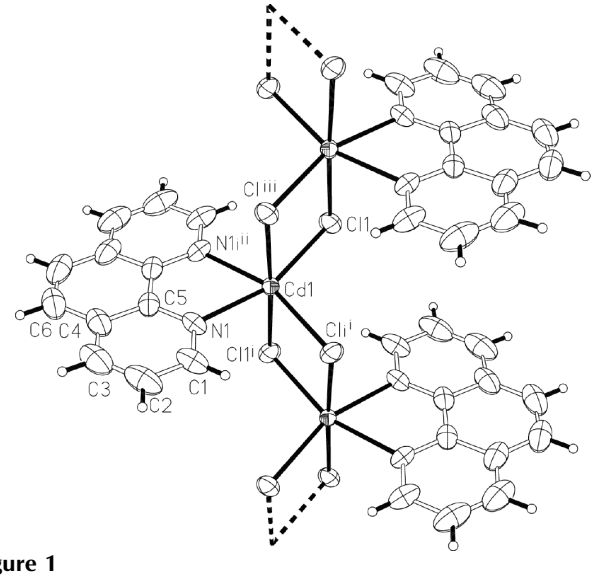


Figure 1
ORTEP (Johnson, 1976) plot of a fragment of $[CdCl_2(C_{12}H_8N_2)]_n$, with displacement ellipsoids drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radii. Symmetry code: (i) $1-y, \frac{1}{2}+z$; (ii) $-x, 1-y, -z$ and (iii) $-x, y, \frac{1}{2}-z$

cadmium maleate. The direct synthesis, with cadmium dichloride and 1,10-phenanthroline in a 1/2 molar stoichiometry, leads to the formation of the monomeric 1/2 adduct (Wang *et al.*, 1996). The connectivity in the 1/1 adduct is similar to that found in the the dipyridine (Paulus, 1969) and tetramethylethylenediamine (Htoon & Ladd, 1976; Li & Mak, 1997) adducts. A 1/1 adduct that exists as a co-crystal with cadium terephthalate, $CdCl_2(C_{12}H_8N_2)$-$Cd(CO_2$-1-C_6H_4-4-$CO_2)$, has also been synthesized by a hydrothermal route (Sun *et al.*, 2001). The structure is similar to that of the 2,2′-bipyridine analog, which has recently been reported (Zhou *et al.* 2003).

Experimental

Sodium maleate (0.14 g, 1 mmol) and 1,10 phenanthroline (0.20 g, 1 mmol) were added to a 1/1 ethanol/water (20 ml) solution of cadmium dichloride 2.5 hydrate (0.23 g, 1 mmol) to give a white product in 50% yield. The mixture was heated at about 333 K until the solid material dissolved completely. Colorless crystals separated from the solution in a few days.

Crystal data

$[Cd(C_{12}H_8N_2)Cl_2]$
$M_r = 363.50$
Monoclinic, $C2/c$
$a = 16.860$ (1) Å
$b = 10.5210$ (7) Å
$c = 7.2325$ (5) Å
$\beta = 110.298$ (1)°
$V = 1203.3$ (1) Å^3
$Z = 4$
$D_x = 2.007$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3213 reflections
$\theta = 2.3$–28.0°
$\mu = 2.23$ mm^{-1}
$T = 223$ K
Cylinder, colorless
0.15 × 0.14 × 0.05 mm

Data collection

Bruker APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan. (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.692$, $T_{max} = 0.897$
5052 measured reflections
1403 independent reflections
1371 reflections with $I > 2\sigma(I)$
$R_{int} = 0.031$
$\theta_{max} = 28.3°$
$h = -21 \rightarrow 22$
$k = -13 \rightarrow 13$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.067$
$wR(F^2) = 0.159$
$S = 1.24$
1403 reflections
78 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.075P)^2 + 10.4379P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 2.23$ e Å^{-3}
$\Delta\rho_{min} = -2.18$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—N1	2.353 (6)	Cd1—Cl1^{iv}	2.753 (2)
Cd1—Cl1	2.552 (2)		
N1—Cd1—N1^{iii}	70.9 (3)	Cl1—Cd1—Cl1^{iv}	96.7 (1)
N1—Cd1—Cl1	161.1 (2)	Cl1—Cd1—Cl1^{ii}	84.9 (1)
N1—Cd1—Cl1^{iv}	92.1 (2)	Cl1—Cd1—Cl1^{iii}	104.4 (1)
N1—Cd1—Cl1^{ii}	85.8 (2)	Cl1^{ii}—Cd1—Cl1^{iii}	96.7 (1)
N1—Cd1—Cl1^{iii}	93.0 (2)		

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

The C—C distances were restrained to 1.39 (1) Å, and the displacement factors of the C atoms were restrained to be approximately isotropic. H atoms were positioned geometrically (C—H 0.93 Å) and they were included in the refinement with U(H) = $1.2U_{eq}$(C) in the riding-model approximation. The final difference Fourier map had its major features near atom Cd1.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXL*97; software used to prepare material for publication: *SHELXL*97.

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