

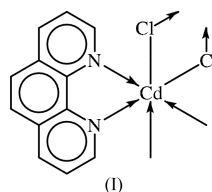
Hong-Bin Chen,<sup>a</sup> Zhao-Hui  
Zhou,<sup>a</sup> Hui-Lin Wan<sup>a</sup> and  
Seik Weng Ng<sup>b\*</sup><sup>a</sup>Department of Chemistry, Xiamen University,  
Xiamen 361005, People's Republic of China,  
and <sup>b</sup>Department of Chemistry, University of  
Malaya, 50603 Kuala Lumpur, Malaysia

Correspondence e-mail: seikweng@um.edu.my

## Key indicators

Single-crystal X-ray study  
 $T = 223\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.012\text{ \AA}$   
 $R$  factor = 0.067  
 $wR$  factor = 0.159  
Data-to-parameter ratio = 18.0For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.**catena-Poly[di- $\mu_2$ -chloro(1,10-phenanthroline)-  
cadmium(II)]**The crystal structure of the 1/1 adduct of cadmium dichloride with 1,10-phenanthroline,  $[\text{CdCl}_2(\text{C}_{12}\text{H}_8\text{N}_2)]_n$ , is based on an infinite chain of  $\text{Cd}_2\text{Cl}_2$  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.Received 27 August 2003  
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## Comment

The 1/1 adduct of cadmium dichloride with 1,10-phenanthroline, (I), features corner-sharing  $\text{Cd}_2\text{Cl}_2$  parallelograms, which are connected through the Cd atoms, leading to a zigzag chain that runs along the  $c$  axis of the unit cell [ $\text{Cd}-\text{Cl}$  2.552 (2) and 2.753 (2) Å]. Both the Cd atom and the phenanthroline molecule lie on a twofold axis.

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

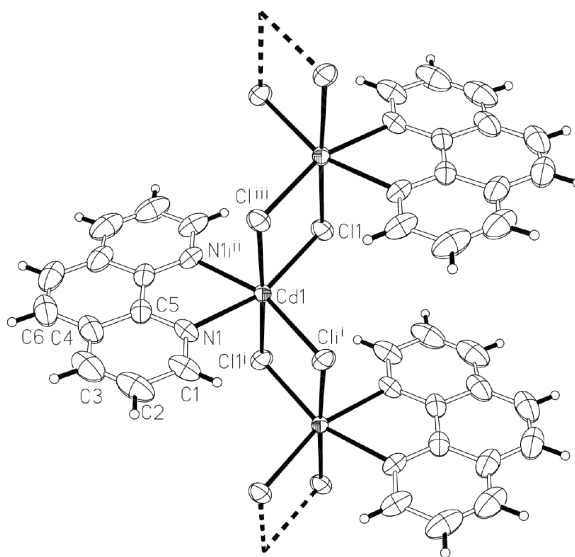


Figure 1

ORTEP (Johnson, 1976) plot of a fragment of  $[\text{CdCl}_2(\text{C}_{12}\text{H}_8\text{N}_2)]_n$ , with displacement ellipsoids drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radii. Symmetry code: 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 cadmium terephthalate,  $\text{CdCl}_2(\text{C}_{12}\text{H}_8\text{N}_2)\text{-Cd}(\text{CO}_2\text{-1-C}_6\text{H}_4\text{-4-CO}_2)$ , 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

$[\text{Cd}(\text{C}_{12}\text{H}_8\text{N}_2)\text{Cl}_2]$	$D_x = 2.007 \text{ Mg m}^{-3}$
$M_r = 363.50$	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 3213 reflections
$a = 16.860(1) \text{ \AA}$	$\theta = 2.3\text{--}28.0^\circ$
$b = 10.5210(7) \text{ \AA}$	$\mu = 2.23 \text{ mm}^{-1}$
$c = 7.2325(5) \text{ \AA}$	$T = 223 \text{ K}$
$\beta = 110.298(1)^\circ$	Cylinder, colorless
$V = 1203.3(1) \text{ \AA}^3$	$0.15 \times 0.14 \times 0.05 \text{ mm}$
$Z = 4$	

#### Data collection

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

#### Refinement

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

**Table 1**

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

Cd1—N1	2.353 (6)	Cd1—Cl1 <sup>iv</sup>	2.753 (2)
Cd1—Cl1	2.552 (2)		
N1—Cd1—N1 <sup>iii</sup>	70.9 (3)	Cl1—Cd1—Cl1 <sup>iv</sup>	96.7 (1)
N1—Cd1—Cl1	161.1 (2)	Cl1—Cd1—Cl1 <sup>iii</sup>	84.9 (1)
N1—Cd1—Cl1 <sup>iv</sup>	92.1 (2)	Cl1—Cd1—Cl1 <sup>iii</sup>	104.4 (1)
N1—Cd1—Cl1 <sup>ii</sup>	85.8 (2)	Cl1 <sup>ii</sup> —Cd1—Cl1 <sup>iii</sup>	96.7 (1)
N1—Cd1—Cl1 <sup>iii</sup>	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)  $\text{\AA}$ , and the displacement factors of the C atoms were restrained to be approximately isotropic. H atoms were positioned geometrically (C—H 0.93  $\text{\AA}$ ) and they were included in the refinement with  $U(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  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: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXL97*; software used to prepare material for publication: *SHELXL97*.

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