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cis-Bis(dicyanamido)bis(1,10-phenanthroline)cadmium(II)

Guo-Zheng Lan, A-Qing Wu, Guo-Cong Guo and Fa-Kun Zheng*

State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, People's Republic of China

Correspondence e-mail: aqwu@ms.fjirsm.ac.cn

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.060
wR factor = 0.132
Data-to-parameter ratio = 16.2

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

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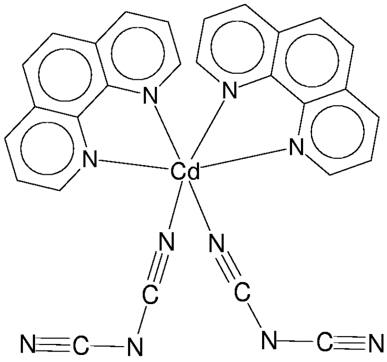
In the title complex, $[Cd(C_2N_3)_2(C_{12}H_8N_2)_2]$, the Cd^{II} atom exhibits a slightly distorted octahedral environment, coordinated by four N atoms of two phenanthroline ligands and two mutually *cis* N-terminal atoms of two dicyanamide ligands. π–π stacking interactions result in the formation of one-dimensional chains extending along [110].

Comment

Investigation of metal–dca complexes {dca is dicyanamide, $[N(CN)_2]^-$} is a fast-growing research field because of the large variety of topologies and magnetic properties shown by complexes of the dca ligand (Miller & Manson, 2001; Batten & Murray, 2003). It is a versatile ligand coordinating to metal ions in various modes: monodentate binding through one nitrile N atom (Marshall *et al.*, 2000), end-to-end bridging through the two nitrile N atoms (Manson, Arif & Miller, 1999; Jensen *et al.*, 1999) and triply bridging three metal atoms using all three N donor atoms (Jensen *et al.*, 2000; Kurmco & Kepert, 1998). These varied coordination possibilities allow the preparation of compounds with a variety of architectures, including mono- and dinuclear complexes, as well as one-, two- and three-dimensional network structures. Complexes $[M(\mathrm{dca})_2]_n$ (M = Mn, Fe, Co, Ni, Cu, Zn and Ag) containing only dca have been synthesized, and display quite limited structural types with rutile-like or two-dimensional (4,4) sheet networks (Manson *et al.*, 1998; Batten *et al.*, 1998). By introducing co-ligands of various types, such as pyridine, bipyridine, 1,10-phenanthroline or 2,2′-biimidazole, many structurally diverse ternary compounds have been synthesized (Marshall *et al.*, 2000; Manson, Arif, Incarvito *et al.*, 1999; Potocnak *et al.*, 1995). As an extension of this research, we report here the synthesis and structure of the title compound, (I).



(I)

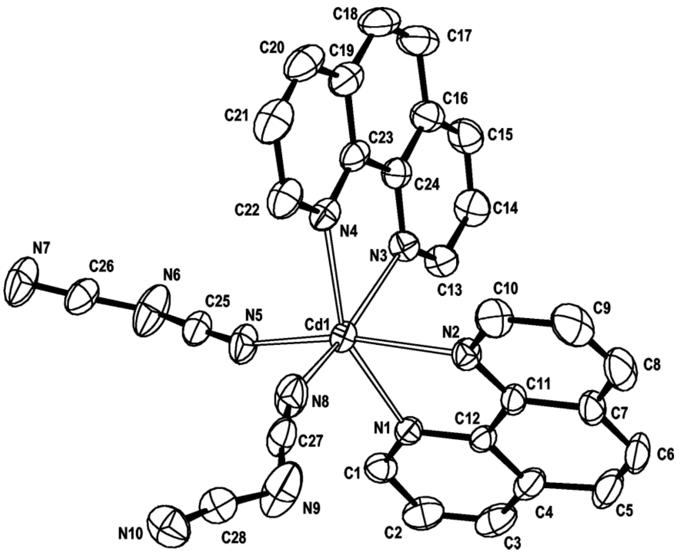


Figure 1
The molecular structure of the title compound, with displacement ellipsoids drawn at the 30% probability level; H atoms have been omitted for clarity.

The structure of (I) consists of discrete molecules (Fig. 1) and is similar to those of the complexes $M(\text{dca})_2(1,10\text{-phen})_2$ (M = Cu, Mn, Zn, and Ni) (Wu *et al.*, 2004; Potocnak *et al.*, 1995; Wang *et al.*, 2000). The Cd^{II} atom is in a slightly distorted octahedral environment, coordinated by four N atoms from the two phen ligands and two N-terminal atoms from two dca ligands. The two dca ligands bind to Cd in a monodentate fashion through their nitrile N atoms, N5 and N8, and are mutually *cis*. The bond lengths of the Cd—N bonds to the phen ligands [mean 2.365 (2) Å] are distinctly longer than those to the nitrile N atoms of dca [mean 2.254 (2) Å]. This difference may be due to steric hindrance involving the bulky phen molecules. The structure is stabilized by weak π–π stacking interactions between phen ligands from adjacent molecules of (I) to form a one-dimensional chain structure extending along [110]. Adjacent rings are inclined at an angle of 1.8 (1)°; the ring centroid-to-centroid distance is 3.816 Å and the perpendicular inter-ring distance is 3.807 Å (Fig. 2). The shortest Cd$^{II}\cdots$Cd^{II} separation along the chain is 8.726 (2) Å. Rings *R*1 (N1/C1–C4/C12) interact with rings *R*2 (C4–C7/C11/C12) on adjacent molecules to give a single one-dimensional chain. This interaction differs markedly from that reported for the coordination polymer formed by the copper complex of phen and a bridging dca ligand (Wu *et al.*, 2003), in which an interleaved double-chain structure was formed.

Experimental

An ethanol solution (10 ml) of 1,10-phen (100 mg, 0.51 mg) was added dropwise, with stirring, to an aqueous solution (6 ml) of $Cd(CH_3COO)_2$ (130 mg, 0.49 mmol) and Na(dca) (88 mg, 0.99 mmol). The mixture was filtered and the filtrate was allowed to stand for several days, yielding transparent colourless block-like crystals (yield 63.5%, based on Cd).

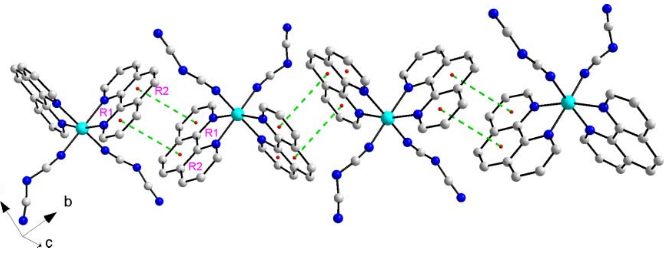


Figure 2
The chain structure of (I), resulting from π–π-stacking interactions (dashed lines), extending along [110].

Crystal data

$[Cd(C_2N_3)_2(C_{12}H_8N_2)_2]$
$M_r = 604.91$
Monoclinic, $P2_1/c$
$a = 9.878\ (2)$ Å
$b = 14.978\ (4)$ Å
$c = 17.764\ (5)$ Å
$\beta = 104.691\ (3)^\circ$
$V = 2542.2\ (11)$ Å^3
$Z = 4$

$D_x = 1.580$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5717 reflections
$\theta = 3.0$–27.5°
$\mu = 0.90$ mm^{-1}
$T = 293\ (2)$ K
Block, colourless
$0.20 \times 0.15 \times 0.10$ mm

Data collection

Rigaku Mercury CCD diffractometer
ω scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2002)
$T_{\min} = 0.777$, $T_{\max} = 0.914$
19 784 measured reflections

5721 independent reflections
4856 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.035$
$\theta_{\max} = 27.5^\circ$
$h = -11 \rightarrow 12$
$k = -14 \rightarrow 19$
$l = -23 \rightarrow 23$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.060$
$wR(F^2) = 0.133$
$S = 1.07$
5721 reflections
353 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0471P)^2 + 4.8527P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.002$
$\Delta\rho_{\max} = 0.79$ e Å^{-3}
$\Delta\rho_{\min} = -0.61$ e Å^{-3}
Extinction correction: none

Table 1
Selected geometric parameters (Å, °).

Cd1—N8	2.251 (2)	Cd1—N2	2.373 (2)
Cd1—N5	2.257 (2)	Cd1—N3	2.4040 (19)
Cd1—N4	2.335 (2)	Cd1—Cd1^{i}	8.7257 (15)
Cd1—N1	2.3484 (17)		
N8—Cd1—N5	98.47 (9)	N4—Cd1—N2	94.61 (7)
N8—Cd1—N4	93.11 (8)	N1—Cd1—N2	70.69 (7)
N5—Cd1—N4	100.32 (8)	N8—Cd1—N3	161.88 (8)
N8—Cd1—N1	105.59 (8)	N5—Cd1—N3	92.27 (8)
N5—Cd1—N1	92.65 (7)	N4—Cd1—N3	70.53 (6)
N4—Cd1—N1	155.44 (6)	N1—Cd1—N3	88.33 (6)
N8—Cd1—N2	88.22 (8)	N2—Cd1—N3	85.50 (7)
N5—Cd1—N2	163.23 (7)		

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

H atoms were placed in idealized positions and refined as riding, with C—H = 0.93 Å and $U_{\rm iso}(H) = 1.2U_{\rm eq}(C)$.

Data collection: *CrystalClear* (Rigaku, 2002); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXTL* (Siemens, 1994); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

Acta Cryst. (2005). E**61**, m1018–m1020 Lan *et al.* • $[Cd(C_2N_3)_2(C_{12}H_8N_2)_2]$ **m1019**

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m1020 Lan *et al.* • $[Cd(C_2N_3)_2(C_{12}H_8N_2)_2]$ *Acta Cryst.* (2005). E**61**, m1018–m1020