Poly[[[(pyrazino[2,3-*f*][1,10]phenanthroline-$\kappa^2 N,N'$)-cadmium(II)]-μ_3-pyridine-2,5-dicarboxylato-$\kappa^3 O,O':N,O:O'':O''$] monohydrate]

Guang-Bo Che,* Jian Wang, Jun Sun, Lu Lu and Zhi-Xin Yu

Department of Chemistry, Jilin Normal University, Siping 136000, People's Republic of China

Correspondence e-mail: guangbochejl@yahoo.com

In the title compound, {[Cd(C$_7$H$_3$NO$_4$)(C$_{14}$H$_8$N$_4$)]·H$_2$O}$_n$, the Cd^{II} atom is seven-coordinated by three N atoms from one pyrazino[2,3-*f*][1,10]phenanthroline molecule and one pyridine-2,5-dicarboxylate (2,5-pdc) ligand, and four O atoms from three different 2,5-pdc anions in a distorted monocapped octahedral coordination geometry. The Cd^{II} atoms are bridged by the 2,5-pdc ligands, forming a layer.

Comment

1,10-Phenanthroline (phen) and its derivatives are important ligands for the formation of metal–organic complexes (Che, Su *et al.*, 2006; Che, Liu, Liu *et al.*, 2006). Pyrazino[2,3-*f*][1,10]-phenanthroline (Pyphen) as a phen derivative possesses an extended delocalized aromatic system. To date, only a few coordination architectures based on Pyphen have been described (Che Liu & Xu, 2006; Che *et al.*, 2006). Our studies continue with the pyridine-2,5-dicarboxylate dianion (2,5-H$_2$pdc) in {[Cd(2,5-pdc)(Pyphen)]·H$_2$O}$_n$, (I).

(I)
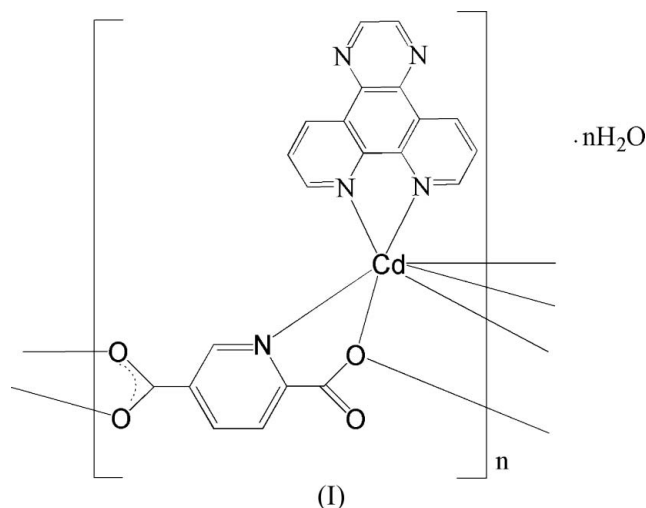
The Cd atom is coordinated by three N atoms from one Pyphen molecule and one 2,5-pdc ligand, and four O atoms from three different 2,5-pdc anions in a distorted monocapped octahedral coordination geometry (Fig. 1). Bond dimensions involving the metal atom are similar to those reported in the literature (Gao *et al.*, 2004). Two Cd atoms are bridged by the 2,5-pdc ligands through the carboxylate μ_2-O atoms, forming a dimeric unit; the dimeric units are further connected by the 2,5-pdc ligands through the chelating carboxylate groups, generating a layer with (4,4)-grids (Fig. 2). Each corner of the (4,4)-grid is occupied by a binuclear subunit. O—H···O hydrogen bonds involving the uncoordinated water molecule
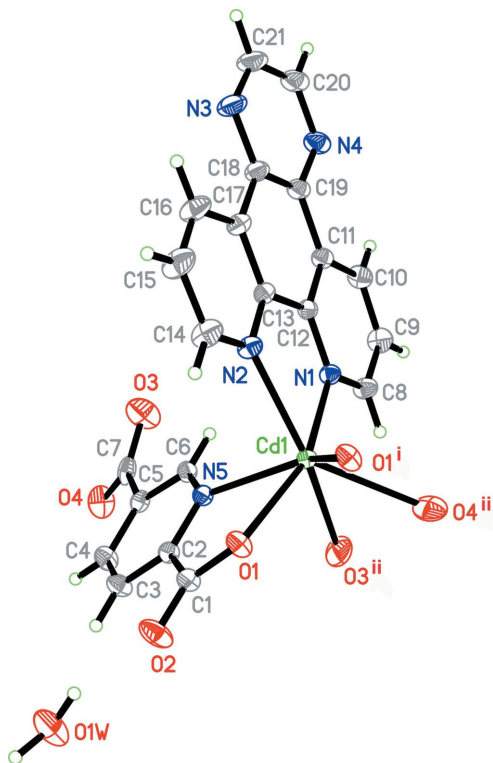
Figure 1
The asymmetric unit of compound (I), together with symmetry-equivalent atoms to complete the coordination of Cd1. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry codes: (i) $1 - x, 1 - y, 1 - z$; (ii) $1 - x, y - \frac{1}{2}, \frac{1}{2} - z$.]

and carboxylate O atoms stabilize the crystal structure (Table 2).

Experimental

The Pyphen ligand was synthesized according to the method of Che, Li *et al.* (2006). A methanol solution (28 ml) of pyrazino[2,3-*f*][1,10]phenanthroline (118 mg, 0.5 mmol) was mixed with an aqueous solution (10 ml) of CdCl$_2$·2.5H$_2$O (114 mg, 0.5 mmol) and 2,5-H$_2$pdc (167 mg, 1 mmol). The mixture was heated to dissolve the reagents. The solution was filtered; crystals separated from the solution after several days in 40% yield.

Crystal data

[Cd(C$_7$H$_3$NO$_4$)(C$_{14}$H$_8$N$_4$)]·H$_2$O
$M_r = 527.76$
Monoclinic, $P2_1/c$
$a = 10.754$ (2) Å
$b = 10.631$ (2) Å
$c = 17.127$ (3) Å
$\beta = 92.64$ (3)°
$V = 1956.0$ (6) Å^3

$Z = 4$
$D_x = 1.792$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.16$ mm^{-1}
$T = 292$ (2) K
Block, colorless
$0.30 \times 0.27 \times 0.23$ mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.670$, $T_{max} = 0.763$

18518 measured reflections
4451 independent reflections
3937 reflections with $I > 2\sigma(I)$
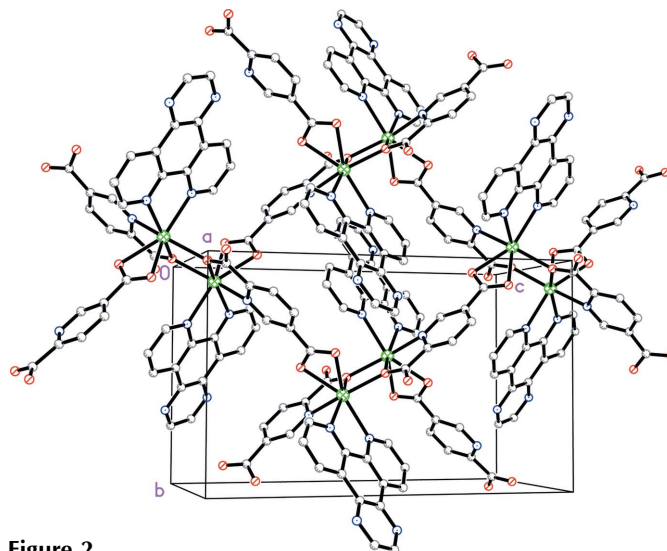$R_{int} = 0.026$
$\theta_{max} = 27.5°$

Figure 2
View of the layer structure of (I). H atoms have been omitted.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.023$
$wR(F^2) = 0.068$
$S = 1.12$
4451 reflections
295 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0334P)^2 + 1.031P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.50$ e Å^{-3}
$\Delta\rho_{min} = -0.46$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—O1^i	2.2625 (16)	Cd1—N1	2.3916 (19)
Cd1—O1	2.3658 (17)	Cd1—N2	2.380 (2)
Cd1—O3^{ii}	2.372 (2)	Cd1—N5	2.3742 (19)
Cd1—O4^{ii}	2.520 (2)		
O1^i—Cd1—O1	69.81 (7)	O1—Cd1—N5	67.76 (6)
O1^i—Cd1—O3^{ii}	119.88 (10)	O3^{ii}—Cd1—N1	92.34 (9)
O1—Cd1—O3^{ii}	88.73 (9)	O3^{ii}—Cd1—N2	154.57 (9)
O1^i—Cd1—O4^{ii}	81.48 (7)	O3^{ii}—Cd1—N5	73.73 (8)
O1—Cd1—O4^{ii}	108.62 (7)	N1—Cd1—O4^{ii}	88.44 (7)
O3^{ii}—Cd1—O4^{ii}	52.55 (8)	N2—Cd1—O4^{ii}	139.53 (7)
O1^i—Cd1—N1	126.53 (7)	N2—Cd1—N1	69.21 (7)
O1—Cd1—N1	158.96 (7)	N5—Cd1—N2	89.21 (7)
O1^i—Cd1—N2	85.52 (7)	N5—Cd1—N1	92.38 (7)
O1—Cd1—N2	102.35 (7)	N5—Cd1—O4^{ii}	126.24 (7)
O1^i—Cd1—N5	134.94 (6)		

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

Table 2
Hydrogen-bond geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O1W—HW12$\cdots$O2	0.86 (3)	1.986 (15)	2.787 (3)	155 (3)
O1W—HW11$\cdots$O4^{iii}	0.874 (10)	1.96 (3)	2.798 (3)	162 (4)

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

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

water H atoms were located in a difference Fourier map, and were refined with a distance restraint of O—H = 0.85 (1) Å; U_{iso}(H) = 1.2 U_{eq}(O).

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTLPlus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

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