

Ya-Guang Sun, En-Jun Gao,\* Xia Liu and Cheng-Chen Wang

Laboratory of Coordination Chemistry,  
 Shenyang Institute of Chemical Technology,  
 Shenyang 110142, People's Republic of China

Correspondence e-mail: ejgao@yahoo.com.cn

Key indicators

Single-crystal X-ray study  
 T = 293 K  
 Mean  $\sigma(C-C)$  = 0.003 Å  
 R factor = 0.020  
 wR factor = 0.048  
 Data-to-parameter ratio = 13.6

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

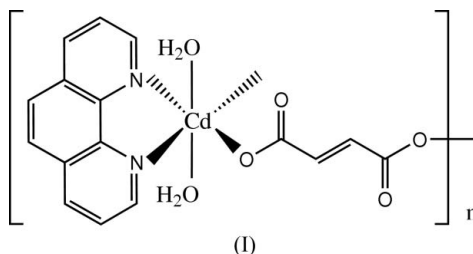
catena-Poly[[diaqua(1,10-phenanthroline- $\kappa^2N,N'$ )-cadmium(II)]- $\mu$ -fumarato- $\kappa^2O:O'$ ]

In the title polymeric complex,  $[Cd(C_4H_2O_4)(C_{12}H_8N_2)(H_2O)_2]_n$ , the Cd<sup>II</sup> ions are bridged by fumarate dianions to form zigzag complex chains.  $\pi$ - $\pi$  stacking is observed between the parallel phenanthroline ligands of neighboring complex chains. The Cd ion is located on a twofold axis and has a distorted octahedral coordination geometry, while the fumarate dianion lies on an inversion center.

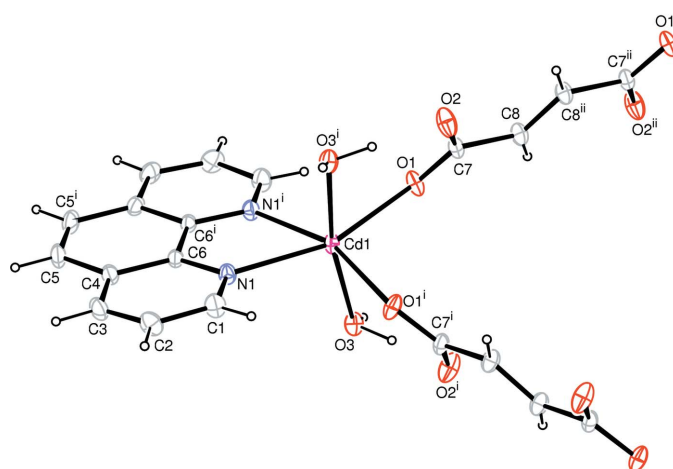
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Comment

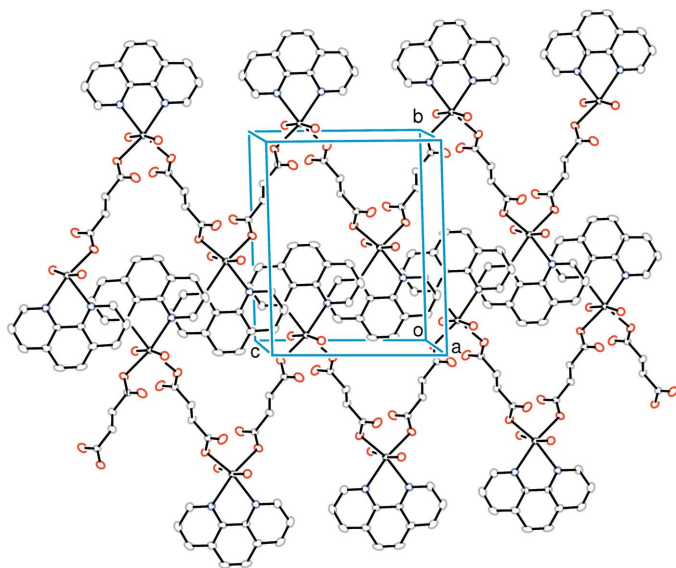
Polynuclear complexes have received much attention in the past decade. Some polynuclear Cd<sup>II</sup> complexes have shown photoluminescent properties (Tao *et al.*, 2000). We prepared the title Cd<sup>II</sup> complex, (I), which displays a polymeric structure.



A segment of the polymeric structure of (I) is shown in Fig. 1. The Cd ion is located on a twofold axis and displays a distorted octahedral coordination geometry (Table 1), formed by two fumarate dianions, a 1,10-phenanthroline (phen) and two water molecules. The fumarate dianions, located on



**Figure 1**  
 A segment of the polymeric structure of (I), with 30% probability displacement ellipsoids (arbitrary spheres for H atoms) [symmetry codes: (i)  $2 - x, y, -z + \frac{1}{2}$ ; (ii)  $-x + \frac{3}{2}, -y + \frac{3}{2}, 1 - z$ ].



**Figure 2**  
A packing diagram for (I), showing  $\pi$ - $\pi$  stacking between phen ligands. H atoms have been omitted.

inversion centers, bridge the neighboring  $\text{Cd}^{\text{II}}$  ions to form zigzag polymeric chains. The polymeric chains are arranged in such a way that the phen ligands of neighboring chains overlap (Fig. 2). The centroid-to-centroid separation of 3.693 (3) Å between N1-containing pyridine rings of parallel phen ligands suggests the existence of  $\pi$ - $\pi$  stacking in the crystal structure of (I).

## Experimental

An aqueous solution (30 ml) containing  $\text{Cd}(\text{NO}_3)_2$  (0.1 mmol), fumaric acid (0.1 mmol),  $\text{Na}_2\text{CO}_3$  (0.2 mmol) and phen (0.1 mmol) was refluxed for 2 h. After cooling to room temperature the solution was filtered. Single crystals of (I) were obtained from the filtrate after 3 d.

### Crystal data

$[\text{Cd}(\text{C}_4\text{H}_2\text{O}_4)(\text{C}_{12}\text{H}_8\text{N}_2)(\text{H}_2\text{O})_2]$   
 $M_r = 442.69$   
 Monoclinic,  $C2/c$   
 $a = 11.760$  (9) Å  
 $b = 13.06$  (1) Å  
 $c = 11.243$  (9) Å  
 $\beta = 114.92$  (1)°  
 $V = 1566$  (2) Å<sup>3</sup>  
 $Z = 4$

$D_x = 1.878$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 Cell parameters from 874 reflections  
 $\theta = 2.5$ – $26.0$ °  
 $\mu = 1.43$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
 Block, yellow  
 $0.32 \times 0.28 \times 0.24$  mm

### Data collection

Bruker SMART CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\text{min}} = 0.628$ ,  $T_{\text{max}} = 0.710$   
 4332 measured reflections

1554 independent reflections  
 1416 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.023$   
 $\theta_{\text{max}} = 26.2$ °  
 $h = -11 \rightarrow 14$   
 $k = -16 \rightarrow 10$   
 $l = -13 \rightarrow 13$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.020$   
 $wR(F^2) = 0.048$   
 $S = 1.04$   
 1554 reflections  
 114 parameters

H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0278P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.003$   
 $\Delta\rho_{\text{max}} = 0.27$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.37$  e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

Cd1—O1	2.3095 (19)	Cd1—N1	2.356 (2)
Cd1—O3	2.311 (2)		
O1—Cd1—O1 <sup>i</sup>	99.78 (10)	O1 <sup>i</sup> —Cd1—N1	95.65 (8)
O1—Cd1—O3	87.21 (7)	O3—Cd1—N1 <sup>i</sup>	84.66 (6)
O1—Cd1—O3 <sup>i</sup>	86.50 (7)	O3—Cd1—N1	103.40 (6)
O1—Cd1—N1	161.80 (6)	O3—Cd1—O3 <sup>i</sup>	170.22 (9)

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

Water H atoms were located in a difference Fourier map and refined as riding, with  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$ . Other H atoms were placed in calculated positions, with C—H = 0.93 Å and refined in riding mode with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 2000); software used to prepare material for publication: SHELXTL.

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