Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Di-μ-succinato-κ^4O:O'-bis[diaqua(1,10-phenanthroline-κ^2N,N')cadmium(II)] dihydrate

Qing-Wei Wang,[a] Xiu-Mei Li,[b]* Guang-Gang Gao[a] and Lin-Fang Shi[a]

[a]Department of Chemistry, Jilin Normal University, Siping 136000, People's Republic of China, and [b]Department of Chemistry, Tonghua Teachers College, Tonghua 134002, People's Republic of China

Correspondence e-mail: lixm20032006@yahoo.com.cn

Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.003 Å
R factor = 0.021
wR factor = 0.056
Data-to-parameter ratio = 14.2

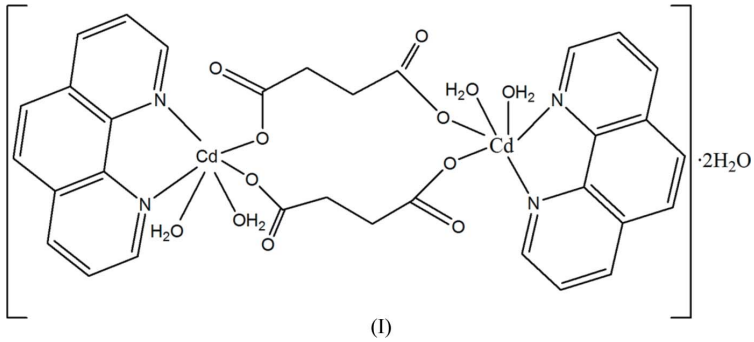
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 16 November 2006
Accepted 17 November 2006

In the centrosymmetric title compound, $[Cd_2(C_4H_4O_4)_2(C_{12}H_8N_2)_2(H_2O)_4]\cdot 2H_2O$, the Cd^{II} atom is six-coordinated in an octahedral environment by two N atoms from one 1,10-phenanthroline, two O atoms from two different succinate and two water molecules. The crystal structure features O—H···O hydrogen bonds between carboxylate O atoms and water molecules as well as π–π stacking interactions between phenanthrolines.

Comment

Metal–organic complexes show a variety of supramolecular architectures (Eddaoudi *et al.*, 2001) and metal succinates are one such class. The succinate anion can connect metal ions to form one-, two- and three-dimensional supramolecular structures (Zheng *et al.*, 2000; Padmanabhan *et al.*, 2005; Ghoshal *et al.*, 2004). 1,10-Phenanthroline in its complexes gives rise to π–π interactions (Chen & Liu, 2002). These two features are combined in the dinuclear title compound, (I).



(I)

The Cd^{II} atom is six-coordinated in an octahedral environment by two N atoms from a phenathroline, two O atoms from two different succinates, and two water molecules (Fig. 1). The compound is dimeric, arising from bridging by the succinates across a center of inversion. A set of π–π interactions between the phenanthroline molecules, the shortest atom-to-atom distance being 3.68 (1) Å, leads to the formation of a linear chain structure. The supramolecular chains are linked into layers by O—H···O hydrogen bonds (Fig. 2 and Table 2).

Experimental

Compound (I) was prepared from a mixture of $Cd(CH_3COO)_2$ (0.133 g, 0.5 mmol), H_2suc (0.118 g, 1.0 mmol), phen (0.099 g, 0.5 mmol) and H_2O (18 ml) in a 30 ml Teflon-lined autoclave under autogenous pressure at 453 K for 3 d. After cooling to room

temperature, pale-yellow crystals suitable for X-ray structure analysis were obtained. Analysis calculated for $C_{32}H_{36}Cd_2N_4O_{14}$: C 72.7, H 5.1, N 14.1%; found: C 72.5, H 4.8, N 113.9%.

Crystal data

$[Cd_2(C_4H_4O_4)_2(C_{12}H_8N_2)_2(H_2O)_4]\cdot 2H_2O$
$M_r = 925.45$
Triclinic, $P\overline{1}$
$a = 8.1775\ (16)$ Å
$b = 8.4059\ (17)$ Å
$c = 13.064\ (3)$ Å
$\alpha = 95.13\ (3)^\circ$
$\beta = 104.18\ (3)^\circ$
$\gamma = 104.86\ (3)^\circ$
$V = 830.4\ (4)$ Å^3
$Z = 1$
$D_x = 1.851$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.36$ mm^{-1}
$T = 292\ (2)$ K
Block, pale yellow
0.27 × 0.23 × 0.21 mm

Data collection

Bruker APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SAINT*; Bruker, 1998)
$T_{min} = 0.661$, $T_{max} = 0.755$
5179 measured reflections
3670 independent reflections
3585 reflections with $I > 2\sigma(I)$
$R_{int} = 0.011$
$\theta_{max} = 28.3^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.021$
$wR(F^2) = 0.056$
$S = 1.13$
3670 reflections
259 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0333P)^2 + 0.2504P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.003$
$\Delta\rho_{max} = 0.36$ e Å^{-3}
$\Delta\rho_{min} = -0.91$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—N1	2.3664 (17)	Cd1—O1*W*	2.3812 (15)
Cd1—N2	2.3661 (16)	Cd1—O2*W*	2.4204 (18)
Cd1—O1	2.2536 (15)	Cd1—O3^{i}	2.2567 (16)
O1—Cd1—O3^{i}	110.17 (6)	N2—Cd1—O1*W*	157.66 (6)
O1—Cd1—N2	95.59 (6)	N1—Cd1—O1*W*	86.82 (6)
O3^{i}—Cd1—N2	116.03 (6)	O1—Cd1—O2*W*	157.09 (7)
O1—Cd1—N1	87.23 (6)	O3^{i}—Cd1—O2*W*	79.63 (7)
O3^{i}—Cd1—N1	159.65 (6)	N2—Cd1—O2*W*	98.41 (7)
N2—Cd1—N1	70.84 (6)	N1—Cd1—O2*W*	80.39 (7)
O1—Cd1—O1*W*	83.12 (6)	O1*W*—Cd1—O2*W*	77.04 (7)
O3^{i}—Cd1—O1*W*	84.98 (6)		

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H*W*12···O2^{ii}	0.82 (3)	1.92 (3)	2.733 (2)	172 (3)
O1*W*—H*W*11···O3^{iii}	0.76 (4)	2.16 (4)	2.855 (3)	153 (3)
O2*W*—H*W*21···O3^{iii}	0.77 (3)	2.13 (3)	2.885 (3)	169 (3)
O2*W*—H*W*22···O3*W*^{iv}	0.78 (3)	1.94 (3)	2.721 (3)	173 (3)
O3*W*—H*W*31···O2	0.84 (4)	1.94 (4)	2.759 (2)	163 (3)
O3*W*—H*W*32···O4^{ii}	0.86 (3)	1.92 (3)	2.777 (2)	171 (3)

Symmetry codes: (ii) $-x+1, -y+1, -z+1$; (iii) $x, y-1, z$; (iv) $x-1, y-1, z$.

All H atoms on C atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$. The H atoms of the water molecules were located in a difference Fourier map and were refined freely.

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: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

We thank Professors Ning-Hai Hu and Heng-Qing Jia of Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, for supporting this work.

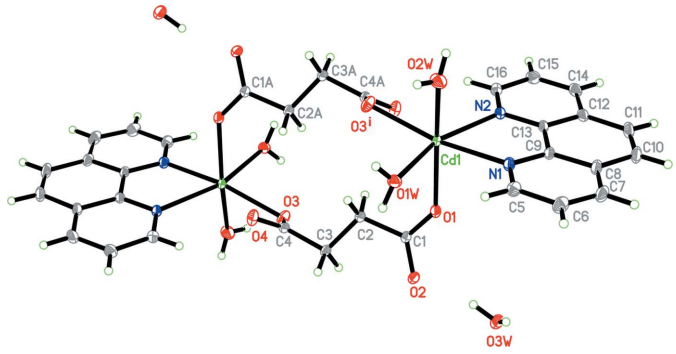


Figure 1
The molecular structure of (I), showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (i) $-x, 1-y, 1-z$.]

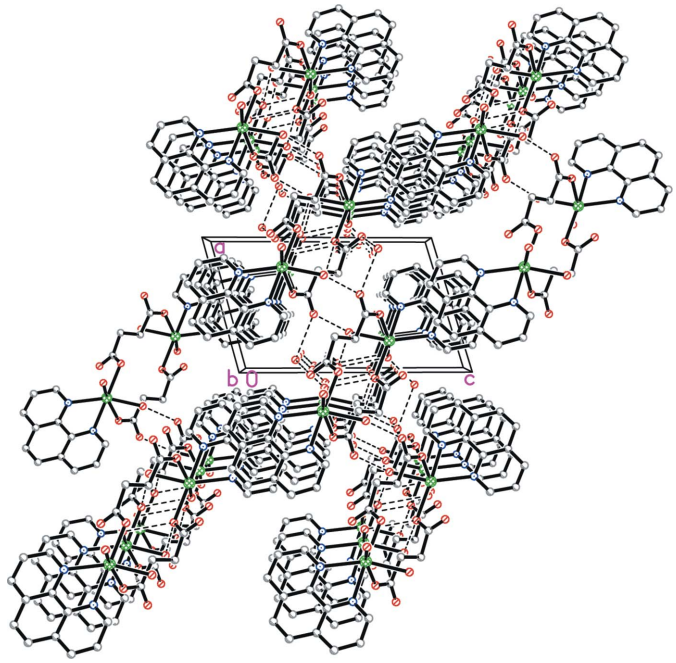


Figure 2
View of the two-dimensional layer, formed *via* π–π stacking and hydrogen-bond interactions (dashed lines), along the *b* axis. H atoms have been omitted.

References

Bruker (1998). *SMART*, *SAINT* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.

Chen, X.-M. & Liu, G.-F. (2002). *Chem. Eur. J.* **8**, 4811–4817.
Eddaoudi, M., Moler, D. B., Li, H., Chen, B., Reineke, T. M., O'Keeffe, M. & Yaghi, O. M. (2001). *Acc. Chem. Res.* **34**, 319–330.
Ghoshal, D., Maji, T. K., Mostafa, G., Sain, S., Lu, T. H., Ribas, J., Zangrando, E. & Chaudhuri, R. (2004). *Dalton Trans.* pp. 1687–1695.
Padmanabhan, M., Kumary, S. M., Huang, X. Y. & Li, **initials?** (2005). *Inorg. Chim. Acta*, **358**, 3537–3544.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Zheng, Y. Q., Sun, J. & Lin, J. L. (2000). *Z. Anorg. Allg. Chem.* **626**, 1501–1504.