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μ-Adipato-$\kappa^4O,O':O'',O'''$-bis[aqua(2,9-dimethyl-1,10-phenanthroline-κ^2N,N)-nitratocadmium(II)] dihydrate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.027
wR factor = 0.068
Data-to-parameter ratio = 13.9

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

In the centrosymmetric binuclear title complex, $[Cd_2(C_6H_8O_4)(NO_3)_2(C_{14}H_{12}N_2)_2(H_2O)_2]$, each Cd atom is seven-coordinated in a CdO_5N_2 environment with a distorted petagonal-bipyramidal geometry. The water molecules act as both donors and acceptors in O—H···O hydrogen bonds, interconnecting the molecules into double chains along the b axis. The packing is further stabilized by π–π interactions between the phenanthroline ring systems.

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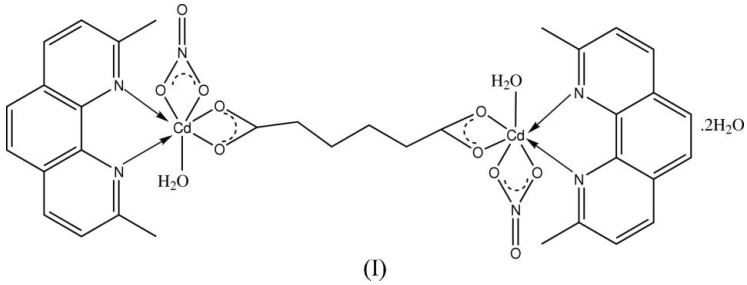
Comment

Recently, we reported the structure of di-μ-adipato-$\kappa^6O,O':O'';O:O',O''$-bis[aqua(1,10-phenanthroline-κ^2N,N)-zinc(II)] (Ding *et al.*, 2005). In our ongoing studies, we synthesized the title compound, (I). An X-ray crystallographic analysis was undertaken to determine the stereochemistry of (I).



(I)

The binuclear cadmium complex molecule in (I) possesses a crystallographically imposed centre of symmetry (Fig. 1). Each Cd^{II} atom is seven-coordinated by two N atoms and five O atoms (Table 1) in a distorted petagonal-bipyramidal

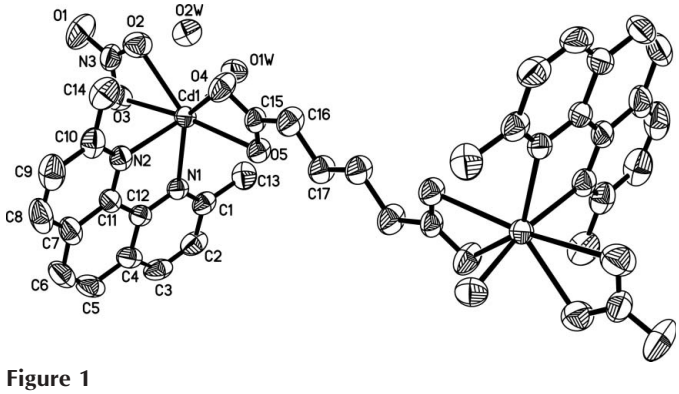


Figure 1
View of (I), showing the atom-numbering scheme and 50% probability displacement ellipsoids. H atoms have been omitted for clarity. Unlabelled atoms are related to labelled atoms by the symmetry code $(-x, -y, -z)$.

geometry. One axial position is occupied by atom O1*W* of a water molecule, with a Cd—O distance of 2.283 (2) Å. The other axial position is occupied by atom N2 of the 2,9-dimethylphenanthroline ligand.

In the crystal structure, the water molecules act as both donors and acceptors to form O—H···O hydrogen bonds (Table 2). These hydrogen bonds link the molecules into double chains along the *c* axis (Fig. 2). The short $Cg1\cdots Cg1^{i}$ distance of 3.508 (2) Å [*Cg*1 is the centroid of the C4–C7/C11/C12 ring; symmetry code: (i) $1-x, y, \frac{1}{2}-z$] indicates the existence of π–π stacking interactions between the phenanthroline ring systems, which stabilize the packing.

Experimental

To a solution of 2,9-dimethyl-1,10-phenanthroline (0.21 g, 1 mmol) and adipic acid (0.73 g, 0.5 mmol) in ethanol (10 ml) was added a solution of cadmium nitrate (0.31 g, 1 mmol) in distilled water (10 ml). The mixture was stirred and refluxed for 2 h. The hot solution was then filtered into another flask containing ethanol (10 ml). Orange crystals appeared over a period of one week by slow evaporation at room temperature.

Crystal data

$[Cd_2(C_6H_8O_4)(NO_3)_2(C_{14}H_{12}N_2)_2(H_2O)_2]$
M_r = 981.54
Monoclinic, *C*2/*c*
a = 24.438 (2) Å
b = 11.2315 (10) Å
c = 13.8799 (12) Å
β = 96.9690 (10)°
V = 3781.6 (6) Å^3
Z = 4
D_x = 1.724 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5950 reflections
θ = 2.4–26.1°
μ = 1.20 mm^{-1}
T = 293 (2) K
Column, orange
0.30 × 0.16 × 0.07 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.715, T_{max} = 0.921
10344 measured reflections
3730 independent reflections
3367 reflections with $I > 2\sigma(I)$
R_{int} = 0.016
θ_{max} = 26.1°
h = −26 → 30
k = −8 → 13
l = −17 → 16

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.068
S = 1.05
3730 reflections
269 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0341P)^2 + 4.9157P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cd1—O1*W*	2.283 (2)	Cd1—O2	2.423 (2)
Cd1—O4	2.321 (2)	Cd1—O5	2.4690 (17)
Cd1—N1	2.330 (2)	Cd1—O3	2.583 (3)
Cd1—N2	2.348 (2)		

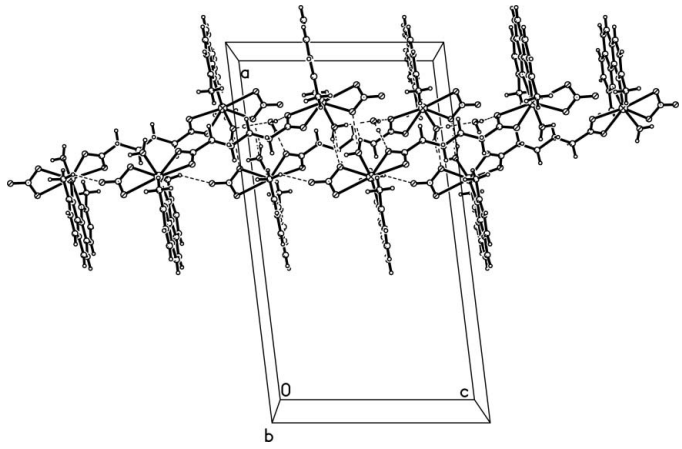


Figure 2
Packing diagram of (I), viewed down the *b* axis. Intermolecular hydrogen bonds are denoted by dashed lines.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*1···O2*W*	0.81 (4)	1.87 (4)	2.681 (4)	177 (4)
O2*W*—H1*W*2···O4^{i}	0.90 (5)	1.85 (5)	2.756 (4)	177 (5)
O2*W*—H2*W*2···O5^{ii}	0.80 (4)	1.99 (4)	2.789 (4)	173 (4)
C14—H14*B*···O1^{iii}	0.96	2.37	3.223 (4)	147

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

C-bound H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.93–0.97 Å and U_{iso}(H) = 1.2–1.5U_{eq}(parent atom). The H atoms of the water molecules were located in a difference Fourier map and refined isotropically.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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