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trans-Diaquatetrakis(4,4′-methylenediphenylamine-*N*)-cadmium(II) dinitrate dihydrate

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The title compound, $[Cd(C_{13}H_{14}N_2)_4(H_2O)_2](NO_3)_2\cdot 2H_2O$, has been prepared from the self-assembly reaction of oligoaniline dadpm (dadpm is diaminodiphenylmethane) and $Cd(NO_3)_2$ in MeOH/H_2O. The Cd^{II} mononuclear complex cation has a center of symmetry, and dadpm acts as a monodentate ligand.

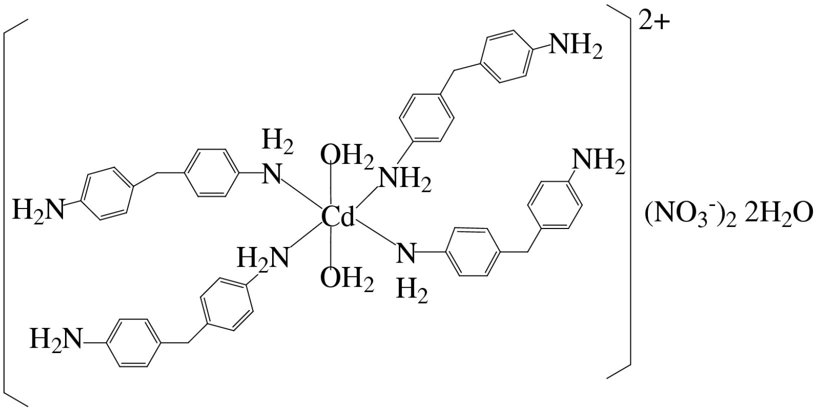
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.044
wR factor = 0.126
Data-to-parameter ratio = 12.8

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

Comment

In recent decades, there has been great interest in the study of metal–organic supramolecular frameworks owing to their intriguing structural diversity and potential application in catalysis, separation and molecular recognition (Piguet *et al.*, 1997; Yaghi *et al.*, 1998; Swiegers & Malefetse, 2000). In the construction of one-, two- and three-dimensional frameworks, the rational design and selection of ligands are crucial for the formation of metal–organic coordination frameworks. For example, many rigid ligands, such as 4,4-bipyridine or polycarboxylic acids, and flexible ligands, such as bipyridine derivatives with spacers, have been extensively employed in the formation of supramolecular architectures (Yang *et al.*, 2001; Wang *et al.*, 2001; Horikoshi *et al.*, 2001). The displacement of oligopyridine by oligoaniline should result in new structural motifs and new topologies, but oligoaniline ligands are seldom employed (Zhang *et al.*, 1999). In this paper, we report the crystal structure of $[Cd(dadpm)_4(H_2O)_2](NO_3)_2.2H_2O$, (I), obtained from the self-assembly of dadpm and $Cd(NO_3)_2$.



(I)

Compound (I) is a mononuclear Cd^{II} complex and dadpm serves as a monodentate ligand (Fig. 1). The Cd atom is coordinated by N atoms from four different dadpm ligands and O atoms from two water molecules, forming a distorted octahedral coordination of CdN_4O_2. The Cd—N and Cd—O

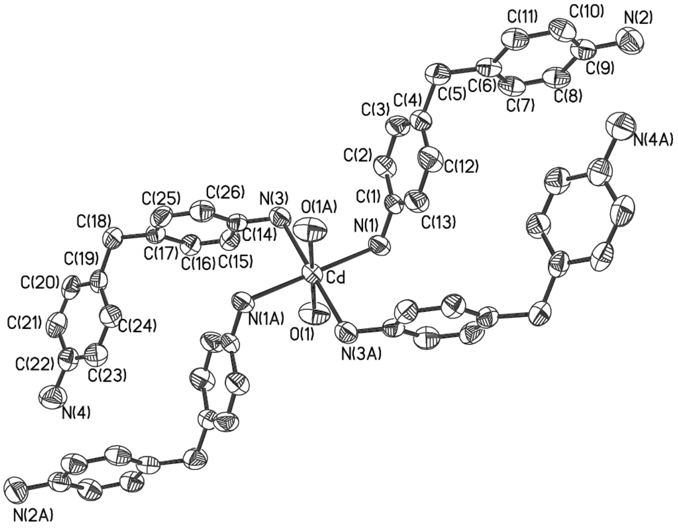


Figure 1
The structure of (I) with NO_3^- and uncoordinated water omitted for clarity. Displacement ellipsoids are plotted at the 50% probability level.

bond distances are 2.363 (3)–2.405 (3) and 2.295 (3) Å, respectively (Table 1).

Experimental

A mixture of $Cd(NO_3)_2$ (0.08 g, 0.25 mmol) and dadpm (0.10 g, 0.50 mmol) in water–methanol (10/20) was stirred for 3 h. The colorless solution was allowed to evaporate slowly for a week, after which time colorless crystals of (I) were obtained.

Crystal data

$[Cd(C_{13}H_{14}N_2)_4(H_2O)_2]$-
$(NO_3)_2 \cdot 2H_2O$
$M_r = 1101.53$
Triclinic, $P\overline{1}$
$a = 9.3189$ (2) Å
$b = 11.6565$ (3) Å
$c = 12.0590$ (1) Å
$\alpha = 80.845$ (1)°
$\beta = 86.638$ (1)°
$\gamma = 89.051$ (1)°
$V = 1290.97$ (4) Å^3
$Z = 1$
$D_x = 1.417$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 68 reflections
$\theta = 1.7$–25.1°
$\mu = 0.49$ mm^{-1}
$T = 293$ (2) K
Columnar, colorless
0.32 × 0.17 × 0.15 mm

Data collection

Smart CCD diffractometer
ω scans
Absorption correction: empirical (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.855$, $T_{max} = 0.929$
6516 measured reflections
4428 independent reflections
3749 reflections with $I > 2\sigma(I)$
$R_{int} = 0.024$
$\theta_{max} = 25.1°$
$h = -11 \rightarrow 10$
$k = -11 \rightarrow 13$
$l = -11 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.126$
$S = 1.10$
4428 reflections
347 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0795P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.35$ e Å^{-3}
$\Delta\rho_{min} = -0.75$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd—O1	2.295 (3)	Cd—N3	2.405 (3)
Cd—N1	2.363 (3)		
O1—Cd—N1	85.56 (12)	N1—Cd—N3	86.30 (11)
O1—Cd—N3	87.97 (12)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—HOA···O12^{i}	0.94 (2)	1.86 (2)	2.796 (5)	174 (5)
O1—HOB···O101^{i}	0.935 (19)	1.76 (2)	2.691 (6)	173 (4)
O101—H01···N4^{ii}	0.875 (18)	2.30 (3)	3.054 (8)	144 (3)
O101—H02···N2^{iii}	0.95 (2)	2.30 (7)	3.074 (6)	138 (8)

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

The positions of the H atoms were generated geometrically (C—H bond fixed at 0.96 Å), assigned isotropic displacement parameters and allowed to ride on their respective parent C atoms, and the positions of the water H atoms were refined with isotropic displacement parameters before the final cycle of least-squares refinement. There are short intermolecular H···H contacts; HOB···H01^{i} = 2.06 Å, H01···H4B^{ii} = 2.09 Å and H02···H2B^{iii} = 1.99 Å (see Table 2 for symmetry codes). However, the assumed H-atom positions are reasonable based on the following angles, O1···H01^{i}—O101^{i} = 63.9°, O101···H4B^{ii}—N4^{ii} = 89.4° and O101···H2B^{iii}—N2^{iii} = 95.9°.

Data collection: *SMART* (Siemens, 1994); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1994); 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*.

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Acta Cryst. (2001). E**57**, m344–m345 Ruihu Wang *et al.* • $[Cd(C_{13}H_{14}N_2)_4(H_2O)_2](NO_3)_2 \cdot 2H_2O$ **m345**