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Key indicators

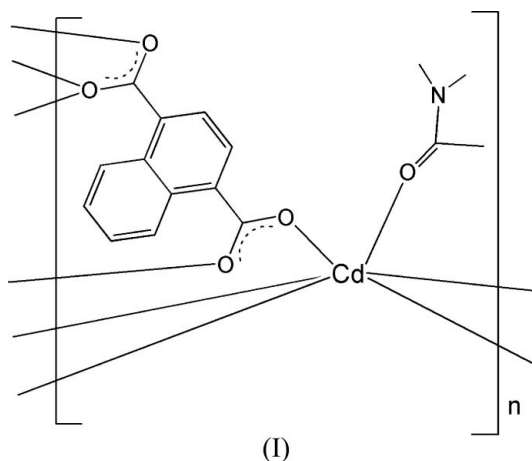
Single-crystal X-ray study
 $T = 292$ K
Mean $\sigma(\text{C}-\text{C}) = 0.005$ Å
 R factor = 0.028
 wR factor = 0.067
Data-to-parameter ratio = 15.7For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Poly[(*N,N*-dimethylacetamide)(μ_5 -naphthalene-1,4-dicarboxylato)cadmium(II)]

In the title compound, $[\text{Cd}(\text{C}_{12}\text{H}_6\text{O}_4)(\text{C}_4\text{H}_9\text{NO})]_n$, each Cd^{II} atom is coordinated by six O atoms from four naphthalene-1,4-dicarboxylate (*L*) ligands (three monodentate and one bidentate) and one O-bonded *N,N*-dimethylacetamide molecule in a very distorted octahedral coordination. Each *L* ligand bridges five Cd^{II} atoms, generating a distinctive three-dimensional coordination polymer.

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Comment

The construction of metal–organic coordination polymers with novel structures and topologies has attracted great interest from chemists due to their potential applications as functional solid materials, as well as their fascinating framework structures (Eddaoudi *et al.*, 2001). Benzene-1,4-dicarboxylate is a rigid rod-like spacer, well known in the construction of metal-organic polymers, and it has shown numerous interesting supramolecular architectures (Batten & Robson, 1998). However, similar ligands such as naphthalene-1,4-dicarboxylate (H_2L^{2-}) have not been so well explored to date (Wang *et al.*, 2006). In this work, the combination of H_2L with Cd^{II} cations in DMA solvent (DMA = *N,N*-dimethylacetamide) resulted in the title compound, $[\text{Cd}(\text{L})(\text{DMA})]_n$, (I), an interesting three-dimensional coordination polymer incorporating a covalently bound non-aqueous solvent molecule.



Selected bond lengths and angles for (I) are given in Table 1. In complex (I), each Cd^{II} atom is six-coordinated by six O atoms from four *L* ligands (three monodentate, one bidentate) and one DMA molecule in a very distorted octahedral, or possibly irregular, coordination. The $\text{Cd}-\text{O}_c$ ($c = \text{carboxylate}$) distances, which range from 2.217 (3) to 2.451 (3) Å (Table 1), are comparable to those observed for $[\text{Cd}(\text{3-PYD})_2(\text{H}_2\text{O})]_n$.

$2\text{H}_2\text{O})_n$ [3-PYD = 3-(3-pyridyl)acrylate] (Li *et al.*, 2005). The C—O distances in the C1/O1/O2 and C10/O4/O5 carboxylate groups suggest delocalized bonding for both groups. In the crystal structure, each *L* ligand bridges five Cd^{II} atoms, generating a distinctive three-dimensional structure (Fig. 2).

Experimental

H_2L (108 mg, 0.5 mmol) was added slowly to an *N,N*-dimethylacetamide solution (15 ml) of $\text{CdCl}_2 \cdot 2.5\text{H}_2\text{O}$ (114 mg, 0.5 mmol) with stirring at 363 K. The resulting solution was filtered and the filtrate was allowed to stand in air at room temperature for several weeks, yielding crystals of (I) (33% yield based on Cd).

Crystal data

$[\text{Cd}(\text{C}_{12}\text{H}_6\text{O}_4)(\text{C}_4\text{H}_9\text{NO})]$	$Z = 4$
$M_r = 413.69$	$D_x = 1.914 \text{ Mg m}^{-3}$
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation
$a = 6.8711 (14) \text{ \AA}$	$\mu = 1.55 \text{ mm}^{-1}$
$b = 14.010 (3) \text{ \AA}$	$T = 292 (2) \text{ K}$
$c = 14.915 (3) \text{ \AA}$	Block, colorless
$V = 1435.7 (5) \text{ \AA}^3$	$0.33 \times 0.31 \times 0.25 \text{ mm}$

Data collection

Rigaku R-Axis RAPID diffractometer	14000 measured reflections
ω scans	3266 independent reflections
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	3029 reflections with $I > 2\sigma(I)$
$T_{\text{min}} = 0.635$, $T_{\text{max}} = 0.687$	$R_{\text{int}} = 0.037$
	$\theta_{\text{max}} = 27.4^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0303P)^2 + 1.3739P]$
$R[F^2 > 2\sigma(F^2)] = 0.028$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.067$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.08$	$\Delta\rho_{\text{max}} = 0.60 \text{ e \AA}^{-3}$
3266 reflections	$\Delta\rho_{\text{min}} = -0.72 \text{ e \AA}^{-3}$
208 parameters	Absolute structure: Flack (1983),
H-atom parameters constrained	1371 Friedel pairs
	Flack parameter: $-0.02 (3)$

Table 1

Selected geometric parameters (\AA , $^\circ$).

C1—O2	1.250 (4)	Cd1—O2	2.268 (3)
C1—O3	1.266 (4)	Cd1—O3 ⁱ	2.259 (2)
C10—O4	1.255 (5)	Cd1—O5 ⁱⁱ	2.373 (3)
C10—O5	1.272 (5)	Cd1—O4 ⁱⁱ	2.451 (3)
Cd1—O1	2.217 (3)	Cd1—O5 ⁱⁱⁱ	2.515 (3)
O1—Cd1—O3 ⁱ	98.94 (11)	O2—Cd1—O4 ⁱⁱ	83.74 (10)
O1—Cd1—O2	83.31 (11)	O5 ⁱⁱ —Cd1—O4 ⁱⁱ	54.58 (9)
O3 ⁱ —Cd1—O2	171.59 (11)	O1—Cd1—O5 ⁱⁱⁱ	84.94 (11)
O1—Cd1—O5 ⁱⁱ	151.76 (11)	O3 ⁱ —Cd1—O5 ⁱⁱⁱ	80.50 (10)
O3 ⁱ —Cd1—O5 ⁱⁱ	85.40 (10)	O2—Cd1—O5 ⁱⁱⁱ	107.82 (10)
O2—Cd1—O5 ⁱⁱ	88.85 (9)	O5 ⁱⁱ —Cd1—O5 ⁱⁱⁱ	123.24 (8)
O1—Cd1—O4 ⁱⁱ	149.84 (11)	O4 ⁱⁱ —Cd1—O5 ⁱⁱⁱ	73.34 (9)
O3 ⁱ —Cd1—O4 ⁱⁱ	97.83 (9)		
Symmetry codes: (i) $x + \frac{1}{2}, -y - \frac{1}{2}, -z$;	(ii) $-x + \frac{1}{2}, -y, z - \frac{1}{2}$;	(iii) $-x + 1, y - \frac{1}{2}, -z + \frac{1}{2}$.	

All H atoms were positioned geometrically and refined as riding, with C—H = 0.93 \AA and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*;

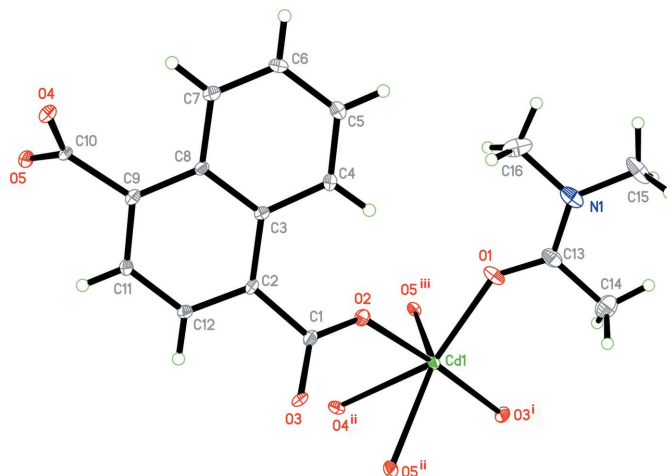


Figure 1

The asymmetric unit of (I), expanded to show the Cd coordination. Displacement ellipsoids are drawn at the 30% probability level for the non-H atoms. [Symmetry codes: (i) $\frac{1}{2} + x, -\frac{1}{2} - y, -z$; (ii) $\frac{1}{2} - x, -y, z - \frac{1}{2}$; (iii) $1 - x, y - \frac{1}{2}, \frac{1}{2} - z$.]

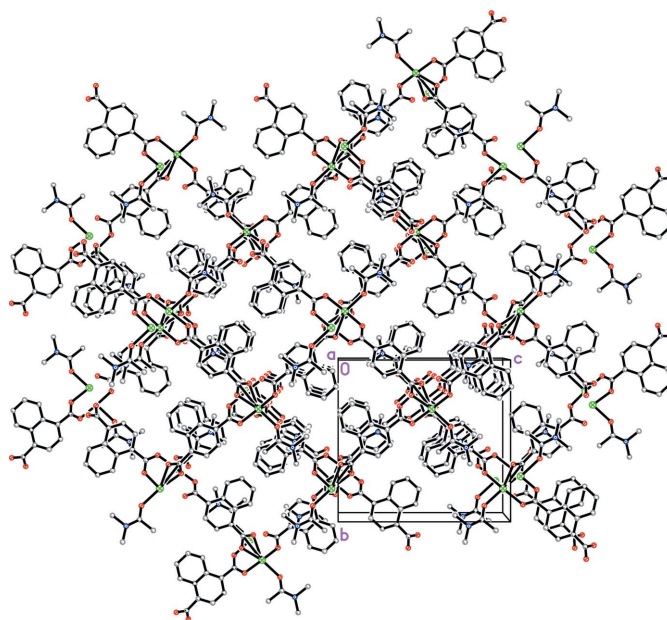


Figure 2

The extended structure of (I).

program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

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