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Poly[(μ_2-4,4′-bipyridine-κ^2N:N')(μ_2-furan-2-carboxylato-κ^2O:O')cadmium(II)]

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.028
wR factor = 0.075
Data-to-parameter ratio = 14.5

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

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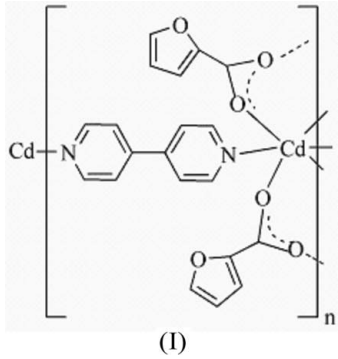
In the crystal structure of the title compound, $[Cd(C_5H_3O_3)_2(C_{10}H_8N_2)]_n$, which was synthesized from the reaction of $Cd(ClO_4)_2\cdot 6H_2O$, furan-2-carboxylic acid and 4,4′-bipyridine in methanol–water, the Cd atom is octahedrally coordinated by two N atoms of two bipyridine ligands and four O atoms of four furan-2-carboxylate ligands. The carboxylate group coordinates in a bridging mode; the Cd atom and 4,4′-bipyridine ligand lie on a crystallographic twofold rotation axis. The compound exhibits a layer structure arising from the bonding modes of the furan-2-carboxylate anion and the 4,4′-bipyridine heterocycle.

Comment

4,4′-Bipyridine is an excellent bridging ligand, and many one-, two- and three-dimensional metal–4,4′-bipy frameworks have beem described in the literature. These frameworks are usually generated by coordination bonds (Li & Lou, 2007). The title compound, (I), is another example of a layer framework.



(I)

The Cd atom of (I) lies on a twofold axis that runs along the N···N vector of the 4,4′-bipyridine ligand. The Cd ion shows octahedral geometry, being coordinated by two N atoms of two bipyridine ligands and four O atoms from four furan-2-carboxylate groups. The furan-2-carboxylate ligand bridges the Cd atoms in a *syn–syn* manner to form a chain. There are rectangular grids with the organic ligands acting as bridges within the layer. Adjacent Cd^{II} centres are doubly bridged by the ligands to form a large eight-membered ring, while four Cd atoms belong to a 26-membered ring (Fig. 2).

Experimental

An aqueous solution (5 ml) of $Cd(ClO_4)_2\cdot 6H_2O$ (1 mmol, 0.422 g) was added to a methanol solution (15 ml) of NaOH (2 mmol, 0.081 g) and furan-2-carboxylic acid (2 mmol, 0.225 g) and 4,4′-bipyridine

(1 mmol, 0.156 g). The mixture was refluxed for 8 h and filtered, and the filtrate was kept in a $CaCl_2$ desiccator. After a few days, colourless crystals were obtained. CHN elemental analysis, calculated: C 48.91, H 2.85, N 5.70%; found: C 48.62, H 2.96, N 5.87%.

Crystal data

$[Cd(C_5H_3O_3)_2(C_{10}H_8N_2)]$
M_r = 490.74
Monoclinic, $C2/c$
a = 16.984 (3) Å
b = 11.686 (2) Å
c = 10.0952 (17) Å
β = 109.455 (11)°
V = 1889.2 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.20 mm^{-1}
T = 293 (2) K
0.20 × 0.16 × 0.14 mm

Data collection

Bruker SMART area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.759, T_{max} = 1.000
(expected range = 0.642–0.846)
5254 measured reflections
1940 independent reflections
1584 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.076
S = 1.06
1940 reflections
134 parameters
12 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—O1	2.1735 (12)	Cd1—N1	2.2735 (19)
Cd1—O2^{i}	2.1844 (12)	Cd1—N2^{ii}	2.3168 (19)
O1—Cd1—O1^{iii}	178.38 (6)	O2^{i}—Cd1—N1	92.95 (3)
O1—Cd1—O2^{i}	89.78 (5)	O1—Cd1—N2^{ii}	90.81 (3)
O1^{iii}—Cd1—O2^{i}	90.31 (5)	O2^{i}—Cd1—N2^{ii}	87.05 (3)
O2^{i}—Cd1—O2^{iv}	174.10 (6)	N1—Cd1—N2^{ii}	180
O1—Cd1—N1	89.19 (3)		

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

H atoms bonded to C atoms were positioned geometrically and treated as riding, with C—H = 0.93 Å and with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2003); software used to prepare material for publication: *SHELXTL*.

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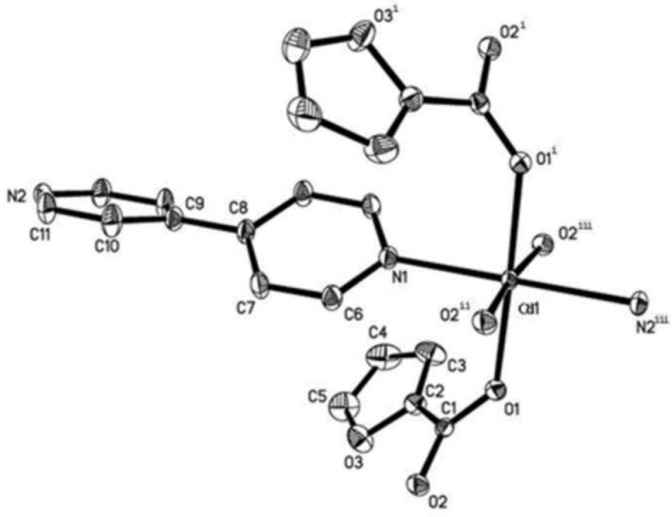

Figure 1
The asymmetric unit of (I), extended to show the complete coordination of Cd and complete ligands. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry codes: (i) $-x, y, -z+\frac{1}{2}$; (ii) $x, -y, z+\frac{1}{2}$; (iii) $-x, -y, -z$.]

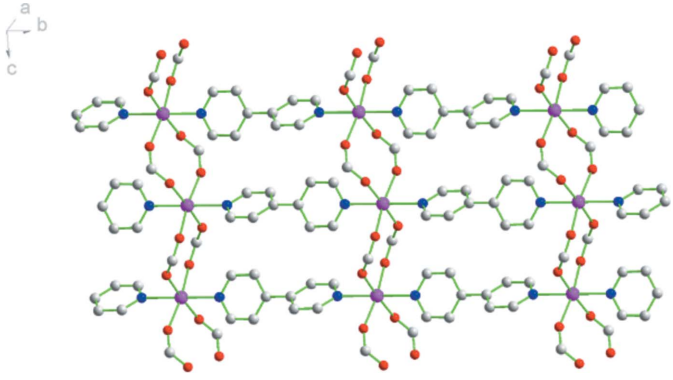

Figure 2
The layer structure of (I). H atoms have been omitted.

References

Bruker (2001). *SMART*. Version 5.624. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2003). *SAINT*. Version 7. Bruker AXS Inc., Madison, Wisconsin, USA.
Li, Y.-F. & Lou, T.-J. (2007). *Acta Cryst.* E**63**, m994–m996.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (2003). *SHELXTL* (Version 6.12) and *SADABS* (Version 2.10). Bruker AXS Inc., Madison, Wisconsin, USA.B