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catena-Poly[di-μ_3-benzoato-tetra-μ_2-benzoato-dipyrroletricadmium(II)]

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.010 Å
R factor = 0.043
wR factor = 0.115
Data-to-parameter ratio = 15.8

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

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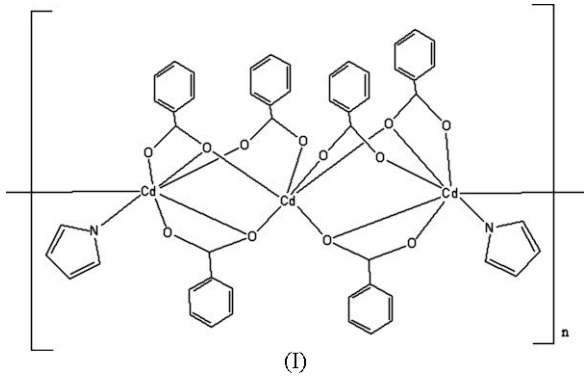
In the title complex, $[Cd_3(C_7H_5O_2)_6(C_4H_4N)_2]_n$, the benzoate groups adopt μ_3 and μ_2 coordination modes to connect neighbouring cadmium(II) ions into one-dimensional chains. One of the Cd atoms lies on a crystallographic twofold axis.

Comment

In recent years, the synthesis of metal–organic framework structures by the modular approach has become an area of intense research activity for potential zeolitic, optoelectronic, magnetic and conducting materials (Kahn & Martinez, 1998; Munakata *et al.*, 1998). In the design and synthesis of polymeric metal–organic frameworks, various synthetic routes with bridging and chelating ligands have been used. Hydrothermal synthesis has been demonstrated to be an effective and powerful technique for the crystal growth of metal–organic framework complexes (Lawandy *et al.*, 1999). In the present research, using benzoic acid and pyrrole ligands, the title one-dimensional complex, (I), $[Cd_3(C_4H_4N)_2(C_7H_5O_2)_6]_n$, has been obtained under hydrothermal conditions and characterized by single-crystal X-ray diffraction.



(I)

The asymmetric unit of (I) is shown in Fig. 1. Selected bond lengths and angles are listed in Table 1. There are two independent Cd atoms in the asymmetric unit, one of which (Cd1) lies on a crystallographic two-fold axis. Atom Cd1 has octahedral geometry, being coordinated by six carboxylate O atoms from six benzoate ligands, while atom Cd2 is linked to Cd1 *via* two μ_3 and one μ_2 benzoate ligands. Atom Cd2 is coordinated by seven atoms, by way of two bis-chelating and two mono-chelating benzoate ligands, and a pyrrole ligand through N. For the Cd1 centre, the Cd—O bond distances vary from 2.235 (4) to 2.324 (4) Å, while for Cd2, these distances are in the range 2.288 (4)–2.515 (4) Å.

The one-dimensional chain structure of (I) is shown in Fig. 2. Within the chains, there are significant C—H···O interactions

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(Table 2), but there are no noticeable interactions between chains.

Experimental

A mixture of $Cd(ClO_4)_2\cdot 6H_2O$ (0.2 mmol. 83.88 mg), benzonitrile (0.3 mmol, 30.03 mg), pyrrole (0.2 mmol, 13.14 mg) and water (9.0 ml), in a 1:1.5:1:2500 molar ratio, was sealed in a 15 ml stainless steel Teflon-lined bomb and heated at 403 K for 72 h, then cooled slowly to 303 K at a rate of 3 K h^{-1}. Colourless crystals of (I) were collected by filtration and washed with ethanol (2 × 5 ml). Analysis calculated for $C_{50}H_{38}N_2O_{12}Cd_3$: C 50.21, H 3.20, N 2.34%; found: C 50.25, H 3.15, N 2.20%.

Crystal data

$[Cd_3(C_7H_5O_2)_6(C_4H_4N)_2]$	D_x = 1.693 Mg m^{-3}
M_r = 1196.02	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 1006 reflections
a = 27.937 (9) Å	θ = 2.4–25.1°
b = 8.828 (3) Å	μ = 1.41 mm^{-1}
c = 19.072 (6) Å	T = 293 (2) K
β = 93.974 (6)°	Block, colourless
V = 4692 (3) $Å^3$	0.24 × 0.20 × 0.18 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	4801 independent reflections
	3118 reflections with $I > 2\sigma(I)$
φ and ω scans	R_{int} = 0.057
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	θ_{max} = 26.4°
	$h = -34 \rightarrow 15$
T_{min} = 0.720, T_{max} = 0.776	$k = -11 \rightarrow 10$
13 090 measured reflections	$l = -23 \rightarrow 23$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.043	$w = 1/[\sigma^2(F_o^2) + (0.0302P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.115	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.04	$\Delta\rho_{max}$ = 0.90 e $Å^{-3}$
4801 reflections	$\Delta\rho_{min}$ = −0.86 e $Å^{-3}$
303 parameters	

Table 1
Selected bond lengths (Å).

Cd1—O6	2.235 (4)	Cd2—O2^{i}	2.302 (4)
Cd1—O3	2.298 (4)	Cd2—O4	2.328 (4)
Cd1—O1	2.324 (4)	Cd2—O2	2.398 (4)
Cd2—N1	2.267 (5)	Cd2—O3	2.456 (4)
Cd2—O5	2.288 (4)	Cd2—O1	2.515 (4)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O6^{ii}	0.93	2.59	3.503 (7)	167
C7—H7···O4^{i}	0.93	2.33	3.217 (7)	159
C22—H22···O5^{i}	0.93	1.89	2.808 (7)	167

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

H atoms were placed in calculated positions (C—H = 0.93 Å) and included in the riding-model approximation, with U_{iso}(H) = $1.2U_{eq}$(C).

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-NT* (Bruker, 1998); software used to prepare material for publication: *SHELXTL-NT* and *PLATON* (Spek, 2003).

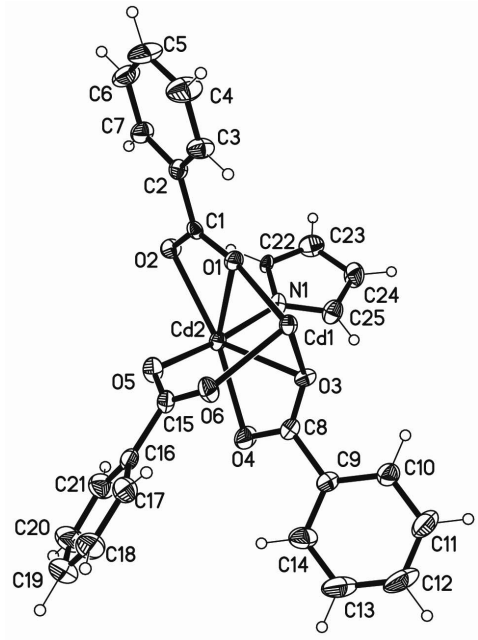

Figure 1
A view of the coordination environment of atom Cd2 of (I), showing the atomic labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted.

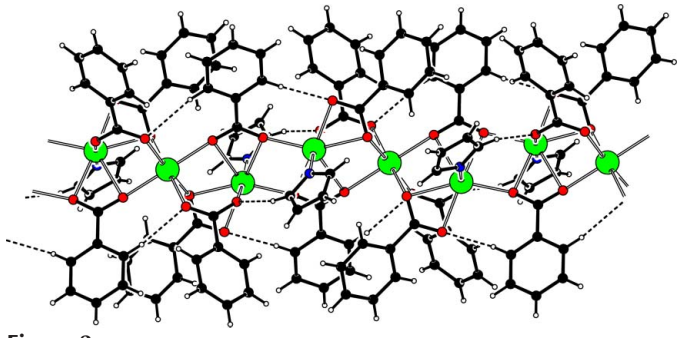

Figure 2
The one-dimensional chain structure of (I), propagating in the *c* direction. Hydrogen bonds are shown as dashed lines. Colour code: green Cd, red O, blue N and black C.

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