

catena-Poly[[bis[4,4'-oxydibenzoato(1-)]-cadmium(II)]- μ -1,2-di-4-pyridylethylene]

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Key indicators

Single-crystal X-ray study
 T = 298 K
 Mean σ (C–C) = 0.007 Å
 R factor = 0.056
 wR factor = 0.123
 Data-to-parameter ratio = 12.9

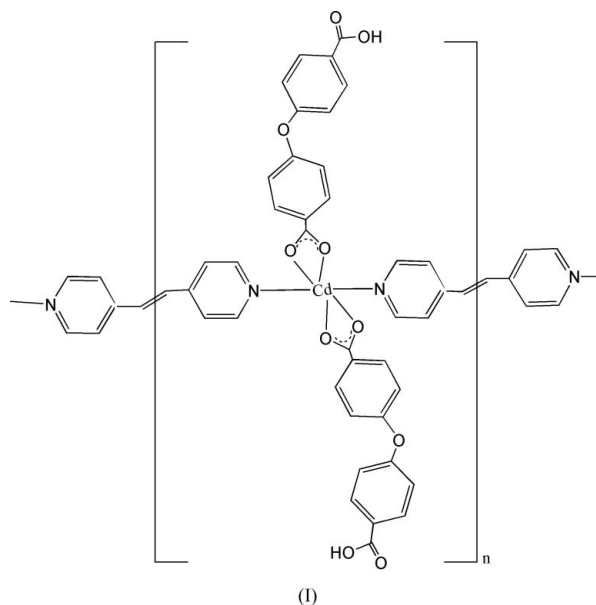
For details of how these key indicators were
 automatically derived from the article, see
<http://journals.iucr.org/e>.

In the title compound, $[\text{Cd}(\text{C}_{14}\text{H}_9\text{O}_5)_2(\text{C}_{12}\text{H}_{10}\text{N}_2)]_n$, the Cd^{II} atom lies at a centre of symmetry and is in a highly distorted octahedral geometry. The 1,2-di-4-pyridylethylene ligand functions as a μ_2 -bridging ligand to form a zigzag chain. The 4,4'-oxydibenzoate(1-) anions protrude on both sides of the chain. O–H...O hydrogen-bond interactions link the chains into a two-dimensional network structure.

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Comment

In contrast to rigid ligands such as 4,4'-biphenyldicarboxylic acid (Long *et al.*, 2003; Zhang *et al.*, 2004), the flexible ligand H_2oba (H_2oba = 4,4'-oxydibenzoic acid) has recently shown interesting properties (Kondo *et al.*, 2004; Wang *et al.*, 2004; Xiao *et al.*, 2005). Meanwhile, 1,2-di-4-pyridylethylene (bpe) is a good rigid N-donor ligand and has been used in the preparation of numerous novel coordination polymers (Hong & You, 2004; Li *et al.*, 2004; Zhao *et al.*, 2005). We report herein the preparation and structure of the title compound, $[\text{Cd}(\text{Hoba})_2(\text{bpe})]_n$, (I), which contains the flexible ligand H_2oba and the rigid ligand bpe.



The Cd^{II} atom in (I) is in an octahedral geometry defined by four O atoms from two Hoba anion and two N atoms from two bpe ligands (Fig. 1). The two carboxyl groups of the H_2oba ligand are in different coordination environments in the crystal structure. One carboxylate group chelates to the Cd^{II} atom and the other one is protonated. The dihedral angle between the two benzene rings of the Hoba anion is 102.3 (2)°. The dihedral angles between the N1-pyridyl ring and two

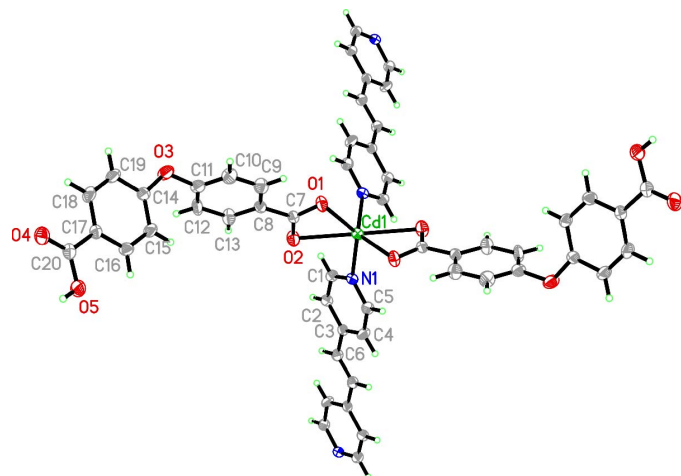


Figure 1
The coordination environment of the Cd atoms in (I), showing the atom numbering and displacement ellipsoids at the 30% probability level. Unlabelled atoms are related to labelled atoms by $-x, y, \frac{3}{2} - z$.

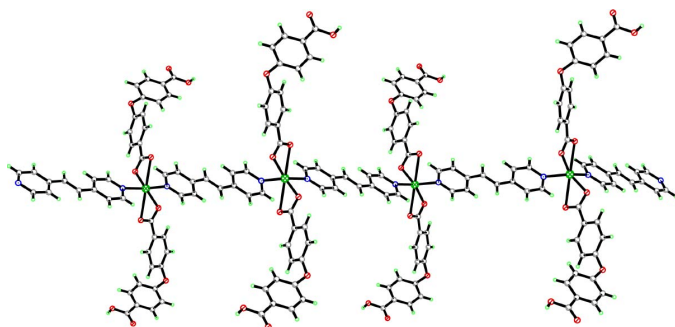


Figure 2
Illustration of a zigzag chain formed by bridging bpe ligands.

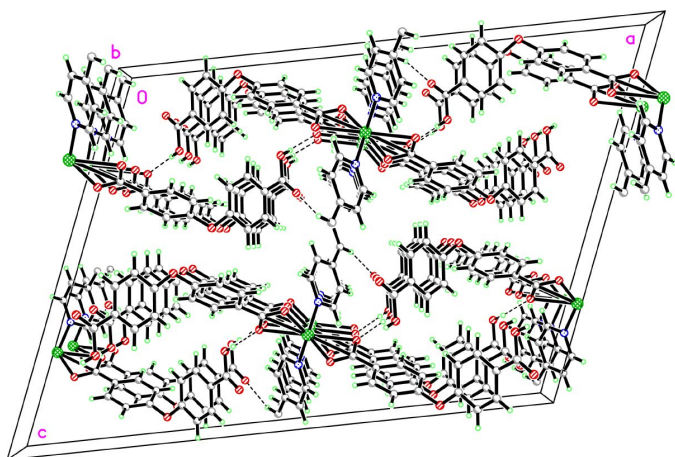


Figure 3
The two-dimensional network structure formed by hydrogen-bond interactions. Dashed lines indicate hydrogen bonds.

benzene rings are $86.7(3)$ (for C8–C13) and $88.2(2)^\circ$ (for C14–C19). The bpe ligands function as bridges to form a zigzag chain. The Hobo anions protrude on both sides of the chain (Fig. 2). In the structure, protonated carboxylate atom O5 forms an intermolecular hydrogen bond with coordinated carboxylate atom O2ⁱ [symmetry code: (i) $-x + \frac{1}{2}, y + \frac{3}{2}, -z + \frac{3}{2}$] of an adjacent chain (Table 2). A two-dimensional network

structure is thus formed by hydrogen-bonding interactions (Fig. 3).

Experimental

4,4'-Oxydibenzoic acid (0.5 mmol, 0.129 g), 3 CdSO₄·8H₂O (0.3 mmol, 0.230 g) and 1,2-di-4-pyridylethylene (0.5 mmol, 0.920 g) were placed in a 20 ml Teflon-lined stainless steel Parr bomb together with water (10 ml). The bomb was heated at 423 K for 6 d. The bomb was cooled slowly to room temperature to yield colorless crystals of (I).

Crystal data

[Cd(C₁₄H₉O₅)₂(C₁₂H₁₀N₂)]
M_r = 809.04
 Monoclinic, C2/c
a = 28.991 (2) Å
b = 5.9448 (5) Å
c = 21.5013 (18) Å
 β = 111.848 (2)°
V = 3439.5 (5) Å³
Z = 4

D_x = 1.562 Mg m⁻³
 Mo K α radiation
 Cell parameters from 2129 reflections
 θ = 2.5–21.7°
 μ = 0.70 mm⁻¹
T = 298 (2) K
 Block, colorless
 0.29 × 0.11 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Bruker, 2002)
T_{min} = 0.823, *T_{max}* = 0.933
 8724 measured reflections

3098 independent reflections
 2784 reflections with *I* > 2 σ (*I*)
R_{int} = 0.033
 θ_{max} = 25.2°
h = -28 → 34
k = -6 → 7
l = -25 → 18

Refinement

Refinement on *F*²
R [*F*² > 2 σ (*F*²)] = 0.056
wR(*F*²) = 0.123
 S = 1.21
 3098 reflections
 241 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0547P)^2 + 3.4154P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta\sigma)_{max} < 0.001$
 $\Delta\rho_{max} = 0.72 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{min} = -0.43 \text{ e } \text{Å}^{-3}$

Table 1

Selected geometric parameters (Å, °).

| | | | |
|--------------------------------------|-------------|--------------------------------------|-------------|
| Cd1–O1 ⁱ | 2.258 (3) | Cd1–N1 ⁱ | 2.268 (3) |
| Cd1–O1 | 2.258 (3) | Cd1–O2 | 2.533 (3) |
| Cd1–N1 | 2.268 (3) | Cd1–O2 ⁱ | 2.533 (3) |
| O1 ⁱ –Cd1–O1 | 101.01 (17) | N1 ⁱ –Cd1–O2 | 99.58 (12) |
| O1 ⁱ –Cd1–N1 | 96.69 (12) | O1 ⁱ –Cd1–O2 ⁱ | 53.60 (10) |
| O1–Cd1–N1 | 134.96 (11) | O1–Cd1–O2 ⁱ | 124.21 (11) |
| O1 ⁱ –Cd1–N1 ⁱ | 134.96 (11) | N1–Cd1–O2 ⁱ | 99.58 (12) |
| O1–Cd1–N1 ⁱ | 96.69 (12) | N1 ⁱ –Cd1–O2 ⁱ | 82.26 (11) |
| N1–Cd1–N1 ⁱ | 99.36 (17) | O2–Cd1–O2 ⁱ | 177.19 (15) |
| O1 ⁱ –Cd1–O2 | 124.21 (11) | O1 ⁱ –Cd1–C7 ⁱ | 26.79 (11) |
| O1–Cd1–O2 | 53.60 (10) | O1–Cd1–C7 ⁱ | 114.27 (11) |
| N1–Cd1–O2 | 82.26 (11) | | |

Symmetry code: (i) $-x, y, \frac{3}{2} - z$.

Table 2

Hydrogen-bonding geometry (Å, °).

| <i>D</i> –H··· <i>A</i> | <i>D</i> –H | H··· <i>A</i> | <i>D</i> ··· <i>A</i> | <i>D</i> –H··· <i>A</i> |
|--------------------------|-------------|---------------|-----------------------|-------------------------|
| O5–H5···O2 ⁱⁱ | 0.82 | 1.87 | 2.652 (4) | 159 |

Symmetry code: (ii) $\frac{1}{2} - x, \frac{3}{2} + y, \frac{3}{2} - z$.

H atoms attached to the C atoms were included in the refinement at calculated positions using a riding-model approximation [C–H = 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$]. The other H atoms were positioned geometrically and allowed to ride on their parent atoms at 0.82 Å, with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINTE* (Bruker, 2002); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2002); software used to prepare material for publication: *SHELXL97*.

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