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Key indicators

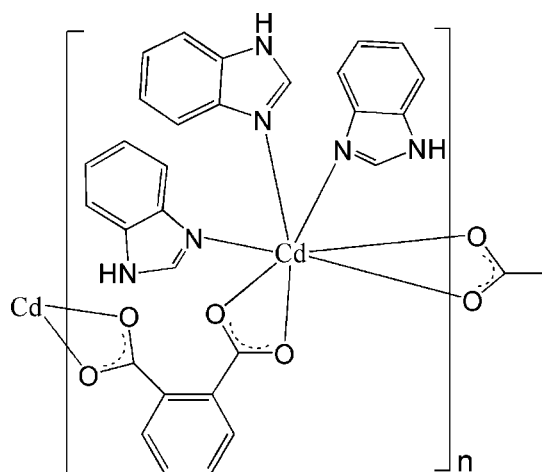
Single-crystal X-ray study
 $T = 293 \text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.005 \text{ \AA}$
 R factor = 0.032
 wR factor = 0.058
Data-to-parameter ratio = 14.8For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.**catena-Poly[[tris(benzimidazole)cadmium(II)]- μ -benzene-1,2-dicarboxylato]**

In the title compound, $[\text{Cd}(\text{C}_8\text{H}_4\text{O}_4)(\text{C}_7\text{H}_6\text{N}_2)_3]_n$, the Cd atom is seven-coordinated by four O atoms from two benzene-1,2-dicarboxylate (1,2-BDC) ligands and three N atoms from three benzimidazole ligands, resulting in a distorted pentagonal-bipyramid geometry. The 1,2-BDC ligands bridge the Cd atoms to form an extended helical chain structure. Neighbouring chains interact through π - π interactions, resulting in a two-dimensional structure.

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Comment

Coordination polymers with a variety of supramolecular structures have been studied extensively because of their novel topologies and potential application as functional materials (Eddaoudi *et al.*, 2002). Benzimidazole-like ligands have been widely used as antiviral compounds, as they have exhibited bioactivity (Katz & Luong, 1999). However, coordination polymers with benzimidazole (bzim) ligands prepared by hydrothermal synthesis have rarely been documented. We selected benzene-1,2-dicarboxylic acid (1,2- H_2BDC) as a linker and bzim as a secondary ligand, generating a new coordination polymer, $[\text{Cd}(\text{bzim})_3(1,2\text{-BDC})]$, (I).



(I)

In compound (I), the Cd atom is coordinated by three N atoms from three bzim ligands and four O atoms from two bridging 1,2-BDC ligands, in a distorted pentagonal-bipyramidal geometry (Fig. 1). Adjacent Cd atoms are connected by a bridging 1,2-BDC ligand, generating a one-dimensional helical chain structure (Fig. 2). Three bzim ligands are bonded to a Cd atom in a T-shaped coordination geometry to minimize the effect of steric hindrance.

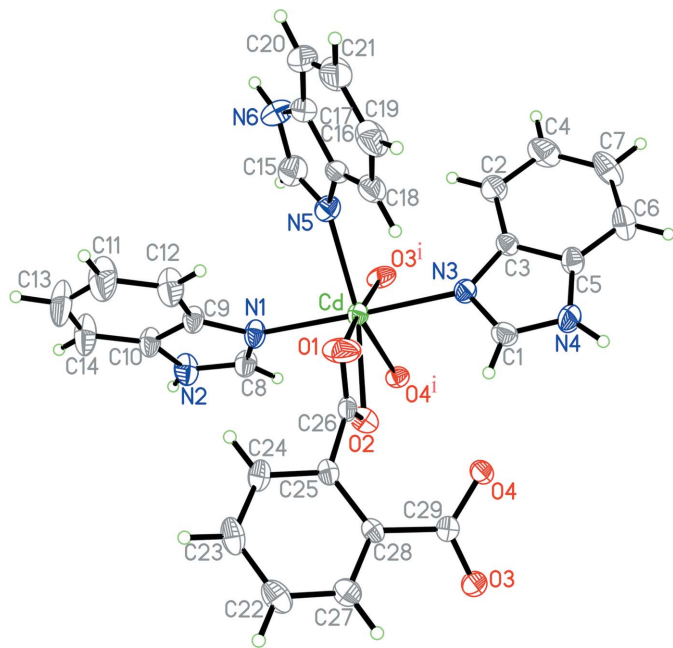


Figure 1
Part of the polymeric structure of (I). Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (i) $\frac{1}{2} - x, \frac{1}{2} + y, \frac{1}{2} - z$.]

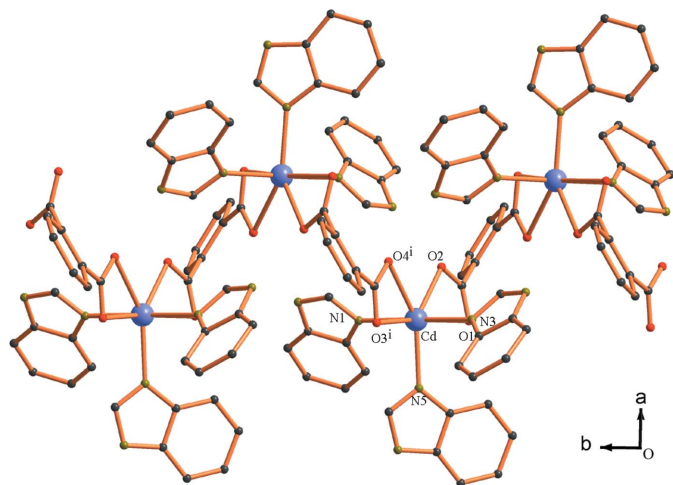


Figure 2
The one-dimensional helical chain in (I), viewed down the *c* axis. H atoms have been omitted for clarity. [Symmetry code: (i) $\frac{1}{2} - x, \frac{1}{2} + y, \frac{1}{2} - z$.]

There are intrachain hydrogen bonds between bzim and 1,2-BDC ligands (Table 2). The average plane-to-plane distance of 3.73 Å between the benzene ring (C9–C14) and its symmetry equivalent at $(-x, 1 - y, -z)$, in an offset fashion, indicates π – π interactions between the two neighbouring chains, which result in a two-dimensional supramolecular structure. It is clear that the π – π interactions and the intrachain N–H...O hydrogen bonds stabilize the structure of (I) (Che, 2006).

Experimental

Benzimidazole (0.35 g, 3 mmol), 1,2-H₂BDC (0.67 g, 1 mmol) and cadmium acetate (0.27 g, 1 mmol) in water (16 ml) were stirred for 30 min and the pH value was then adjusted to 7.1. The mixture, with a

total volume of 21 ml, was heated at 413 K for 5 d in a sealed 25 ml Teflon-lined stainless steel vessel under autogenous pressure. After the reaction mixture had been slowly cooled to room temperature at a rate of 5 K h⁻¹, pale-yellow crystals of (I) were collected by filtration, washed with distilled water and dried in air (yield 51% based on Cd).

Crystal data

[Cd(C₈H₄O₄)(C₇H₆N₂)₃]
M_r = 630.93
 Monoclinic, *P*2₁/*n*
a = 13.285 (3) Å
b = 9.3058 (18) Å
c = 22.913 (5) Å
 β = 105.296 (4)°
V = 2732.3 (10) Å³

Z = 4
D_x = 1.534 Mg m⁻³
 Mo *K*α radiation
 μ = 0.85 mm⁻¹
T = 293 (2) K
 Column, pale yellow
 0.17 × 0.08 × 0.07 mm

Data collection

Bruker SMART APEXII CCD
 area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan
 (SADABS; Sheldrick, 1996)
T_{min} = 0.912, *T_{max}* = 0.933

14148 measured reflections
 5339 independent reflections
 3698 reflections with *I* > 2σ(*I*)
R_{int} = 0.056
 θ_{max} = 26.0°

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.032
wR (*F*²) = 0.058
S = 0.96
 5339 reflections
 361 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0051P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.46 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\text{min}} = -0.46 \text{ e } \text{Å}^{-3}$

Table 1

Selected geometric parameters (Å, °).

N1–Cd	2.319 (3)	O2–Cd	2.363 (2)
N3–Cd	2.321 (2)	O3–Cd ⁱ	2.414 (2)
N5–Cd	2.334 (2)	O4–Cd ⁱ	2.5500 (19)
O1–Cd	2.733 (3)		
N1–Cd–N3	177.04 (9)	N3–Cd–O4 ⁱⁱ	89.89 (8)
N1–Cd–N5	90.13 (9)	N5–Cd–O4 ⁱⁱ	142.88 (8)
N3–Cd–N5	89.16 (9)	O2–Cd–O4 ⁱⁱ	80.66 (7)
N1–Cd–O2	91.39 (8)	O3 ⁱⁱⁱ –Cd–O4 ⁱⁱ	52.94 (6)
N3–Cd–O2	91.11 (8)	N1–Cd–O1	98.13 (9)
N5–Cd–O2	136.47 (8)	N3–Cd–O1	84.70 (9)
N1–Cd–O3 ⁱⁱⁱ	88.68 (9)	N5–Cd–O1	86.55 (8)
N3–Cd–O3 ⁱⁱⁱ	88.44 (9)	O2–Cd–O1	50.20 (6)
N5–Cd–O3 ⁱⁱⁱ	89.93 (8)	O3 ⁱⁱⁱ –Cd–O1	172.33 (8)
O2–Cd–O3 ⁱⁱⁱ	133.59 (7)	O4 ⁱⁱ –Cd–O1	130.28 (6)
N1–Cd–O4 ⁱⁱ	88.93 (8)		

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

Table 2

Hydrogen-bond 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>
N2–H2A...O4 ⁱⁱⁱ	0.86	2.13	2.849 (3)	141
N4–H4A...O2 ⁱ	0.86	1.99	2.756 (3)	148

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

All H atoms were positioned geometrically and refined as riding atoms, with C–H = 0.93 Å and N–H = 0.86 Å, and with *U*_{iso}(H) = 1.2*U*_{eq}(C,N).

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINTE* (Bruker, 2001); 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, 2001); software used to prepare material for publication: *SHELXTL*.

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