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Bis(benzimidazole-*κN*)bis(salicylato-κ^2O,O')-cadmium(II) monohydrate

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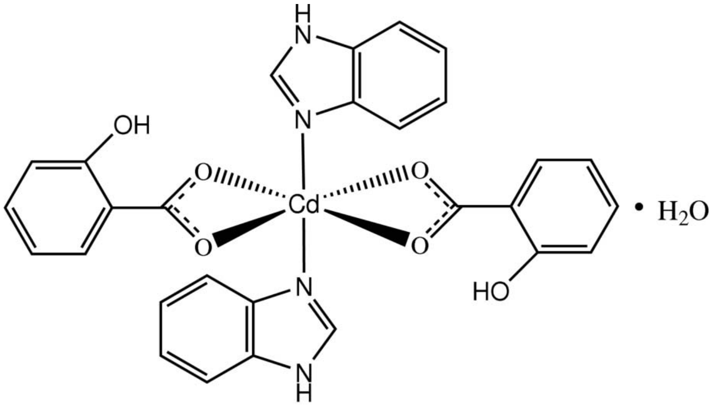
In the title compound, $[Cd(C_7H_5O_3)_2(C_7H_6N_2)_2]\cdot H_2O$, the Cd^{II} ion is surrounded by two salicylate anions and two benzimidazole molecules in a strongly distorted octahedral *cis*-CdN_2O_4 geometry. The partially overlapped arrangement and the face-to-face distances of 3.22 (3) and 3.34 (2) Å suggest π–π stacking between the benzimidazole ligands of neighbouring molecules.

Key indicators
Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.008 Å
R factor = 0.046
wR factor = 0.096
Data-to-parameter ratio = 13.5

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

Comment

The π–π stacking effect is an important intermolecular non-covalent interaction and is correlated with electron transfer in some biological systems (Deisenhofer & Michel, 1989). As part of an ongoing investigation into π–π stacking in metal complexes (Pan & Xu, 2004; Liu *et al.*, 2004), we have prepared the title Cd^{II} complex, (I), and present its structure here.



(I)

The molecular structure of (I) is illustrated in Fig. 1. The Cd^{II} atom is coordinated by two chelating salicylate anions and two monodentate benzimidazole (bzim) molecules, with a strongly distorted octahedral coordination geometry (Table 1). A search of the Cambridge Structural Database (Version 5.26, update of May 2005; Allen, 2002) indicates that four Cd^{II} complexes chelated by two salicylate anions have been crystallographically authenticated to date and all display seven-coordination geometry (Charles & Griffith, 1983; Huo *et al.*, 2004; Venkatasubramanian *et al.*, 1972; Mazurier *et al.*, 2000), unlike the situation in (I), where no other coordinating atoms (*i.e.* those with lone pairs) occur within 4 Å of Cd.

The crystal structure of the corresponding six-coordinated Cu^{II} complex, $[Cu(C_7H_6N_2)_2(C_7H_5O_3)_2]_n$, has been reported previously (Li *et al.*, 2005). The hydroxyl group of the

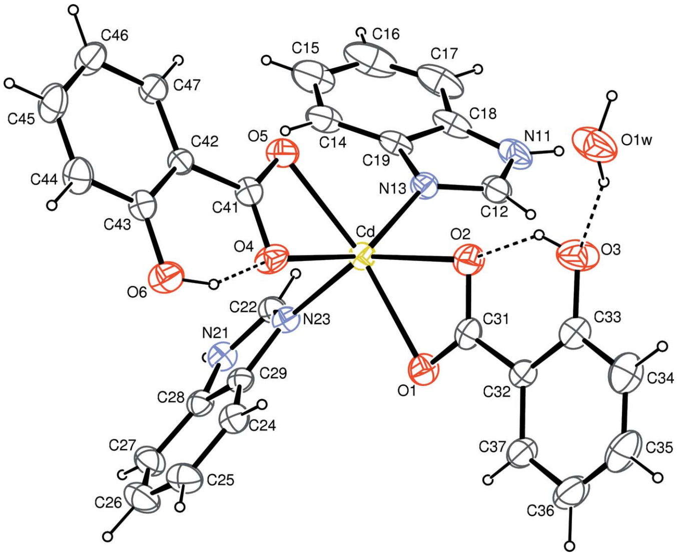


Figure 1
The molecular structure of (I), with 30% probability displacement ellipsoids (arbitrary spheres for H atoms). Dashed lines indicate the hydrogen bonding.

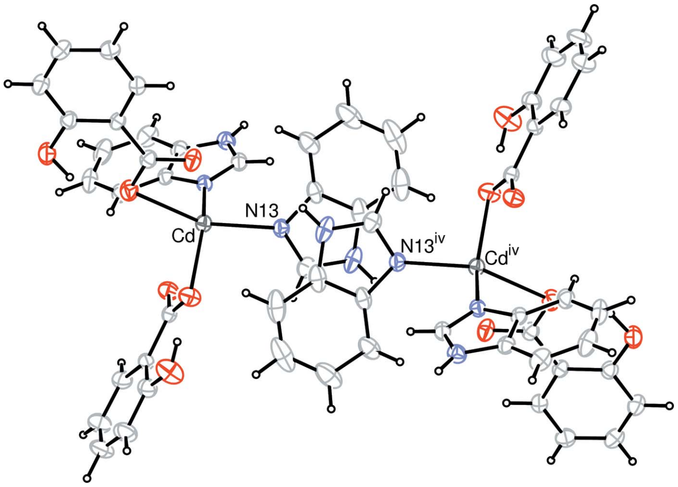


Figure 2
A diagram showing the π–π stacking between parallel N13-bzim ligands in (I) [symmetry code: (iv) $-x, 1 - y, 2 - z$].

salicylate moiety bridges neighbouring Cu atoms to form one-dimensional polymeric chains, while one carboxyl group of the salycilate coordinates monodentately to the Cu atom. The completely different structure for the Cu^{II} complex is evidently correlated with the Jahn–Teller distortion for Cu^{2+}, which results in the longer $Cu—O_H$ (hydroxyl) bonds in the axial direction.

In (I), a partially overlapped arrangement is observed between parallel N13-bzim and $N13^{iv}$-bzim ligands [symmetry code: (iv) $-x, 1 - y, 2 - z$] (Fig. 2) and between parallel N21-bzim and $N21^{iii}$-bzim ligands [symmetry code: (iii) $-x, 1 - y, 1 - z$] (Fig. 3). The face-to-face distances of 3.22 (3) Å between N13-bzim and $N13^{iv}$-bzim ligands and 3.34 (2) Å between N23-bzim and $N23^{iii}$-bzim ligands strongly suggest the existence of π–π stacking.

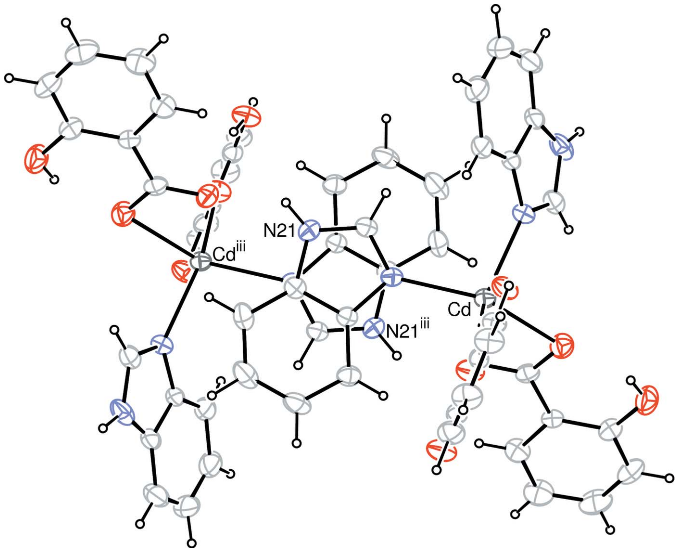


Figure 3
A diagram showing the π–π stacking between parallel N21-bzim ligands in (I) [symmetry code: (iii) $-x, 1 - y, 1 - z$].

The hydroxyl groups of the salicylate ligand participate in intermolecular O—H···O hydrogen bonds to carboxyl groups, while the bzim ligands link to neighbouring complexes *via* intermolecular N—H···O hydrogen bonding (Fig. 4). Bifurcated hydrogen bonding involving atom H21 occurs in the crystal of (I) (Table 2).

Experimental

$CdCl_2$ (1 mmol), salicylic acid (2 mmol), bzim (2 mmol) and Na_2CO_3 (1 mmol) were dissolved in a water (15 ml)/ethanol (5 ml) solution. The mixture was refluxed for 4 h and filtered after cooling to room temperature. Colourless single crystals of (I) were obtained from the filtrate after 1 d.

Crystal data

$[Cd(C_7H_5O_3)_2(C_7H_6N_2)_2]\cdot H_2O$
$M_r = 640.91$
Triclinic, $P\bar{1}$
$a = 9.336$ (3) Å
$b = 11.370$ (3) Å
$c = 13.967$ (4) Å
$\alpha = 81.154$ (4)°
$\beta = 89.470$ (4)°
$\gamma = 69.204$ (4)°
$V = 1367.8$ (7) Å^3
$Z = 2$
$D_x = 1.556$ Mg m^{-3}
$D_m = 1.558$ Mg m^{-3}
D_m measured by flotation in dibromoethane/cyclohexane
Mo $K\alpha$ radiation
Cell parameters from 6836 reflections
$\theta = 2.5$–24.6°
$\mu = 0.85$ mm^{-1}
$T = 295$ (2) K
Block, colourless
0.45 × 0.38 × 0.29 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.678$, $T_{max} = 0.778$
7395 measured reflections
4894 independent reflections
3657 reflections with $I > 2\sigma(I)$
$R_{int} = 0.037$
$\theta_{max} = 25.2°$
$h = -11 \rightarrow 11$
$k = -12 \rightarrow 13$
$l = -11 \rightarrow 16$

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Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.096$
$S = 1.01$
4894 reflections
362 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0302P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.55$ e Å^{-3}
$\Delta\rho_{min} = -0.59$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997)
Extinction coefficient: 0.0028 (6)

Table 1
Selected geometric parameters (Å, °).

Cd—O1	2.389 (3)	Cd—O5	2.388 (3)
Cd—O2	2.362 (3)	Cd—N13	2.235 (3)
Cd—O4	2.372 (3)	Cd—N23	2.236 (3)
N13—Cd—N23	101.12 (13)	O2—Cd—O5	108.91 (12)
N13—Cd—O2	90.96 (12)	O4—Cd—O5	54.85 (10)
N23—Cd—O2	146.99 (12)	N13—Cd—O1	116.40 (12)
N13—Cd—O4	146.59 (12)	N23—Cd—O1	92.05 (12)
N23—Cd—O4	92.15 (12)	O2—Cd—O1	55.30 (11)
O2—Cd—O4	94.32 (11)	O4—Cd—O1	93.32 (10)
N13—Cd—O5	92.29 (12)	O5—Cd—O1	145.47 (11)
N23—Cd—O5	101.25 (11)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1A···O5^{i}	0.92	1.89	2.782 (5)	164
O1W—H1B···O3	0.96	1.98	2.887 (6)	157
O3—H3A···O2	0.86	1.83	2.543 (6)	139
O6—H6A···O4	0.93	1.72	2.546 (5)	147
N11—H11···O1W^{ii}	0.86	1.91	2.764 (6)	175
N21—H21···O6^{ii}	0.86	2.43	3.003 (5)	124
N21—H21···O1^{iii}	0.86	2.42	2.994 (5)	125

Symmetry codes: (i) $1 - x, 1 - y, 2 - z$; (ii) $x - 1, y, z$; (iii) $-x, 1 - y, 1 - z$.

H atoms on aromatic rings were placed in calculated positions, with C—H = 0.93 Å and N—H = 0.86 Å, and refined as riding, with $U_{iso}(H) = 1.2U_{eq}$(carrier). Water and hydroxyl H atoms were located in a difference Fourier map and refined as riding in their as-found positions relative to their parent O atoms, with $U_{iso}(H) = 1.5U_{eq}(O)$.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

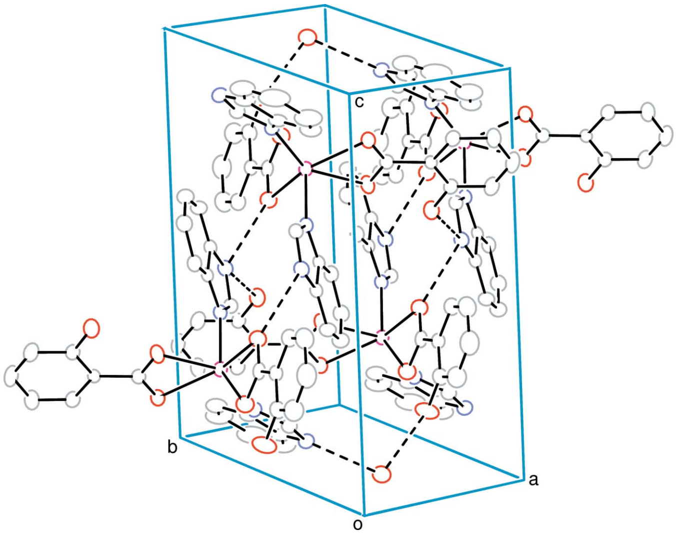

Figure 4
A unit-cell packing diagram for (I), showing the intermolecular hydrogen bonding (dashed lines). H atoms have been omitted.

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