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Tris(1*H*-benzimidazole-κN^3)(thiodiacetato-$\kappa^3 O,S,O'$)-cadmium(II) dihydrate

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In the title complex, $[Cd(C_4H_4O_4S)(C_7H_6N_2)_3]\cdot 2H_2O$, the Cd^{II} atom is surrounded by three benzimidazole ligands and one thiodiacetate dianion to complete a distorted octahedral CdN_3O_2S coordination geometry. The tridentate TDA chelates to the Cd^{II} atom in a facial mode. A C—H$\cdots\pi$ interaction and hydrogen bonding between neighboring complexes help to stabilize the crystal structure.

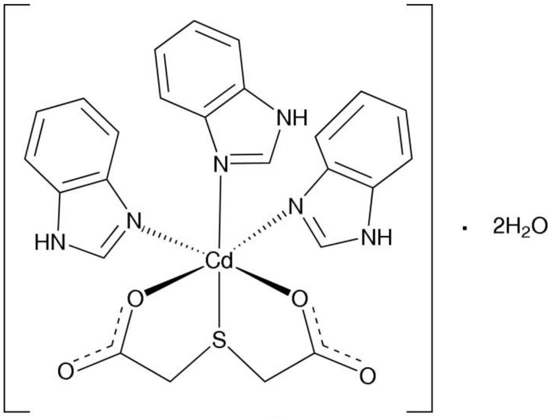
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.011 Å
R factor = 0.067
wR factor = 0.167
Data-to-parameter ratio = 13.8

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

Comment

As part of our ongoing investigations on non-covalent interactions in metal complexes, the title Cd^{II} compound, (I), incorporating benzimidazole (BZIM) ligands has been prepared and its X-ray crystal structure is presented here.



(I)

The Cd^{II} atom assumes a distorted octahedral coordination geometry formed by three BZIM ligands and one tridentate thiodiacetate dianion (TDA) (Fig. 1). The molecular structure is similiar to that for $[Cd(BZIM)_3(iminodiacetato)]\cdot 2H_2O$ (Su & Xu, 2005). The TDA chelates to the Cd^{II} atom in a facial configuration, a feature commonly found in metal–TDA complexes (Baggio *et al.*, 1999; Pan *et al.*, 2005*a*,*b*).

Each carboxyl group coordinates in a monodentate fashion to the Cd^{II} atom, and the uncoordinated carboxyl O atom is hydrogen bonded to the uncoordinated water molecule (Fig. 1). Each five-membered chelate ring has an envelope conformation, with the Cd atom in the flap position and lying 0.571 (12) and 1.086 (10) Å out of the mean planes formed by the other four atoms.

No π–π stacking occurs in the crystal structure of (I), but a C—H$\cdots\pi$ interaction is observed involving BZIM ligands of neighboring complexes (Fig. 2). The H$\cdots$*Cg* (*Cg* is the ring centroid) separations and C—H$\cdots$*Cg* angles range from 2.65

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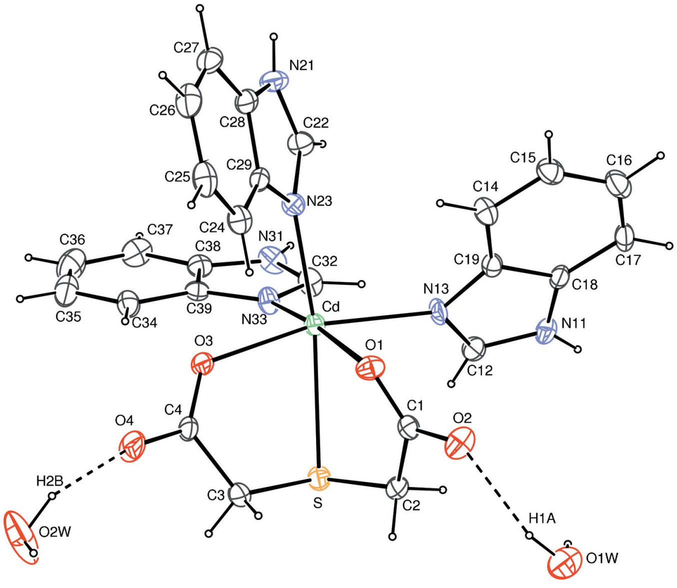

Figure 1
The molecular structure of (I) with 20% probability displacement ellipsoids (arbitrary spheres for H atoms). Dashed lines indicate hydrogen bonds.

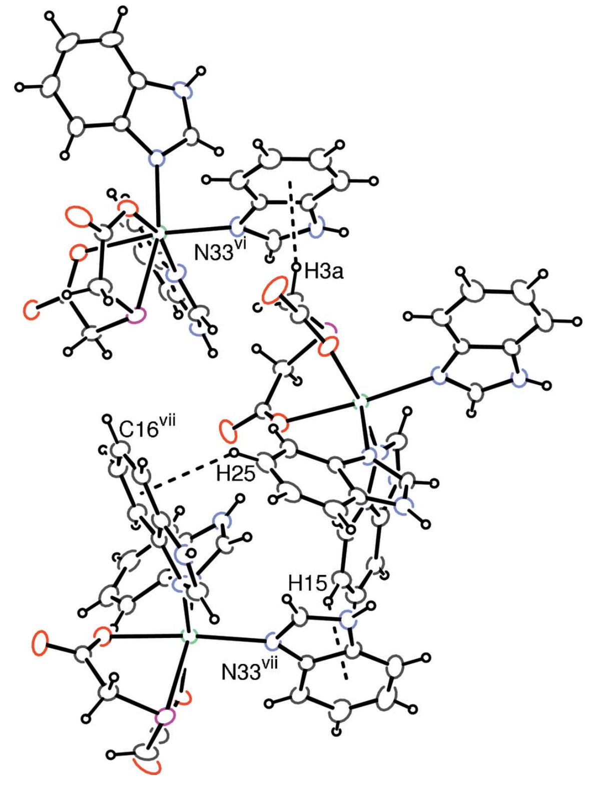

Figure 2
The intermolecular C—H$\cdots\pi$ interactions (dashed lines) in (I) [symmetry codes: (vi) $-\frac{1}{2}+x, y, \frac{1}{2}-z$; (vii) $-\frac{1}{2}+x, \frac{1}{2}-y, -z$].

to 2.82 Å and 139 to 157°. Neighboring complexes are linked to each other *via* N—H$\cdots$O hydrogen bonding between BZIM and carboxyl groups (Table 2).

Experimental

$CdCl_2\cdot2.5H_2O$ (0.46 g, 2 mmol), Na_2CO_3 (0.21 g, 2 mmol) and H_2TDA (0.30 g, 2 mmol) were dissolved in a water–ethanol solution (20 ml, 1:3 *v*/*v*). Benzimidazole (0.24 g, 2 mmol) was added and the mixture was refluxed for 4 h and then filtered. Colorless crystals were obtained after one week.

Crystal data

$[Cd(C_4H_4O_4S)(C_7H_6N_2)_3]\cdot2H_2O$
$M_r = 650.98$
Orthorhombic, *Pbca*
$a = 10.6042\ (3)$ Å
$b = 20.1157\ (8)$ Å
$c = 25.9795\ (8)$ Å
$V = 5541.7\ (3)$ Å^3
$Z = 8$
$D_x = 1.560$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 29359 reflections
$\theta = 2.3$–$25.0°$
$\mu = 0.91$ mm^{-1}
$T = 295\ (2)$ K
Platelet, colorless
0.26 × 0.22 × 0.07 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.782$, $T_{max} = 0.929$
36430 measured reflections
4866 independent reflections
4125 reflections with $I > 2\sigma(I)$
$R_{int} = 0.071$
$\theta_{max} = 25.2°$
$h = -12 \rightarrow 12$
$k = -24 \rightarrow 24$
$l = -31 \rightarrow 31$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.067$
$wR(F^2) = 0.167$
$S = 1.33$
4866 reflections
352 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0561P)^2 + 17.5824P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.74$ e Å^{-3}
$\Delta\rho_{min} = -0.97$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd—O1	2.390 (5)	Cd—N23	2.268 (6)
Cd—O3	2.272 (4)	Cd—N33	2.308 (6)
Cd—N13	2.313 (5)	Cd—S	2.7365 (18)
O1—Cd—O3	86.10 (19)	O3—Cd—S	74.89 (12)
O1—Cd—N13	82.8 (2)	N13—Cd—N23	98.6 (2)
O1—Cd—N23	95.72 (17)	N13—Cd—N33	94.2 (2)
O1—Cd—N33	171.32 (19)	N23—Cd—N33	92.8 (2)
O1—Cd—S	73.33 (11)	N13—Cd—S	93.37 (15)
O3—Cd—N13	165.82 (19)	N23—Cd—S	162.70 (14)
O3—Cd—N23	91.32 (18)	N33—Cd—S	98.77 (16)
O3—Cd—N33	95.39 (19)		

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

D—H$\cdots$*A*	*D*—H	H$\cdots$*A*	*D*$\cdots$*A*	*D*—H$\cdots$*A*
O1*W*—H1*A*$\cdots$O2	0.89	2.01	2.786 (8)	144
O1*W*—H1*B*$\cdots$O2*W*^{i}	0.99	2.00	2.899 (10)	149
O2*W*—H2*A*$\cdots$O1*W*^{ii}	0.98	1.90	2.817 (10)	155
O2*W*—H2*B*$\cdots$O4	0.94	1.86	2.752 (11)	158
N11—H11$\cdots$O4^{iii}	0.86	1.93	2.768 (9)	164
N21—H21$\cdots$O1^{iv}	0.86	2.38	3.172 (8)	154
N21—H21$\cdots$O2^{iv}	0.86	2.36	3.021 (7)	134
N31—H31$\cdots$O2^{v}	0.86	1.94	2.766 (8)	161

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

The water H atoms were located in a difference Fourier map and refined as riding in their as-found relative positions, with a fixed $U_{\rm iso}$ value of 0.08 Å^2. Other H atoms were placed in calculated positions, with C—H = 0.97 (methylene) or 0.93 Å (aromatic) and N—H = 0.86 Å, and were included in the final cycles of refinement in riding mode, with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$ of the carrier atoms.

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).

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