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Benzimidazolium bis(1*H*-benzimidazole-κN^3)-chloro(oxydiacetato-$\kappa^3 O,O',O''$)cadmium(II)

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Key indicators

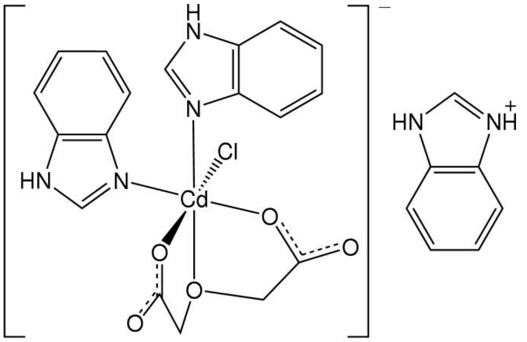
Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
R factor = 0.021
wR factor = 0.053
Data-to-parameter ratio = 16.9

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

The title compound, $(C_7H_7N_2)[Cd(C_4H_4O_5)Cl(C_7H_6N_2)_2]$, is composed of Cd^{II}-containing complex anions and benzimidazolium (HBZIM) cations. The Cd^{II} atom is coordinated by a tridentate oxydiacetate (ODA) dianion, a chloride anion and two benzimidazole (BZIM) molecules, forming a distorted octahedral CdN_2O_3Cl coordination geometry. The ODA dianion chelates facially to the Cd^{II} atom. The face-to-face distances of 3.444 (12) and 3.386 (5) Å between partially overlapped BZIM rings and between HBZIM rings, respectively, indicate the existence of π–π stacking in the crystal structure.

Comment

As part of our ongoing investigations of π–π stacking in metal complexes incorporating benzimidazole (BZIM) ligands (Su *et al.*, 2005), the title Cd^{II} complex, (I) (Fig. 1), has been prepared and its crystal structure is presented here.



(I)

The Cd^{II}-containing complex anion displays a distorted octahedral CdN_2O_3Cl coordination geometry, formed by a tridentate oxydiacetate (ODA) dianion, a chloride anion and two BZIM molecules. The ODA dianion chelates to the Cd^{II} atom in a facial configuration, the two five-membered chelate rings being nearly perpendicular to each other (Fig. 1). The O1-ring displays an envelope configuration, with atom O3 at the flap position, displaced by 0.239 (2) Å from the mean plane of the other atoms. Conversely, the O4-ring is twisted about the Cd—O3 bond, and the Cd atom lies 0.832 (6) Å out of the plane formed by atoms C3, C4 and O4, while atom O3 is displaced by −0.341 (5) Å with respect to the same three atoms.

The molecular packing is illustrated in Fig. 2, showing the parallel arrangement of BZIM molecules and benzimidazolium (HBZIM) cations in the crystal structure of (I). The parallel N33-HBZIM and N33^{v}-HBZIM [symmetry code: (v) $-x, -y, 1-z$] cations overlap their imidazole rings, whereas

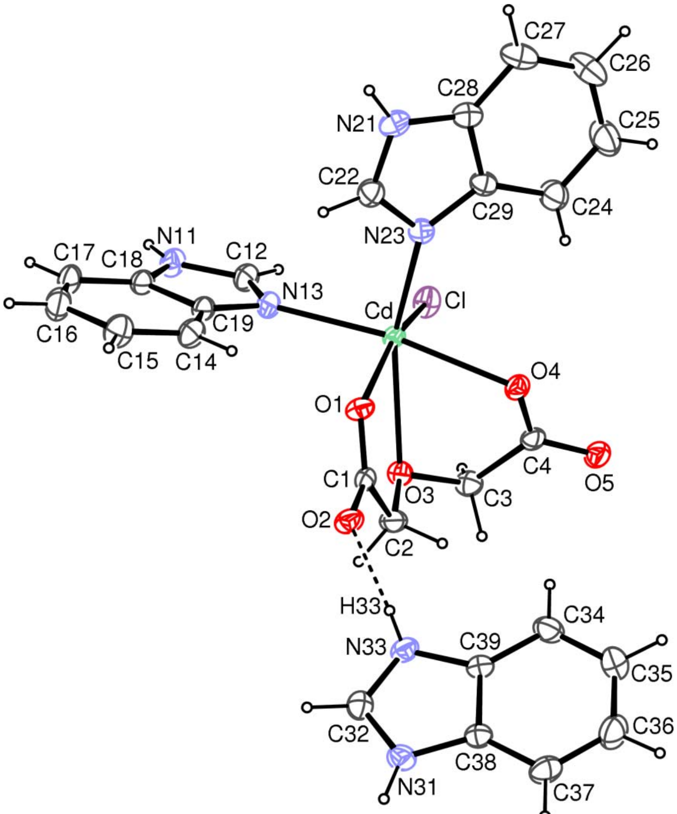


Figure 1
The molecular structure of (I), with 30% probability displacement ellipsoids (spheres of arbitrary radii for H atoms). The dashed line indicates a hydrogen-bonding interaction.

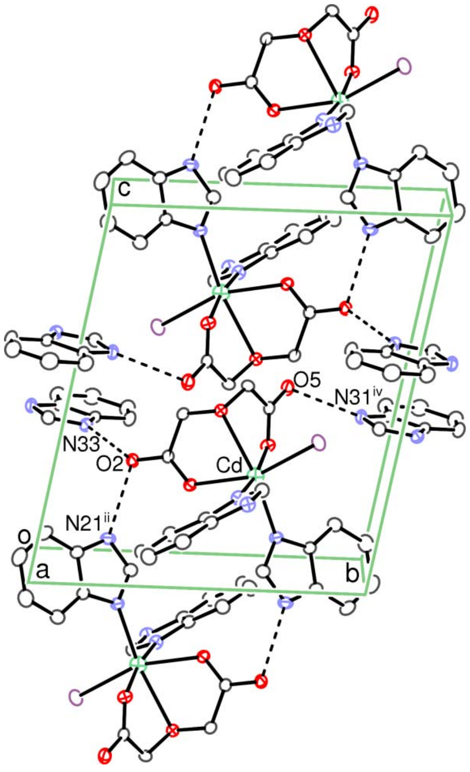


Figure 2
The packing in (I), showing the hydrogen bonding (dashed lines). [Symmetry codes: (ii) $1 - x, 1 - y, -z$; (iv) $x, 1 + y, z$.]

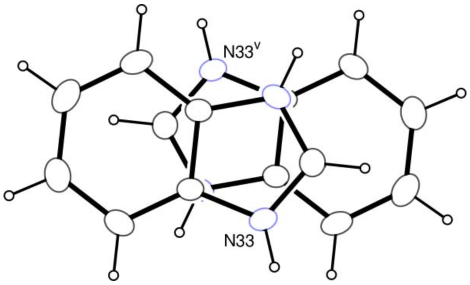


Figure 3
A diagram showing π–π stacking between HBZIM cations. [Symmetry code: (v) $-x, -y, 1 - z$.]

the parallel C19-BZIM and C19^{vi}—BZIM [symmetry code: (vi) $2 - x, 1 - y, -z$] molecules overlap their benzene rings, as shown in Figs. 3 and 4. The face-to-face distances of 3.386 (5) and 3.444 (12) Å between imidazole rings and between benzene rings, respectively, reflect the π–π stacking interactions in the crystal structure of (I).

Neighbouring Cd^{II} complex anions are linked through N—H$\cdots$O hydrogen bonds. N—H$\cdots$O hydrogen-bond interactions are also observed between Cd^{II} complex anions and HBZIM cations (Table 2 and Fig. 2).

Experimental

All starting chemicals were of analytical grade and were used as received. H_2ODA (0.13 g, 1 mmol), Na_2CO_3 (0.11 g, 1 mmol), BZIM (0.24 g, 2 mmol) and $CdCl_2 \cdot 2.5H_2O$ (0.23 g, 1 mmol) were dissolved in a water–ethanol mixture (20 ml, 3:1). The solution was refluxed for 4 h, cooled to room temperature and filtered. The filtrate was kept at room temperature. Colourless single crystals of (I) were obtained from the filtrate after about one week.

Crystal data

$(C_7H_7N_2)[Cd(C_4H_4O_5)Cl(C_7H_6N_2)_2]$
$M_r = 635.34$
Triclinic, $P\overline{1}$
$a = 9.016$ (2) Å
$b = 11.1672$ (14) Å
$c = 13.243$ (3) Å
$\alpha = 78.47$ (1)°
$\beta = 80.58$ (3)°
$\gamma = 84.82$ (1)°
$V = 1286.5$ (5) Å^3
$Z = 2$
$D_x = 1.640$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 8625 reflections
$\theta = 2.0$–26.0°
$\mu = 1.00$ mm^{-1}
$T = 295$ (2) K
Block, colourless
0.40 × 0.30 × 0.28 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.670$, $T_{max} = 0.754$
12674 measured reflections
5825 independent reflections
5419 reflections with $I > 2\sigma(I)$
$R_{int} = 0.020$
$\theta_{max} = 27.5°$
$h = -10 \rightarrow 11$
$k = -14 \rightarrow 14$
$l = -17 \rightarrow 17$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.021$
$wR(F^2) = 0.053$
$S = 1.08$
5825 reflections
344 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0336P)^2 + 1.1911P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.003$
$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.38$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0114 (5)

m1232 *et al.* • $(C_7H_7N_2)[Cd(C_4H_4O_5)Cl(C_7H_6N_2)_2]$ *Acta Cryst.* (2005). E**61**, m1231–m1233

Table 1
Selected geometric parameters (Å, °).

Cd—O1	2.2909 (12)	Cd—N13	2.3235 (15)
Cd—O3	2.4975 (13)	Cd—N23	2.2708 (15)
Cd—O4	2.3727 (13)	Cd—Cl	2.5213 (5)
O1—Cd—O3	68.92 (4)	O3—Cd—Cl	91.61 (3)
O1—Cd—O4	88.49 (4)	O4—Cd—N13	171.42 (5)
O1—Cd—N13	89.05 (5)	O4—Cd—N23	94.40 (5)
O1—Cd—N23	95.46 (5)	O4—Cd—Cl	86.95 (4)
O1—Cd—Cl	160.20 (3)	N13—Cd—N23	94.01 (6)
O3—Cd—O4	66.84 (5)	N13—Cd—Cl	92.62 (4)
O3—Cd—N13	104.63 (5)	N23—Cd—Cl	104.10 (4)
O3—Cd—N23	155.08 (5)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N11—H11···O4^{i}	0.86	1.97	2.769 (2)	155
N21—H21···O2^{ii}	0.86	1.95	2.786 (2)	165
N31—H31···O5^{iii}	0.86	1.83	2.670 (2)	164
N33—H33···O2	0.86	1.83	2.673 (2)	168

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

H atoms were positioned geometrically, with C—H = 0.93 (aromatic) or 0.97 Å (methylene) and N—H = 0.86 Å, and included in the final cycles of refinement in the riding model, with the constraint $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(carrier) applied.

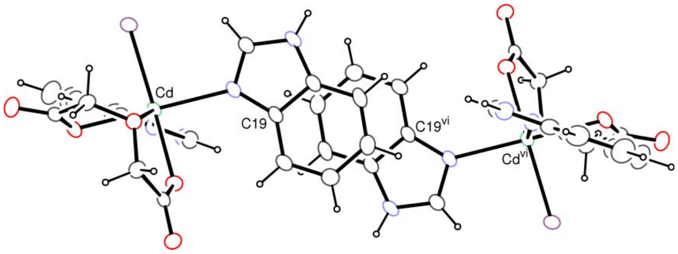


Figure 4
A diagram showing π–π stacking between BZIM molecules of neighboring Cd^{II} complex anions. [Symmetry code: (vi) $2-x, 1-y, -z$.]

Data collection: *PROCESS-AUTO* (Rigaku Corporation, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC & Rigaku Corporation, 2002); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Acta Cryst. (2005). E**61**, m1231–m1233 *et al.* • $(C_7H_7N_2)[Cd(C_4H_4O_5)Cl(C_7H_6N_2)_2]$ **m1233**