Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis(8-aminoquinoline-κ^2N,N')-diperchloratocadmium(II)

L.-M. Guo, H. Xu and X.-M. Ren*

Key Laboratory of Anhui Province for Functional Coordination Compounds, Anqing Normal College, Anqing 246011, People's Republic of China
Correspondence e-mail: xmren_nju@yahoo.com.cn

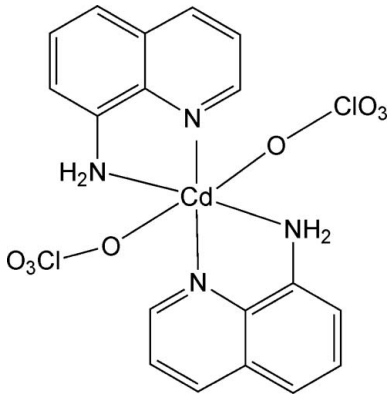
Received 20 April 2007; accepted 27 April 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.026; wR factor = 0.076; data-to-parameter ratio = 25.1.

In the crystal structure of the title compound, $[Cd(ClO_4)_2(C_9H_8N_2)_2]$, the Cd atom is coordinated by four N atoms of two 8-aminoquinoline ligands and two O atoms of two perchlorate anions, within a strongly distorted octahedron and with the Cd atom located on a centre of inversion. These complexes are connected *via* N—H···O hydrogen bonding into a channel structure.

Related literature

For related literature, see: Dietrich *et al.* (2005).



Experimental

Crystal data

$[Cd(ClO_4)_2(C_9H_8N_2)_2]$
M_r = 599.65
Monoclinic, $P2_1/c$
a = 9.1653 (5) Å
b = 8.9841 (6) Å
c = 12.9597 (7) Å
β = 107.933 (3)°
V = 1015.28 (10) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.40 mm^{-1}
T = 293 (2) K
0.25 × 0.20 × 0.10 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.72, T_{max} = 0.86
15078 measured reflections
3868 independent reflections
3312 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.076
S = 0.91
3868 reflections
154 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—N2	2.2727 (13)	Cd1—O1	2.4705 (14)
Cd1—N1	2.2829 (11)		
N2—Cd1—N1	75.47 (4)	N2^i—Cd1—O1	88.28 (5)
N2^i—Cd1—N1	104.53 (4)	N1—Cd1—O1	92.34 (5)
N2—Cd1—O1	91.72 (5)	N1^i—Cd1—O1	87.66 (5)

Symmetry code: (i) $-x, -y+1, -z+1$.

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2B···O4^{ii}	0.90	2.29	3.123 (2)	153
N2—H2A···O3^{iii}	0.90	2.17	3.0520 (19)	165

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1996); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXL97*.

We thank the Natural Science Foundation of Anhui Province in China (project No. 044-J-04011, 2004kj266) for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NC2036).

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 doi:10.1107/S1600536807021125

supplementary materials

Acta Cryst. (2007). E**63**, m1579 [**doi:10.1107/S1600536807021125**]

Bis(8-aminoquinoline-κ^2N,N')diperchloratocadmium(II)

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Comment

The crystal structure of the title compound, (I), consists of discrete complexes, in which the cadmium atoms are coordinated by four nitrogen atoms of two symmetry related 8-aminoquinoline ligands and two oxygen atoms of two symmetry related perchlorate anions (Figure 1). The perchlorate anions and the 8-aminoquinoline ligands are located in general positions, whereas the cadmium atoms are located on centres of inversion. The Cd—N and Cd—O bond lengths are in the normal ranges (Dietrich *et al.*, 2005) and the Cd coordination polyhedron can be described as a strongly distorted octehedra (Table 1).

The complexes are connected *via* N—H···O hydrogen bonding between the amino hydrogen atoms and the oxygen atoms of the perchlorate anions (Table 2). From this arrangement channels are formed, which elongated in the direction of the *b* axis (Figure 2).

Experimental

A solution of 8-aminoquinoline (288 mg, 2 mmol) in 5 ml of MeOH was added to a solution of $Cd(ClO_4)_2$ (320 mg, 1.03 mmol) in 15 ml MeOH. The mixture was stirred for 30 min at room temperature and then filtered off. On slow evaporation of the solvent from the filtrate light yellow crystals of the title compound has grown, which were filtered off, washed with a small amount of MeOH and dried on air. The yield is about 60% based on 8-aminoquinoline.

Refinement

All H atoms were placed in geometrically calculated positions (C—H 0.93 Å; N—H 0.90 Å) with U_{iso} = 1.2 U_{eq} of the parent atom.

Figures

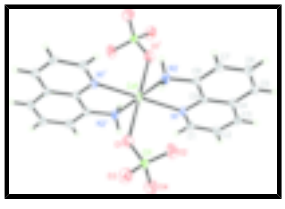

Fig. 1. : The structure of complex I, showing 30% probability displacement ellipsoids and the numbering scheme (Symmetry codes: i = −*x*, 1 − *y*, 1 − *z*).

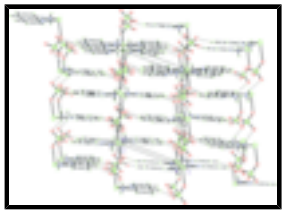

Fig. 2. : Crystal structure of I with view in the direction of the *b* axis (hydrogen bonding is shown as dashed lines).

Bis(8-aminoquinoline-κ^2N,N')diperchloratocadmium(II)

Crystal data

$[Cd(ClO_4)_2(C_9H_8N_2)_2]$	$Z = 2$
$M_r = 599.65$	$F_{000} = 596$
Monoclinic, $P2_1/c$	$D_x = 1.962$ Mg m^{-3}
$a = 9.1653$ (5) Å	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$b = 8.9841$ (6) Å	$\mu = 1.40$ mm^{-1}
$c = 12.9597$ (7) Å	$T = 293$ (2) K
$\beta = 107.933$ (3)º	Block, yellow
$V = 1015.28$ (10) Å^3	0.25 × 0.20 × 0.10 mm

Data collection

Siemens SMART CCD area-detector diffractometer	3868 independent reflections
Radiation source: fine-focus sealed tube	3312 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.024$
$T = 293$(2) K	$\theta_{max} = 33.2$º
φ and ω scans	$\theta_{min} = 2.8$º
Absorption correction: multi-scan (SADABS; Bruker, 2000)	$h = -13\rightarrow14$
$T_{min} = 0.72$, $T_{max} = 0.86$	$k = -13\rightarrow10$
15078 measured reflections	$l = -19\rightarrow19$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.026$	$w = 1/[\sigma^2(F_o^2) + (0.0499P)^2 + 0.2558P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.076$	$(\Delta/\sigma)_{max} < 0.001$
$S = 0.91$	$\Delta\rho_{max} = 0.49$ e Å^{-3}
3868 reflections	$\Delta\rho_{min} = -0.46$ e Å^{-3}
154 parameters	Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0098 (9)
Secondary atom site location: difference Fourier map	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cd1	0.0000	0.5000	0.5000	0.03503 (6)
Cl1	−0.03922 (4)	0.51775 (4)	0.21116 (3)	0.03284 (8)
O1	0.04819 (19)	0.49130 (16)	0.32274 (11)	0.0571 (4)
O2	−0.16350 (16)	0.61644 (17)	0.20631 (13)	0.0634 (4)
O3	0.06260 (17)	0.58105 (19)	0.15859 (11)	0.0614 (4)
O4	−0.09602 (18)	0.38130 (17)	0.15848 (14)	0.0690 (4)
N1	−0.25539 (12)	0.45338 (14)	0.42306 (9)	0.0302 (2)
N2	−0.10913 (13)	0.72903 (14)	0.46380 (11)	0.0378 (2)
H2A	−0.0753	0.7867	0.5232	0.078 (8)*
H2B	−0.0805	0.7717	0.4102	0.066 (7)*
C1	−0.32304 (17)	0.32218 (16)	0.40086 (12)	0.0365 (3)
H1A	−0.2615	0.2378	0.4107	0.044*
C2	−0.48220 (17)	0.30340 (18)	0.36342 (12)	0.0393 (3)
H2C	−0.5247	0.2089	0.3478	0.047*
C3	−0.57413 (16)	0.42566 (18)	0.35012 (11)	0.0372 (3)
H3B	−0.6802	0.4151	0.3261	0.045*
C4	−0.50747 (14)	0.56864 (17)	0.37304 (10)	0.0309 (2)
C5	−0.59541 (16)	0.70000 (19)	0.36404 (12)	0.0393 (3)
H5A	−0.7019	0.6947	0.3401	0.047*
C6	−0.52495 (18)	0.83408 (19)	0.39019 (13)	0.0431 (3)
H6A	−0.5837	0.9196	0.3859	0.052*
C7	−0.36400 (17)	0.84453 (17)	0.42377 (12)	0.0387 (3)
H7A	−0.3177	0.9372	0.4408	0.046*
C8	−0.27456 (15)	0.72045 (15)	0.43182 (10)	0.0305 (2)
C9	−0.34533 (14)	0.57849 (14)	0.40875 (9)	0.0272 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.01856 (8)	0.04247 (9)	0.04189 (9)	0.00338 (4)	0.00610 (5)	0.00340 (5)
Cl1	0.02699 (15)	0.03779 (15)	0.03309 (15)	−0.00214 (10)	0.00826 (11)	0.00169 (10)
O1	0.0423 (8)	0.0965 (12)	0.0340 (6)	0.0167 (6)	0.0137 (5)	0.0137 (5)

O2	0.0452 (7)	0.0625 (9)	0.0761 (9)	0.0215 (6)	0.0094 (6)	0.0025 (7)
O3	0.0524 (8)	0.0837 (10)	0.0523 (7)	−0.0165 (7)	0.0219 (6)	0.0159 (7)
O4	0.0554 (9)	0.0563 (8)	0.0960 (11)	−0.0182 (7)	0.0245 (8)	−0.0259 (8)
N1	0.0219 (5)	0.0355 (5)	0.0325 (5)	0.0015 (4)	0.0076 (4)	−0.0007 (4)
N2	0.0249 (5)	0.0379 (6)	0.0480 (6)	−0.0029 (4)	0.0076 (4)	−0.0002 (5)
C1	0.0317 (6)	0.0366 (6)	0.0412 (7)	−0.0016 (5)	0.0111 (5)	−0.0038 (5)
C2	0.0331 (7)	0.0433 (7)	0.0410 (7)	−0.0102 (5)	0.0106 (5)	−0.0074 (5)
C3	0.0236 (6)	0.0553 (8)	0.0316 (6)	−0.0063 (5)	0.0070 (4)	−0.0039 (5)
C4	0.0210 (5)	0.0451 (7)	0.0260 (5)	0.0022 (4)	0.0064 (4)	0.0011 (4)
C5	0.0235 (6)	0.0569 (9)	0.0369 (6)	0.0104 (5)	0.0082 (5)	0.0050 (6)
C6	0.0362 (7)	0.0482 (8)	0.0457 (8)	0.0157 (6)	0.0137 (6)	0.0073 (6)
C7	0.0375 (7)	0.0361 (6)	0.0420 (7)	0.0065 (5)	0.0117 (5)	0.0029 (5)
C8	0.0249 (5)	0.0356 (6)	0.0306 (5)	0.0015 (4)	0.0077 (4)	0.0014 (4)
C9	0.0203 (5)	0.0373 (6)	0.0241 (4)	0.0021 (4)	0.0069 (4)	0.0010 (4)

Geometric parameters (Å, °)

Cd1—N2	2.2727 (13)	C1—C2	1.399 (2)
Cd1—N2^{i}	2.2727 (13)	C1—H1A	0.9300
Cd1—N1	2.2829 (11)	C2—C3	1.363 (2)
Cd1—N1^{i}	2.2829 (11)	C2—H2C	0.9300
Cd1—O1	2.4705 (14)	C3—C4	1.414 (2)
Cd1—O1^{i}	2.4705 (14)	C3—H3B	0.9300
Cl1—O4	1.4216 (14)	C4—C5	1.414 (2)
Cl1—O2	1.4296 (13)	C4—C9	1.4167 (17)
Cl1—O3	1.4317 (13)	C5—C6	1.359 (2)
Cl1—O1	1.4408 (14)	C5—H5A	0.9300
N1—C1	1.3216 (18)	C6—C7	1.407 (2)
N1—C9	1.3722 (17)	C6—H6A	0.9300
N2—C8	1.4455 (17)	C7—C8	1.3685 (19)
N2—H2A	0.9000	C7—H7A	0.9300
N2—H2B	0.9000	C8—C9	1.4203 (18)
N2—Cd1—N2^{i}	180.0	Cd1—N2—H2B	109.3
N2—Cd1—N1	75.47 (4)	H2A—N2—H2B	108.0
N2^{i}—Cd1—N1	104.53 (4)	N1—C1—C2	123.53 (14)
N2—Cd1—N1^{i}	104.53 (4)	N1—C1—H1A	118.2
N2^{i}—Cd1—N1^{i}	75.47 (4)	C2—C1—H1A	118.2
N1—Cd1—N1^{i}	180.00 (3)	C3—C2—C1	119.01 (14)
N2—Cd1—O1	91.72 (5)	C3—C2—H2C	120.5
N2^{i}—Cd1—O1	88.28 (5)	C1—C2—H2C	120.5
N1—Cd1—O1	92.34 (5)	C2—C3—C4	119.69 (13)
N1^{i}—Cd1—O1	87.66 (5)	C2—C3—H3B	120.2
N2—Cd1—O1^{i}	88.28 (5)	C4—C3—H3B	120.2
N2^{i}—Cd1—O1^{i}	91.72 (5)	C5—C4—C3	122.86 (13)
N1—Cd1—O1^{i}	87.66 (5)	C5—C4—C9	119.27 (13)
N1^{i}—Cd1—O1^{i}	92.34 (5)	C3—C4—C9	117.85 (13)

O1—Cd1—O1^{i}	180.0	C6—C5—C4	120.27 (13)
O4—Cl1—O2	110.16 (10)	C6—C5—H5A	119.9
O4—Cl1—O3	108.06 (10)	C4—C5—H5A	119.9
O2—Cl1—O3	111.10 (10)	C5—C6—C7	120.58 (14)
O4—Cl1—O1	110.37 (10)	C5—C6—H6A	119.7
O2—Cl1—O1	109.61 (9)	C7—C6—H6A	119.7
O3—Cl1—O1	107.50 (9)	C8—C7—C6	121.05 (14)
Cl1—O1—Cd1	136.44 (9)	C8—C7—H7A	119.5
C1—N1—C9	118.63 (12)	C6—C7—H7A	119.5
C1—N1—Cd1	127.44 (10)	C7—C8—C9	119.43 (12)
C9—N1—Cd1	113.65 (9)	C7—C8—N2	121.96 (13)
C8—N2—Cd1	111.53 (9)	C9—C8—N2	118.61 (11)
C8—N2—H2A	109.3	N1—C9—C4	121.27 (12)
Cd1—N2—H2A	109.3	N1—C9—C8	119.39 (11)
C8—N2—H2B	109.3	C4—C9—C8	119.34 (12)

Symmetry codes: (i) −*x*, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2B···O4^{ii}	0.90	2.29	3.123 (2)	153
N2—H2A···O3^{iii}	0.90	2.17	3.0520 (19)	165

Symmetry codes: (ii) −*x*, *y*+1/2, −*z*+1/2; (iii) *x*, −*y*+3/2, *z*+1/2.

Fig. 1

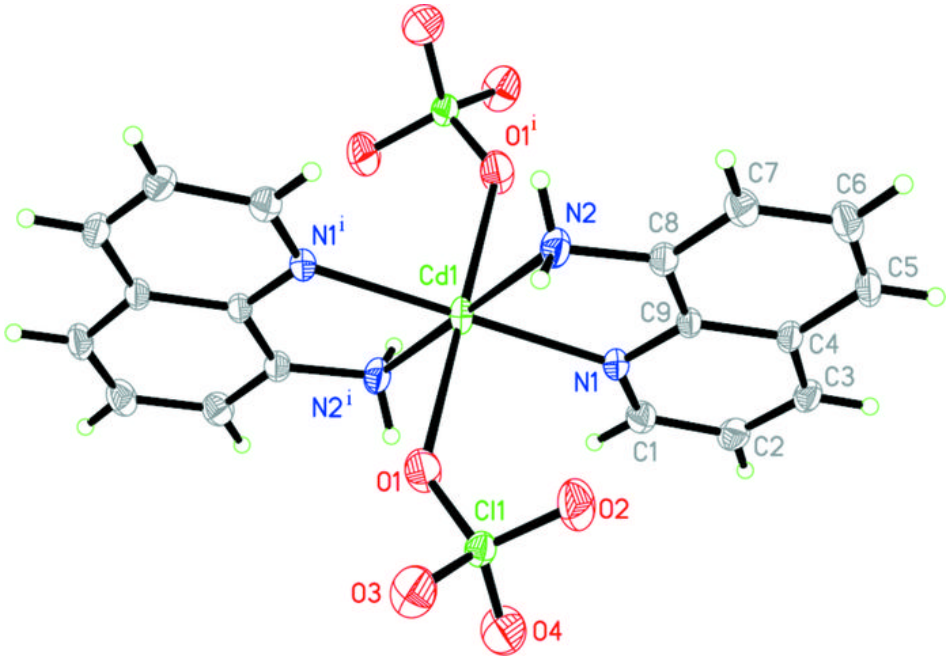

Fig. 2