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trans-Tetrakis(3-aminopyridine)dichlorocadmium(II)

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Key indicators

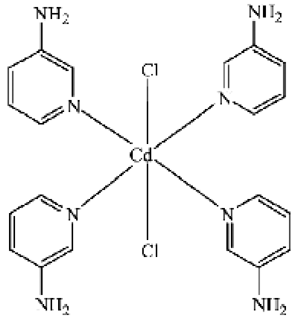
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.029
wR factor = 0.106
Data-to-parameter ratio = 14.7

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

The hydrothermal reaction of 3-aminopyridine and cadmium(II) chloride in alkaline aqueous solution gave rise to the title complex, $[CdCl_2(C_5H_6N_2)_4]$. The Cd^{II} atom is six-coordinate with a distorted octahedral geometry and the Cl^- ions are in *trans* positions. The Cd atom lies on an inversion centre and the asymmetric unit contains two aminopyridine ligands and one Cl^- ion.

Comment

d^{10}-Metal complexes have been found to exhibit intriguing structural and photoluminescent properties (Dai *et al.*, 2002; Ouyang *et al.*, 2003; Tao *et al.*, 2003). While attempting to prepare a cadmium complex containing 3-aminopyridine ligands *via* a hydrothermal reaction, we did not obtain the expected compound but instead obtained the title compound, (I). This complex has now been characterized by elemental analysis and single-crystal diffraction analysis, and we report here the preparation and crystal structure of (I) (Fig. 1).



(I)

X-ray analysis reveals that (I) possesses a mononuclear structure with the Cd atom on an inversion centre, and the asymmetric unit contains two aminopyridine molecules and one Cl^- ion. The Cd atom is coordinated octahedrally (Table 1) by four N atoms from four 3-aminopyridine ligands and two Cl^- ions in *trans* positions. The Cd1—N bond lengths are in the range 2.373 (3)–2.401 (3) Å. The N—Cd—N angles involving neighbouring atoms range from 83.68 (9) to 96.32 (9)°, while the Cl—Cd—Cl angle is 180°. One Cl^- ion acts as an acceptor for a weak N2—H2*B*···Cl1^{ii} intermolecular interaction [symmetry code: (ii) $1-x$, $-y$, $-z$; Table 2].

Experimental

$CdCl_2 \cdot 2.5H_2O$ (0.34 g, 1.5 mmol), 3-aminopyridine (0.19 g, 2 mmol) and NaSCN (0.16 g, 2 mmol) were mixed in H_2O (20 ml) and heated

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at 433 K for 3 d in a sealed 30 ml Teflon-lined stainless steel vessel under autogenous pressure. After the reaction mixture had been slowly cooled to room temperature, yellow prismatic crystals of (I) were produced, which were collected by filtration, washed with distilled water and dried in air (yield 65%, based on Cd). Analysis calculated for $C_{20}H_{24}CdCl_2N_8$: C 42.91, H 4.32, N 20.02%; found: C 42.78, H 4.56, N 20.32%.

Crystal data

$[CdCl_2(C_5H_6N_2)_4]$
$M_r = 559.77$
Triclinic, $P\bar{1}$
$a = 7.7792$ (3) Å
$b = 8.7583$ (3) Å
$c = 10.2481$ (2) Å
$\alpha = 71.159$ (2)°
$\beta = 69.668$ (2)°
$\gamma = 67.949$ (1)°
$V = 591.76$ (3) Å^3

$Z = 1$
$D_x = 1.571$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 142 reflections
$\theta = 2.2$–25.1°
$\mu = 1.17$ mm^{-1}
$T = 293$ (2) K
Prism, yellow
0.46 × 0.30 × 0.24 mm

Data collection

Siemens SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.566$, $T_{\max} = 0.755$
3146 measured reflections

2081 independent reflections
2028 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.016$
$\theta_{\max} = 25.1°$
$h = -9 \rightarrow 7$
$k = -10 \rightarrow 10$
$l = -12 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.106$
$S = 0.99$
2081 reflections
142 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.44$ e Å^{-3}
$\Delta\rho_{\min} = -0.71$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cl1—Cd1	2.6312 (8)	Cd1—N3	2.373 (3)
N1—Cd1	2.401 (3)		
N3—Cd1—N3^{i}	180	N1—Cd1—Cl1^{i}	90.63 (6)
N3—Cd1—N1	83.68 (9)	N3—Cd1—Cl1	91.17 (6)
N3^{i}—Cd1—N1	96.32 (9)	N1—Cd1—Cl1	89.37 (6)
N1—Cd1—N1^{i}	180	Cl1^{i}—Cd1—Cl1	180
N3—Cd1—Cl1^{i}	88.83 (6)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2B···Cl1^{i}	0.86	2.52	3.347 (4)	162

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

H atoms were placed in idealized positions, with C—H = 0.93 and N—H = 0.86 Å, and allowed to ride on their respective parent C atoms, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}$(C,N).

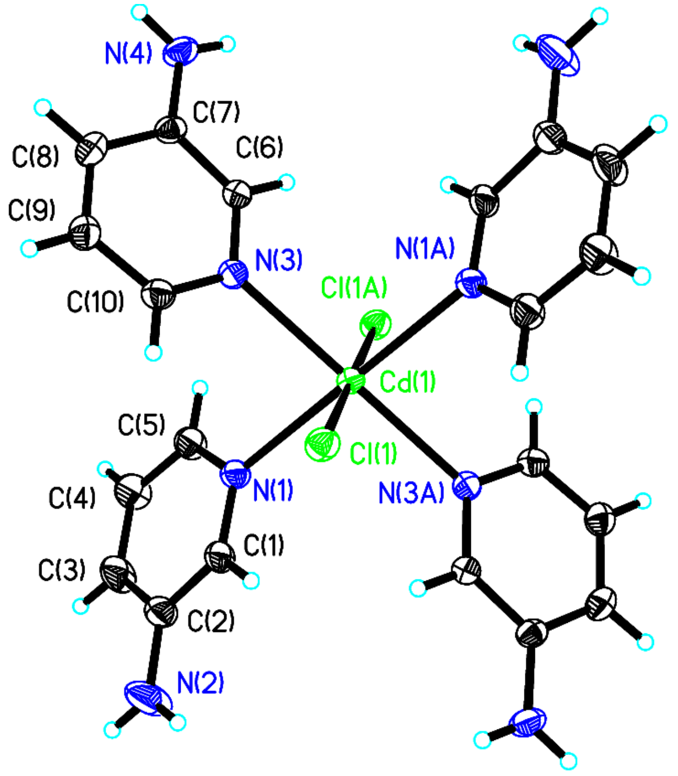

Figure 1
A view of (I), showing the atom-numbering scheme and with 30% probability displacement ellipsoids [symmetry code: (i) $-x, -y, -z$].

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART* and *SAINT* (Siemens, 1994); data reduction: *XPREP* in *SHELXTL* (Siemens, 1994); program(s) used to solve structure: *SHELXTL*; program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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