Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Tris(3,3′-diamino-2,2′-bipyridine)cadmium(II) dinitrate

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Received 27 June 2006
Accepted 4 August 2006

Key indicators

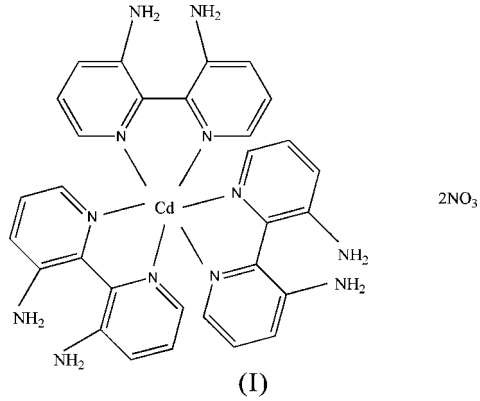
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.023
wR factor = 0.060
Data-to-parameter ratio = 13.8

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

In the title compound, $[Cd(C_{10}H_{10}N_4)_3](NO_3)_2$, the Cd^{II} atom lies on the intersection of a threefold axis and three twofold axes, and is coordinated by the six N atoms from the three 3,3′-diamino-2,2′-bipyridine ligands, with a Cd—N distance of 2.328 (2) Å. The crystal packing is stabilized by intermolecular N—H···O hydrogen bonds between the amino groups and nitrate anions.

Comment

2,2′-Bipyridine and its derivatives are often used as ligands in the synthesis of complexes with metals, which have various applications, for example, in dye-sensitized solar cells (Kuang *et al.*, 2006). In our work with complexes containing bipyridine and its derivatives, we have synthesized the Ni^{II} complex with 3,3′-diamino-2,2′-bipyridine (Min *et al.*, 2006). Here we report the structure of the related Cd^{II} complex, *viz.* the title compound, (I).



(I)

In (I) (Fig. 1), the Cd^{II} atom, located on the intersection of a threefold axis and three twofold axes, has a distorted octahedral CdN_6 coordination geometry (Table 1). Atom N3 of the nitrate anion lies on a threefold axis. In the 3,3′-diamino-2,2′-bipyridine ligand, each pyridine ring is essentially planar with a maximum deviation of 0.046 (4) Å for atom C4; the dihedral angle between the two pyridine rings is 36.41 (17)°. The deviation from planarity for each ligand is expected in terms of steric relief, just as in the Ni^{II} complex (Min *et al.*, 2006). Intermolecular N—H···O hydrogen bonds between the amino groups and nitrate anions (Table 2) stabilize the crystal packing.

Experimental

$Cd(NO_3)_2·6H_2O$ (0.0390 g, 0.113 mmol) in water (10 ml) was added to 3,3′-diamino-2,2′-bipyridine (0.0105 g, 0.0564 mmol) in acetonitrile

(5 ml), and the solution was stirred for a few minutes. Yellow crystals of (I) were obtained after allowing the solution to stand at room temperature for one week.

Crystal data

$[Cd(C_{10}H_{10}N_4)_3](NO_3)_2$
M_r = 795.08
Trigonal, *R*32
a = 14.8206 (15) Å
c = 13.248 (3) Å
V = 2520.1 (6) Å^3
Z = 3
D_x = 1.572 Mg m^{-3}
Mo *Kα* radiation
μ = 0.72 mm^{-1}
T = 298 (2) K
Block, yellow
0.60 × 0.45 × 0.42 mm

Data collection

Bruker SMART APEX CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.673, T_{max} = 0.753
4406 measured reflections
1074 independent reflections
1070 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 25.7°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.060
S = 1.11
1074 reflections
78 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.041P)^2 + 0.3368P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}
Absolute structure: Flack (1983), 470 Friedel pairs
Flack parameter: −0.06 (3)

Table 1
Selected geometric parameters (Å, °).

Cd1—N1	2.328 (2)		
N1—Cd1—N1^{iv}	165.53 (9)	N1^{i}—Cd1—N1^{v}	98.03 (6)
N1—Cd1—N1^{v}	93.68 (9)	N1—Cd1—N1^{i}	71.82 (9)

Symmetry codes: (i) *y*, *x*, −*z*; (iv) *x* − *y*, −*y*, −*z*; (v) −*x*, −*x* + *y*, −*z*.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O1	0.86	2.14	2.985 (4)	166

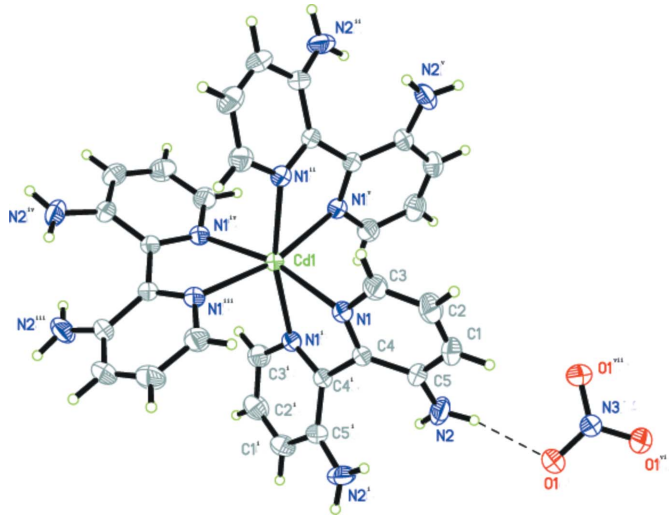


Figure 1
The structure of (I), showing the atom-numbering scheme, with displacement ellipsoids drawn at the 30% probability level [symmetry codes: (i) *y*, *x*, −*z*; (ii) −*y*, *x* − *y*, *z*; (iii) −*x* + *y*, −*x*, *z*; (iv) *x* − *y*, −*y*, −*z*; (v) −*x*, −*x* + *y*, −*z*; (vi) −*y* + 1, *x* − *y* + 1, *z* (vii) −*x* + *y*, −*x* + 1, *z*]. The dashed line indicates a hydrogen bond.

The H atoms were placed in calculated positions (C—H = 0.93 Å and N—H = 0.86 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C,N).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

The authors thank the Natural Science Foundation of Shandong Province of China (grant No. Y2005B25).

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