Azidobis(2,2′-bipyridine)cadmium(II)

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In the title compound, $[Cd(N_3)_2(C_{10}H_8N_2)_2]$, the cadmium(II) ion is coordinated by two N atoms from two azide groups and four N atoms from two 2,2′-bipyridine ligands. The coordination geometry of the cadmium(II) ion is distorted octahedral. The packing is stabilized by intermolecular C—H···N hydrogen-bond interactions.

Comment

The toxic effects of cadmium in the form of Cd^{2+} ions are well established and documented (Flick *et al.*, 1971). The ions have been found to induce various pathological conditions, such as cardiovascular diseases, hypertension and cancer (Schroeder & Balassa, 1965). It is also known, however, that most of the Cd^{2+} in biological systems is not in the form of free Cd^{2+} ions, but is coordinated by the abundance of biological ligands therein (Hung, 1982). Therefore, the coordination chemistry of Cd^{2+} ions with such ligands is of interest. Furthermore, the azide anion is a good inorganic ligand in the synthesis of coordinated compounds. It has been selected for its versatility in allowing ferro- or antiferromagnetic coupling, according to its coordination mode (end-on = EO or end-to-end = EE) to transition metals. In this paper, we report the crystal structure of the title azidobis(2,2′-bipyridine)cadmium(II) complex, (I).

(I)
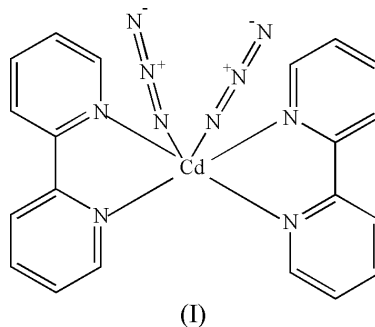
In (I), the Cd atom is chelated by two 2,2′-bipyridine ligands, and additionally coordinated by two azide anions in a *cis* arrangement. The cadmium ion has a distorted octahedral environment. The two 2,2′-bipyridine ligands are bonded in bidentate mode to cadmium, forming five-membered chelate rings. The dihedral angle formed by the least-squares planes through the two chelate rings is 77.6 (1)°. The angle formed by the least-squares lines through the azide anions is 17.3 (2)°. The Cd—N(bipyridine) bond distances fall in the range of values reported in the literature. Bond lengths and angles in the azide groups are normal (Table 1).

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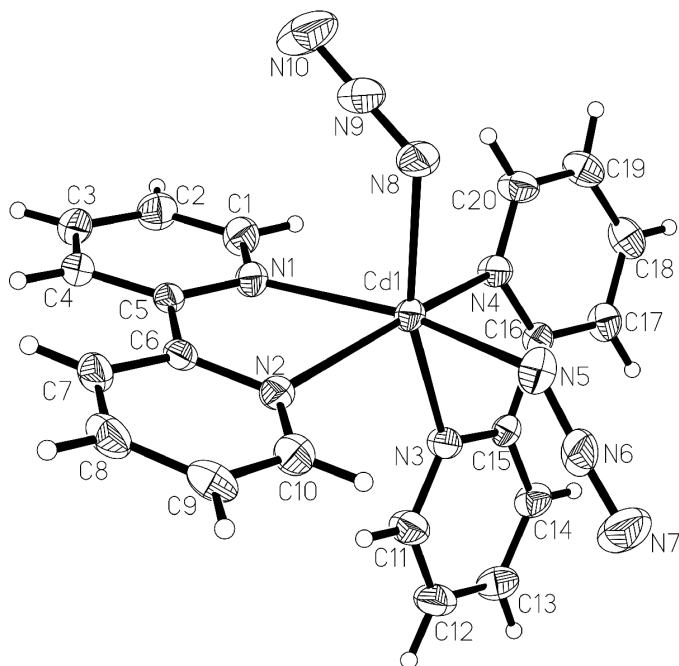
Figure 1
The structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme.

In the crystal structure, there are some weak C—H···N intermolecular hydrogen-bond interactions stabilizing the structure (Table 2).

Experimental

The title compound was prepared by the reaction of 2,2′-bipyridine (1.56 g, 10 mmol) with CdCl$_2$ (0.92 g, 5 mmol) and sodium azide (0.66 g, 10 mmol) by means of hydrothermal synthesis in a stainless steel reactor with a Teflon liner at 393 K for 24 h.

Crystal data

[Cd(N$_3$)$_2$(C$_{10}$H$_8$N$_2$)$_2$]	D_x = 1.680 Mg m^{-3}
M_r = 508.83	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 25
a = 17.099 (3) Å	reflections
b = 14.758 (3) Å	θ = 4–14°
c = 8.0020 (16) Å	μ = 1.12 mm^{-1}
β = 95.00 (3)°	T = 293 (2) K
V = 2011.6 (7) Å^3	Block, yellow
Z = 4	0.35 × 0.28 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer	R_{int} = 0.014
ω scans	θ_{max} = 26.1°
Absorption correction: ψ scan (North *et al.*, 1968)	$h = -20 \rightarrow 20$
	$k = -17 \rightarrow 0$
T_{min} = 0.690, T_{max} = 0.800	$l = 0 \rightarrow 9$
4247 measured reflections	3 standard reflections
3950 independent reflections	every 100 reflections
2776 reflections with $I > 2\sigma(I)$	intensity decay: none

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0318P)^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.025	$+ 0.9972P]$
$wR(F^2)$ = 0.071	where $P = (F_o^2 + 2F_c^2)/3$
S = 1.07	$(\Delta/\sigma)_{max}$ = 0.001
3950 reflections	$\Delta\rho_{max}$ = 0.58 e Å^{-3}
281 parameters	$\Delta\rho_{min}$ = -0.41 e Å^{-3}
H-atom parameters constrained	Extinction correction: *SHELXL*97
	Extinction coefficient: 0.0041 (3)

Table 1
Selected geometric parameters (Å, °).

Cd1—N1	2.426 (2)	Cd1—N8	2.178 (3)
Cd1—N2	2.406 (2)	N5—N6	1.175 (4)
Cd1—N3	2.276 (2)	N6—N7	1.140 (4)
Cd1—N4	2.442 (2)	N8—N9	1.193 (4)
Cd1—N5	2.362 (3)	N9—N10	1.160 (5)
N1—Cd1—N2	70.24 (8)	N5—N6—N7	177.4 (4)
N3—Cd1—N4	67.16 (8)	N8—N9—N10	177.6 (4)
N5—Cd1—N8	91.33 (11)		

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4A···N9^i	0.93	2.50	3.301 (4)	145
C11—H11A···N7^{ii}	0.93	2.59	3.231 (5)	127
C14—H14A···N6^{iii}	0.93	2.50	3.290 (4)	143
C17—H17A···N5^{iii}	0.93	2.58	3.507 (4)	173
C19—H19A···N10^{iv}	0.93	2.61	3.421 (5)	146

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

The H atoms were positioned geometrically (C—H = 0.93Å) and allowed to ride on their attached atoms, with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *NRCVAX* (Gabe *et al.*, 1989); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL-PC* (Sheldrick, 1990); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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