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Diaquabis(4,4′-bipyridine *N*,*N*′-dioxide-κ*O*)-bis(dicyanamido)cadmium(II)

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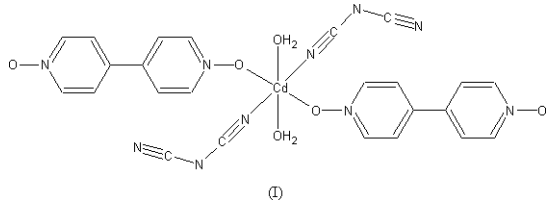
Key indicators

Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.005 Å
R factor = 0.034
wR factor = 0.082
Data-to-parameter ratio = 11.1

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

The structure of the title compound, $[Cd(dca)_2(bpno)_2(H_2O)_2]$, contains a Cd atom coordinated by bpno (4,4′-bipyridine *N*,*N*′-dioxide, $C_{10}H_8N_2O_2$), dca [dca is dicyanamide, $N(CN)_2^-$] and two water molecules. The central Cd^{II} ion is located at an inversion center, coordinated by two N atoms from dca, two O atoms from bpno and two O atoms from water molecules, in an approximately octahedral geometry. This discrete structure is further extended to form a two-dimensional layer structure involving weak hydrogen bonds. The compound is isostructural with its cobalt analog [Aneta, Zdirad, Augustin, Jiri & Marius (2003). *Polyhedron*, **22**, 789–794].



(I)

Experimental

$Cd(NO_3)_2·4H_2O$ (0.039 g, 0.125 mmol) and dca (0.023 g, 0.250 mmol) were dissolved in methanol (20 ml) and water (1:1). After stirring the mixture for about 20 min, bpno (0.056 g, 0.25 mmol) was added. The mixture was heated with continuous stirring for about 15 min. Colorless prismatic crystals of the title complex were grown from the solution by slow evaporation at room temperature over a period of several days (yield 58%, based on Cd). Analysis calculated (%): C 43.84, H 3.04, N 21.31; found (%): C 43.79, H 3.56, N 21.29.

Crystal data

$[Cd(C_2N_3)_2(C_{10}H_8N_2O_2)_2(H_2O)_2]$
M_r = 656.90
Triclinic, $P\overline{1}$
a = 8.2040 (9) Å
b = 8.850 (1) Å
c = 9.667 (1) Å
α = 70.868 (1)°
β = 79.068 (2)°
γ = 73.184 (2)°
V = 631.25 (12) Å^3
Z = 1
D_x = 1.728 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 2950 reflections
θ = 2.2–25.1°
μ = 0.93 mm^{-1}
T = 273 (2) K
Prism, colorless
0.21 × 0.18 × 0.16 mm

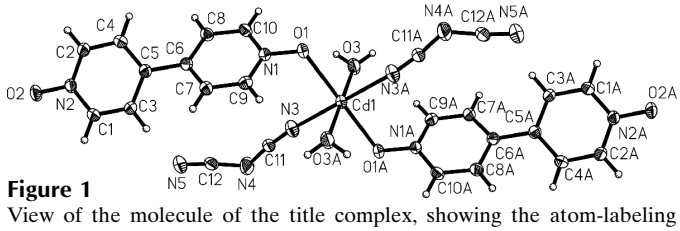


Figure 1
View of the molecule of the title complex, showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 35% probability level. H atoms are represented by circles of arbitrary size. Atoms labeled with the suffix *A* are at the symmetry position (1 − *x*,1 − *y*,1 − *z*).

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Data collection

Bruker SMART CCD diffractometer	2180 independent reflections
φ and ω scans	2100 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$R_{int} = 0.021$
$T_{min} = 0.766$, $T_{max} = 0.860$	$\theta_{max} = 25.1^\circ$
3235 measured reflections	$h = -9 \rightarrow 9$
	$k = -10 \rightarrow 9$
	$l = -10 \rightarrow 11$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0209P)^2 + 1.282P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.034$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.082$	$\Delta\rho_{max} = 0.51$ e Å^{-3}
$S = 1.12$	$\Delta\rho_{min} = -0.43$ e Å^{-3}
2180 reflections	Extinction correction: *SHELXL*97
196 parameters	Extinction coefficient: 0.0090 (18)
H atoms treated by a mixture of independent and constrained refinement	

H atoms bonded to C atoms were placed at calculated idealized positions using a riding model [C—H = 0.93 Å and $U_{iso} = 1.2U_{eq}$(C)]. Those bonded to O atoms were located in a difference Fourier synthesis and refined freely.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1994); data reduction: *SAINT* and *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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