Crystal structure of diaqua(bis(2-aminopyridine))dinitratocadmium(II) monohydrate, $[Cd(H_2O)_2(C_{10}H_{12}N_4)_2(NO_3)_2] \cdot H_2O$

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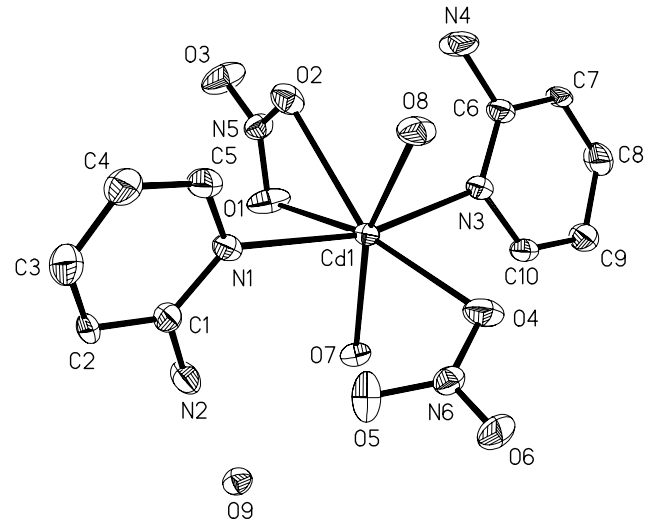

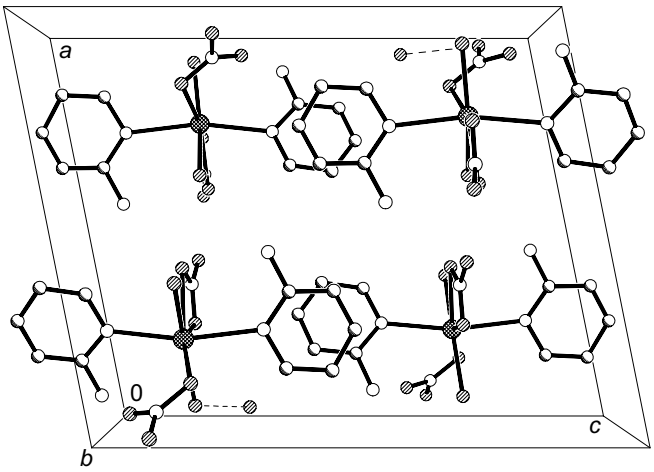

Abstract

$C_{10}H_{18}CdN_6O_9$, monoclinic, $P12_1/c1$ (no. 14), a = 13.451(2) Å, b = 7.869(1) Å, c = 16.699(3) Å, β = 101.330(2)°, V = 1733.1 Å^3, Z = 4, $R_{gt}(F)$ = 0.032, $wR_{ref}(F^2)$ = 0.088, T = 298 K.

Source of material

All commercially available reagents were used as supplied. Cadmium(II) nitrate (1 mmol) was added to the solution of 2-aminopyridine (2 mmol) in a 10 mL of ethanol. The mixture was stirred continuously for 3 h at refluxing temperature, evaporating some ethanol, then the product was collected by filtration (yield 68 %). Single crystals suitable for X-ray determination were obtained by evaporation from ethanol solution after two weeks.

Elemental analysis – found: C, 24.89 %; H, 4.00 %; N, 17.68 %; calc. for $C_{10}H_{18}N_6O_9Cd$: C, 25.07 %, H, 3.76 %, N, 17.55 %. IR data are available in the CIF.

Discussion

During the search of molecule-based materials with interesting properties such as catalytical, clathration, magnetic and photophysical properties, much attention has been focused on the synthesis of one-, two- and three-dimensionally extended solids involving cadmium [1,2], as its d^{10} configuration permits a wide variety of coordination numbers and environments. Rigid ligands such as pyridine groups are frequently used to construct these materials.

The crystal structure of the title compound consists of a neutral complex, $[Cd(2\text{-aminopyridine})_2(NO_3)_2(H_2O)_2]$, and an uncoordinated water molecule. The Cd(II) center is seven-coordinated by two N donor atoms of 2-aminopyridine, three O donor atoms of bidentate NO_3^- and monodentate NO_3^- and two O donor atoms of water (figure, top). The distances of the Cd—O bonds and Cd—N bonds are in the range of 2.303(2) Å – 2.637(4) Å and 2.363(4) Å – 2.400(3) Å, respectively. They are similar to the Cd—O and Cd—N bond lengths reported previously. The pyridine rings in the molecule do not show any unusual features, and the bond lengths and bond angles are within the range of normal values. The dihedral angle of plane N1-C1-C2-C3-C4-C5 with plane C6-C7-C8-C9-C10-N3 is 33.9°, which indicates that the two planes in the molecule are not coplanar and which is most probably duo to the hydrogen bonding requirement. The complex molecules and the uncoordinated water molecules are interlinked via hydrogen bonds of the types O–H···O and N–H···N. A three-dimensional network is formed by interactions of the hydrogen bonds and π-π stacking of the 2-aminopyridine rings (figure, bottom).

Table 1. Data collection and handling.

Crystal:	colorless block, size 0.34 × 0.47 × 0.57 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	13.19 cm^{-1}
Diffractometer, scan mode:	Bruker SMART CCD, φ/ω
$2\theta_{max}$:	50.02°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	8382, 3056
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 2686
$N(param)_{refined}$:	236
Program:	SHELXTL [3]

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Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(2A)	4*e*	0.0636	–0.1848	–0.0120	0.053
H(2B)	4*e*	0.1011	–0.1421	0.0756	0.053
H(4A)	4*e*	0.4980	–0.0205	0.4219	0.077
H(4B)	4*e*	0.4460	–0.0051	0.3349	0.077
H(7A)	4*e*	0.0427	–0.0153	0.2013	0.038
H(7B)	4*e*	0.0836	–0.1730	0.2236	0.038
H(8A)	4*e*	0.3867	0.3447	0.2246	0.057
H(8B)	4*e*	0.4349	0.1895	0.2293	0.057
H(9A)	4*e*	0.0160	0.8574	0.8082	0.044
H(9B)	4*e*	0.0501	0.9218	0.7414	0.044
H(2)	4*e*	0.1530	–0.1266	–0.1112	0.040
H(3)	4*e*	0.2932	–0.0158	–0.1435	0.066
H(4)	4*e*	0.4227	0.0876	–0.0451	0.065
H(5)	4*e*	0.3998	0.0905	0.0877	0.057
H(7)	4*e*	0.4160	–0.0081	0.5273	0.039
H(8)	4*e*	0.2682	0.0230	0.5689	0.062
H(9)	4*e*	0.1174	0.0663	0.4766	0.057
H(10)	4*e*	0.1234	0.0723	0.3401	0.046

Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cd(1)	4*e*	0.24764(2)	0.03670(3)	0.20504(2)	0.0213(2)	0.0282(2)	0.0272(2)	0.00027(9)	0.0012(1)	–0.0013(1)
N(1)	4*e*	0.2647(2)	–0.0107(5)	0.0687(2)	0.028(2)	0.044(2)	0.030(2)	–0.001(1)	0.001(1)	–0.003(2)
N(2)	4*e*	0.1095(2)	–0.1425(5)	0.0259(2)	0.042(2)	0.058(2)	0.034(2)	–0.015(2)	0.006(1)	–0.011(2)
N(3)	4*e*	0.2696(2)	0.0331(4)	0.3511(2)	0.026(2)	0.040(2)	0.030(2)	0.001(1)	–0.000(1)	–0.003(1)
N(4)	4*e*	0.4434(3)	–0.0069(6)	0.3859(2)	0.030(2)	0.134(4)	0.027(2)	0.018(2)	–0.002(2)	0.000(2)
N(5)	4*e*	0.3643(2)	–0.2859(4)	0.2254(2)	0.029(2)	0.031(2)	0.042(2)	0.004(1)	0.007(1)	0.001(2)
N(6)	4*e*	0.1041(2)	0.3297(4)	0.1488(2)	0.028(2)	0.034(2)	0.045(2)	0.000(1)	0.010(1)	–0.000(2)
O(1)	4*e*	0.2710(2)	–0.2958(5)	0.2162(2)	0.025(1)	0.063(2)	0.081(2)	0.003(1)	0.011(1)	0.014(2)
O(2)	4*e*	0.4042(2)	–0.1440(3)	0.2198(2)	0.044(2)	0.028(2)	0.049(2)	–0.006(1)	–0.003(1)	–0.001(1)
O(3)	4*e*	0.4193(2)	–0.4122(4)	0.2417(3)	0.043(2)	0.030(2)	0.115(3)	0.013(1)	0.022(2)	0.011(2)
O(4)	4*e*	0.1642(2)	0.3038(4)	0.2157(2)	0.037(2)	0.047(2)	0.058(2)	0.002(1)	–0.009(1)	0.008(2)
O(5)	4*e*	0.0922(3)	0.2159(4)	0.0960(2)	0.095(2)	0.041(2)	0.046(2)	–0.003(2)	0.031(2)	–0.008(2)
O(6)	4*e*	0.0576(2)	0.4625(4)	0.1367(2)	0.056(2)	0.045(2)	0.063(2)	0.028(2)	0.004(2)	0.003(2)
O(7)	4*e*	0.0899(2)	–0.0839(3)	0.1963(2)	0.024(1)	0.035(1)	0.038(2)	0.002(1)	0.006(1)	0.005(1)
O(8)	4*e*	0.3774(2)	0.2383(4)	0.2182(2)	0.030(1)	0.033(2)	0.076(2)	–0.009(1)	0.004(1)	–0.003(2)
O(9)	4*e*	0.0671(2)	0.8660(4)	0.7855(2)	0.035(1)	0.043(2)	0.034(1)	0.004(1)	0.010(1)	0.003(1)
C(1)	4*e*	0.1938(3)	–0.0773(5)	0.0076(2)	0.036(2)	0.034(2)	0.035(2)	0.007(2)	0.003(2)	–0.004(2)
C(2)	4*e*	0.2036(3)	–0.0807(5)	–0.0709(2)	0.034(2)	0.046(2)	0.019(2)	–0.000(2)	0.003(2)	–0.008(2)
C(3)	4*e*	0.2866(4)	–0.0172(7)	–0.0891(3)	0.059(3)	0.073(3)	0.037(3)	0.004(2)	0.017(2)	–0.003(2)
C(4)	4*e*	0.3633(4)	0.0466(7)	–0.0316(3)	0.042(2)	0.076(4)	0.049(3)	–0.002(2)	0.020(2)	0.000(3)
C(5)	4*e*	0.3486(3)	0.0473(6)	0.0472(3)	0.031(2)	0.065(3)	0.045(3)	–0.003(2)	0.005(2)	–0.006(2)
C(6)	4*e*	0.3542(3)	0.0116(5)	0.4093(2)	0.027(2)	0.047(2)	0.029(2)	0.002(2)	–0.001(2)	–0.001(2)
C(7)	4*e*	0.3558(3)	0.0076(5)	0.4897(2)	0.023(2)	0.054(2)	0.017(2)	0.004(2)	–0.004(1)	–0.001(2)
C(8)	4*e*	0.2689(4)	0.0266(7)	0.5134(3)	0.054(3)	0.075(4)	0.026(2)	–0.001(2)	0.006(2)	–0.008(2)
C(9)	4*e*	0.1783(3)	0.0519(6)	0.4589(3)	0.035(2)	0.070(3)	0.039(2)	–0.004(2)	0.010(2)	–0.010(2)
C(10)	4*e*	0.1830(3)	0.0547(6)	0.3781(3)	0.023(2)	0.055(3)	0.037(2)	0.001(2)	0.002(2)	–0.007(2)

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