Crystal structure of aqua(2,2′-bipyridine-κ^2N:N')(nitrato)-(4-amino-benzoato)cadmium(II) nitrate, $[Cd(H_2O)(NO_3)(C_{10}H_8N_2)(C_7H_7NO_2)][NO_3]$

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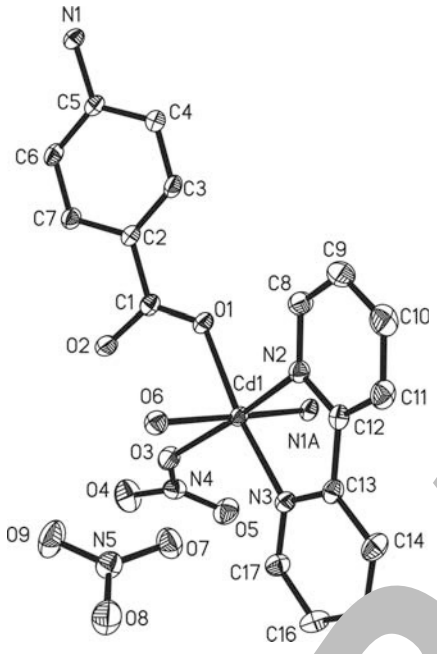
Received October 23, 2009, accepted and available on-line November 4, 2009; CCDC no. 1267/2818



Abstract

$C_{17}H_{17}CdN_5O_9$, monoclinic, $P12_1/$ (no. 14, a = 14.355(1) Å, b = 8.5015(8) Å, [illegible] = 16.431(2) Å, β = 93.570(1)°, V = 2001.2 Å^3, [illegible], $R_{gt}(F)$ = 0.025, $wR_{ref}(F^2)$ = 0.062, T = 293 K.

Source of material

A mixture of $CdCO_3$ (1 [illegible] mmol, 0.1729 g), 4-a[illegible]obenzoic acid (2.0 mmol, 0.278 g), [illegible]O (10 [illegible] 0.55 mmol), 2,2′-bipyridine (1.0 mmol, 0.156 g), [illegible] vo[illegible]ps of acetic acid with the pH value of about 3.0, was [illegible]n a 25 [illegible] Teflon-lined reaction vessel at 160 °C for 3 days, [illegible]ctio[illegible] mixture was cooled to room tempe[illegible]r a perio[illegible]8 h. The product was collected b[illegible]ratio[illegible] washed with H$_2$O and air-dried, colorless block-sh[illegible] crysta[illegible] suitable for X-ray differaction analysis were obtai[illegible].

Experimental det[illegible]

H atoms bonded to C[illegible]ms were placed geometrically and treated as riding with d(C—H) = 0.93 Å and U_{iso}(H) = 1.2 U_{eq}(C). The water H atoms found from difference Fourier maps were included in the refinement with restraints of d(O—H) = 0.82 - 0.826 Å and U_{iso}(H) = 1.5 U_{eq}(O).

Discussion

Metal coordina[illegible] polym[illegible]rs have be[illegible]died extensively in the recent years [illegible] their i[illegible]esting network topologies and material properties [1[illegible]. [illegible]theless, [illegible]ordination polymers with 4-aminobe[illegible]ate liga[illegible]ntai[illegible] neutral donor groups, are rather [illegible].

The [illegible]m centres are co[illegible]inated by three oxygen (one from th[illegible]ami[illegible]oate ligands, one from a nitrare and one from wa[illegible]r) and th[illegible]ogen atoms in a distorted octahedronal manner. Each 4-amin[illegible]ate ligand coordinate one cadmium ion as monodentate ligan[illegible] *via* one oxygen atom and another one *via* the nitrogen atom, leading to a one-dimensional infinite chain with Cd···Cd distances of 9.448 Å. The cadmium atoms are linked *via* two 4-am[illegible]benzoate ligands. The chains are parallel to [illegible]. The [illegible]est Cd···Cd distance between two neighbouring ch[illegible] Å.

Table 1. Data collection and handling.

Crystal:	colorless block, size 0.21 × 0.27 × 0.37 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	11.55 cm^{-1}
Diffractometer, scan mode:	Bruker SMART CCD, φ/ω
$2\theta_{max}$:	51°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	14006, 3726
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 3208
$N(param)_{refined}$:	290
Programs:	SHELXS-97 [4], SHELXL-97 [5], SHELXTL [6]

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

Atom	Site	x	y	z	U_{iso}
H(2)	4*e*	0.8529	0.6582	0.8378	0.069
H(1W)	4*e*	0.6512	0.5144	0.7747	0.055
H(2W)	4*e*	0.6281	0.6413	0.7273	0.055
H(1A)	4*e*	0.9474	0.0630	1.1608	0.037
H(1B)	4*e*	0.9276	–0.0667	1.1052	0.037
H(3)	4*e*	0.8541	0.1447	0.8604	0.039
H(4)	4*e*	0.8758	–0.0311	0.9671	0.039
H(6A)	4*e*	0.9194	0.3301	1.1225	0.040
H(7)	4*e*	0.8979	0.5054	1.0160	0.040
H(8)	4*e*	0.7449	0.1793	0.7367	0.046
H(9)	4*e*	0.6525	–0.0287	0.6940	0.057
H(10)	4*e*	0.5601	–0.0055	0.5734	0.060
H(11)	4*e*	0.5648	0.2254	0.4985	0.051
H(14)	4*e*	0.5837	0.4448	0.4311	0.052
H(15)	4*e*	0.5992	0.6916	0.3735	0.060
H(16)	4*e*	0.6852	0.8831	0.4452	0.054
H(17)	4*e*	0.7568	0.8207	0.5699	0.044

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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*	0.77935(2)	0.52439(3)	0.68257(1)	0.0283(1)	0.0284(1)	0.0203(1)	–0.00157(9)	–0.00150(8)	–0.00044(9)
O(1)	4*e*	0.83867(9)	0.4099(2)	0.78738(7)	0.0413(7)	0.0363(7)	0.0218(7)	0.0003(6)	–0.0028(5)	0.0013(6)
O(2)	4*e*	0.8636(1)	0.6036(2)	0.87839(8)	0.076(1)	0.0334(8)	0.0280(7)	–0.0026(7)	–0.0013(7)	0.0016(6)
O(3)	4*e*	0.83510(9)	0.7387(2)	0.73175(8)	0.0504(8)	0.0352(8)	0.0319(7)	–0.0136(6)	0.0036(6)	–0.0013(6)
O(4)	4*e*	0.9269(1)	0.9354(2)	0.7592(1)	0.063(1)	0.056(1)	0.069(1)	–0.0193(8)	–0.0092(9)	–0.0244(9)
O(5)	4*e*	0.9270(1)	0.8241(2)	0.64123(9)	0.059(1)	0.053(1)	0.0450(9)	–0.0127(8)	0.0146(7)	0.0050(7)
O(1W)	4*e*	0.67099(9)	0.5914(2)	0.75117(8)	0.0336(7)	0.0401(8)	0.0358(7)	0.0005(6)	0.0043(6)	0.0008(6)
O(7)	4*e*	0.5265(1)	0.7238(2)	0.64966(9)	0.0443(8)	0.0520(9)	0.0507(9)	[illegible]	0.0024(7)	–0.0105(7)
O(8)	4*e*	0.3981(1)	0.8558(2)	0.65256(9)	0.0473(9)	0.090(1)	0.0461(	[illegible]	–0.0105(7)	–0.0106(9)
O(9)	4*e*	0.4915(1)	0.8441(2)	0.75943(9)	0.058(1)	0.103(2)	0.034	0.011(1)	0.0077(7)	–0.0149(9)
N(1)	4*e*	0.9051(1)	0.0249(2)	1.12316(9)	0.0314(8)	0.0382(9)	0.0	0.0007(7)	.0016(6)	0.0032(7)
N(2)	4*e*	0.7108(1)	0.3233(2)	0.64659(9)	0.0318(8)	0.0312(9)	0.027	0.0016(6)	.0006(6)	–0.0021(7)
N(3)	4*e*	0.7146(1)	0.6020(2)	0.57553(9)	0.0280(8)	0.0319(9)	0.0253(8)	004(6)	.0001(6)	0.0009(7)
N(4)	4*e*	0.8986(1)	0.8341(2)	0.7104(1)	0.0344(9)	0.0325(9)	038(1)	[illegible]	-0.0068(7)	0.0022(8)
N(5)	4*e*	0.4722(1)	0.8069(2)	0.6880(1)	0.0362(9)	0.047(1)	0.038(1)	–0.0	0.0005(7)	–0.0003(8)
C(1)	4*e*	0.8572(1)	0.4539(2)	0.8580(1)	0.0282(9)	0.037(1)	0.026	–0.0002(	0.0036(7)	0.0011(8)
C(2)	4*e*	0.8723(1)	0.3432(2)	0.9268(1)	0.0296(9)	0.035(1)	[illegible]	–0.0007(8)	0.0023(7)	0.0009(8)
C(3)	4*e*	0.8667(1)	0.1821(2)	0.9132(1)	0.038(1)	0.0 (1)	[illegible]	2(8)	0.0001(7)	–0.0035(8)
C(4)	4*e*	0.8797(1)	0.0765(2)	0.9770(1)	0.038(1)	0 (1)	0.	06(8)	0.0032(8)	–0.0010(8)
C(5)	4*e*	0.8986(1)	0.1323(2)	1.0561(1)	0.0249(9)	8(1)	0.022	0002(7)	0.0028(7)	0.0032(8)
C(6)	4*e*	0.9058(1)	0.2929(2)	1.0699(1)	0.039(1)	(1)	0.0202(9)	0.0069(8)	0.0003(7)	–0.0022(8)
C(7)	4*e*	0.8929(1)	0.3979(2)	1.0062(1)	0.040(1)	0.	0.027(1)	–0.0046(8)	0.0016(8)	–0.0021(8)
C(8)	4*e*	0.7079(1)	0.1886(2)	0.6884(1)	0.045(1)	0.036(	0.034(1)	–0.0032(9)	–0.0021(9)	0.0028(9)
C(9)	4*e*	0.6529(2)	0.0633(3)	0.6634(1)	0.059(	0.033(1)	0(1)	–0.009(1)	0.004(1)	0.001(1)
C(10)	4*e*	0.5983(2)	0.0772(3)	0.5917(1)	0.0	0.041(1)	(1)	–0.017(1)	–0.002(1)	–0.010(1)
C(11)	4*e*	0.6007(1)	0.2150(3)	0.5473(1)	0 (1)	0.046(1)	0.037(1)	–0.009(1)	–0.0056(9)	–0.008(1)
C(12)	4*e*	0.6573(1)	0.3372(2)	0.5761(1)	0 9(9)	0.036(1)	0.028(1)	–0.0019(8)	0.0018(7)	–0.0056(8)
C(13)	4*e*	0.6627(1)	0.4911(2)	0.5345(1)	0 (9)	0.041(1)	0.026(1)	–0.0007(8)	–0.0010(7)	–0.0030(8)
C(14)	4*e*	0.6188(2)	0.5223(3)	0.4587(1)	0.	0.056(1)	0.032(1)	–0.007(1)	–0.0086(9)	–0.001(1)
C(15)	4*e*	0.6277(2)	0.6693(3)	0.4246(1)	0.04	0.069(	0.031(1)	–0.000(1)	–0.0102(9)	0.011(1)
C(16)	4*e*	0.6792(2)	0.7827(3)	0.4667(1)	0.046(1)	[illegible]	0.039(1)	0.001(1)	–0.0028(9)	0.016(1)
C(17)	4*e*	0.7216(1)	0.7442(2)	0.54	0.037(1)	(1)	0.035(1)	–0.0015(8)	–0.0022(8)	0.0037(9)

Acknowledgments. This work was supported by the Construct m of th Key Disciplines in Hunan Province, Distinguished Young C ar Hunan Province (2008), Distinguished Young Cadreman of Heng mal University (2007) and Hengyang Bureau of Sci & Technolog t no. 2009KJ29).

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