Crystal structure of diaqua(4,4′-bipyridine-*N*,*N*′)-bis(2-benzoylbenzoato)-cadmium(II) dihydrate, $Cd(C_{14}H_9O_3)_2(C_{10}H_8N_2)(H_2O)_2 \cdot 2H_2O$

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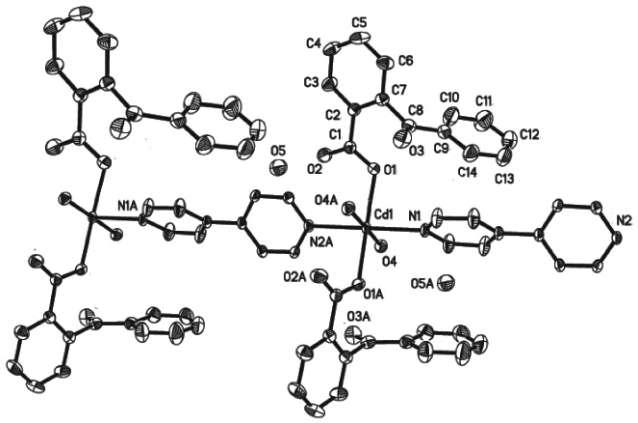
Received March 22, 2011, accepted and available on-line June 16, 2011; CCDC no. 1267/3469



Abstract

$C_{38}H_{34}CdN_2O_{10}$, monoclinic, *P*12/*c*1 (no. 13), *a* = 12.923(3) Å, *b* = 11.651(2) Å, *c* = 13.133(3) Å, β = 115.88(3)°, *V* = 1779.1 Å^3, *Z* = 2, $R_{gt}(F)$ = 0.032, $wR_{ref}(F^2)$ = 0.079, *T* = 293 K.

Source of material

A mixture of 2-benzoylbenzoic acid (2.03 mmol), 4,4′-bipyridine (1.21 mmol) and cadmium acetate (1.00 mmol) was dissolved in the mixed solvent of ethanol (10 ml) and *N*,*N*-dimethylformamide (1 ml). The reaction was kept at 343 K for 6 h. Afterwards the system was filtrated, and the filtrate was allowed to stand at room temperature. Slow evaporation for three days afforded a few pale-yellow grain-shaped single crystals suitable for X-ray diffraction analysis.

Experimental details

Hydrogen atoms bound to carbon atoms were positioned geometrically with *d*(C—H) = 0.93 Å and refined as riding, with U_{iso}(H) = 1.2 U_{eq}(C).

Discussion

4,4′-bipyridine is an excellent bridging ligand, it coordinates most transitional metals via N atom to produce a series of complexes possessing novel structures [1-5]. 2-Benzoylbenzoic acid is a main raw material of anthraquinone dyes intermediates. It is used to manufacture anthraquinone and 1-aminoanthra- quinone. As ligand, 2-benzoylbenzoic acid can coordinate metal ions to generate complexes.

In the molecule of the title complex, two neighboring Cd(II) ions are linked by 4,4′-bipyridine, forming a chain structure. The Cd(II) ion is coordinated by two aqua oxygen atoms, two oxygen atoms from two 2-benzoylbenzoates and two nitrogen atoms of different 4,4′-bipyridine ligands to form a distorted CdN_2O_4 octahedron, where O1, N1, O1A and N2A are located at the equatorial plane, and O4 and O4A occupy the axial positions. The bond angles of the equatorial plane are ∠O1–Cd1–N1 = 89.30(3)°, ∠N1–Cd1–O1A = 89.30(3)°, ∠O1A–Cd1–N2A = 90.69(3)° and ∠N2A–Cd1–O1 = 90.70(3)°. The angles ∠O–Cd1–O and ∠O–Cd1–N are within the range of 85.14(5)° to 178.61(6)° and 89.16(3)° to 90.84(3)°, respectively. The average lengths are *d*(Cd1—N) = 2.3011 Å. *d*(Cd1—O1) = 2.2686 Å and *d*(Cd1—O4) = 2.3830 Å, which shows that the coordination ability of O4 in water is weaker than that of O1 from 2-benzoylbenzoate. Additionally, there exist O–H···O hydrogen bonding interaction involving the oxygen atoms of 2-benzoylbenzoate ligands and water molecules with the distances in the range of 2.681(2)-2.903(2) Å.

Table 1. Data collection and handling.

Crystal:	yellow grain, size 0.10 × 0.18 × 0.20 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	6.75 cm^{-1}
Diffractometer, scan mode:	Rigaku Saturn CCD area detector, ω/φ
$2\theta_{max}$:	50.04°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	13738, 3142
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2869
$N(param)_{refined}$:	234
Programs:	SHELXS-97, SHELXL-97, SHELXTL [6]

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

Atom	Site	*x*	*y*	*z*	U_{iso}
H(4A)	4*g*	0.5518	0.8176	0.0574	0.051
H(4B)	4*g*	0.4376	0.7904	0.0410	0.051
H(3)	4*g*	0.0817	0.8925	–0.1419	0.065
H(4)	4*g*	–0.1110	0.9210	–0.1937	0.072
H(5)	4*g*	–0.1880	0.8688	–0.0730	0.076
H(6)	4*g*	–0.0733	0.7910	0.1007	0.066
H(10)	4*g*	0.0854	0.5733	0.0778	0.098
H(11)	4*g*	0.1011	0.3802	0.1261	0.132
H(12)	4*g*	0.1813	0.3282	0.3134	0.120
H(13)	4*g*	0.2549	0.4636	0.4515	0.099
H(14)	4*g*	0.2425	0.6562	0.4055	0.082
H(15)	4*g*	0.4718	0.5548	0.3829	0.070
H(16)	4*g*	0.4679	0.3594	0.3853	0.071
H(19)	4*g*	0.6324	0.1841	0.2090	0.042
H(20)	4*g*	0.6310	–0.0112	0.2136	0.042
H(5A)	4*g*	0.7145	0.1077	0.5808	0.080
H(5B)	4*g*	0.6592	0.0114	0.5095	0.080

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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)	2*f*	½	0.77066(1)	¼	0.03489(8)	0.01611(8)	0.03602(8)	0	0.01423(6)	0
O(1)	4*g*	0.3065(1)	0.7683(1)	0.1448(1)	0.0325(6)	0.0483(8)	0.0465(7)	–0.0041(5)	0.0122(5)	0.0129(6)
O(2)	4*g*	0.2898(1)	0.8450(1)	–0.0172(1)	0.0480(6)	0.084(1)	0.0532(7)	0.0071(7)	0.0278(5)	0.0192(7)
O(3)	4*g*	0.1776(1)	0.8323(1)	0.2799(1)	0.082(1)	0.068(1)	0.0396(7)	–0.0041(8)	0.0171(7)	–0.0115(7)
O(4)	4*g*	0.5089(1)	0.7737(1)	0.0726(1)	0.0484(6)	0.0404(7)	0.0470(6)	–0.0004(5)	0.0291(5)	0.0015(5)
N(1)	2*f*	½	0.5742(2)	¼	0.047(1)	0.017(1)	0.047(1)	0	0.0235(8)	0
N(2)	2*f*	½	–0.0308(2)	¼	0.0352(9)	0.020(1)	0.037(1)	0	0.0125(8)	0
C(1)	4*g*	0.2492(1)	0.8121(2)	0.0480(1)	0.0394(8)	0.0336(9)	0.0400(8)	–0.0002(8)	0.0162(7)	0.0016(8)
C(2)	4*g*	0.1231(1)	0.8258(2)	0.0132(1)	0.0388(8)	0.037(1)	0.0332(8)	0.0024(8)	0.0141(7)	–0.0005(7)
C(3)	4*g*	0.0511(2)	0.8723(2)	–0.0921(2)	0.051(1)	0.071(1)	0.0405(9)	0.010(1)	0.0194(8)	0.0100(9)
C(4)	4*g*	–0.0644(2)	0.8890(2)	–0.1236(2)	0.049(1)	0.081(2)	0.040(1)	0.020(1)	0.0104(9)	0.008(1)
C(5)	4*g*	–0.1099(2)	0.8584(2)	–0.0516(2)	0.0363(9)	0.089(2)	0.055(1)	0.016(1)	0.0115(9)	–0.009(1)
C(6)	4*g*	–0.0411(2)	0.8121(2)	0.0525(2)	0.0427(9)	0.076(2)	0.049(1)	–0.001(1)	0.0236(8)	–0.005(1)
C(7)	4*g*	0.0756(1)	0.7967(2)	0.0863(1)	0.0389(8)	0.038(1)	0.0357(8)	–0.0012(8)	0.0135(7)	–0.0050(7)
C(8)	4*g*	0.1459(2)	0.7587(2)	0.2067(2)	0.0414(9)	0.055(1)	0.0369(9)	–0.0057(8)	0.0183(7)	–0.0028(8)
C(9)	4*g*	0.1598(2)	0.6346(2)	0.2357(2)	0.0429(9)	0.059(1)	0.047(1)	–0.0030(9)	0.0184(8)	0.0091(9)
C(10)	4*g*	0.1193(2)	0.5519(2)	0.1536(2)	0.098(2)	0.056(2)	0.061(1)	–0.010(1)	0.007(1)	0.006(1)
C(11)	4*g*	0.1282(3)	0.4360(2)	0.1823(3)	0.124(2)	0.054(2)	0.104(2)	–0.016(2)	0.007(2)	0.006(2)
C(12)	4*g*	0.1772(2)	0.4053(3)	0.2937(3)	0.087(2)	0.071(2)	0.124(2)	–0.003(2)	0.028(2)	0.043(2)
C(13)	4*g*	0.2201(2)	0.4860(2)	0.3759(2)	0.080(2)	0.093(2)	0.076(1)	0.017(1)	0.036(1)	0.041(1)
C(14)	4*g*	0.2125(2)	0.6012(2)	0.3487(2)	0.070(1)	0.083(2)	0.054(1)	0.010(1)	0.030(1)	0.017(1)
C(15)	4*g*	0.4831(2)	0.5147(2)	0.3274(2)	0.098(1)	0.028(1)	0.066(1)	–0.0003(9)	0.051(1)	–0.0049(8)
C(16)	4*g*	0.4815(2)	0.3971(2)	0.3299(2)	0.102(1)	0.029(1)	0.064(1)	–0.004(1)	0.051(1)	0.0006(8)
C(17)	2*f*	½	0.3348(2)	¼	0.040(1)	0.019(1)	0.038(1)	0	0.0155(9)	0
C(18)	2*f*	½	0.2079(2)	¼	0.035(1)	0.019(1)	0.030(1)	0	0.0094(9)	0
C(19)	4*g*	0.5787(1)	0.1460(1)	0.2261(1)	0.0397(8)	0.0231(8)	0.0470(9)	–0.0038(7)	0.0227(7)	0.0003(7)
C(20)	4*g*	0.5767(1)	0.0290(1)	0.2281(1)	0.0380(7)	0.0247(9)	0.0453(9)	0.0024(7)	0.0216(7)	–0.0026(7)
O(5)	4*g*	0.6572(1)	0.0866(1)	0.5208(1)	0.0564(8)	0.084(1)	0.0560(8)	–0.0001(8)	0.0208(6)	–0.0222(8)

Acknowledgments. This work was supported by Hengyang Bureau of Science & Technology (grant no. 2009KJ26) and the Construct Program of the Key Disciplines in Hunan Province.

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