Crystal structure of bis[2-(1*H*-benzimidazol-2-yl)benzoato-κ^2N,O]-(1,10-phenanthroline)Cd(II), $Cd(C_{14}H_9N_2O_2)_2(C_{12}H_8N_2)$

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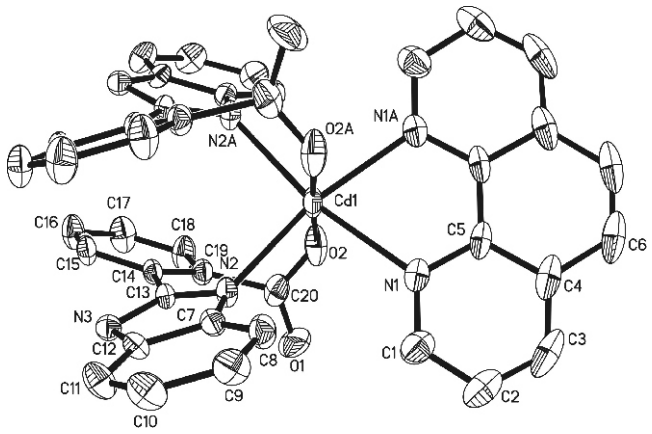

Abstract

$C_{40}H_{26}CdN_6O_4$, hexagonal, $P6_2$ (no. 171), a = 12.2812(2) Å, c = 18.7740(4) Å, V = 2452.3 Å^3, Z = 3, $R_{gt}(F)$ = 0.029, $wR_{ref}(F^2)$ = 0.059, T = 293 K.

Source of material

The mixture of 2-(1H-benzimidazol-2-yl)benzoic acid (L, 0.047 g, 0.2 mmol), $Cd(Ac)_2 \cdot 2H_2O$ (0.026 g, 0.1 mmol), 1,10-phenanthroline (phen, 0.1 g, 0.019 g), 5 mL distilled H_2O and 5 mL CH_3OH were sealed in a 25 mL Teflon-lined stainless reactor and heated at 140 °C for 3 d under autogeneous pressure, then cooled to room temperature. Upon cooling to room temperature, colorless crystals were obtained and washed with distilled water (yield 36 %).

Experimental details

H atoms of C atoms and N atoms were positioned geometrically with d(C—H) = 0.93 Å and d(N—H) = 0.86 Å and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C,N). The Flack parameter of 0.04 proves the correctness of the absolute crystal structure.

Discussion

To our best knowledge, only one Zn(II) coordination polymer based on L has been reported so far [1]. Differing from the reported architecture, we have synthsized a Cd(II) coordination polymer based on L, $Cd(Ac)_2$ and phen.

The asymmetric unit of the title crystal structure consitsts of one Cd(II) ion, two L and a phen molecule. Cd(II) ion adopts slightly distorted octahedral environment, which is formed by four N atoms and two O atoms from two L and a phen molecule. The distances Cd—O(N) are in the range of 2.313-2.354 Å. Neighbouring molecules of L interact through C–H···O hydrogen bonds and π-π interactions of aromatic ring to form a three-dimensional structure.

Table 1. Data collection and handling.

Crystal:	colorless block, size 0.02 × 0.02 × 0.03 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	7.22 cm^{-1}
Diffractometer, scan mode:	Oxford Diffraction Gemini R Ultra, ω
$2\theta_{max}$:	58.4°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	7429, 3149
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2088
$N(param)_{refined}$:	231
Programs:	SHELXS-97, SHELXL-97 [2]

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

Atom	Site	x	y	z	U_{iso}
H(1)	6*c*	0.2466	0.5057	0.0841	0.081
H(2)	6*c*	0.1505	0.5134	-0.0200	0.093
H(3)	6*c*	0.2362	0.5089	-0.1271	0.103
H(6)	6*c*	0.4106	0.5029	-0.1963	0.105
H(8)	6*c*	0.1922	0.2868	0.1385	0.061
H(9)	6*c*	0.0059	0.1202	0.1782	0.070
H(10)	6*c*	-0.0525	0.1060	0.2961	0.072
H(11)	6*c*	0.0644	0.2613	0.3761	0.066
H(15)	6*c*	0.4992	0.6061	0.4095	0.055
H(16)	6*c*	0.6726	0.7862	0.4491	0.071
H(17)	6*c*	0.7779	0.9539	0.3717	0.081
H(18)	6*c*	0.7136	0.9367	0.2563	0.071
H(3')	6*c*	0.2945	0.4947	0.3813	0.047

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)	3*b*	½	½	0.14228(2)	0.0479(2)	0.0742(3)	0.0221(1)	0.0266(2)	0	0
C(1)	6*c*	0.2823(4)	0.5045(4)	0.0407(3)	0.073(3)	0.067(3)	0.067(3)	0.039(3)	-0.016(3)	-0.010(2)
C(2)	6*c*	0.2240(5)	0.5091(3)	-0.0218(3)	0.084(3)	0.060(3)	0.090(4)	0.037(2)	-0.037(3)	-0.008(3)

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Table 3. Continued.

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(3)	6*c*	0.2756(6)	0.5074(4)	-0.0852(3)	0.125(5)	0.053(3)	0.066(3)	0.035(3)	-0.052(3)	-0.007(2)
C(4)	6*c*	0.3875(5)	0.5032(4)	-0.0886(2)	0.105(4)	0.041(3)	0.040(2)	0.025(3)	-0.020(2)	-0.002(2)
C(5)	6*c*	0.4422(3)	0.5011(3)	-0.0229(2)	0.076(3)	0.036(2)	0.028(2)	0.019(2)	-0.009(2)	-0.001(2)
C(6)	6*c*	0.4470(5)	0.5016(5)	-0.1531(2)	0.132(6)	0.068(3)	0.032(2)	0.028(4)	-0.015(2)	0.006(2)
C(7)	6*c*	0.2402(3)	0.3781(3)	0.2340(2)	0.038(2)	0.045(2)	0.035(2)	0.020(2)	0.002(2)	-0.002(2)
C(8)	6*c*	0.1670(3)	0.2828(4)	0.1856(2)	0.053(2)	0.058(2)	0.038(2)	0.024(2)	-0.004(2)	-0.008(2)
C(9)	6*c*	0.0575(4)	0.1837(4)	0.2097(2)	0.048(2)	0.052(2)	0.064(3)	0.016(2)	-0.009(2)	-0.012(2)
C(10)	6*c*	0.0215(4)	0.1762(4)	0.2811(2)	0.043(2)	0.045(2)	0.074(3)	0.008(2)	0.010(2)	0.002(2)
C(11)	6*c*	0.0901(4)	0.2669(4)	0.3290(2)	0.047(2)	0.049(2)	0.055(3)	0.013(2)	0.016(2)	-0.000(2)
C(12)	6*c*	0.2008(3)	0.3689(3)	0.3045(2)	0.035(2)	0.038(2)	0.038(2)	0.017(2)	0.006(2)	-0.004(2)
C(13)	6*c*	0.3841(3)	0.5427(3)	0.2882(1)	0.039(2)	0.039(2)	0.027(2)	0.020(2)	0.005(1)	0.004(1)
C(14)	6*c*	0.4990(3)	0.6603(3)	0.3083(2)	0.039(2)	0.042(2)	0.026(2)	0.019(2)	0.006(2)	0.006(2)
C(15)	6*c*	0.5420(3)	0.6729(4)	0.3782(2)	0.047(2)	0.056(2)	0.027(2)	0.019(2)	0.007(2)	0.005(2)
C(16)	6*c*	0.6456(4)	0.7805(4)	0.4023(2)	0.055(2)	0.063(3)	0.033(2)	0.009(2)	-0.003(2)	-0.006(2)
C(17)	6*c*	0.7086(4)	0.8798(4)	0.3560(2)	0.055(3)	0.059(3)	0.052(2)	0.000(2)	-0.003(2)	-0.011(2)
C(18)	6*c*	0.6693(4)	0.8692(3)	0.2871(2)	0.058(3)	0.048(2)	0.042(2)	0.005(2)	-0.001(2)	0.007(2)
C(19)	6*c*	0.5655(3)	0.7613(3)	0.2614(2)	0.041(2)	0.049(2)	0.031(2)	0.020(2)	0.003(2)	0.006(2)
C(20)	6*c*	0.5361(3)	0.7628(4)	0.1824(2)	0.040(2)	0.060(3)	0.044(2)	0.009(2)	0.008(2)	0.022(2)
N(1)	6*c*	0.3874(3)	0.4983(3)	0.0404(2)	0.061(2)	0.050(2)	0.037(2)	0.024(2)	-0.006(2)	-0.002(1)
N(2)	6*c*	0.3549(2)	0.4876(2)	0.2253(1)	0.037(2)	0.044(2)	0.028(1)	0.012(1)	0.001(1)	-0.001(1)
N(3)	6*c*	0.2937(2)	0.4748(2)	0.3373(1)	0.043(2)	0.039(2)	0.028(1)	0.015(1)	0.008(1)	-0.002(1)
O(1)	6*c*	0.4895(3)	0.8252(4)	0.1636(2)	0.106(3)	0.168(3)	0.078(2)	0.098(3)	0.021(2)	0.064(2)
O(2)	6*c*	0.5732(3)	0.7070(3)	0.1402(1)	0.086(2)	0.067(2)	0.034(1)	0.018(2)	0.010(2)	0.010(1)

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References

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