Crystal structure of aqua(1,10-phenanthroline-*N,N'*)(2-nitrobenzoato-*O*)-(2-nitrobenzoato-*O,O'*)cadmium(II), $\text{Cd}(\text{H}_2\text{O})(\text{NO}_2\text{C}_6\text{H}_4\text{COO})_2(\text{C}_{12}\text{H}_8\text{N}_2)$

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Received September 6, 2005, accepted and available on-line December 2, 2005; CCDC no. 1267/1641

Abstract

$\text{C}_{26}\text{H}_{18}\text{CdN}_4\text{O}_9$, triclinic, $P\bar{1}$ (no. 2), $a = 10.2989(8)$ Å, $b = 11.5069(9)$ Å, $c = 11.821(1)$ Å, $\alpha = 96.048(2)^\circ$, $\beta = 103.245(1)^\circ$, $\gamma = 109.525(1)^\circ$, $V = 1259.7$ Å³, $Z = 2$, $R_{\text{gt}}(F) = 0.048$, $wR_{\text{ref}}(F^2) = 0.110$, $T = 298$ K.

Source of material

The title compound was prepared by mixing hot ethanol-water (1:1 v/v, 50 ml) solution of CdO (0.064 g, 0.5 mmol), *o*-nitrobenzoic acid (0.167 g, 1.0 mmol) and 1,10-phenanthroline (0.09 g, 0.5 mmol), and stirring for one day. After allowing the solution to evaporate at room temperature, colorless prismatic crystals were obtained after ten days.

Experimental details

The H atoms attached to C atoms were positioned geometrically and refined using a riding model ($d(\text{C}-\text{H}) = 0.93$ Å, $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$). The water H atoms were located from Fourier difference map and refined isotropically with the O—H distances restrained at 0.79(2) Å and $U_{\text{iso}}(\text{H}) = 1.5 U_{\text{eq}}(\text{O})$.

Discussion

The title compound is the only reported cadmium complex constructed by 2-nitrobenzoate ligand, in which the carboxylate groups exhibit two different coordination modes, monodentate and chelate. The center Cd(II) atom is six-coordinated by three carboxylate O atoms from two 2-nitrobenzoate ligands and two N atoms from 1,10-phenanthroline, with Cd—O distances falling in the range 2.233(3) Å – 2.644(3) Å and Cd—N distances being 2.307(3) Å and 2.318(3) Å, respectively, as well as a water molecule (Cd—O1w distance of 2.280(3) Å). The structure of title compound is similar to $[\text{Zn}(\text{C}_7\text{H}_4\text{NO}_4)_2(\text{C}_{12}\text{H}_8\text{N}_2)(\text{H}_2\text{O})]$ [1]. There are strong intermolecular hydrogen bond involving the carboxylate O8 atom as an acceptor and the coordinated water O1w atom as a donor, resulting in the formation of a hydrogen bonded dimer. There is also an intramolecular hydrogen bond between the other H atom of the water molecule and the uncoordinated O4 atom of the other carboxylate group.

Table 1. Data collection and handling.

Crystal:	colorless prism, size 0.32 × 0.48 × 0.60 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ :	9.30 cm ⁻¹
Diffractometer, scan mode:	Bruker P4, ω
$2\theta_{\text{max}}$:	56.5°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	7905, 5499
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2\sigma(I_{\text{obs}})$, 5305
$N(\text{param})_{\text{refined}}$:	369
Program:	SHELXTL [2]

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U_{iso}
H(1A)	2i	-0.0435	0.5787	0.7239	0.048
H(2A)	2i	-0.1310	0.6919	0.8373	0.056
H(3A)	2i	0.0206	0.8769	0.9662	0.065
H(4A)	2i	0.2646	0.9510	0.9817	0.061
H(8A)	2i	0.5432	0.6063	0.8946	0.058
H(9A)	2i	0.7195	0.6749	1.0720	0.071
H(10A)	2i	0.8795	0.5764	1.1197	0.078
H(11A)	2i	0.8671	0.4094	0.9855	0.069
H(15A)	2i	-0.1119	0.3029	0.5848	0.060
H(16A)	2i	-0.3316	0.1376	0.5189	0.075
H(17A)	2i	-0.3591	-0.0344	0.3877	0.076
H(19A)	2i	-0.2465	-0.1495	0.2655	0.077
H(20A)	2i	-0.0532	-0.1518	0.2098	0.077
H(22A)	2i	0.2072	-0.0401	0.2130	0.077
H(23A)	2i	0.4127	0.1365	0.2812	0.080
H(24A)	2i	0.4178	0.3036	0.4098	0.067
H(1WA)	2i	0.344(3)	0.546(4)	0.430(4)	0.05(1)
H(1WB)	2i	0.312(4)	0.601(3)	0.507(3)	0.05(2)

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Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
Cd(1)	2i	0.21555(3)	0.38837(2)	0.55607(2)	0.0336(2)	0.0333(2)	0.0347(2)	0.0071(1)	0.0042(1)	-0.0048(1)
C(1)	2i	0.0194(4)	0.6533(4)	0.7755(3)	0.040(2)	0.044(2)	0.036(2)	0.015(2)	0.009(2)	0.009(2)
C(2)	2i	-0.0333(5)	0.7212(4)	0.8436(4)	0.040(2)	0.061(3)	0.047(2)	0.024(2)	0.016(2)	0.015(2)
C(3)	2i	0.0572(5)	0.8319(5)	0.9207(4)	0.060(3)	0.065(3)	0.051(2)	0.035(2)	0.024(2)	0.005(2)
C(4)	2i	0.2024(5)	0.8761(4)	0.9303(4)	0.053(2)	0.049(2)	0.050(2)	0.020(2)	0.016(2)	-0.004(2)
C(5)	2i	0.2529(4)	0.8061(4)	0.8617(3)	0.038(2)	0.040(2)	0.038(2)	0.015(2)	0.010(2)	-0.000(2)
C(6)	2i	0.1644(4)	0.6942(3)	0.7826(3)	0.037(2)	0.036(2)	0.031(2)	0.014(2)	0.009(1)	0.005(1)
C(7)	2i	0.2163(4)	0.6216(4)	0.7004(3)	0.039(2)	0.039(2)	0.035(2)	0.015(2)	0.006(2)	-0.002(2)
C(8)	2i	0.6069(5)	0.5650(4)	0.9122(4)	0.041(2)	0.050(2)	0.044(2)	0.009(2)	0.014(2)	-0.005(2)
C(9)	2i	0.7130(5)	0.6064(5)	1.0186(4)	0.051(3)	0.064(3)	0.038(2)	-0.003(2)	0.014(2)	-0.013(2)
C(10)	2i	0.8093(5)	0.5482(5)	1.0471(4)	0.053(3)	0.078(3)	0.034(2)	-0.002(2)	-0.001(2)	0.008(2)
C(11)	2i	0.8011(5)	0.4483(5)	0.9679(4)	0.045(2)	0.065(3)	0.054(3)	0.012(2)	0.003(2)	0.025(2)
C(12)	2i	0.6938(4)	0.4060(4)	0.8613(4)	0.040(2)	0.038(2)	0.041(2)	0.010(2)	0.008(2)	0.010(2)
C(13)	2i	0.5939(4)	0.4623(3)	0.8310(3)	0.033(2)	0.040(2)	0.030(2)	0.007(2)	0.011(1)	0.007(2)
C(14)	2i	0.4730(4)	0.4235(3)	0.7185(3)	0.033(2)	0.032(2)	0.034(2)	0.008(1)	0.008(1)	-0.002(1)
C(15)	2i	-0.1221(4)	0.2330(4)	0.5312(4)	0.040(2)	0.051(2)	0.058(3)	0.016(2)	0.013(2)	0.011(2)
C(16)	2i	-0.2549(5)	0.1335(5)	0.4920(5)	0.039(2)	0.066(3)	0.081(4)	0.015(2)	0.019(2)	0.022(3)
C(17)	2i	-0.2707(5)	0.0320(5)	0.4149(5)	0.038(2)	0.056(3)	0.077(3)	-0.001(2)	0.002(2)	0.024(3)
C(18)	2i	-0.1544(5)	0.0257(4)	0.3753(4)	0.044(2)	0.034(2)	0.049(2)	0.003(2)	-0.001(2)	0.012(2)
C(19)	2i	-0.1608(6)	-0.0803(4)	0.2946(5)	0.064(3)	0.029(2)	0.068(3)	-0.005(2)	-0.005(2)	0.001(2)
C(20)	2i	-0.0458(6)	-0.0810(4)	0.2607(4)	0.086(4)	0.030(2)	0.055(3)	0.010(2)	0.002(3)	-0.006(2)
C(21)	2i	0.0879(5)	0.0232(4)	0.3001(4)	0.067(3)	0.033(2)	0.040(2)	0.018(2)	0.004(2)	0.001(2)
C(22)	2i	0.2097(6)	0.0280(5)	0.2645(5)	0.090(4)	0.052(3)	0.055(3)	0.035(3)	0.021(3)	-0.004(2)
C(23)	2i	0.3316(6)	0.1323(5)	0.3052(5)	0.073(3)	0.067(3)	0.063(3)	0.027(3)	0.030(3)	-0.002(3)
C(24)	2i	0.3339(5)	0.2324(5)	0.3828(4)	0.047(2)	0.056(3)	0.058(3)	0.013(2)	0.019(2)	-0.004(2)
C(25)	2i	-0.0243(4)	0.1294(3)	0.4183(3)	0.036(2)	0.029(2)	0.038(2)	0.007(1)	-0.001(2)	0.008(1)
C(26)	2i	0.0983(4)	0.1278(3)	0.3792(3)	0.048(2)	0.031(2)	0.033(2)	0.013(2)	0.003(2)	0.003(1)
N(1)	2i	-0.0098(3)	0.2316(3)	0.4948(3)	0.036(2)	0.039(2)	0.038(2)	0.014(1)	0.003(1)	0.004(1)
N(2)	2i	0.2217(4)	0.2311(3)	0.4202(3)	0.039(2)	0.038(2)	0.039(2)	0.007(1)	0.007(1)	-0.003(1)
N(3)	2i	0.6859(5)	0.2971(4)	0.7810(4)	0.063(2)	0.044(2)	0.067(3)	0.025(2)	0.011(2)	0.011(2)
N(4)	2i	0.4098(4)	0.8553(4)	0.8811(3)	0.045(2)	0.050(2)	0.051(2)	0.011(2)	0.010(2)	-0.016(2)
O(1)	2i	0.4635(4)	0.9565(4)	0.8531(4)	0.058(2)	0.061(2)	0.085(3)	0.000(2)	0.028(2)	-0.004(2)
O(1W)	2i	0.2759(3)	0.5442(3)	0.4516(3)	0.039(2)	0.049(2)	0.043(2)	0.014(1)	0.009(1)	0.002(1)
O(2)	2i	0.4769(4)	0.7975(4)	0.9288(4)	0.051(2)	0.077(3)	0.093(3)	0.029(2)	-0.003(2)	-0.006(2)
O(3)	2i	0.1342(3)	0.5086(3)	0.6591(3)	0.048(2)	0.040(2)	0.058(2)	0.009(1)	0.016(1)	-0.009(1)
O(4)	2i	0.3302(3)	0.6763(3)	0.6778(3)	0.049(2)	0.053(2)	0.064(2)	0.006(1)	0.026(2)	-0.013(2)
O(5)	2i	0.7929(5)	0.2700(5)	0.7934(5)	0.093(3)	0.096(3)	0.127(4)	0.068(3)	0.003(3)	-0.003(3)
O(6)	2i	0.5756(4)	0.2406(3)	0.7020(4)	0.069(2)	0.045(2)	0.087(3)	0.019(2)	0.007(2)	-0.017(2)
O(7)	2i	0.3490(3)	0.3701(3)	0.7280(2)	0.033(1)	0.050(2)	0.043(2)	0.005(1)	0.009(1)	0.007(1)
O(8)	2i	0.4977(3)	0.4551(3)	0.6259(2)	0.040(2)	0.057(2)	0.035(1)	0.012(1)	0.011(1)	0.007(1)

References

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