Crystal structure of bis(salicylato)(neocuproin)cadmium(II), $\text{Cd}(\text{C}_7\text{H}_5\text{O}_3)_2(\text{C}_{14}\text{H}_{12}\text{N}_2)$

Pascale Lemoine^{*I}, Dung Nguyen-Huy^{II} and Bernard Viossat^I

^I Laboratoire de Cristallographie et RMN Biologiques, UMR 8015 CNRS, Faculté des Sciences Pharmaceutiques et Biologiques de Paris Descartes, 4, avenue de l'Observatoire 75270 Paris Cedex 06, France

^{II} Université de Paris XI, Faculté des Sciences Pharmaceutiques et Biologiques, Laboratoire de Cristallographie Bioinorganique, 5, rue J. B. Clément, 92296 Châtenay-Malabry Cedex, France

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Table 1. Data collection and handling.

Crystal:	colorless parallelepiped, size 0.16 × 0.18 × 0.25 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	9.24 cm ⁻¹
Diffractometer, scan mode:	Enraf-Nonius CAD4, ω/θ
$2\theta_{\max}$:	49.96°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	8709, 4365
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 3100
$N(\text{param})_{\text{refined}}$:	334
Programs:	SIR92 [5], SHELXL-97 [6] CAMERON [7], WinGX [8]

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

Atom	Site	x	y	z	U_{iso}
H(3)	4e	0.3344	0.8303	0.7207	0.134
H(4)	4e	0.0380	0.8519	0.6394	0.116
H(5)	4e	-0.0580	0.9734	0.6065	0.141

Table 2. Continued.

Atom	Site	x	y	z	U_{iso}
H(6)	4e	0.0497	1.0896	0.6219	0.117
H(7)	4e	0.2602	1.0873	0.6756	0.092
H(13)	4e	0.6376	0.8490	0.4864	0.126
H(14)	4e	0.7817	0.7121	0.3958	0.134
H(15)	4e	0.9343	0.6365	0.4952	0.157
H(16)	4e	0.9991	0.6487	0.6719	0.145
H(17)	4e	0.9126	0.7460	0.7544	0.112
H(23)	4e	0.8717	0.9998	1.1560	0.080
H(24)	4e	1.0045	1.0968	1.1424	0.082
H(25)	4e	1.0716	1.1963	1.0294	0.086
H(26)	4e	1.0568	1.2474	0.8732	0.087
H(27)	4e	0.9479	1.2513	0.6795	0.082
H(28)	4e	0.7964	1.2019	0.5420	0.079
H(35A)	4e	0.6178	0.9513	1.0036	0.130
H(35B)	4e	0.7246	0.9006	1.0737	0.130
H(35C)	4e	0.6879	0.8910	0.9528	0.130
H(36A)	4e	0.6642	1.0386	0.5080	0.110
H(36B)	4e	0.6116	1.1248	0.4829	0.110
H(36C)	4e	0.5689	1.0711	0.5610	0.110

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	4e	0.65318(2)	0.97540(2)	0.75493(2)	0.0408(2)	0.0550(2)	0.0589(2)	-0.0061(1)	0.0042(1)	-0.0062(1)
O(1)	4e	0.4649(3)	0.9010(2)	0.7595(3)	0.060(2)	0.096(3)	0.089(2)	0.019(2)	0.015(2)	0.015(2)
C(1)	4e	0.4100(4)	0.9644(3)	0.7260(3)	0.048(2)	0.076(3)	0.052(2)	0.000(2)	0.008(2)	-0.008(2)
O(2)	4e	0.4662(3)	1.0250(2)	0.7162(3)	0.051(2)	0.075(2)	0.120(3)	-0.010(2)	0.020(2)	-0.017(2)
C(2)	4e	0.2749(4)	0.9666(3)	0.6938(3)	0.045(2)	0.079(3)	0.046(2)	-0.005(2)	0.011(2)	-0.001(2)
O(3)	4e	0.2605(4)	0.8251(3)	0.7007(4)	0.119(3)	0.092(3)	0.131(4)	-0.014(3)	0.049(3)	0.004(3)
C(3)	4e	0.2080(5)	0.8975(3)	0.6823(4)	0.072(3)	0.088(4)	0.065(3)	-0.014(3)	0.023(2)	0.000(3)
C(4)	4e	0.0827(5)	0.8988(5)	0.6482(4)	0.065(3)	0.146(6)	0.079(4)	-0.037(4)	0.021(3)	-0.015(4)
C(5)	4e	0.0263(5)	0.9714(6)	0.6276(5)	0.050(3)	0.23(1)	0.067(4)	-0.001(5)	0.012(3)	0.000(5)
C(6)	4e	0.0906(5)	1.0414(5)	0.6373(4)	0.074(3)	0.143(6)	0.072(3)	0.041(4)	0.015(3)	0.020(4)
C(7)	4e	0.2159(4)	1.0403(3)	0.6698(4)	0.061(3)	0.101(4)	0.068(3)	0.023(3)	0.017(2)	0.013(3)
C(11)	4e	0.7414(3)	0.8515(2)	0.6707(4)	0.046(2)	0.046(2)	0.078(3)	-0.011(2)	0.016(2)	-0.002(2)
O(11)	4e	0.6611(3)	0.8977(2)	0.6140(2)	0.069(2)	0.059(2)	0.067(2)	0.013(1)	0.005(2)	-0.004(1)
O(12)	4e	0.7757(3)	0.8618(2)	0.7665(2)	0.062(2)	0.068(2)	0.068(2)	-0.002(2)	0.003(2)	-0.003(2)
O(13)	4e	0.6640(4)	0.8168(2)	0.4525(3)	0.142(4)	0.084(3)	0.087(3)	0.006(3)	0.032(3)	-0.008(2)
C(12)	4e	0.7933(4)	0.7881(2)	0.6203(4)	0.055(2)	0.044(2)	0.095(3)	-0.007(2)	0.032(2)	0.002(2)
C(13)	4e	0.7544(5)	0.7765(3)	0.5150(5)	0.086(3)	0.050(3)	0.107(4)	-0.008(2)	0.048(3)	-0.007(3)
C(14)	4e	0.8078(7)	0.7192(4)	0.4673(6)	0.132(6)	0.081(4)	0.151(6)	-0.017(4)	0.084(5)	-0.030(4)
C(15)	4e	0.8978(8)	0.6742(4)	0.5270(9)	0.132(7)	0.070(4)	0.23(1)	0.003(4)	0.114(8)	-0.013(6)
C(16)	4e	0.9380(6)	0.6818(4)	0.6332(8)	0.082(4)	0.067(4)	0.230(9)	0.014(3)	0.071(6)	0.034(5)
C(17)	4e	0.8864(4)	0.7397(3)	0.6828(6)	0.055(3)	0.055(3)	0.176(6)	0.005(2)	0.044(3)	0.020(3)
N(21)	4e	0.7755(3)	1.0211(2)	0.9091(2)	0.040(2)	0.058(2)	0.050(2)	-0.001(1)	0.006(1)	-0.001(2)
C(22)	4e	0.7827(4)	0.9917(3)	1.0025(3)	0.053(2)	0.072(3)	0.054(2)	0.000(2)	0.012(2)	0.001(2)
C(23)	4e	0.8684(4)	1.0208(3)	1.0912(3)	0.058(3)	0.088(3)	0.049(2)	0.005(2)	0.006(2)	0.000(2)
C(24)	4e	0.9461(4)	1.0790(3)	1.0834(3)	0.053(2)	0.091(3)	0.054(3)	0.000(2)	0.001(2)	-0.017(2)
C(25)	4e	1.0137(4)	1.1757(3)	0.9719(4)	0.053(2)	0.078(3)	0.077(3)	-0.021(2)	0.009(2)	-0.027(3)
C(26)	4e	1.0046(4)	1.2066(3)	0.8795(4)	0.063(3)	0.067(3)	0.088(4)	-0.025(2)	0.023(2)	-0.020(3)
C(27)	4e	0.8985(4)	1.2100(3)	0.6895(4)	0.074(3)	0.056(2)	0.081(3)	-0.012(2)	0.032(3)	-0.002(2)
C(28)	4e	0.8092(4)	1.1803(3)	0.6079(4)	0.078(3)	0.056(3)	0.063(3)	0.002(2)	0.020(2)	0.005(2)
C(29)	4e	0.7371(4)	1.1173(3)	0.6237(3)	0.057(2)	0.055(2)	0.052(2)	0.005(2)	0.010(2)	-0.001(2)
N(30)	4e	0.7535(3)	1.0848(2)	0.7153(2)	0.042(2)	0.049(2)	0.053(2)	0.000(1)	0.006(1)	-0.002(2)
C(31)	4e	0.8403(3)	1.1146(2)	0.7987(3)	0.042(2)	0.044(2)	0.055(2)	0.000(2)	0.012(2)	-0.011(2)
C(32)	4e	0.9151(4)	1.1777(2)	0.7889(3)	0.053(2)	0.051(2)	0.073(3)	-0.007(2)	0.021(2)	-0.011(2)
C(33)	4e	0.9390(3)	1.1127(3)	0.9868(3)	0.043(2)	0.064(3)	0.056(2)	-0.002(2)	0.006(2)	-0.017(2)
C(34)	4e	0.8516(3)	1.0815(2)	0.9002(3)	0.038(2)	0.049(2)	0.056(2)	0.001(2)	0.009(2)	-0.009(2)
C(35)	4e	0.6956(5)	0.9280(4)	1.0087(4)	0.074(3)	0.110(4)	0.072(3)	-0.020(3)	0.015(2)	0.019(3)
C(36)	4e	0.6364(4)	1.0851(3)	0.5361(3)	0.077(3)	0.075(3)	0.055(3)	-0.005(3)	0.000(2)	0.003(2)

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