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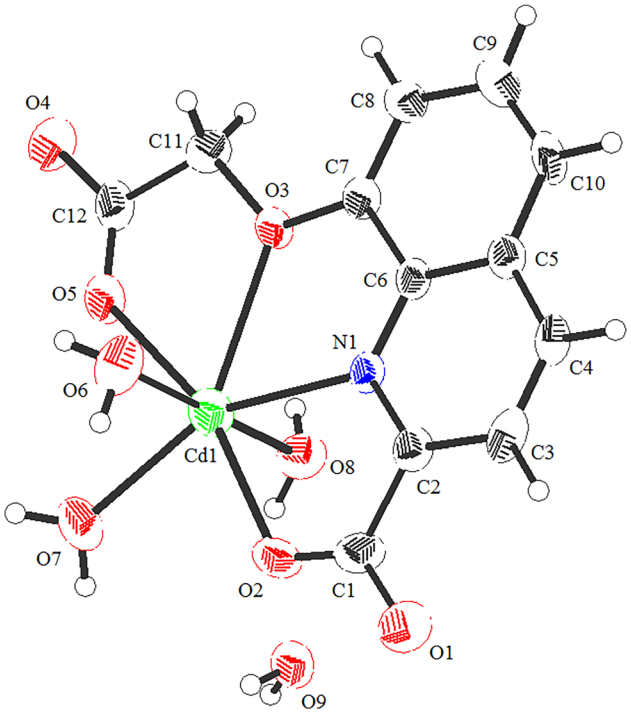
Crystal structure of [triaqua-(8-carboxymethoxy-quinoline-2-carboxylate-κ^4N,O,O,O)cadmium(II)] monohydrate, $C_{12}H_{15}NO_9Cd$



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Abstract

$C_{12}H_{15}NO_9Cd$, triclinic, $P\bar{1}$ (no. 2), a = 7.5263(5) Å, b = 8.0953(3) Å, c = 12.4005(8) Å, α = 86.814(4)°, β = 79.845(5)°, γ = 86.140(4)°, V = 741.28(7) Å^3, Z = 2, $R_{gt}(F)$ = 0.0759, $wR_{ref}(F^2)$ = 0.2248, T = 295 K.

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Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.15 × 0.13 × 0.11 mm
Wavelength:	Cu *K*α radiation (1.54184 Å)
μ:	12.3 mm^{-1}
Diffractometer, scan mode:	XtaLAB Synergy, ω
θ_{max}, completeness:	77.1°, 99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	8374, 2922, 0.108
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 2635
$N(param)_{refined}$:	218
Programs:	Bruker [1], Olex2 [2], SHELX [3], Diamond [4]

Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

1 Source of materials

The title complex was synthesized as following: 0.1336 g 8-carboxymethoxy-quinoline-2-carboxylic acid (0.5 mmol), 0.040 g NaOH (1.0 mmol) and 0.0771 g cadmium nitrate tetrahydrate (0.25 mmol), were added to a solution of ethanol–water (30 ml, v:v = 1:1) with stirring. The reaction mixture reacted for 6 h at 70 °C. After cooling to room temperature, the filtrate was transferred to a small flask. The colorless needle crystals of the title complex were obtained after 15 days.

2 Experimental details

The hydrogen atoms were positioned geometrically (C–H = 0.95–0.99 Å, O–H = 0.85–0.87 Å). Their U_{iso} values were set to 1.2U_{eq} or 1.5U_{eq} of the parent atoms.

3 Comment

The deprotonoated anion of the, 8-carboxymethoxyquinoline-2-carboxylic acid showed excellent coordination abilities

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
C1	0.3080 (11)	0.5684 (11)	0.2203 (8)	0.0367 (18)
C2	0.3419 (10)	0.6194 (10)	0.3307 (6)	0.0296 (15)
C3	0.2190 (11)	0.5875 (11)	0.4285 (8)	0.0401 (19)
H3	0.110923	0.534042	0.426935	0.048*
C4	0.2583 (11)	0.6350 (10)	0.5262 (7)	0.0349 (17)
H4	0.175747	0.615150	0.592321	0.042*
C5	0.4197 (10)	0.7129 (10)	0.5296 (6)	0.0302 (15)
C6	0.5325 (10)	0.7387 (9)	0.4279 (6)	0.0257 (14)
C7	0.6977 (10)	0.8177 (10)	0.4243 (6)	0.0304 (15)
C8	0.7418 (13)	0.8646 (11)	0.5211 (7)	0.0402 (19)
H8	0.851926	0.915929	0.520102	0.048*
C9	0.6266 (13)	0.8374 (12)	0.6196 (7)	0.043 (2)
H9	0.659376	0.872008	0.685002	0.052*
C10	0.4684 (12)	0.7631 (11)	0.6260 (7)	0.0382 (18)
H10	0.392177	0.745397	0.694783	0.046*
C11	0.9494 (10)	0.9329 (11)	0.3065 (7)	0.0363 (17)
H11A	1.038494	0.885502	0.351369	0.044*
H11B	0.912682	1.047488	0.328725	0.044*
C12	1.0322 (10)	0.9333 (11)	0.1855 (7)	0.0342 (17)
Cd1	0.68674 (7)	0.73115 (8)	0.15633 (5)	0.0404 (3)
N1	0.4948 (8)	0.6930 (8)	0.3303 (5)	0.0258 (12)
O1	0.1713 (10)	0.4903 (10)	0.2203 (7)	0.0559 (19)
O2	0.4219 (8)	0.6039 (8)	0.1378 (5)	0.0403 (14)
O3	0.7954 (8)	0.8349 (9)	0.3226 (5)	0.0393 (14)
O4	1.1721 (8)	1.0150 (9)	0.1632 (6)	0.0491 (16)
O5	0.9624 (8)	0.8615 (8)	0.1211 (5)	0.0383 (13)
O6	0.5511 (9)	0.9894 (9)	0.1330 (7)	0.0476 (16)
H6A	0.639024	1.041224	0.097359	0.071*
H6B	0.487085	0.971386	0.085314	0.071*
O7	0.7530 (14)	0.7112 (10)	−0.0314 (6)	0.062 (2)
H7A	0.791299	0.785865	−0.079098	0.093*
H7B	0.735298	0.630695	−0.068619	0.093*
O8	0.8277 (8)	0.4752 (8)	0.1815 (5)	0.0381 (13)
H8A	0.931587	0.486766	0.197633	0.057*
H8B	0.850278	0.426923	0.120758	0.057*
O9	0.7464 (8)	0.2558 (8)	0.0387 (5)	0.0379 (13)
H9A	0.681590	0.318088	−0.000848	0.057*
H9B	0.822249	0.199228	−0.008604	0.057*

through tetradentate O,O,N,O-chelate modes. Its Mn(II), Co(II), Ni(II), and Cu(II) complexes shows excellent properties such as its mononuclear Co(II) complex exhibits the typical field-induced slow magnetic relaxation behavior and binding ability of CT–DAN. Its one-dimensional zig–zag chain Ni(II) complex can be considered a quantum antiferromagnet [5,6]. Our research group has been engaged in the synthesis and structural characterization of related metal complexes [7–10].

The molecular structure and atom-labeling scheme of the title Cd(II) complex is shown in the Figure. The title complex contains one Cd(II) ion, one 8-carboxymethoxy-quinoline-2-carboxylate ligand, three coordinated water molecules, and one uncoordinated water molecules. The Cd(II) ion is hepta-coordinated with three oxygen atoms (O2, O3 and O5) and one nitrogen atom (N1) of 8-carboxymethoxy-quinoline-2-carboxylate ligand, and three oxygen atoms (O6, O7 and O8) of three coordinated water molecules, forming a distorted pentagonal bipyramidal. The nitrogen (N1), three oxygen atoms (O2, O3 and O5) of 8-carboxymethoxy-quinoline-2-carboxylate ligand and one oxygen atom (O7) of coordinated water molecule form the basal plane, and two oxygen atoms (O6 and O8) of two coordinated water molecules are at the axial position. The bond lengths of Cd–O are 2.290(7)–2.551(6) Å, and the Cd–N bond length is 2.393(6) Å, which is coincident with other Cd(II) complexes [11,12]. The dihedral angles of ring 1 (Cd1–O2–C1–C2–N1–Cd1), and ring 2 (Cd1–O3–C7–C6–N1–Cd1) is 0.38°, and ring 2 and ring 3 (Cd1–O3–C11–C12–O5–Cd1) are and 3.72°, respectively, indicating that the Cd(II) complex molecule is coplanar. The Cd(II) complex molecules form 3D network by the O–H···O hydrogen bonds.

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Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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