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Crystal structure of (2-carboxy-4-(3-carboxy-5-carboxylatophenoxy)benzoato- $\kappa^2 O, O'$)bis(1,10-phenantroline- $\kappa^2 N, N'$)cobalt(II), $C_{40}H_{24}N_4O_9Co$

Table 1: Data collection and handling.

Crystal:	Red block
Size:	0.41 × 0.35 × 0.30 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.57 mm ⁻¹
Diffractometer, scan mode:	SuperNova, ω
$\theta_{\max}$, completeness:	25.5°, 99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	31165, 6024, 0.093
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 4766
$N(\text{param})_{\text{refined}}$:	489
Programs:	CrysAlis ^{PRO} [1], SHELX [2, 3]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	0.57734(3)	0.80008(3)	0.27407(2)	0.03101(13)
N1	0.46295(18)	0.94146(17)	0.20460(15)	0.0350(5)
N2	0.69826(19)	0.91169(17)	0.20993(15)	0.0348(5)
N3	0.56647(18)	0.82431(17)	0.42642(15)	0.0346(5)
N4	0.44865(18)	0.69962(17)	0.34495(16)	0.0353(5)
O1	0.72250(15)	0.64727(13)	0.27432(12)	0.0356(4)
O2	0.63450(16)	0.70029(15)	0.14071(12)	0.0435(5)
O3	1.06406(15)	0.29048(15)	0.17620(12)	0.0424(5)
O4	0.7890(2)	0.4602(2)	−0.16348(15)	0.0744(7)
O5	0.95184(19)	0.31295(18)	−0.15942(14)	0.0644(6)
H5	0.9507	0.3143	−0.2204	0.097*
O6	0.7921(2)	0.0712(2)	0.40498(18)	0.0848(8)
O7	0.8180(2)	0.0547(2)	0.56304(16)	0.0738(7)
H7	0.8507	0.0861	0.5971	0.111*
O8	0.9087(2)	0.1479(2)	0.66528(15)	0.0741(7)
O9	0.98763(19)	0.3062(2)	0.64932(14)	0.0656(6)
C1	0.8149(2)	0.8951(2)	0.2144(2)	0.0460(7)
H1	0.8492	0.8294	0.2550	0.055*
C2	0.8879(3)	0.9715(3)	0.1609(2)	0.0565(8)
H2	0.9694	0.9569	0.1656	0.068*
C3	0.8382(3)	1.0682(3)	0.1016(2)	0.0605(9)
H3	0.8859	1.1202	0.0654	0.073*
C4	0.7145(3)	1.0896(2)	0.0951(2)	0.0453(7)
C5	0.6483(2)	1.0084(2)	0.15118(18)	0.0348(6)
C6	0.6540(3)	1.1885(3)	0.0352(2)	0.0631(9)
H6	0.6971	1.2437	−0.0021	0.076*
C7	0.5355(3)	1.2030(3)	0.0316(2)	0.0594(9)
H7A	0.4988	1.2679	−0.0084	0.071*
C8	0.4652(3)	1.1214(2)	0.08783(19)	0.0412(7)
C9	0.5224(2)	1.0238(2)	0.14745(18)	0.0329(6)
C10	0.3407(3)	1.1324(3)	0.0890(2)	0.0532(8)

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Abstract

$C_{40}H_{24}N_4O_9Co$, triclinic, $P\bar{1}$ (no. 2), $a = 11.5623(9)$ Å, $b = 11.5732(12)$ Å, $c = 13.4379(11)$ Å, $\alpha = 82.003(8)^\circ$, $\beta = 77.597(7)^\circ$, $\gamma = 76.048(8)^\circ$, $V = 1697.1(3)$ Å³, $Z = 2$, $R_{\text{gt}}(F) = 0.0462$, $wR_{\text{ref}}(F^2) = 0.1021$, $T = 293(2)$ K.

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

Source of material

A mixture of $Co(OAc)_2 \cdot 6H_2O$ (0.1 mmol, 30.2 mg), 1,10-phenanthroline (0.1 mmol, 15 mg) and 4-(3,5-

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Table 2 (continued)

Atom	x	y	z	U_{iso}^*/U_{eq}
H10	0.2990	1.1957	0.0508	0.064*
C11	0.2824(3)	1.0507(3)	0.1459(2)	0.0524(8)
H11	0.2003	1.0575	0.1472	0.063*
C12	0.3456(2)	0.9561(2)	0.2028(2)	0.0451(7)
H12	0.3039	0.9005	0.2414	0.054*
C13	0.6281(2)	0.8842(2)	0.4659(2)	0.0466(7)
H13	0.6736	0.9331	0.4218	0.056*
C14	0.6272(3)	0.8767(3)	0.5701(2)	0.0599(9)
H14	0.6723	0.9190	0.5949	0.072*
C15	0.5598(3)	0.8071(3)	0.6355(2)	0.0597(9)
H15	0.5589	0.8015	0.7053	0.072*
C16	0.4918(3)	0.7439(2)	0.5981(2)	0.0460(7)
C17	0.4990(2)	0.7546(2)	0.49226(19)	0.0338(6)
C18	0.4176(3)	0.6692(3)	0.6605(2)	0.0595(9)
H18	0.4114	0.6625	0.7311	0.071*
C19	0.3566(3)	0.6086(3)	0.6201(2)	0.0583(9)
H19	0.3087	0.5610	0.6631	0.070*
C20	0.3637(2)	0.6157(2)	0.5119(2)	0.0425(7)
C21	0.4349(2)	0.6883(2)	0.44819(19)	0.0327(6)
C22	0.3025(2)	0.5534(2)	0.4646(3)	0.0554(8)
H22	0.2538	0.5042	0.5041	0.066*
C23	0.3148(3)	0.5656(3)	0.3616(3)	0.0590(9)
H23	0.2744	0.5255	0.3296	0.071*
C24	0.3888(2)	0.6391(2)	0.3040(2)	0.0484(7)
H24	0.3969	0.6464	0.2332	0.058*
C25	0.7141(2)	0.6318(2)	0.18528(18)	0.0320(6)
C26	0.8002(2)	0.5293(2)	0.13241(17)	0.0291(6)
C27	0.8905(2)	0.4580(2)	0.18067(17)	0.0305(6)
H27	0.8968	0.4728	0.2453	0.037*
C28	0.9712(2)	0.3645(2)	0.13206(17)	0.0293(6)
C29	0.9655(2)	0.3443(2)	0.03455(17)	0.0314(6)
H29	1.0218	0.2829	0.0016	0.038*
C30	0.8751(2)	0.4164(2)	−0.01425(17)	0.0309(6)
C31	0.7913(2)	0.5081(2)	0.03565(17)	0.0328(6)
H31	0.7294	0.5550	0.0041	0.039*
C32	0.8663(3)	0.3992(2)	−0.11957(19)	0.0417(7)
C33	1.0379(2)	0.2719(2)	0.28384(18)	0.0351(6)
C34	0.9590(2)	0.2006(2)	0.32866(19)	0.0371(6)
H34	0.9240	0.1661	0.2874	0.045*
C35	0.9294(2)	0.1782(2)	0.43465(18)	0.0340(6)
C36	0.9811(2)	0.2334(2)	0.49552(18)	0.0370(6)
C37	1.0618(3)	0.3050(3)	0.4465(2)	0.0501(8)
H37	1.0969	0.3413	0.4864	0.060*
C38	1.0920(2)	0.3242(3)	0.3406(2)	0.0471(7)
H38	1.1472	0.3712	0.3097	0.056*
C39	0.8407(3)	0.0966(3)	0.4676(2)	0.0503(8)
C40	0.9569(3)	0.2280(3)	0.6122(2)	0.0488(8)

dicarboxyphenoxy)phthalic acid (H4dic) (50 mg, 0.1 mmol), was dissolved in 10 mL H₂O. Then the solution was heated in a 23 mL autoclave under autogenous pressure at 393 K for two days. After cooling to room temperature crystals formed.

Experimental details

Coordinates of hydrogen atoms were calculated. Their U_{iso} values were set to $1.2U_{eq}$ of the parent atoms.

Comment

Mixed ligands-MOFs can be constructed from metal ions and carboxylic acid and nitrogen-containing ligands. Among organic aromatic multicarboxylates like the ether oxygen tetraacetates can yield predetermined networks and have been widely utilized to construct MOFs [4–7]. On the other hand, 1,10-phenanthroline serves as ligand for coordination polymers [8–10].

In the mononuclear title complex, unexpectedly obtained, there are one Co(II) ion, one H2dic ligand, and two the 1,10-phenanthroline ligands in the asymmetric unit. Co1 is six-coordinated with a distorted octahedral geometry by two O atoms from one H2dic, and four N atoms from the 1,10-phenanthroline ligands (see the figure). The Co–O bond lengths are 2.1247(16) Å; 2.1635(16) Å and the Co–N ones are in the range of 2.078(2) to 2.100(2) Å.

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