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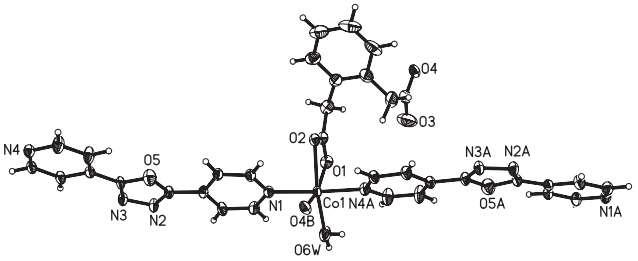
Crystal structure of poly[aqua(μ$_2$-2,5-bis(4-pyridyl)-1,3,4-oxadiazole-κ^2*N*,*N*)(μ$_2$-1,3-phenylenediacetato-κ^3*O*,*O*′:*O*″)cobalt(II)], $C_{22}H_{18}CoN_4O_6$



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Abstract

$C_{22}H_{18}CoN_4O_6$, monoclinic, $P2_1/c$ (no. 14), $a = 8.540(2)$ Å, $b = 11.371(3)$ Å, $c = 23.441(5)$ Å, $\beta = 95.298(3)°$, $V = 2266.6(9)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0652$, $wR_{ref}(F^2) = 0.1743$, $T = 293(2)$ K.

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Tables 1–3 contain details of the measurement method and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

O-phenylenediacetic acid (H_2phda) (19 mg, 0.1 mmol), 2,5-bis(4-pyridyl)-1,3,4-oxadiazole (bpo) (22 mg, 0.1 mmol), $Co(OAc)_2{\cdot}4H_2O$ (24 mg, 0.1 mmol) and KOH (5.6 mg, 0.1 mmol) were added to water (12 mL) in a Teflon-lined stainless steel vessel. The mixture was heated at 433 K for 3 d, and then slowly cooled down to room temperature. Pink block crystals of the title complex were obtained.

Table 1: Data collection and handling.

Crystal:	Pink, block, size 0.27×0.38×0.41 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	8.03 cm^{-1}
Diffractometer, scan mode:	CCD area detector, φ and ω scans
$2\theta_{max}$:	51°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	10014, 4119
$N(param)_{refined}$:	298
Programs:	Bruker programs [12], SHELX [13]

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

Atom	Site	*x*	*y*	*z*	U_{iso}
H(1W)	4*e*	0.2882	−0.0171	−0.0303	0.135
H(2W)	4*e*	0.2552	0.0946	−0.0388	0.135
H(2A)	4*e*	−0.2518	0.1594	0.1014	0.065
H(2B)	4*e*	−0.1516	0.1631	0.1606	0.065
H(4)	4*e*	−0.1490	0.3307	0.2170	0.076
H(5)	4*e*	−0.2333	0.5150	0.2366	0.103
H(6)	4*e*	−0.3810	0.6197	0.1667	0.119
H(7)	4*e*	−0.4254	0.5450	0.0764	0.099
H(9A)	4*e*	−0.2389	0.3051	0.0212	0.093
H(9B)	4*e*	−0.3516	0.4102	0.0042	0.093
H(11)	4*e*	0.3738	−0.0570	0.0980	0.053
H(12)	4*e*	0.5437	−0.1047	0.1763	0.052
H(14)	4*e*	0.5214	0.2311	0.2269	0.046
H(15)	4*e*	0.3628	0.2697	0.1458	0.050
H(19)	4*e*	0.8482	0.2983	0.3611	0.070
H(20)	4*e*	0.9913	0.3884	0.4355	0.071
H(21)	4*e*	1.1486	0.0889	0.4943	0.047
H(22)	4*e*	1.0049	−0.0108	0.4231	0.048

Experimental details

The hydrogen atoms were placed on calculated positions using a riding model (AFIX 3, 23 and 43 options of the SHELX program [13]).

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Table 3: Fractional coordinates and atomic displacement parameters (Å^2).

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Co(1)	4*e*	0.21718(7)	0.17439(5)	0.04070(3)	0.0330(4)	0.0316(3)	0.0304(4)	0.0040(3)	−0.0071(3)	−0.0010(3)
N(1)	4*e*	0.3510(5)	0.1105(3)	0.1137(2)	0.042(3)	0.036(2)	0.037(2)	0.004(2)	−0.005(2)	−0.001(2)
N(2)	4*e*	0.7182(5)	−0.0669(3)	0.2777(2)	0.047(3)	0.042(2)	0.039(3)	−0.001(2)	−0.014(2)	0.002(2)
N(3)	4*e*	0.8147(5)	−0.0427(3)	0.3263(2)	0.043(3)	0.036(2)	0.040(3)	−0.002(2)	−0.012(2)	−0.001(2)
N(4)	4*e*	1.0875(5)	0.2477(3)	0.4719(2)	0.042(2)	0.029(2)	0.040(2)	0.003(2)	−0.006(2)	0.002(2)
O(1)	4*e*	0.0057(4)	0.1036(3)	0.0660(2)	0.058(2)	0.030(2)	0.051(2)	−0.008(2)	−0.001(2)	−0.006(2)
O(2)	4*e*	0.0767(4)	0.2792(3)	0.0970(1)	0.035(2)	0.033(2)	0.041(2)	−0.006(1)	−0.004(2)	−0.003(1)
O(3)	4*e*	−0.4449(6)	0.1640(6)	−0.0076(3)	0.068(4)	0.141(5)	0.142(5)	0.022(3)	0.016(4)	−0.057(4)
O(4)	4*e*	−0.6022(4)	0.2879(3)	0.0328(2)	0.032(2)	0.057(2)	0.055(2)	0.004(2)	−0.001(2)	0.009(2)
O(5)	4*e*	0.7231(5)	0.1286(4)	0.2954(2)	0.066(3)	0.058(2)	0.066(3)	0.001(2)	−0.010(2)	0.006(2)
O(6W)	4*e*	0.2850(6)	0.0472(4)	−0.0120(2)	0.122(4)	0.086(3)	0.053(3)	0.060(3)	−0.034(3)	−0.032(2)
C(1)	4*e*	−0.0201(6)	0.1948(4)	0.0938(2)	0.040(3)	0.030(2)	0.039(3)	−0.009(2)	−0.004(2)	−0.001(2)
C(2)	4*e*	−0.1698(7)	0.2025(5)	0.1239(3)	0.054(4)	0.054(3)	0.053(4)	−0.017(3)	0.006(3)	0.000(3)
C(3)	4*e*	−0.2295(6)	0.3247(5)	0.1340(2)	0.030(3)	0.078(4)	0.047(3)	−0.012(3)	0.008(3)	−0.006(3)
C(4)	4*e*	−0.2038(7)	0.3740(6)	0.1880(3)	0.050(4)	0.076(4)	0.065(4)	−0.009(3)	0.015(3)	−0.015(4)
C(5)	4*e*	−0.2557(9)	0.4832(7)	0.2002(4)	0.072(5)	0.097(6)	0.092(6)	−0.007(4)	0.028(5)	−0.036(5)
C(6)	4*e*	−0.341(1)	0.5461(8)	0.1584(5)	0.075(6)	0.095(6)	0.134(9)	0.013(5)	0.051(6)	−0.026(6)
C(7)	4*e*	−0.3682(8)	0.5010(7)	0.1046(4)	0.046(4)	0.092(6)	0.113(7)	0.022(4)	0.022(4)	0.017(5)
C(8)	4*e*	−0.3119(6)	0.3896(6)	0.0906(3)	0.029(3)	0.077(4)	0.066(4)	−0.005(3)	0.006(3)	0.002(3)
C(9)	4*e*	−0.3351(7)	0.3437(7)	0.0299(3)	0.030(3)	0.150(7)	0.054(4)	−0.008(4)	0.003(3)	0.013(4)
C(10)	4*e*	−0.4702(7)	0.2585(7)	0.0174(3)	0.041(4)	0.091(5)	0.056(4)	0.011(3)	0.001(3)	0.003(4)
C(11)	4*e*	0.4057(6)	0.0020(4)	0.1240(2)	0.051(3)	0.038(3)	0.041(3)	−0.001(2)	−0.006(3)	0.001(2)
C(12)	4*e*	0.5074(6)	−0.0280(4)	0.1712(2)	0.045(3)	0.033(3)	0.050(3)	0.005(2)	−0.013(3)	0.005(2)
C(13)	4*e*	0.5543(6)	0.0592(4)	0.2109(2)	0.033(3)	0.039(3)	0.033(3)	−0.007(2)	−0.004(2)	0.004(2)
C(14)	4*e*	0.4953(6)	0.1710(4)	0.2008(2)	0.039(3)	0.040(3)	0.035(3)	0.001(2)	−0.005(2)	−0.003(2)
C(15)	4*e*	0.3981(6)	0.1931(4)	0.1523(2)	0.041(3)	0.041(3)	0.041(3)	0.005(2)	−0.007(2)	−0.004(2)
C(16)	4*e*	0.6655(6)	0.0376(4)	0.2610(2)	0.038(3)	0.028(2)	0.037(3)	−0.004(2)	−0.008(2)	0.001(2)
C(17)	4*e*	0.8156(6)	0.0728(4)	0.3358(2)	0.035(3)	0.032(2)	0.037(3)	0.005(2)	−0.012(2)	0.004(2)
C(18)	4*e*	0.9091(6)	0.1330(4)	0.3828(2)	0.034(3)	0.033(2)	0.038(3)	0.002(2)	−0.004(2)	0.000(2)
C(19)	4*e*	0.9083(7)	0.2531(4)	0.3879(2)	0.081(4)	0.032(3)	0.054(4)	0.011(3)	−0.031(3)	0.002(3)
C(20)	4*e*	0.9960(8)	0.3069(5)	0.4325(3)	0.080(5)	0.035(3)	0.055(4)	0.005(3)	−0.025(3)	0.000(3)
C(21)	4*e*	1.0870(6)	0.1319(4)	0.4670(2)	0.035(3)	0.036(2)	0.044(3)	0.004(2)	−0.009(2)	0.005(2)
C(22)	4*e*	1.0012(6)	0.0709(4)	0.4242(2)	0.038(3)	0.034(2)	0.046(3)	0.004(2)	−0.008(2)	0.001(2)

Discussion

The design and construction of Co(II)-based metal-organic frameworks (MOFs) is of current interest in the fields of supramolecular chemistry and crystal engineering [1–5]. It is well known that flexible multicarboxylate acids, such as o-phenylenediacetic acid (H_2phda) [6–9], are widely used to link metals to produce MOFs. On the other hand, exo-bidentate rodlike N,N′-donor ligands can have significant influence on the assembly systems of multicarboxylate ligands and metal centers. 2,5-bis(4-pyridyl)-1,3,4-oxadiazole (bpo) with certain spacers between the two 4-pyridyl rings may also lead to fascinating architectures with interesting properties [10, 11]. The crystal structure of the title complex comprises a phda ligand, a Co(II) ion and a bpo molecule per asymmetric unit (figure). Both carboxylate groups of the former acid are deprotonated. The Co(II) ion is six coordinated and resides in a distorted octahedral coordination geometry with three carboxylate oxygen atoms from two phda ligands, two nitrogen atoms from bpo ligands and one water molecule. The Co—N bond lengths are 2.070(4) and 2.098(4) Å and the Co—O ones are in the range of 2.021(4)–2.212(3) Å. Each phda ligand acts as a μ_2-bridge linking two Co(II) ions, in which one carboxylate group adopts a monodentate mode while another one adopts a chelating mode coodinating to one Co(II) ion. Based on the previous connection, the adjacent Co(II) ions are bridged by phda and bpo ligands to form a 2D 4^4 layer. Such 2D layers are further connected by hydrogen bonds, between the coordinated water molecules and the carboxylate oxygen groups of the phda ligands ($d(O\cdots O) = 2.779(7)$ Å), to form a 3D supramolecular architecture.

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