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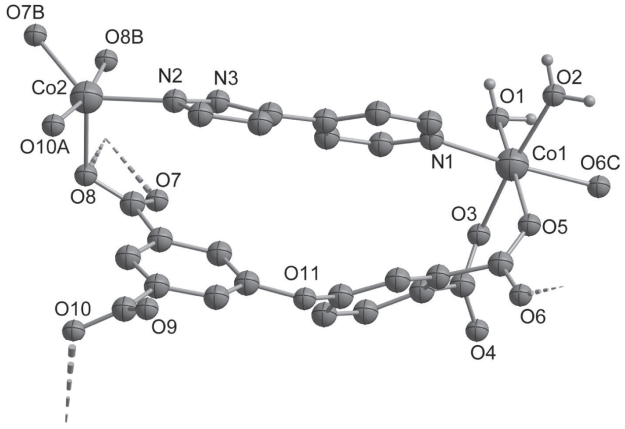
Crystal structure of poly[diaqua-μ_5-4-(3,5-dicarboxylato-κ^3O^1:O^2:O^3-phenoxy)phthalato-κ^3O^5,O^7:O^8)(μ_2-4-(1*H*-pyrazol-5-yl)pyridine-κ^2N:N')dicobalt(II)] $C_{24}H_{16}N_3O_{11}Co_2$



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Abstract

$C_{24}H_{16}N_3O_{11}Co_2$, monoclinic, $P2_1/n$, $a = 7.3343(2)$ Å, $b = 42.2275(12)$ Å, $c = 7.5118(2)$ Å, $\beta = 100.988(3)°$, $V = 2283.82(11)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0365$, $wR_{ref}(F^2) = 0.1142$, $T = 293(2)$ K.

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The crystal structure is shown in the figure. Tables 1–3 contain details of the measurement method and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

A mixture of $Co(NO_3)_2{\cdot}6H_2O$ (29 mg, 0.1 mmol), 4-(3,5-dicarboxyphenoxy)phthalic acid (35 mg, 0.1 mmol), 4-(1H-pyrazol-5-yl)pyridine (55 mg, 0.1 mmol) was dissolved in 10 mL H_2O. Then the solution was heated in a 25 mL Teflon-lined autoclave under autogenous pressure at 413 K for 4 days. After cooling to room temperature red block crystals formed.

Table 1: Data collection and handling.

Crystal:	Colourless, block, size 0.28×0.38×0.42 mm
Wavelength:	Cu K_α radiation (1.54178 Å)
μ:	120.55 cm^{-1}
Diffractometer, scan mode:	multiwire proportional, φ and ω scans
$2\theta_{max}$:	147.28°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	8489, 4456
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 4032
$N(param)_{refined}$:	361
Programs:	SHELX [10]

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*	−0.1838	0.7807	0.2340	0.046
H(2W)	4*e*	−0.0981	0.8019	0.1589	0.046
H(3W)	4*e*	0.2771	0.7608	0.1958	0.063
H(4W)	4*e*	0.2727	0.7366	0.3148	0.063
H(3)	4*e*	0.5948	0.8209	0.9608	0.033
H(5)	4*e*	0.2780	0.8946	1.0504	0.036
H(6)	4*e*	0.0150	0.8644	0.9482	0.032
H(10)	4*e*	0.9075	0.9053	1.2122	0.031
H(12)	4*e*	0.7882	0.9917	0.9972	0.036
H(14)	4*e*	0.4370	0.9187	0.8460	0.033
H(18)	4*e*	0.8884	0.8836	0.6438	0.039
H(19)	4*e*	0.9954	0.9393	0.6449	0.041
H(21)	4*e*	0.2605	0.8982	0.4753	0.035
H(22)	4*e*	0.0731	0.8543	0.4407	0.035
H(23)	4*e*	0.4967	0.7983	0.4538	0.039
H(24)	4*e*	0.6963	0.8405	0.4776	0.039

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Table 3: 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*	0.09364(6)	0.78151(1)	0.46284(6)	0.0229(2)	0.0173(2)	0.0208(2)	−0.0012(2)	−0.0002(2)	0.0009(2)
Co(2)	4*e*	0.74300(8)	0.99912(1)	0.51501(8)	0.0413(3)	0.0245(3)	0.0515(4)	−0.0129(2)	−0.0247(3)	0.0146(2)
N(1)	4*e*	0.2652(3)	0.82204(6)	0.4465(3)	0.027(1)	0.021(1)	0.030(1)	−0.0013(9)	0.007(1)	0.0016(9)
N(2)	4*e*	0.7389(4)	0.95078(6)	0.5137(3)	0.035(1)	0.026(1)	0.031(1)	−0.011(1)	−0.002(1)	0.001(1)
N(3)	4*e*	0.5891(4)	0.93141(6)	0.4629(3)	0.032(1)	0.022(1)	0.028(1)	−0.0061(9)	0.000(1)	0.0014(9)
O(1)	4*e*	−0.1181(3)	0.79705(5)	0.2562(3)	0.035(1)	0.031(1)	0.024(1)	−0.0013(9)	0.0005(8)	0.0026(8)
O(2)	4*e*	0.2366(4)	0.75705(6)	0.2899(4)	0.056(2)	0.032(1)	0.044(1)	0.008(1)	0.023(1)	−0.000(1)
O(3)	4*e*	−0.0644(3)	0.80167(6)	0.6320(3)	0.0231(9)	0.047(1)	0.022(1)	−0.0029(9)	0.0007(8)	−0.0062(9)
O(4)	4*e*	−0.1384(3)	0.80140(7)	0.9019(3)	0.035(1)	0.061(2)	0.031(1)	−0.018(1)	0.011(1)	−0.006(1)
O(5)	4*e*	0.2679(3)	0.76516(5)	0.7001(3)	0.038(1)	0.0202(9)	0.031(1)	0.0024(8)	−0.0124(9)	−0.0016(8)
O(6)	4*e*	0.4486(3)	0.76237(5)	0.9735(3)	0.038(1)	0.021(1)	0.027(1)	0.0082(8)	−0.0045(9)	−0.0006(8)
O(7)	4*e*	0.3193(3)	0.96894(6)	0.6885(3)	0.035(1)	0.033(1)	0.043(1)	−0.0021(9)	−0.014(1)	0.007(1)
O(8)	4*e*	0.5487(4)	1.00223(6)	0.6921(4)	0.053(2)	0.028(1)	0.047(1)	−0.006(1)	−0.013(1)	0.014(1)
O(9)	4*e*	1.1811(3)	0.94635(6)	1.2933(4)	0.035(1)	0.032(1)	0.058(2)	−0.007(1)	−0.017(1)	0.012(1)
O(10)	4*e*	1.0214(4)	0.99026(6)	1.3205(4)	0.043(1)	0.034(1)	0.048(1)	−0.006(1)	−0.018(1)	−0.010(1)
O(11)	4*e*	0.6293(3)	0.87587(5)	1.0687(4)	0.036(1)	0.019(1)	0.057(2)	−0.0089(9)	−0.018(1)	0.008(1)
C(1)	4*e*	0.3469(4)	0.77729(6)	0.8481(4)	0.021(1)	0.019(1)	0.026(1)	−0.000(1)	0.001(1)	0.001(1)
C(2)	4*e*	0.3195(4)	0.81194(6)	0.8871(4)	0.023(1)	0.018(1)	0.023(1)	−0.000(1)	−0.001(1)	0.000(1)
C(3)	4*e*	0.4776(4)	0.82988(7)	0.9521(4)	0.023(1)	0.022(1)	0.034(2)	−0.001(1)	−0.005(1)	0.002(1)
C(4)	4*e*	0.4604(4)	0.86100(7)	1.0035(4)	0.031(1)	0.021(1)	0.028(2)	−0.007(1)	−0.007(1)	0.004(1)
C(5)	4*e*	0.2882(5)	0.87418(7)	1.0072(4)	0.038(2)	0.020(1)	0.029(2)	−0.002(1)	−0.001(1)	−0.004(1)
C(6)	4*e*	0.1315(4)	0.85606(7)	0.9447(4)	0.027(1)	0.025(1)	0.029(1)	0.002(1)	0.003(1)	−0.001(1)
C(7)	4*e*	0.1443(4)	0.82555(6)	0.8764(4)	0.023(1)	0.019(1)	0.020(1)	−0.002(1)	0.000(1)	0.001(1)
C(8)	4*e*	−0.0298(4)	0.80795(6)	0.7987(4)	0.018(1)	0.022(1)	0.025(1)	0.001(1)	0.002(1)	0.001(1)
C(9)	4*e*	0.6606(4)	0.90722(7)	1.0379(4)	0.032(1)	0.019(1)	0.027(1)	−0.006(1)	0.000(1)	−0.000(1)
C(10)	4*e*	0.8268(4)	0.91877(7)	1.1375(4)	0.026(1)	0.022(1)	0.026(1)	−0.002(1)	−0.005(1)	0.000(1)
C(11)	4*e*	0.8716(4)	0.95049(7)	1.1250(4)	0.028(1)	0.025(1)	0.025(1)	−0.005(1)	−0.005(1)	0.001(1)
C(12)	4*e*	0.7582(4)	0.97043(7)	1.0051(4)	0.033(2)	0.021(1)	0.030(2)	−0.007(1)	−0.006(1)	0.003(1)
C(13)	4*e*	0.5982(4)	0.95801(7)	0.8964(4)	0.028(1)	0.024(1)	0.026(1)	−0.002(1)	−0.004(1)	0.003(1)
C(14)	4*e*	0.5464(4)	0.92657(7)	0.9150(4)	0.026(1)	0.026(1)	0.027(1)	−0.006(1)	−0.006(1)	−0.002(1)
C(15)	4*e*	1.0403(5)	0.96266(7)	1.2528(4)	0.034(2)	0.025(1)	0.033(2)	−0.010(1)	−0.009(1)	0.005(1)
C(16)	4*e*	0.4823(5)	0.97754(7)	0.7534(4)	0.035(2)	0.026(2)	0.032(2)	−0.000(1)	−0.009(1)	0.000(1)
C(17)	4*e*	0.6334(4)	0.90110(7)	0.5103(4)	0.030(1)	0.025(1)	0.027(1)	−0.002(1)	0.006(1)	0.001(1)
C(18)	4*e*	0.8180(4)	0.90102(8)	0.5958(5)	0.029(2)	0.030(2)	0.038(2)	−0.001(1)	0.002(1)	0.003(1)
C(19)	4*e*	0.8764(5)	0.93228(8)	0.5952(4)	0.029(2)	0.036(2)	0.033(2)	−0.008(1)	−0.003(1)	0.001(1)
C(20)	4*e*	0.5024(4)	0.87442(7)	0.4817(4)	0.029(1)	0.022(1)	0.024(1)	−0.002(1)	0.003(1)	0.003(1)
C(21)	4*e*	0.3117(4)	0.87817(7)	0.4702(4)	0.030(2)	0.021(1)	0.038(2)	0.001(1)	0.006(1)	0.002(1)
C(22)	4*e*	0.2005(4)	0.85157(7)	0.4510(4)	0.024(1)	0.026(1)	0.037(2)	0.000(1)	0.003(1)	0.002(1)
C(23)	4*e*	0.4489(4)	0.81867(7)	0.4572(5)	0.030(2)	0.022(1)	0.047(2)	0.001(1)	0.009(1)	−0.001(1)
C(24)	4*e*	0.5702(4)	0.84392(8)	0.4729(5)	0.025(1)	0.025(2)	0.048(2)	−0.000(1)	0.009(1)	0.000(1)

Discussion

The keen interest in the design and synthesis of coordination polymers (CPs) stems not only because of their potential applications in gas storage, molecular sieves, catalysis, drug delivery, nonlinear optics, and molecular sensing, but also because of impressive structural topologies [1–3]. Over the past decades, numerous CPs have been successfully constructed, and crystal engineering has reached a relatively mature level that some CPs with specific topologies can be designed by the judicious selection of metal ions and organic ligands [4]. However, it still remains a great and long-term challenge to predict exactly the molecular structure and property of coordination polymers because of many subtle factors involved in the formation and crystallization process such as the geometries of the metal ions (node) and ligands (linker), supramolecular interaction, and reaction conditions [5]. One strategy is to perform reactions with mixed-ligands such as polycarboxylate and N-containing ligands in the same system, and a great number of novel intriguing structures are obtained [6–9], which indicates that the introduction of N-containing auxiliary ligands into a metal-polycarboxylate system often leads to structural diversity and affords novel frameworks.

The asymmetric unit of the title structure contains two Co(II) ions, and 4-(3,5-dicarboxylato-phenoxy)phthalato as

well as 4-(1H-pyrazol-5-yl)pyridine as bridging ligands to construct a coordination polymer. Co1 is six-coordinated by three oxygen atoms from the tetracarboxylato ligands, by one nitrogen atom from the N-heterocyclic ligand and by two coordinated water molecules. The Co—O bond lengths range from 2.060(2) to 2.146(2) Å, the Co—N bond lengths is 2.141(2) Å. The Cobalt atom Co2 is five-coordinated by four oxygen atoms from the tetracarboxylato ligands, and by one nitrogen atom. The Co—O bond lengths range from 1.975(2) to 2.394(3) Å, the Co—N bond lengths is 2.041(3) Å. The bond angles of O—Co1—O are in the range of 84.38(9)°–174.22(10)°. The bond angles of O—Co2—O are in the range of 58.67(9)°–168.22(10)°. In addition, there is a complex network of intermolecular hydrogen bonds. These interactions result in an infinite three dimensional architecture.

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