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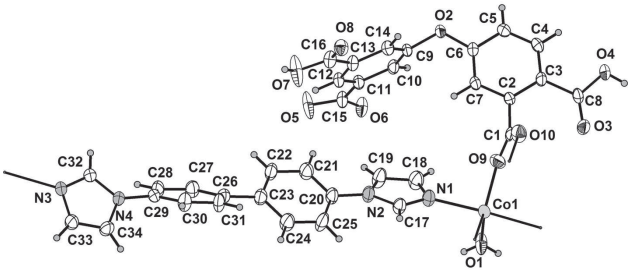
Crystal structure of *catena-poly*-[aqua-(2-carboxy-5-(3-carboxy-5-carboxylatophenoxy)benzoato-κ*O*)(μ$_2$-4,4′-di(1*H*-imidazol-1-yl)-1,1′-biphenyl-κ^2*N*:*N*′)cobalt(II)], $C_{34}H_{24}N_4O_{10}Co$



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Abstract

$C_{34}H_{24}N_4O_{10}Co$, triclinic, $P\bar{1}$, $a = 11.0862(19)$ Å, $b = 11.770(2)$ Å, $c = 12.370(2)$ Å, $\alpha = 83.124(2)°$, $\beta = 70.915(2)°$, $\gamma = 86.075(2)°$, $V = 1513.7(4)$ Å^3, $Z = 2$, $R_{gt}(F) = 0.0458$, $wR_{ref}(F^2) = 0.1505$, $T = 293(2)$ K.

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The asymmetric unit of the crystal structure is shown in the figure. Tables 1 and 2 contain details of the measurement method and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

A mixture of $Co(NO_3)_2 \cdot 6H_2O$ (0.1 mmol, 29 mg), 4,4′-di(1H-imidazol-1-yl)-1,1′-biphenyl (0.1 mmol, 28 mg), 5-(3′,4′-dicarboxylphenoxy)-isophthalic acid (0.1 mmol, 35 mg), was dissolved in 8 mL H_2O. The solution was heated in a 25 mL Teflon-lined autoclave under autogenous pressure at 433 K for 4 days. After cooling to room temperature red block crystals were obtained.

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Table 1: Data collection and handling.

Crystal:	Red, blocks, Size 0.43 × 0.35 × 0.27 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	6.4 cm^{-1}
Diffractometer, scan mode:	CCD, φ and ω
$2\theta_{max}$, completeness:	51°, >99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	16987, 5632, 0.048
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 4229
$N(param)_{refined}$:	444
Programs:	SHELX [7], Bruker programs [8]

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.90871(4)	0.40773(4)	0.61729(4)	0.02582(16)
N1	0.8320(3)	0.5168(2)	0.7480(2)	0.0344(7)
N2	0.7965(3)	0.6237(3)	0.8907(3)	0.0353(7)
N3	0.9732(3)	1.2835(2)	1.4962(2)	0.0300(6)
N4	0.9786(3)	1.1500(2)	1.3840(2)	0.0315(7)
O1	0.8219(3)	0.2783(2)	0.7255(2)	0.0641(10)
H1W	0.7981	0.2078	0.7170	0.096*
H2W	0.7758	0.2658	0.7996	0.096*
O2	0.4516(2)	0.8290(2)	0.54936(19)	0.0331(6)
O3	0.7916(2)	0.4277(2)	0.2748(2)	0.0408(6)
O4	0.6709(3)	0.4999(2)	0.1685(2)	0.0456(7)
H4	0.6980	0.4428	0.1348	0.068*
O5	0.2949(3)	0.7826(3)	1.0617(2)	0.0630(10)
O6	0.2485(2)	0.6579(2)	0.9645(2)	0.0396(6)
O7	0.6205(3)	1.0494(3)	0.8812(2)	0.0757(11)
H7	0.6701	1.0971	0.8831	0.113*
O8	0.7183(2)	1.0800(2)	0.6921(2)	0.0351(6)
O9	0.7892(2)	0.4810(2)	0.5376(2)	0.0428(7)
O10	0.9139(2)	0.5807(2)	0.3811(2)	0.0412(6)
C1	0.8073(3)	0.5491(3)	0.4480(3)	0.0286(8)
C2	0.6897(3)	0.6048(3)	0.4273(3)	0.0242(7)
C3	0.6493(3)	0.5868(3)	0.3345(3)	0.0282(8)
C4	0.5434(4)	0.6489(3)	0.3200(3)	0.0368(9)
H4A	0.5158	0.6368	0.2590	0.044*
C5	0.4790(3)	0.7272(3)	0.3931(3)	0.0357(9)
H5	0.4083	0.7679	0.3821	0.043*

Table 2 (continued)

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
C6	0.5202(3)	0.7451(3)	0.4834(3)	0.0265(7)
C7	0.6224(3)	0.6840(3)	0.5023(3)	0.0272(7)
H7A	0.6469	0.6954	0.5652	0.033*
C8	0.7132(3)	0.4973(3)	0.2578(3)	0.0304(8)
C9	0.4692(3)	0.8414(3)	0.6547(3)	0.0280(8)
C10	0.3905(3)	0.7823(3)	0.7523(3)	0.0291(8)
H10	0.3348	0.7295	0.7465	0.035*
C11	0.3949(3)	0.8020(3)	0.8594(3)	0.0280(7)
C12	0.4790(3)	0.8823(3)	0.8641(3)	0.0303(8)
H12	0.4829	0.8968	0.9352	0.036*
C13	0.5569(3)	0.9410(3)	0.7653(3)	0.0299(8)
C14	0.5524(3)	0.9200(3)	0.6581(3)	0.0310(8)
H14	0.6047	0.9586	0.5908	0.037*
C15	0.3065(3)	0.7418(3)	0.9684(3)	0.0322(8)
C16	0.6403(3)	1.0310(3)	0.7740(3)	0.0353(8)
C17	0.8858(3)	0.5698(3)	0.8070(3)	0.0334(8)
H17	0.9733	0.5705	0.7935	0.040*
C18	0.7023(4)	0.5360(3)	0.7959(4)	0.0468(10)
H18	0.6400	0.5084	0.7714	0.056*
C19	0.6792(4)	0.6009(3)	0.8840(4)	0.0458(11)
H19	0.5998	0.6253	0.9308	0.055*
C20	0.8187(3)	0.6956(3)	0.9674(3)	0.0353(8)
C21	0.7282(4)	0.7773(3)	1.0137(3)	0.0425(10)
H21	0.6519	0.7838	0.9971	0.051*
C22	0.7495(4)	0.8502(3)	1.0849(3)	0.0401(9)
H22	0.6871	0.9051	1.1157	0.048*
C23	0.8625(3)	0.8428(3)	1.1109(3)	0.0363(9)
C24	0.9527(4)	0.7577(3)	1.0635(4)	0.0470(11)
H24	1.0290	0.7503	1.0801	0.056*
C25	0.9313(4)	0.6853(4)	0.9937(4)	0.0473(11)
H25	0.9924	0.6292	0.9638	0.057*
C26	0.8897(3)	0.9249(3)	1.1815(3)	0.0338(8)
C27	0.7959(3)	0.9629(3)	1.2774(3)	0.0378(9)
H27	0.7132	0.9370	1.2981	0.045*
C28	0.8245(3)	1.0388(3)	1.3423(3)	0.0373(9)
H28	0.7612	1.0628	1.4064	0.045*
C29	0.9452(3)	1.0787(3)	1.3127(3)	0.0300(8)
C30	1.0398(4)	1.0448(3)	1.2166(3)	0.0400(9)
H30	1.1214	1.0733	1.1953	0.048*
C31	1.0116(4)	0.9677(3)	1.1524(3)	0.0402(9)
H31	1.0756	0.9442	1.0884	0.048*
C32	0.9184(3)	1.2461(3)	1.4279(3)	0.0319(8)
H32	0.8475	1.2813	1.4120	0.038*
C33	1.0724(3)	1.2068(3)	1.4967(3)	0.0383(9)
H33	1.1277	1.2110	1.5386	0.046*
C34	1.0781(3)	1.1252(3)	1.4285(3)	0.0386(9)
H34	1.1369	1.0642	1.4139	0.046*

Experimental details

Carbon-bound H atoms were placed in calculated positions (C–H 0.95 Å) and were included in the refinement in the riding model approximation, with U_{iso}(H) set to 1.2U_{eq}(C). The H atoms of the hydroxyl groups were allowed to rotate with a fixed angle around the C—O bond (HFIX 147 in the SHELX program suite [7]), with U_{iso}(H) set to 1.5U_{eq}(O). The hydrogen atoms of the water molecule were located on a difference Fourier map and refined with U_{iso}(H) set to 1.5U_{eq}(O).

Discussion

In recent years, research on coordination complexes has made considerable progress in the fields of crystal engineering, owing to their intriguing architectures and functional applications, such as gas storage [1], catalysis [2], magnetism [3] and luminescence [4]. Studies have been focused on the rational design of novel frameworks and the relationships between their structures and properties. The coordination complexes constructed from organic ligands and metal ions through a self-assembly route has been explored, and many efforts have been devoted to use different organic ligands as co-ligands to bridge metal ions to form structures, such as chain structures and 2- or 3-D networks [5]. However, it is still a challenge to obtain predictable frameworks with properties assembled by coordination bonds [6].

The asymmetric unit of the title structure contains one Co(II) ion, 4,4′-di(1*H*-imidazol-1-yl)-1,1′-biphenyl and one 2-carboxy-5-(3-carboxy-5-carboxylatophenoxy)benzoate dianion. The neutral diimidazole ligand acts as a bridging ligand to construct a one-dimensional coordination polymer. The dianionic benzoato ligand is coordinated to one cobalt(II) by one of its carboxylate groups only. The cobalt atom is five-coordinated by two oxygen atoms from two anionic ligands, by two nitrogen atoms from two 4,4′-di(1H-imidazol-1-yl)-1,1′-biphenyl ligands and by one oxygen atom from the coordinated water molecule. The Co—O bond lengths range from 1.977(3)-1.991(2) Å, the Co—N bond lengths is 2.106(3) Å. The bond angles of O—Co—O are in the range of 108.16(13)° to 140.69(11)°. In addition, there are intermolecular hydrogen bonds between coordinated water molecules with adjacent anions: d(O(1)-H(1W)$\cdots$O(8)#4) = 2.801(3) Å, d(O(1)-H(2W)$\cdots$O(5)#5) = 2.563(4) Å. Additionally, there are hydrogen bonds between the anions: d(O(4)-H(4)$\cdots$O(6)#6) = 2.549(3) Å, d(O(7)-H(7)$\cdots$O(5)#7) = 2.512(4) Å. Symmetry codes: #4 x, $y-1$, z; #5 $-x+1$, $-y+1$, $-z+2$; #6 $-x+1$, $-y+1$, $-z+1$; #7 $-x+1$, $-y+2$, $-z+2$. Thus these interactions result in the infinite three dimensional structure.

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