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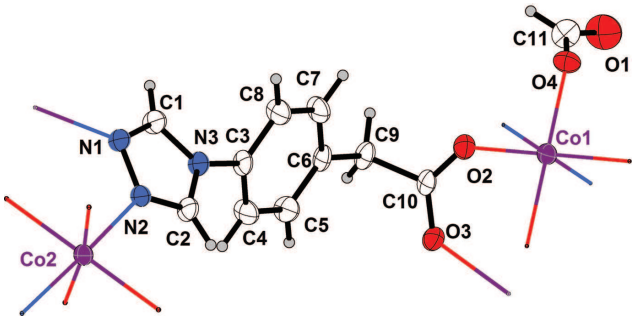
Crystal structure of poly[(μ_4-(4*H*-1,2,4-triazol-4-yl)phenyl)acetato-κ^4*N*,*N*′,*O*,*O*′)(formiato-κ^1*O*)cobalt(II)], $C_{11}H_9CoN_3O_4$



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Abstract

$C_{11}H_9CoN_3O_4$, monoclinic, *C*2/*c* (no. 15), $a = 12.6503(9)$ Å, $b = 8.0959(6)$ Å, $c = 22.9723(14)$ Å, $\beta = 99.424(6)°$, $V = 2321.0(3)$ Å^3, $Z = 8$, $R_{gt}(F) = 0.0370$, $wR_{ref}(F^2) = 0.1101$, $T = 293(2)$ K.

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

Source of material

A mixture of 4-(1,2,4-triazol-4-yl)phenylacetic acid (Htpa, 0.020 g, 0.1 mmol), $Co(NO_3)_2{\cdot}6\,H_2O$ (0.060 g, 0.2 mmol), DMF (4 mL), EtOH (1 mL) and H_2O (1 mL) was added to a 23 mL Teflon bomb, and then heated to 120 °C for 48 h. After cooling to room temperature, pink crystals of the titled complex with block shape were obtained by filtration and washed with water and ethanol for several times.

Table 1: Data collection and handling.

Crystal:	Pink block
Size:	0.22 × 0.18 × 0.07 mm
Wavelength:	Cu *Kα* radiation (1.54184 Å)
μ:	11.8 mm^{-1}
Diffractometer, scan mode:	SuperNova, ω
θ_{max}, completeness:	73.6°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	4247, 2265, 0.030
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 2098
$N(param)_{refined}$:	174
Programs:	Olex2 [1], SHELX [2], CrysAlis^{PRO} [3]

Experimental details

H atoms bonded to C atoms from organic ligands were positioned geometrically and refined using a riding model, with C—H = 0.93 Å, with U_{iso}(H) = 1.2 times U_{eq}(C).

Comment

The rational design and fabrication of coordination polymers (CPs) that composed metal ion/cluster as nodes and organic ligands as connectors have flourished as an emerging area of research because of their beautiful structures as well as their potential applications in many important domains [4–6]. In general, the final properties of CPs are highly dependent on their structures, which are high related to their synthetic conditions and the selected building blocks [7]. Compared with the metal ion/cluster, the effect of organic ligands is more predictable. Organic ligands with *N*- and/or *O*-donors have been extensively used to build novel MOFs with interesting structures and properties [8]. Recent literatures have revealed that the bifunctional organic ligands combining the carboxylate and triazole groups in one unit are good candidates for building CPs with interesting structures and promising bioactivities, which could be applied for the growth inhibition of human osteogenic sarcoma cells [9].

Single-crystal X-ray diffraction analysis revealed that the title complex crystallizes in the monoclinic system with space group *C*2/*c* and demonstrates a three-dimensional framework structure. The asymmetric unit of the title structure contains two crystallographically independent Co(II) ions, one

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.500000	0.500000	0.500000	0.02391(17)
Co2	0.250000	0.32206(7)	0.500000	0.02309(17)
O1	0.7222(2)	0.3586(4)	0.62216(12)	0.0623(7)
O2	0.49955(15)	0.2629(3)	0.46799(8)	0.0330(4)
O3	0.33401(15)	0.1558(2)	0.45756(8)	0.0328(4)
O4	0.66409(15)	0.4822(2)	0.53536(8)	0.0326(4)
N1	0.45607(17)	0.0836(3)	0.08058(9)	0.0289(5)
N2	0.36193(17)	0.1696(3)	0.07882(9)	0.0266(4)
N3	0.42762(17)	0.1178(3)	0.17072(9)	0.0300(5)
C1	0.4935(2)	0.0535(4)	0.13590(11)	0.0326(6)
H1	0.556434	−0.003975	0.149392	0.039*
C2	0.3460(2)	0.1881(3)	0.13318(11)	0.0298(5)
H2	0.287546	0.241469	0.144490	0.036*
C3	0.4360(2)	0.0987(4)	0.23366(10)	0.0299(5)
C4	0.3511(2)	0.0330(4)	0.25645(12)	0.0374(6)
H4	0.287262	0.007874	0.231797	0.045*
C5	0.3622(2)	0.0048(4)	0.31686(12)	0.0368(6)
H5	0.304940	−0.038729	0.332604	0.044*
C6	0.4575(2)	0.0408(3)	0.35402(10)	0.0287(5)
C7	0.5414(2)	0.1095(4)	0.32991(11)	0.0365(6)
H7	0.605015	0.136701	0.354426	0.044*
C8	0.5312(2)	0.1380(4)	0.26964(12)	0.0374(6)
H8	0.587814	0.182956	0.253696	0.045*
C9	0.4690(2)	0.0069(3)	0.41928(11)	0.0319(6)
H9A	0.543409	−0.016302	0.434957	0.038*
H9B	0.426948	−0.089607	0.425771	0.038*
C10	0.4312(2)	0.1546(3)	0.45157(10)	0.0263(5)
C11	0.7134(3)	0.3713(4)	0.56971(13)	0.0407(7)
H11	0.747095	0.289325	0.551068	0.049*

tpa-ligand and one $HCOO^-$ group derived from the decomposition of DMF. Both Co(II) atoms (Co1 and Co2, occupancy 0.5) locating on the special sites of the space group are six-coordinated with two N atoms from two tpa-ligands and three carboxyl O atoms from three tpa-ligands as well as one O atom of the $HCOO^-$ group, shaping a distorted octahedral geometry. The Co(II)—O bond distances are in the range of 2.055(2) to 2.107(2) Å and the Co(II)—N bond length is 2.129(2) Å. As for the tpa^- ligand, it binds with four Co(II) ions using its two carboxyl O atoms and two triazolyl N atoms to behave as a four-connected node. The adjacent Co(II) ions are connected with each other *via* the carboxyl oxygen atoms and triazolyl groups along the *a* axis to afford the 1D chain-like secondary building unit chains, which are further joint *via* the tpa-ligands to shape a three-dimensional framework structure.

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