Crystal structure of (μ-benzene-1,3-diacetato-κ^2O:O')-(μ-1,3-di(1*H*-imidazol-4-yl)benzene-κ^2N:N')cobalt(II), $Co(C_{10}H_8O_4)(C_{12}H_{10}N_4)$

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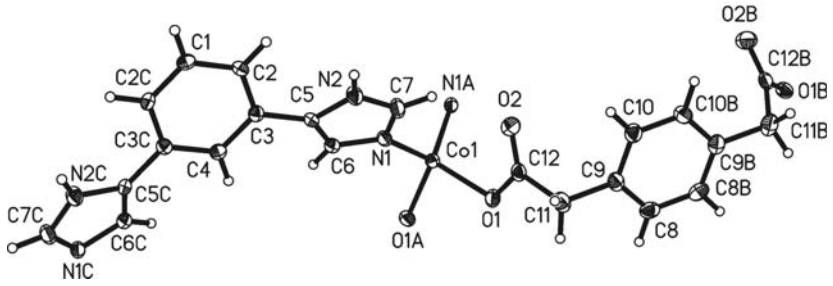

Abstract

$C_{22}H_{18}CoN_4O_4$, orthorhombic, *Ima*2 (no. 46), a = 21.27(1) Å, b = 7.817(4) Å, c = 11.698(6) Å, V = 1944.9 Å^3, Z = 4, $R_{gt}(F)$ = 0.034, $wR_{ref}(F^2)$ = 0.073, T = 298 K.

Source of material

All reagents and solvents were used as obtained commercially without further purification. A mixture of 1,3-di(1*H*-imidazol-4-yl)benzene (L, 0.1 mmol), $CoCl_2$ (0.05 mmol), 1,4-phenylenediacetic acid (H_2PHAD, 0.1 mmol) and NaOH (0.2 mmol) was dissolved in 10 ml distilled water. Then the solution was placed in a Teflon-lined stainless vessel (25 ml). The vessel was sealed and heated at 373 K for 72 h under autogenous pressure and then cooled down to room temperature. The resulting solution was filtered and purple block-shaped single crystals suitable for X-ray diffraction were obtained.

Discussion

The rational design and synthesis of new supramolecular frameworks with covalent and weak intra/intermolecular interactions have brought forth architectures with intriguing structure motifs [1-3]. It is well-known that aromatic polycarboxylates, especially the N-heterocyclic carboxylates, are excellent candidates for preparing novel complexes, because of their versatile coordination modes and potential hydrogen bonding donors and acceptors. Recent studies further demonstrated that mixed organic ligands, especially the mixed polycarboxylate and N-containing ones, with more tunable factors are good candidates for the construction of novel complexes [4,5].

In the title complex, the Co(II) atom is four-coordinated by two carboxylate oxygen atoms from two different $PHAD^{2-}$ and two imidazole nitrogen atoms from two different L ligands in slightly distorted tetrahedral manner. The Co—N bond length is 2.019(2) Å and the Co—O one is 1.989(2) Å, while the bond angles around the Co atoms are in the range of 93.17(9)° - 122.2(1)°. Each L acts as linear terminal bidentate ligand interlinking two cobalt ions and giving an infinite chain with Co···Co distance of 10.635 Å. The $PHAD^{2-}$ ligand uses its two carboxylate groups to bridge the adjacent cobalt ions forming the double chain. There are N–H···O and O–H···O hydrogen bonding interactions in the title crystal structure.

Table 1. Data collection and handling.

Crystal:	purple block, size 0.10 × 0.12 × 0.15 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	9.22 cm^{-1}
Diffractometer, scan mode:	Bruker SMART APEX CCD, φ/ω
$2\theta_{max}$:	51.96°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	5010, 1941
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1771
$N(param)_{refined}$:	144
Programs:	SHELXS-97, SHELXL-97, SHELXTL [6]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(1)	4*b*	¾	0.5096	0.9791	0.037
H(2)	8*c*	0.6564	0.4356	0.8942	0.035
H(4)	4*b*	¾	0.2198	0.6348	0.034
H(6)	8*c*	0.6448	0.0675	0.5953	0.034
H(7)	8*c*	0.4906	0.3217	0.6627	0.046
H(8)	8*c*	0.3043	0.2745	0.1963	0.047
H(10)	8*c*	0.3038	0.4749	0.5099	0.044
H(11A)	8*c*	0.4019	0.4857	0.3729	0.057
H(11B)	8*c*	0.4012	0.3484	0.2754	0.057
H(2A)	8*c*	0.5740	0.4462	0.7680	0.044

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Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Co(1)	4*a*	½	0	0.50519(6)	0.0232(2)	0.0346(3)	0.0251(2)	–0.0043(2)	0	0
C(1)	4*b*	¾	0.4503(5)	0.9102(3)	0.037(2)	0.034(2)	0.023(2)	0	0	–0.009(2)
C(2)	8*c*	0.6941(1)	0.4064(3)	0.8592(2)	0.025(2)	0.036(2)	0.026(2)	0.003(1)	0.006(1)	–0.001(1)
C(3)	8*c*	0.6933(1)	0.3187(3)	0.7558(2)	0.026(2)	0.025(1)	0.028(2)	–0.000(1)	–0.001(1)	0.001(1)
C(4)	4*b*	¾	0.2768(5)	0.7046(3)	0.031(2)	0.029(2)	0.025(2)	0	0	–0.002(2)
C(5)	8*c*	0.6337(1)	0.2732(4)	0.7011(2)	0.022(1)	0.034(2)	0.024(1)	0.000(1)	0.004(1)	0.001(1)
C(6)	8*c*	0.6172(1)	0.1477(4)	0.6258(2)	0.026(1)	0.033(2)	0.026(2)	0.001(1)	0.002(1)	–0.003(1)
C(7)	8*c*	0.5323(1)	0.2862(4)	0.6623(3)	0.024(2)	0.049(2)	0.043(2)	0.004(1)	–0.003(1)	–0.008(2)
C(8)	8*c*	0.2827(1)	0.3151(4)	0.2599(3)	0.051(2)	0.035(2)	0.032(2)	0.005(1)	0.005(2)	0.006(2)
C(9)	8*c*	0.3161(1)	0.3743(4)	0.3529(3)	0.031(2)	0.031(2)	0.045(2)	0.005(1)	0.003(1)	0.013(1)
C(10)	8*c*	0.2823(1)	0.4341(4)	0.4462(3)	0.033(2)	0.041(2)	0.037(2)	0.001(1)	–0.004(1)	–0.005(1)
C(11)	8*c*	0.3868(1)	0.3727(5)	0.3524(3)	0.035(2)	0.050(2)	0.057(2)	0.009(2)	0.007(2)	0.023(2)
C(12)	8*c*	0.4159(1)	0.2412(4)	0.4344(3)	0.023(1)	0.037(2)	0.039(2)	–0.004(1)	–0.003(1)	0.003(1)
N(1)	8*c*	0.5541(1)	0.1561(3)	0.6013(2)	0.023(1)	0.033(1)	0.029(1)	–0.001(1)	0.002(1)	–0.005(1)
N(2)	8*c*	0.5782(1)	0.3600(3)	0.7231(2)	0.028(1)	0.042(2)	0.040(2)	0.006(1)	–0.001(1)	–0.016(1)
O(1)	8*c*	0.4499(1)	0.1237(3)	0.3877(2)	0.030(1)	0.038(1)	0.035(1)	0.005(1)	–0.0051(9)	–0.003(1)
O(2)	8*c*	0.4074(1)	0.2495(3)	0.5369(2)	0.047(1)	0.061(2)	0.037(1)	0.010(1)	–0.002(1)	0.000(1)

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