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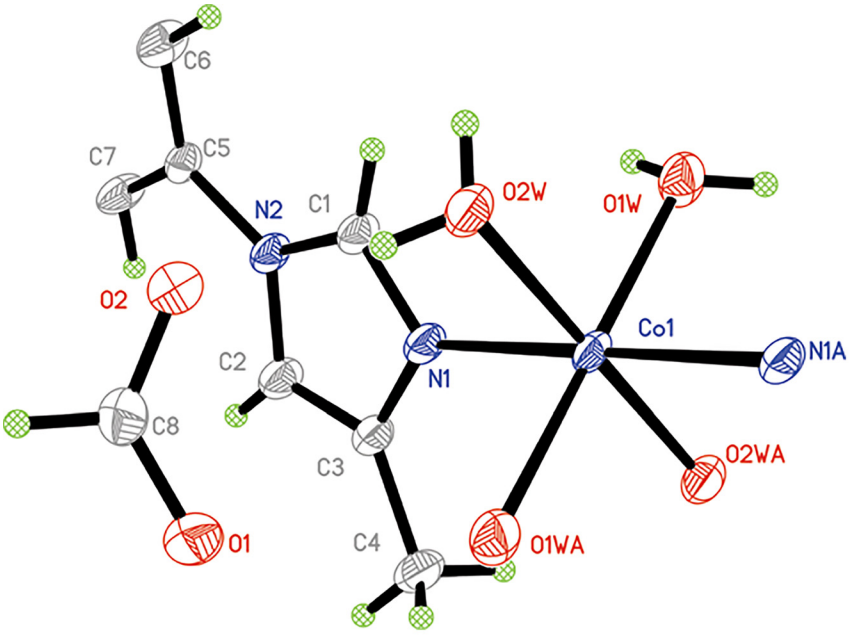
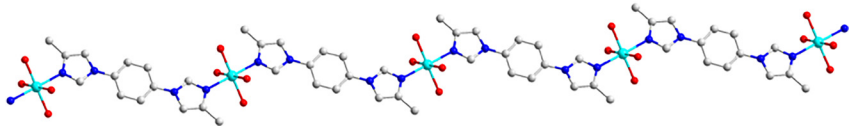
The crystal structure of *catena*-poly[[tetraaqua [(μ_2-1,4-di(4-methyl-1-imidazolyl)benzene] cobalt(II)]bis(formate)], $C_{16}H_{24}CoN_4O_8$





https://doi.org/10.1515/ncrs-2024-0044
Received January 26, 2024; accepted March 1, 2024;
published online March 18, 2024

Abstract

$C_{16}H_{24}CoN_4O_8$, triclinic, $P\bar{1}$ (no. 2), a = 7.4371(8) Å, b = 7.6451(9) Å, c = 9.9156(12) Å, α = 69.830(6)°, β = 71.245(5)°, γ = 79.653(5)°, V = 499.60(10) Å^3, Z = 1, $R_{gt}(F)$ = 0.0247, w$R_{ref}(F^2)$ = 0.0630, T = 293(2) K.

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CCDC no.: 2007704

The molecular structure and 1D chain are shown in Figure 1a and b. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Red block
Size:	0.20 × 0.16 × 0.10 mm
Wavelength:	MoKα radiation (0.71073 Å)
μ:	0.91 mm^{-1}
Diffractometer, scan mode:	φ and ω
θ_{max}, completeness:	26.0°, 99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	7379, 1956, 0.017
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma\,(I_{obs})$, 1923
$N(param)_{refined}$:	144
Programs:	Bruker [1], SHELX [2–4]

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Co1	1.000000	0.500000	1.000000	0.02866 (10)
C1	0.7997 (2)	0.7300 (2)	0.76120 (17)	0.0335 (3)
H1	0.698638	0.753080	0.839032	0.040*
C2	0.9742 (2)	0.7324 (3)	0.53683 (19)	0.0408 (4)
H2	1.017103	0.755371	0.433694	0.049*
C3	1.0701 (2)	0.6300 (2)	0.63785 (19)	0.0370 (4)
C4	1.2636 (3)	0.5310 (3)	0.6080 (2)	0.0529 (5)
H4A	1.307061	0.533120	0.505232	0.079*
H4B	1.258300	0.403782	0.671930	0.079*
H4C	1.350031	0.592224	0.627592	0.079*
C5	0.6486 (2)	0.9015 (2)	0.55737 (17)	0.0302 (3)
C6	0.4706 (2)	0.9236 (3)	0.65215 (19)	0.0426 (4)
H6A	0.450064	0.872581	0.755142	0.051*
C7	0.6789 (2)	0.9783 (3)	0.40521 (19)	0.0414 (4)
H7	0.799207	0.964647	0.340706	0.050*
C8	0.6760 (3)	0.1843 (3)	0.8556 (2)	0.0485 (4)
H8	0.615093	0.155313	0.798334	0.058*
H1WA	1.004 (4)	0.793 (3)	1.077 (3)	0.066 (7)*
H2WA	0.631 (4)	0.527 (4)	1.096 (3)	0.067 (8)*
N1	0.95879 (18)	0.62875 (18)	0.77987 (14)	0.0327 (3)
N2	0.80114 (17)	0.79569 (18)	0.61646 (14)	0.0317 (3)
O1	0.84181 (19)	0.11475 (19)	0.84781 (16)	0.0512 (3)
O2	0.5830 (2)	0.2861 (2)	0.9292 (2)	0.0645 (4)
O1W	0.9324 (2)	0.76114 (17)	1.04079 (15)	0.0454 (3)
H1WB	0.913133	0.842063	0.966086	0.068*
O2W	0.71260 (17)	0.44855 (19)	1.07878 (14)	0.0391 (3)
H2WB	0.688799	0.396408	1.027456	0.059*

1 Source of materials

All chemicals were purchased from commercial sources and used as received. A mixture of 0.05 mmol $Co(NO_3)_2{\cdot}6H_2O$ (15.0 mg, 0.05 mmol), 1,4-di(4-methyl-1-imidazolyl)benzene (20.8 mg, 0.1 mmol), $HCOONa{\cdot}2H_2O$ (10.4 mg, 0.1 mmol), H_2O (4.0 mL) and DMF (4.0 mL) was heated in a 16 mL capacity Teflon-lined reaction vessel at 393 K for three days, the reaction mixture was cooled to room temperature over a period of 40 h. The product was collected by filtration, washed with H_2O and air-dried.

2 Experimental details

The structure was solved by Direct Methods with the Shelxs-2018 program. All the H atoms were located in the difference electron density maps but were placed in idealized positions and allowed to ride on the carrier atoms, with O–H = (0.8200–0.86(5) Å), C–H = 0.93 and 0.96 Å for aryl H and methyl H aotms, respectively, and U_{iso}(H) = 1.2U_{eq}(C) or U_{iso}(H) = 1.5U_{eq}(C_{methyl}).

3 Comment

Imidazole derivatives have been found to possess wide spread biological activities, many of them have been developed as medical and functional materials [5, 6]. Many crystal structures of cobalt(II) compounds with 1,4-di(1-imidazolyl) benzene have been determined so far [7, 8]. However, 1,4-di(4-methyl-1-imidazolyl)benzene is similar to the 1,4-di (1-imidazolyl)benzene, only a few structures were reported so far [9, 10].

In the title compound, the central Co^{II} ion is six-coordinated by two N atoms from two different 1,4-di(4-methyl-1-imidazolyl)benzene ligands and four O atoms from four water molecules in an octahedral coordination geometry (Figure 1a). The Co atoms are linked by the 1,4-di(4-methyl-1-imidazolyl)benzene ligands, forming an extended one-dimensional chain (Figure 1b). There are two free formate counter anions in the structure, stabilized by hydrogen bonds. The $HCOO^-$ anion interacts indirectly through the coordinated water molecules to generate a two-dimensional layer.

Author contribution: All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.
Research funding: This work was supported by the Scientific Research Fund of Hunan Provincial Education Department (No. 23C0232).
Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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