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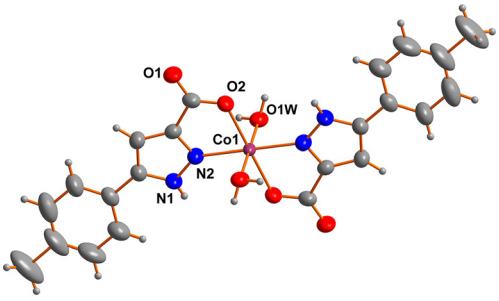
# The crystal structure of diaqua-bis[5-(4-methylphenyl)-1*H*-pyrazole-3-carboxylato-κ$^2$N,O]-cobalt(II), $C_{11}H_{11}Co_{0.5}N_2O_3$

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**Abstract**

$C_{11}H_{11}Co_{0.5}N_2O_3$, Triclinic, $P\bar{1}$, $a$ = 4.8354(4) Å, $b$ = 6.2696(3) Å, $c$ = 18.3717(12)(4) Å, $\alpha$ = 92.763(5)°, $\beta$ = 94.079(7)°, $\gamma$ = 103.858(6)°, $V$ = 538.15(6) Å$^3$, $Z$ = 2, $R_{gt}(F)$ = 0.050, w$R_{ref}(F^2)$ = 0.125, $T$ = 293 K.

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The molecular structure is shown in the figure. Table 1 contains the crystallographic data. The list of the atoms including atomic coordinates and displacement parameters can be found in the cif-file attached to this article.

## 1 Experimental details

Single crystals were placed on a Rigaku XtaLAB-Synergy-R diffractometer with graphite-monochromated MoKα radiation ($\lambda$ = 0.71073 Å).[1] The crystal structure was solved using the Direct Methods and refined. The complex structures were calculated using OLEX2 1.5 and SHELXL 2018/3.[2,3] Hydrogens atoms were positioned geometrically and refined using riding mode.

## 2 Source of material

The ligand 5-(4-methylphenyl)-1*H*-pyrazole-3-carboxylic acid ($H_2L$) was synthesized according literature reported.[4] Dissolve $Co(CH_3COO)_2{\cdot}4H_2O$ (0.1 mmol, 0.0249 g) in 2 mL distilled water and 5-(4-methylphenyl)-1*H*-pyrazole-3-carboxylic acid ($H_2L$) (0.1 mmol, 0.0202 g) in 5 mL methanol. Add the salt solution, $H_2L$ methanol solution, and ethyl acetate into a test tube in descending order of density, seal and react at room temperature for two weeks. Orange crystals were filtered, washed with $CH_3OH$ and dried at room temperature.

## 3 Comment

Pyrazole carboxylic acids provide ample oxygen and nitrogen atoms as coordination sites and can form diverse coordination patterns.[5] Consequently, these compounds have been widely studied, leading to the synthesis of many coordination polymers.[5–7] Studies on phenyl-substituted pyrazole carboxylic acids as building units for coordination polymers are relatively rare compared with other pyrazole carboxylic acids. Introducing phenyl groups provides two key advantages: (1) expanding the ligand's spatial dimensions and (2) facilitating π–π stacking and C–H–π interactions.[8] Strategic methyl substitution on the phenyl ring

**Table 1:** Data collection and handling.

| | |
|---|---|
| Crystal: | Plate |
| Size: | 0.42 × 1.27 × 0.12 mm |
| Wavelength: | MoKα radiation (0.71073 Å) |
| $\mu$: | 0.85 mm$^{-1}$ |
| Diffractometer, scan mode: | Rigaku Synergy-R, $\omega$ scans |
| $\theta_{max}$, completeness: | 30.8°, 100 % |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$, $R_{int}$: | 5.71, 2,604, 0.081 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\ \sigma(I_{obs})$, 1,918 |
| $N(param)_{refined}$: | 161 |
| Programs: | Rigaku,[1] SHELX,[2] Olex2[3] |

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fine-tunes electron density and modulates conformational flexibility through steric effects.[9,10]

Diaqua-bis[5-(4-methylphenyl)-1*H*-pyrazole-3-carboxylatok$^2$N,O]-cobalt(II) crystallized in triclinic system with $P\bar{1}$ space group and exhibits a 0D single-molecule structure. Each crystallographic independence unit comprises a half of Co(II), one $HL^-$ ligand, and one water molecule. The coordination geometry can be described as a slightly distorted octahedron, the N2 and O2 atoms in the two symmetrical ligands form the equatorial plane, and O1W atoms in the coordination water occupy the axial positions. The Co–O bond lengths range from 2.0914 to 2.1713 Å, and the Co–N bond length is 2.066 Å. Bond angles around the Co(II) ion vary from 77.86(7)° to 180°. The N atoms from the pyrazole ring and O atoms from the carboxyl group in each $H_2L$ ligand chelate with the $Co^{2+}$ center, forming a 0D single-molecule structure. The $H_2L$ ligand in the asymmetric unit adopts the $\mu_1$–$N^1$, $O^1$ coordination mode, and the two ligands are symmetrically arranged around Co. Adjacent single molecules form a one-dimensional chain via hydrogen bonds (N1–H1–O1W, 2.070 Å) between pyrazole N atoms and coordinated water O atoms. Further, these chains assemble into a two-dimensional network through hydrogen bonds (O1W–H1WA–O1, 1.80 Å) between carboxylic acid O atoms and coordinated water O atoms.

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