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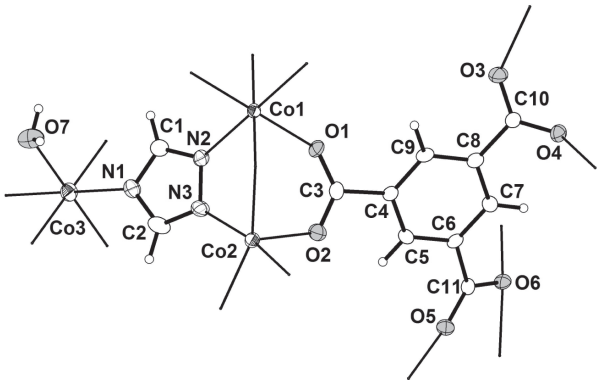
# Crystal structure of *poly*-[aqua-($\mu_7$-benzene-1,3,5-tricarboxylato)-($\mu_3$-1,2,4-triazol-1-ido)dicobalt(II)], $C_{11}H_7Co_2N_3O_7$

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## Abstract

$C_{11}H_7Co_2N_3O_7$, triclinic, $P\bar{1}$ (no. 2), $a = 7.8744(6)$ Å, $b = 9.2561(9)$ Å, $c = 9.6688(9)$ Å, $\alpha = 65.775(9)°$, $\beta = 87.625(7)°$, $\gamma = 73.654(8)°$, $V = 614.48(11)$ Å$^3$, $Z = 2$, $R_{gt}(F) = 0.0537$, $wR_{ref}(F^2) = 0.1458$, $T = 296$ K.

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A representative part of the coordination polymer forming the crystal structure is shown in the figure ($' = x, 1 + y, z$). Tables 1 and 2 contain details of the measurement method and a list of the atoms including atomic coordinates and displacement parameters.

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

| | |
|---|---|
| Crystal: | Red block<br>Size 0.30 × 0.20 × 0.20 mm |
| Wavelength: | Mo $K\alpha$ radiation (0.71073 Å) |
| $\mu$: | 27.5 cm$^{-1}$ |
| Diffractometer, scan mode: | Xcalibur, $\omega$-scans |
| $2\theta_{max}$, completeness: | 52.8°, >99% |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$, $R_{int}$: | 4241, 2504, 0.045 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\ \sigma(I_{obs})$, 1921 |
| $N(param)_{refined}$: | 211 |
| Programs: | SHELX [2], CrysAlis$^{PRO}$ [3], OLEX2 [4] |

## Source of material

A mixture of $CoCl_2{\cdot}2H_2O$ (0.1 mmol, 0.024 g), 1,2,4 triazole (Htrz) (13.9 mg, 0.2 mmol), and benzene-1,3,5-tricarboxylic acid ($H_3$btc) (21.0 mg, 0.1 mmol) was dissolved in 5 mL DMF and 2 mL EtOH. The mixture was then transferred into a 20 mL vial and heated to 80 °C, and hold for 60 h. Then the reactant mixture was cooled at a rate of 10 °C/min to lead to the formation of crystals in 36% yield based on Co(II) ion.

## Experimental details

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

## Discussion

There is a general interest in 1,2,4-triazoles [1].

Structural analysis suggests that there are three crystallographically independent Co(II) ions, one deprotonated trz$^-$ ligand and one deprotonated btc$^{3-}$ ligand in the asymmetric unit. Co1 (occupancy 1/2) is six-coordinated by four carboxylic O atoms from four different btc$^{3-}$ ligands and two N atoms from two different trz$^-$ ligands, forming a octahedral coordination; Co2 is five-connected with four carboxylic O atoms from four different btc$^{3-}$ ligands and one N atom from one trz$^-$ ligand; Co3 (occupancy 1/2) is six-coordinated again

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

| Atom | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Co1 | 0.5000 | 1.0000 | 0.5000 | 0.0157(3) |
| Co2 | 0.75945(9) | 0.72355(8) | 0.83856(8) | 0.0186(2) |
| Co3 | 0.0000 | 1.0000 | 1.0000 | 0.0237(3) |
| O6 | 0.7519(5) | −0.0598(4) | 0.6320(4) | 0.0184(8) |
| O5 | 0.8277(5) | −0.0172(4) | 0.8252(4) | 0.0239(9) |
| O3 | 0.7504(5) | 0.5901(4) | 0.0683(4) | 0.0273(9) |
| O4 | 0.9644(5) | 0.3515(4) | 0.1351(4) | 0.0223(8) |
| O2 | 0.7485(6) | 0.5723(4) | 0.7342(4) | 0.0273(9) |
| O1 | 0.5886(5) | 0.7607(4) | 0.5168(4) | 0.0232(9) |
| N2 | 0.3943(6) | 0.9428(5) | 0.7063(5) | 0.0189(10) |
| O7 | −0.0245(6) | 1.2535(5) | 0.9027(5) | 0.0359(11) |
| H7A | −0.0830 | 1.2986 | 0.8159 | 0.054* |
| H7B | 0.0784 | 1.2679 | 0.8915 | 0.054* |
| N1 | 0.2270(6) | 0.9508(5) | 0.8921(5) | 0.0265(11) |
| N3 | 0.4912(6) | 0.8334(5) | 0.8394(5) | 0.0247(11) |
| C11 | 0.7906(7) | 0.0325(6) | 0.6871(6) | 0.0170(11) |
| C10 | 0.8440(7) | 0.4548(6) | 0.1662(6) | 0.0166(11) |
| C6 | 0.7876(7) | 0.2053(5) | 0.5782(6) | 0.0167(11) |
| C7 | 0.8257(7) | 0.2468(6) | 0.4289(6) | 0.0176(11) |
| H7 | 0.8643 | 0.1640 | 0.3941 | 0.021* |
| C5 | 0.7401(7) | 0.3251(6) | 0.6326(6) | 0.0167(11) |
| H5 | 0.7165 | 0.2968 | 0.7340 | 0.020* |
| C8 | 0.8072(7) | 0.4117(6) | 0.3285(6) | 0.0189(11) |
| C4 | 0.7266(7) | 0.4922(6) | 0.5351(6) | 0.0181(11) |
| C3 | 0.6828(7) | 0.6208(6) | 0.6002(6) | 0.0197(11) |
| C9 | 0.7530(7) | 0.5338(6) | 0.3826(6) | 0.0200(12) |
| H9 | 0.7341 | 0.6442 | 0.3159 | 0.024* |
| C1 | 0.2387(7) | 1.0106(6) | 0.7438(6) | 0.0234(12) |
| H1 | 0.1472 | 1.0918 | 0.6732 | 0.028* |
| C2 | 0.3887(8) | 0.8411(7) | 0.9461(7) | 0.0334(15) |
| H2 | 0.4232 | 0.7776 | 1.0493 | 0.040* |

by two carboxylic O atoms from two different $btc^{3-}$ ligands and two N atom from two different $trz^{-}$ ligands, and the remaining sites are finished by two water molecules. The Co—O bond distances fall in the range of 2.052(2)–2.293(2) Å and the Co—N distances are in the range of 2.047(3)–2.068(3) Å. Cationic cobalt(II), anionic ligands and the neutral water ligands form a three-dimensional coordination polymer. The compactly packing of the whole framework results in its little solvent accessible void. From a topological point of view, each Co ion could be judged as a separate node, the trz ligand could be considered as a 3-connected node, the $btc^{3-}$ ligand could be viewed as a 7-connected node, so the whole framework can be viewed as a 5-nodal (3,4,5,6,7)-connected net with Point symbol of $\{4.6^2\}2\{4^6.6^1 4.8\}2\{4^6.6^4\}2\{4^8.6^7\}\{6^5.8\}$.

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