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The crystal structure of *catena*-poly[bis(μ_2 -1,2-bis((1*H*-imidazol-1-yl)methyl)benzene- $\kappa^2 N:N'$)-bis(nitrato- κO)copper(II)], $C_{28}H_{28}N_{10}O_6Cu$

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Abstract

$C_{28}H_{28}N_{10}O_6Cu$, triclinic, $P\bar{1}$ (no. 2), $a = 8.6869(7)$ Å, $b = 9.0094(6)$ Å, $c = 9.5839(8)$ Å, $\alpha = 74.288(7)^\circ$, $\beta = 87.672(9)^\circ$, $\gamma = 76.110(7)^\circ$, $V = 700.69(11)$ Å³, $Z = 1$, $R_{gt}(F) = 0.0492$, $wR_{ref}(F^2) = 0.0979$, $T = 293(2)$ K.

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Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

A mixture of $Cu(NO_3)_2 \cdot 3 H_2O$ (0.05 mmol), 2,2-bis((2'-carboxy-[1,1'-biphenyl]-4-yl)methyl)isoindolin-2-ium chloride

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Table 1: Data collection and handling.

Crystal:	Purple block
Size:	0.34 × 0.20 × 0.15 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.84 mm ⁻¹
Diffractometer, scan mode:	Xcalibur, ω
θ_{max} , completeness:	29.5°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int} :	5920, 3203, 0.035
Criterion for I_{obs} , $N(hkl)_{gt}$:	$I_{obs} > 2 \sigma(I_{obs})$, 2607
$N(param)_{refined}$:	205
Programs:	CrysAlis ^{PRO} [1], SHELX [2, 3], Diamond [4]

(0.05 mmol), 1,2-bis((1*H*-imidazol-1-yl)methyl)benzene (0.05 mmol), 1*H*-pyrazole (0.05 mmol), NaOH (0.2 mmol) and 5.5 mL of DMF/EtOH/MeOH/H₂O (1:1:2:1.5) was sealed in a 20 mL vial and heated at 358 K for 15 days. Purple block crystals were collected.

Experimental details

H atoms were placed in calculated positions and were included in the refinement in the riding model approximation, with $U_{iso}(H)$ set to 1.2 $U_{eq}(C)$.

Comment

In recent years, 1,2-bis((1*H*-imidazol-1-yl)methyl)benzene has been widely applied in the formation of many kinds of metal coordination complexes [5–10]. In this study it was used to prepare a new Cu²⁺ coordination polymer.

The asymmetric unit of the title structure has one 1,2-bis((1*H*-imidazol-1-yl)methyl)benzene ligand, one nitrate anion, one half of a Cu(II) cation. The nitrate ion is coordinated to the Cu(II) ion. Cu1 forms a distorted octahedral geometry, with four imidazole nitrogen atoms in the equatorial plane and two oxygen atoms of nitrate ions in axial positions. The Cu1–N2 and Cu1–N4 bond lengths

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	x	y	z	U _{iso} [*] /U _{eq}
Cu1	0.000000	0.500000	1.000000	0.02377 (14)
O1	0.0352 (3)	0.7872 (3)	0.9029 (2)	0.0436 (6)
O2	0.0824 (3)	1.0169 (3)	0.8078 (3)	0.0552 (7)
O3	0.2379 (3)	0.8481 (3)	0.9718 (3)	0.0702 (8)
N1	0.2175 (3)	0.3420 (3)	0.4075 (2)	0.0264 (5)
N2	0.0978 (2)	0.4657 (3)	0.1966 (2)	0.0244 (5)
N3	0.3969 (2)	0.2327 (2)	0.8542 (2)	0.0219 (5)
N4	0.2090 (2)	0.3952 (3)	0.9365 (2)	0.0227 (5)
N5	0.1171 (3)	0.8839 (3)	0.8966 (2)	0.0283 (5)
C1	0.4753 (3)	0.1961 (3)	0.5342 (3)	0.0244 (6)
C2	0.5607 (3)	0.1336 (3)	0.6661 (3)	0.0210 (5)
C3	0.7248 (3)	0.1084 (3)	0.6676 (3)	0.0266 (6)
H3	0.781464	0.065099	0.755294	0.032*
C4	0.8052 (3)	0.1470 (3)	0.5397 (3)	0.0342 (7)
H4	0.915180	0.128954	0.541394	0.041*
C5	0.7211 (4)	0.2119 (4)	0.4109 (3)	0.0371 (7)
H5	0.774146	0.240384	0.325162	0.044*
C6	0.5580 (4)	0.2355 (3)	0.4073 (3)	0.0334 (7)
H6	0.502664	0.278310	0.318923	0.040*
C7	0.2975 (3)	0.2148 (3)	0.5295 (3)	0.0314 (7)
H7A	0.276010	0.115715	0.524112	0.038*
H7B	0.253997	0.235957	0.618900	0.038*
C8	0.1560 (3)	0.3263 (3)	0.2877 (3)	0.0276 (6)
H8	0.154588	0.229540	0.271104	0.033*
C9	0.1236 (3)	0.5760 (3)	0.2617 (3)	0.0323 (7)
H9	0.094762	0.685487	0.222273	0.039*
C10	0.1973 (4)	0.5010 (3)	0.3917 (3)	0.0355 (7)
H10	0.228363	0.548149	0.457533	0.043*
C11	0.4808 (3)	0.0913 (3)	0.8101 (3)	0.0255 (6)
H11A	0.406033	0.029134	0.802674	0.031*
H11B	0.560257	0.026333	0.883930	0.031*
C12	0.2476 (3)	0.2596 (3)	0.9012 (3)	0.0252 (6)
H12	0.180521	0.191683	0.907874	0.030*
C13	0.3397 (3)	0.4571 (3)	0.9123 (3)	0.0310 (7)
H13	0.347101	0.552487	0.928392	0.037*
C14	0.4567 (3)	0.3579 (3)	0.8614 (3)	0.0331 (7)
H14	0.557777	0.372017	0.836168	0.040*

(2.014(2) and 1.989(2) Å, respectively) in the equatorial plane are shorter than the Cu1–O1 bond length (2.590 Å) of the axis. A one dimensional polynuclear chain of the complex is formed by the connection of the ligand to two neighboring Cu(II) ions (see the Figure). The lattice

constants of the title complex were almost the same as the reported copper complex [10].

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