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Methanol(2-methyl-1*H*-imidazole-κN^3)(pyridine-2,6-dicarboxylato-$\kappa^3 N,O,O'$)copper(II)

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In the title compound, $[Cu(C_7H_3NO_4)(C_4H_6N_2)(CH_4O)]$, the Cu atom lies in the centre of an N_2O_2 square plane, and the methanol molecule is apically coordinated. The coordination geometry is best described as distorted square-pyramidal. There are intermolecular hydrogen bonds in the crystal structure, which mediate the formation of layers.

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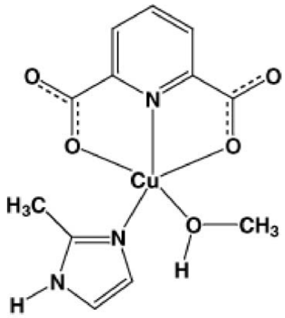
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.033
wR factor = 0.088
Data-to-parameter ratio = 13.6

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

We report here the isolation of a new copper(II) complex, (I). The crystal structure shows that the bond distances and angles in (I) have normal values. The Cu atom lies in the centre of a square plane which consists of two O atoms and two N atoms (O1, O3, N1 and N2). The average bond distances of Cu—O and Cu—N are 2.0286 (17) and 1.921 (17) Å, respectively. The Cu atom deviates from the plane (O1/O3/N1/N2) by 0.1013 (8) Å towards the apically coordinated methanol molecule; the Cu1—O5 bond length is 2.2685 (17) Å. The coordination geometry is best described as distorted square-pyramidal.



(I)

There are intermolecular hydrogen bonds in the structure of (I), mediating the formation of layers. The hydrogen bonds result in a two-dimensional network, parallel to the (001) plane. Each molecule participates as both donor and acceptor in such contacts (Fig. 2 and Table 1).

Experimental

Pyridine-2,6-dicarboxylic acid was prepared according to the literature (Singer & McElvain, 1935). The pyridine-2,6-dicarboxylate copper(II) complex hexahydrate was prepared by the following procedure. To a heated aqueous solution (60 ml) of pyridine-2,6-dicarboxylic acid (334.2 mg, 2 mmol) was added 1 *M* NaOH (4 ml) and copper(II) oxide (318.1 mg, 4 mmol). The mixture was stirred at 373 K for 18 h and then filtered several times. After two weeks, blue crystals were obtained. This intermediate (312.7 mg, 1 mmol) was dissolved in a heated methanol solution of 2-methylimidazole (50 ml). The solution was refluxed for 12 h, and then filtered. After

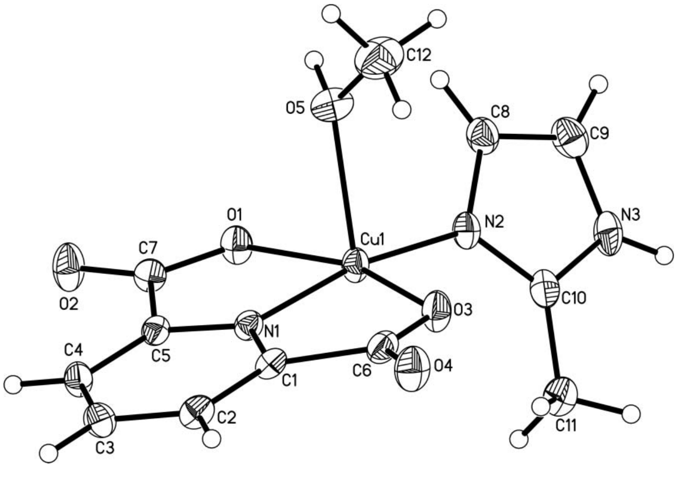


Figure 1
The structure of the title complex, with displacement ellipsoids drawn at the 50% probability level.

five weeks, blue prismatic crystals of (I) were obtained from the filtered solution.

Crystal data

$[Cu(C_7H_3NO_4)(C_4H_6N_2)(CH_4O)]$
$M_r = 342.79$
Monoclinic, $P2_1/n$
$a = 8.5226$ (10) Å
$b = 12.2353$ (15) Å
$c = 13.2586$ (16) Å
$\beta = 105.095$ (2)°
$V = 1334.9$ (3) Å^3
$Z = 4$

$D_x = 1.706$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3156 reflections
$\theta = 2.3$–$27.4°$
$\mu = 1.66$ mm^{-1}
$T = 293$ (2) K
Prism, blue
$0.30 \times 0.28 \times 0.14$ mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min} = 0.61$, $T_{max} = 0.79$
7005 measured reflections

2619 independent reflections
2242 reflections with $I > 2\sigma(I)$
$R_{int} = 0.048$
$\theta_{max} = 26.0°$
$h = -10 \rightarrow 9$
$k = -15 \rightarrow 15$
$l = -16 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.088$
$S = 0.99$
2619 reflections
192 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.05P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.39$ e Å^{-3}
$\Delta\rho_{min} = -0.33$ e Å^{-3}

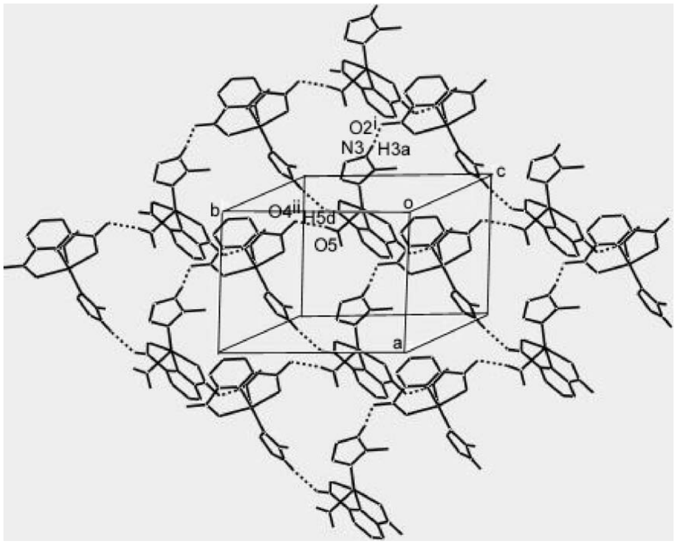


Figure 2
A view of a layer in (I). Dashed lines indicate hydrogen bonds. H atoms not involved in hydrogen bonding have been omitted. [Symmetry codes: (i) $-\frac{1}{2} - x, -\frac{1}{2} + y, \frac{1}{2} - z$; (ii) $\frac{1}{2} - x, \frac{1}{2} + y, \frac{1}{2} - z$.]

Table 1
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···O2^i	0.86	1.99	2.806 (3)	158
O5—H5D···O4^{ii}	0.85	1.83	2.673 (3)	170

Symmetry codes: (i) $-\frac{1}{2} - x, y - \frac{1}{2}, \frac{1}{2} - z$; (ii) $\frac{1}{2} - x, \frac{1}{2} + y, \frac{1}{2} - z$.

All H atoms were positioned geometrically (C—H 0.93–0.96 Å) and refined as riding, with U_{iso}(H) = 1.2 or 1.5 times U_{eq}(parent atom).

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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References

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