

## Diammine(pyridine-2,6-dicarboxylato)copper(II)

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In the crystal structure of the title compound,  $[\text{Cu}(\text{C}_7\text{H}_3\text{NO}_4)(\text{NH}_3)_2]$ , the Cu atom is coordinated in a square-pyramidal geometry by a pyridine-2,6-dicarboxylate ligand acting in an  $N,O,O'$ -tridentate chelating mode, and by two N atoms from two ammine ligands. A further long Cu—O bond involving a symmetry-related molecule generates chains of molecules in the  $a$ -axis direction.

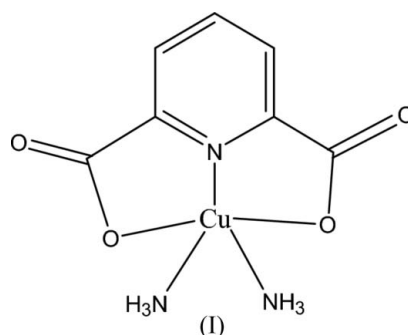
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## Key indicators

Single-crystal X-ray study  
 $T = 295 \text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$   
 $R$  factor = 0.037  
 $wR$  factor = 0.104  
Data-to-parameter ratio = 13.8For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

## Comment

The multifunctional ligand  $\text{H}_2\text{PDC}$  (pyridine-2,6-dicarboxylic acid) is of particular interest for obtaining metal organic frameworks because of its potential coordinating sites, from a carboxylic acid group, which when deprotonated results in a divalent anion, and a neutral aromatic nitrogen coordinating site (Eubank *et al.*, 2005). In the molecule of the title compound, the central  $\text{Cu}^{\text{II}}$  atom is chelated by a  $\text{PDC}^{2-}$  ligand and two ammine ligands, giving a square pyramidal coordination geometry (Fig. 1). In addition, as shown in Fig. 2, a weak interaction between  $\text{Cu}^{\text{II}}$  and an O atom from a symmetry-related molecule (Table 1) connects molecules into one-dimensional chains in the  $a$ -axis direction. In the crystal structure, intermolecular hydrogen bonds connect the one-dimensional molecular chains into a two-dimensional framework perpendicular to the  $b$  axis (Table 2 and Fig. 3).



## Experimental

Following the procedure described by Constable *et al.*, (1990),  $\text{H}_2\text{PDC}$  (0.083 g, 0.5 mmol) was added with 1 ml of concentrated ammonia to an aqueous solution (15 ml) of copper(II) oxalate (0.075 g, 0.5 mmol). The mixture was placed in a 25 ml Teflon-lined Parr bomb and heated at 433 K for 38 h. The bomb was then cooled to room temperature at  $5 \text{ K h}^{-1}$ . Crystals were obtained in about 30% yield. Analysis calculated for  $\text{C}_7\text{H}_3\text{N}_3\text{O}_4\text{Cu}$ : C 32.00, H 3.45, N 15.99%; found: C 31.98, H 3.50, N 16.02%. IR (KBr,  $\text{cm}^{-1}$ ): 3378 ( $m$ ), 3065 ( $w$ ), 1605 ( $vs$ ), 1565 ( $m$ ), 1556 ( $m$ ), 1482 ( $s$ ), 1417 ( $s$ ).

## Crystal data

$[\text{Cu}(\text{C}_7\text{H}_3\text{NO}_4)(\text{NH}_3)_2]$   
 $M_r = 262.72$   
 Triclinic,  $P\bar{1}$   
 $a = 4.8654(6) \text{ \AA}$   
 $b = 9.1161(11) \text{ \AA}$   
 $c = 10.0916(12) \text{ \AA}$   
 $\alpha = 76.927(2)^\circ$   
 $\beta = 86.987(2)^\circ$   
 $\gamma = 86.618(2)^\circ$   
 $V = 434.88(9) \text{ \AA}^3$

$Z = 2$   
 $D_x = 2.006 \text{ Mg m}^{-3}$   
 Mo  $K\alpha$  radiation  
 Cell parameters from 58  
 reflections  
 $\theta = 2.2\text{--}26.0^\circ$   
 $\mu = 2.51 \text{ mm}^{-1}$   
 $T = 295(2) \text{ K}$   
 Block, blue  
 $0.26 \times 0.18 \times 0.11 \text{ mm}$

## Data collection

Bruker APEX area-detector  
 diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan  
 (SADABS; Bruker, 2002)  
 $T_{\min} = 0.558$ ,  $T_{\max} = 0.755$   
 2693 measured reflections

1901 independent reflections  
 1772 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.014$   
 $\theta_{\max} = 27.8^\circ$   
 $h = -6 \rightarrow 5$   
 $k = -11 \rightarrow 11$   
 $l = -12 \rightarrow 13$

## Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.037$   
 $wR(F^2) = 0.104$   
 $S = 1.08$   
 1901 reflections  
 138 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0653P)^2 + 0.365P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.83 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -0.81 \text{ e \AA}^{-3}$

Table 1

 Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

Cu1—N1	1.911 (2)	Cu1—O3	2.049 (2)
Cu1—N3	1.962 (3)	Cu1—N2	2.319 (2)
Cu1—O2	2.021 (2)	O1—Cu1 <sup>i</sup>	2.925 (2)
N1—Cu1—N3	169.27 (11)	O2—Cu1—O3	160.08 (9)
N1—Cu1—O2	80.68 (9)	N1—Cu1—N2	100.57 (9)
N3—Cu1—O2	104.03 (10)	N3—Cu1—N2	89.13 (10)
N1—Cu1—O3	79.60 (9)	O2—Cu1—N2	90.40 (9)
N3—Cu1—O3	94.95 (10)	O3—Cu1—N2	95.96 (9)

 Symmetry code: (i)  $x - 1, y, z$ .

Table 2

 Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D\text{—}H\cdots A$	$D\text{—}H$	$H\cdots A$	$D\cdots A$	$D\text{—}H\cdots A$
N2—H2A <sup>i</sup> ⋯O3 <sup>i</sup>	0.89	1.95	2.765 (3)	152
N2—H2B <sup>ii</sup> ⋯O4 <sup>ii</sup>	0.89	1.91	2.739 (3)	155
N2—H2C <sup>iii</sup> ⋯N3 <sup>iii</sup>	0.89	2.55	3.148 (4)	126
N3—H3A <sup>iii</sup> ⋯O2 <sup>iii</sup>	0.89	2.41	3.204 (4)	149
N3—H3B <sup>iv</sup> ⋯O1 <sup>iv</sup>	0.89	2.18	3.007 (3)	154

 Symmetry codes: (i)  $x - 1, y, z$ ; (ii)  $-x + 1, -y, -z + 1$ ; (iii)  $x + 1, y, z$ ; (iv)  $-x, -y, -z$ .

H atoms were placed in calculated positions ( $\text{C—H} = 0.93 \text{ \AA}$ ;  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  and  $\text{N—H} = 0.89 \text{ \AA}$ ;  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{N})$ ), and were included in the refinement in a riding-model approximation.

Data collection: SMART (Bruker, 2002); cell refinement: SAINT (Bruker, 2002); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEPII (Johnson, 1976) and PLATON (Spek, 2003); software used to prepare material for publication: SHELXL97.

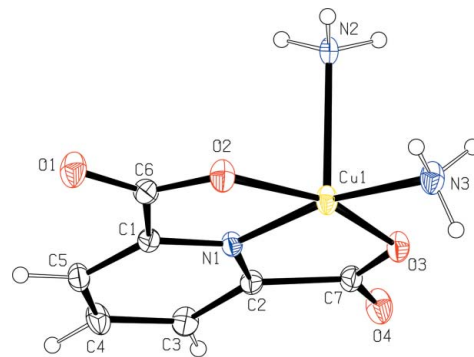


Figure 1

View of (I), showing 30% displacement ellipsoids and H atoms drawn as spheres of arbitrary radii.

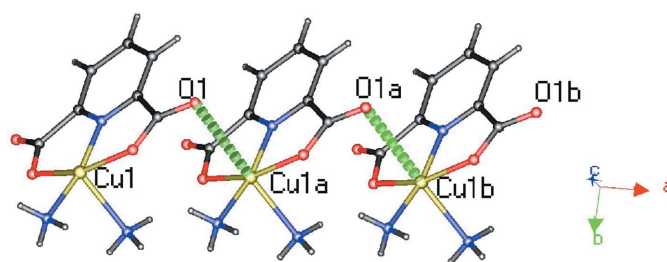


Figure 2

Section of a one-dimensional chain of molecules of (I) connected by weak Cu—O bonds (shown as green dashed lines). The atoms labeled with suffixes a and b are related by the symmetry operators  $-1 + x, y, z$  and  $-2 + x, y, z$  respectively.

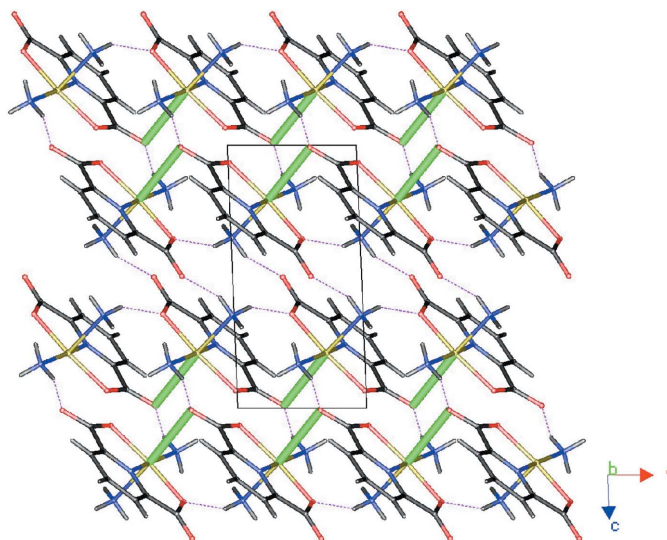


Figure 3

View of the hydrogen bonding in (I), shown as dashed lines. Thick green lines indicate the long Cu—O bonds.

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## References

Bruker (2002). SADABS, SAINT and SMART. Bruker AXS Inc., Madison, Wisconsin, USA.

Constable, E. C., Lewis, J., Liptrot, M. C. & Raithby, P. R. (1990). *Inorg. Chim. Acta*, **178**, 47–54.

Eubank, J. F., Walsh, R. D. & Eddaoudi, M. (2005). *Chem. Commun.* pp. 2095–2097.

Johnson, C. K. (1976). *ORTEP II*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.