

Jaroslava Maroszová, Petra Stachová, Zuzana Vasková, Dušan Valigura and Marian Koman\*

Department of Inorganic Chemistry, Slovak University of Technology, Radlinského 9, SK-812 37 Bratislava, Slovak Republic

Correspondence e-mail: jaroslava.maroszova@stuba.sk

## Key indicators

Single-crystal X-ray study  
 $T = 293$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å  
Disorder in main residue  
 $R$  factor = 0.042  
 $wR$  factor = 0.111  
Data-to-parameter ratio = 15.1For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.(3,5-Dinitrobenzoato- $\kappa O$ )bis[(2-pyridyl)-methanol- $\kappa^2 N, O$ ]copper(II) 3,5-dinitrobenzoate

In the title compound,  $[\text{Cu}(\text{C}_7\text{H}_3\text{N}_2\text{O}_6)(\text{C}_6\text{H}_7\text{NO})_2](\text{C}_7\text{H}_3\text{N}_2\text{O}_6)$ , the  $\text{Cu}^{\text{II}}$  atom is coordinated by two chelating 2-pyridylmethanol ligands and a monodentate 3,5-dinitrobenzoate anion, forming a square-pyramidal coordination polyhedron. The cation and neighbouring anion are connected by two very strong  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds to form an ion pair.

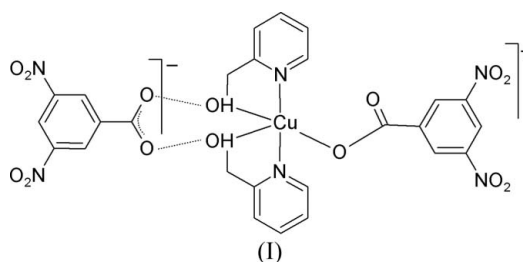
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## Comment

As a part of our systematic study of copper(II) carboxylate complexes with biologically interesting molecular ligands, we report here the crystal structure of the title compound, (I).



The asymmetric unit of (I) is made up of a  $[\text{Cu}(\text{C}_6\text{H}_7\text{NO})_2(\text{C}_7\text{H}_3\text{N}_2\text{O}_6)]^+$  cation and a  $\text{C}_7\text{H}_3\text{N}_2\text{O}_6^-$  anion. The (2-pyridyl)methanol ligand (also known as 2-pyridylcarbinol and abbreviated as 2-pycarb) prefers a chelating mode, in contrast with the bridging mode found for (3-pyridyl)methanol (known as ronicol) in copper(II) complexes (Stachová *et al.*, 2005). The 3,5-dinitrobenzoate ligand is monodentate, coordinating through a carboxylate O atom to give a complex cation with distorted square-pyramidal geometry and a  $\text{CuO}_2\text{N}_2\text{O}'$  coordination polyhedron. The basal plane is formed by carboxylate atom O1 from the coordinating 3,5-dinitrobenzoate ligand, atom O31 from one

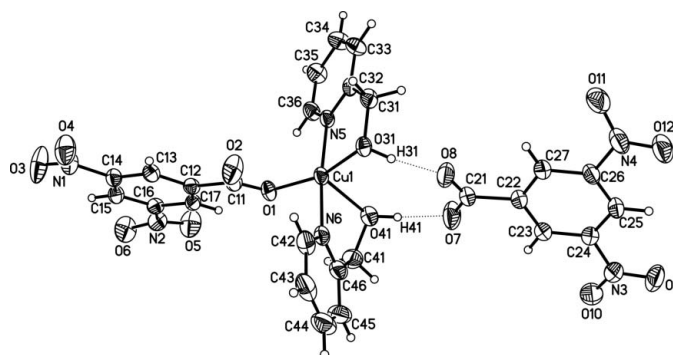


Figure 1

The asymmetric unit of (I). Displacement ellipsoids are drawn at the 40% probability level. Dotted lines represent  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds.

2-pycarb ligand and two mutually *trans* pyridine atoms, N5 and N6, from two 2-pycarb ligands. The apical position of the coordination polyhedron is occupied by atom O41 of a 2-pycarb ligand, with a Cu—O distance longer than those in the basal plane (Table 1). The Cu1—O2 distance of 2.735 (2) Å is longer than the Cu1—O1 distance. Also, the C11—O2 distance is significantly shorter than the C11—O1 distance. These confirm that atom O2 is not involved in coordination and the ligand is monodentate. Atom Cu1 is displaced out of the basal plane by 0.120 (1) Å in the direction of the apical O41 atom. The 3,5-dinitrobenzoate anion is uncoordinated. With the exception of the C—O distances in the carboxylate groups, there are no significant differences in bond lengths or angles between the coordinated and uncoordinated anions and the values are comparable with those observed for bis(1,3-diaminopropane)-3,5-dinitrobenzoatocopper(II) 3,5-dinitrobenzoate (Sundberg *et al.*, 1994).

Two very strong hydrogen bonds link atoms O7 and O8 of the uncoordinated 3,5-dinitrobenzoate anion to hydroxyl atoms H41 and H31 of the coordinated 2-pycarb ligands (Table 2), giving rise to ion-pair formation. Similar hydrogen bonding is reported for bis(triethanolamine)copper(II) diacetate (Krabbes *et al.*, 1999). In the closely related benzoatobis(dimethylaminoethanol)copper(II) benzoate (Turpeinen *et al.*, 1985), the carboxylate anions form hydrogen bonds with hydroxyl H atoms of the coordinated ligands. Similar but weaker hydrogen bonds are found in copper(II) complexes containing coordinated NH groups (Sen *et al.*, 2000, Sundberg & Klinga, 1994).

### Experimental

(2-Pyridyl)methanol (2 mmol) was added to copper(II) acetate (1 mmol) in aqueous solution (20 ml). 3,5-Dinitrobenzoic acid (2 mmol) was then added. The powdery blue product was filtered off and dried at room temperature. Blue prismatic crystals of (I) suitable for X-ray analysis were obtained from the mother liquor after slow room-temperature crystallization over a period of a few weeks.

#### Crystal data

[Cu(C<sub>7</sub>H<sub>3</sub>N<sub>2</sub>O<sub>6</sub>)(C<sub>6</sub>H<sub>7</sub>NO)<sub>2</sub>]  
(C<sub>7</sub>H<sub>3</sub>N<sub>2</sub>O<sub>6</sub>)  
*M<sub>r</sub>* = 704.02  
Triclinic, P $\bar{1}$   
*a* = 9.870 (1) Å  
*b* = 12.181 (1) Å  
*c* = 12.732 (1) Å  
 $\alpha$  = 95.29 (1)°  
 $\beta$  = 108.68 (1)°  
 $\gamma$  = 91.80 (1)°  
*V* = 1440.9 (2) Å<sup>3</sup>

*Z* = 2  
*D<sub>x</sub>* = 1.623 Mg m<sup>-3</sup>  
Mo K $\alpha$  radiation  
Cell parameters from 25 reflections  
 $\theta$  = 4.2–12.0°  
 $\mu$  = 0.84 mm<sup>-1</sup>  
*T* = 293 (2) K  
Prism, blue  
0.55 × 0.45 × 0.30 mm

#### Data collection

Siemens P4 diffractometer  
 $\varphi$  scans  
Absorption correction:  $\psi$  scan  
(XEMP; Siemens, 1990)  
*T<sub>min</sub>* = 0.641, *T<sub>max</sub>* = 0.777  
7697 measured reflections  
6556 independent reflections  
5266 reflections with *I* > 2 $\sigma$ (*I*)

*R<sub>int</sub>* = 0.029  
 $\theta_{\text{max}}$  = 27.5°  
*h* = -1 → 12  
*k* = -15 → 15  
*l* = -16 → 16  
2 standard reflections every 100 reflections  
intensity decay: none

#### Refinement

Refinement on *F*<sup>2</sup>  
*R*[*F*<sup>2</sup> > 2 $\sigma$ (*F*<sup>2</sup>)] = 0.042  
*wR*(*F*<sup>2</sup>) = 0.111  
*S* = 1.04  
6556 reflections  
433 parameters  
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0601P)^2 + 0.292P]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
( $\Delta/\sigma$ )<sub>max</sub> = 0.001  
 $\Delta\rho_{\text{max}}$  = 0.52 e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}}$  = -0.63 e Å<sup>-3</sup>

Table 1

Selected geometric parameters (Å, °).

Cu1—O1	1.967 (2)	Cu1—O41	2.301 (2)
Cu1—N5	1.972 (2)	O1—C11	1.274 (3)
Cu1—N6	1.993 (2)	O2—C11	1.224 (3)
Cu1—O31	2.000 (2)		
O1—Cu1—N5	92.43 (7)	N6—Cu1—O31	93.16 (7)
O1—Cu1—N6	93.46 (7)	O1—Cu1—O41	96.50 (7)
N5—Cu1—N6	173.81 (7)	N5—Cu1—O41	99.99 (7)
O1—Cu1—O31	162.24 (7)	N6—Cu1—O41	77.45 (8)
N5—Cu1—O31	81.75 (7)	O31—Cu1—O41	101.02 (6)

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O31—H31...O8	0.87	1.65	2.512 (2)	173
O41—H41...O7	0.93	1.71	2.631 (3)	174

Atoms H31 and H41 were located in a difference Fourier map and their positions were not refined. The remaining H atoms were placed in geometrically calculated positions and allowed to ride on their parent atoms, with C—H distances of 0.93 (aromatic) or 0.97 Å (methylene). The *U<sub>iso</sub>* value for all H atoms was fixed at 0.05 Å<sup>2</sup>. Atom O11 of an NO<sub>2</sub> group is disordered over two positions, O11A and O11B. The occupancy factors were initially refined to 0.502 (2) and 0.498 (2), but later fixed at 0.5 each.

Data collection, cell refinement and data reduction: XSCANS (Siemens, 1994); program(s) used to solve structure: SHELXS86 (Sheldrick, 1985); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 (Farrugia, 1997); publication material: WinGX (Farrugia, 1999).

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