

Xu-Yan Ma, Xin-Dian Dong,  
Yan-Ping Li and Zhi-Gang  
Zhang\*Institute of Molecular Science, Chemical Biology  
and Molecular Engineering Laboratory of the  
Education Ministry, Shanxi University, Taiyuan,  
Shanxi 030006, People's Republic of China

Correspondence e-mail: zgzhang@sxu.edu.cn

## Key indicators

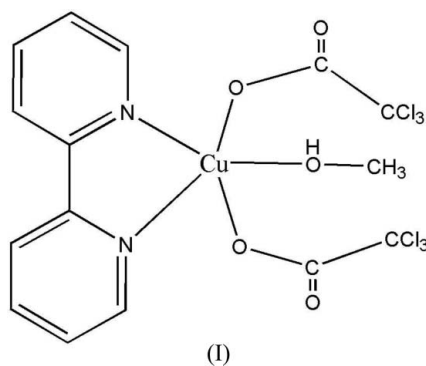
Single-crystal X-ray study  
 $T = 293$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.006$  Å  
 $R$  factor = 0.049  
 $wR$  factor = 0.123  
Data-to-parameter ratio = 14.0For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.(2,2'-Bipyridyl)methanolbis(trichloroacetato)-  
copper(II)

In the title compound,  $[\text{Cu}(\text{C}_2\text{Cl}_3\text{O}_2)_2(\text{C}_{10}\text{H}_8\text{N}_2)(\text{CH}_4\text{O})]$ , the  $\text{Cu}^{\text{II}}$  cation is coordinated by bipyridyl N atoms, two trichloroacetato O atoms and one methanol O atom in a distorted tetragonal pyramidal geometry. In the crystal structure, intermolecular  $\text{O}-\text{H}\cdots\text{O}$ ,  $\text{C}-\text{H}\cdots\text{O}$  and  $\pi-\pi$  interactions are found.

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## Comment

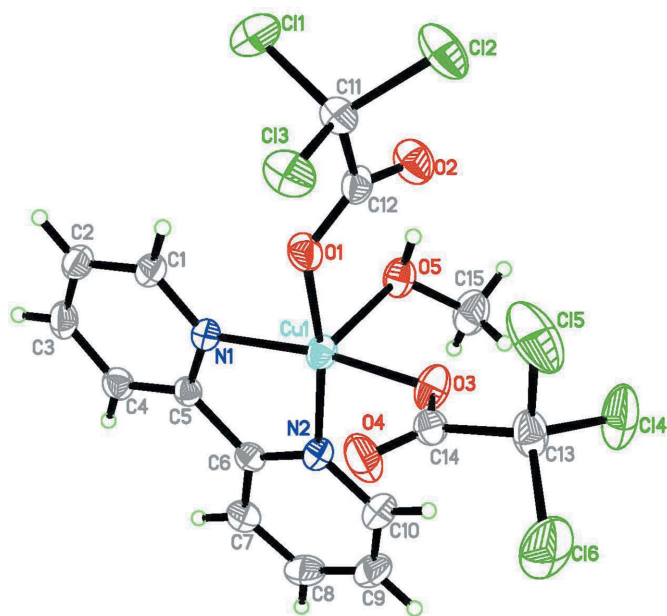
Copper(II) complexes containing heterocyclic ligands have attracted considerable attention in nucleic acid chemistry. Chakravarty and co-workers, for example, have used several copper(II) complexes of diimines to cleave DNA by double-strand scission under physiological conditions (Dhar *et al.*, 2003). We have therefore prepared and characterized the title copper complex, (I).



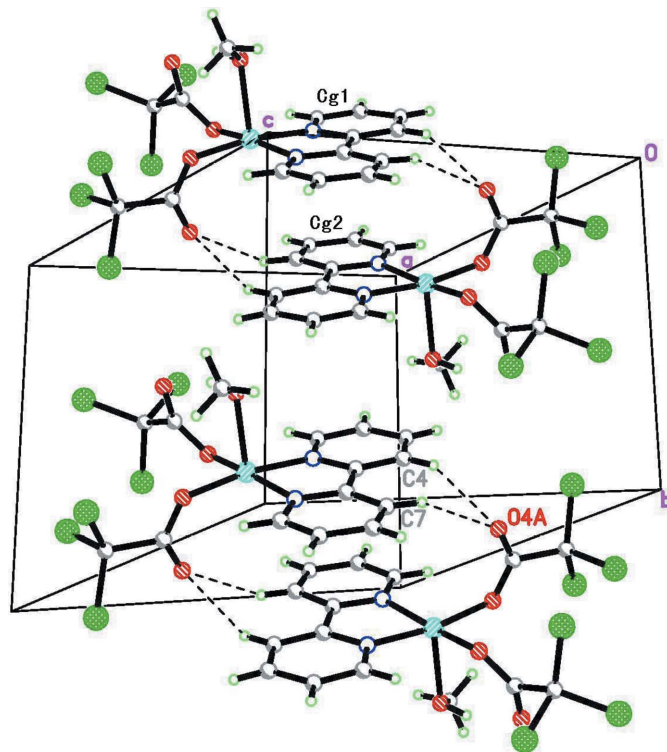
In (I), the  $\text{Cu}^{\text{II}}$  ion has a distorted tetragonal pyramidal geometry. The coordination of the  $\text{Cu}^{\text{II}}$  cation is composed of two bipyridyl N atoms and two O atoms of the trichloroacetate anion in basal positions and one methanol O atom in the apical position (Fig. 1 and Table 1). In the crystal structure, pairs of complexes are connected into dimers *via* intermolecular  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonding and  $\pi-\pi$  interactions between the bipyridyl rings [ $\text{Cg}1(x, y-1, z)\cdots\text{Cg}1(-x+1, -y+1, -z+1) = 3.677$  Å;  $\text{Cg}1$  is the centroid of atoms C1–C5, N1; Fig. 2 and Table 2]. The  $\text{O}-\text{H}$  hydrogen of the methanol molecule forms an intermolecular hydrogen bond to the trichloroacetate atom O2 (Table 2).

## Experimental

All chemicals were of reagent grade and commercially available from the Beijing Chemical Reagents Company of China, and were used without further purification. At room temperature, an aqueous solution (10 ml) of  $\text{CuCl}_2\cdot 2\text{H}_2\text{O}$  (0.1094 g, 0.64 mmol) was added dropwise to an aqueous solution (10 ml) of  $\text{Na}_2\text{CO}_3$  (0.0848 g,



**Figure 1**  
The molecular structure of the title compound, showing the atom labeling and 30% probability displacement ellipsoids.



**Figure 2**  
The crystal structure of (I), with C...H—O hydrogen bonds shown as dashed lines. [Symmetry code: (A)  $1 - x, 2 - y, 1 - z$ .]

0.8 mmol). The pale-blue precipitate was filtered off and washed with demineralized water. The precipitate was dispersed in water/methanol (1:1) solution and trichloroacetic acid (0.2941 g, 1.8 mmol) was added. After the precipitate had dissolved, bipyridine (0.0936 g, 0.6 mmol) was added and the mixture was stirred for 4 h. After slow evaporation of the solvent at room temperature for about a week, blue crystals of the title compound formed.

*Crystal data*

[Cu(C<sub>2</sub>Cl<sub>3</sub>O<sub>2</sub>)<sub>2</sub>(C<sub>10</sub>H<sub>8</sub>N<sub>2</sub>)(CH<sub>4</sub>O)]  
*M<sub>r</sub>* = 576.51  
 Triclinic, *P* $\bar{1}$   
*a* = 9.278 (3) Å  
*b* = 9.863 (3) Å  
*c* = 12.356 (3) Å  
 $\alpha$  = 76.540 (3)°  
 $\beta$  = 76.941 (3)°  
 $\gamma$  = 87.618 (4)°

*V* = 1071.1 (5) Å<sup>3</sup>  
*Z* = 2  
*D<sub>x</sub>* = 1.787 Mg m<sup>-3</sup>  
 Mo *K*α radiation  
 $\mu$  = 1.80 mm<sup>-1</sup>  
*T* = 293 (2) K  
 Block, blue  
 0.40 × 0.40 × 0.30 mm

*Data collection*

Bruker SMART CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 2000)  
*T<sub>min</sub>* = 0.533, *T<sub>max</sub>* = 0.615  
 (expected range = 0.505–0.583)

4439 measured reflections  
 3695 independent reflections  
 3233 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.016  
 $\theta_{max}$  = 25.0°

*Refinement*

Refinement on *F*<sup>2</sup>  
*R*[*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.049  
*wR*(*F*<sup>2</sup>) = 0.123  
*S* = 1.06  
 3695 reflections  
 263 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0584P)^2 + 1.0108P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{max} = 0.003$   
 $\Delta\rho_{max} = 0.66 \text{ e \AA}^{-3}$   
 $\Delta\rho_{min} = -0.56 \text{ e \AA}^{-3}$

**Table 1**

Selected bond lengths (Å).

|        |           |        |           |
|--------|-----------|--------|-----------|
| Cu1—O3 | 1.945 (3) | Cu1—N1 | 2.000 (3) |
| Cu1—O1 | 1.949 (3) | Cu1—O5 | 2.293 (3) |
| Cu1—N2 | 1.988 (3) |        |           |

**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> |
|-------------------------|-------------|---------------|-----------------------|-------------------------|
| O5—H11...O2             | 0.82        | 1.93          | 2.699 (5)             | 155                     |
| C4—H4...O4 <sup>i</sup> | 0.93        | 2.42          | 3.247 (6)             | 148                     |
| C7—H7...O4 <sup>i</sup> | 0.93        | 2.49          | 3.336 (7)             | 151                     |

Symmetry code: (i)  $-x + 1, -y + 2, -z + 1$ .

H atoms attached to C atoms were placed in geometrically idealized positions and refined using a riding model, with *Csp*<sup>3</sup>—H = 0.96 Å [*U<sub>iso</sub>*(H) = 1.5*U<sub>eq</sub>*(C)] and *Csp*<sup>2</sup>—H = 0.93 Å [*U<sub>iso</sub>*(H) = 1.2*U<sub>eq</sub>*(C)]. The O—H H atom was located in a difference Fourier map, repositioned geometrically and refined as riding with O—H = 0.82 Å and *U<sub>iso</sub>*(H) = 1.2*U<sub>eq</sub>*(O).

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 2000); software used to prepare material for publication: SHELXTL.

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