

## Tetraaquabis(4-pyridylthioacetato)copper(II)

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## Key indicators

Single-crystal X-ray study

$T = 298\text{ K}$

Mean  $\sigma(\text{C}-\text{C}) = 0.007\text{ \AA}$

$R$  factor = 0.059

w $R$  factor = 0.186

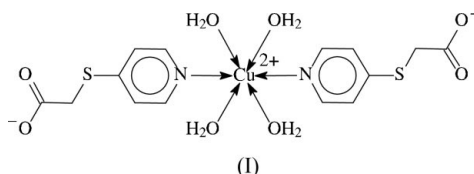
Data-to-parameter ratio = 14.4

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

The Cu atom in the zwitterionic title compound,  $[\text{Cu}(\text{C}_7\text{H}_6\text{NO}_2\text{S})_2(\text{H}_2\text{O})_4]$ , lies on a center of symmetry. It is linked to the pyridyl N atoms of two anionic groups and to four water molecules in an octahedral arrangement. The compound is isostructural with the Ni analog, whose structure has been reported [Zhang, Fang, Wu & Ng (2004). *Acta Cryst. E* **60**, m135–m136].

## Comment

The Cu atom in the centrosymmetric zwitterionic title compound,  $[\text{Cu}(\text{C}_7\text{H}_6\text{NO}_2\text{S})_2(\text{H}_2\text{O})_4]$ , (I), is linked to the pyridyl N atoms of two anionic groups and to four water molecules in an octahedral environment. The compound is isostructural with the Ni analog (Zhang *et al.*, 2004a), whose structure has been described in detail.



The Mn, Co and Zn pyridylthioacetates have different formulations (Qin *et al.*, 2004; Zhang *et al.*, 2003, 2004b).

## Experimental

Copper(II) chloride (0.11 g, 0.8 mmol), (4-pyridylthio)acetic acid (0.09 g, 0.6 mmol), 4,4'-bipyridine (0.06 g, 0.4 mmol) and water (7 ml) in a 4:3:2:1500 molar ratio were mixed and the pH of the solution was adjusted to 8 by adding 2N sodium hydroxide. The mixture was transferred to a 15 ml Teflon-lined stainless-steel reactor, which was heated at 433 K for 108 h. Blue crystals of the title compound were recovered in about 60% yield.

## Crystal data

$[\text{Cu}(\text{C}_7\text{H}_6\text{NO}_2\text{S})_2(\text{H}_2\text{O})_4]$

$M_r = 471.98$

Monoclinic,  $P2_1/a$

$a = 7.481\text{ (1)\ \AA}$

$b = 10.453\text{ (2)\ \AA}$

$c = 12.123\text{ (2)\ \AA}$

$\beta = 107.435\text{ (2)^\circ}$

$V = 904.4\text{ (3)\ \AA}^3$

$Z = 2$

$D_x = 1.733\text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation

Cell parameters from 1559 reflections

$\theta = 2.7\text{--}26.4^\circ$

$\mu = 1.49\text{ mm}^{-1}$

$T = 298\text{ (2)\ K}$

Prism, blue

$0.20 \times 0.16 \times 0.05\text{ mm}$

## Data collection

Bruker SMART APEX area-detector diffractometer

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan

(SADABS; Bruker, 2002)

$T_{\text{min}} = 0.529$ ,  $T_{\text{max}} = 0.929$

4867 measured reflections

1953 independent reflections

1671 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.03$

$\theta_{\text{max}} = 27.1^\circ$

$h = -9 \rightarrow 9$

$k = -13 \rightarrow 13$

$l = -10 \rightarrow 15$

Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.059$   
 $wR(F^2) = 0.186$   
 $S = 1.20$   
 1953 reflections  
 136 parameters

H atoms treated by a mixture of independent and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0727P)^2 + 3.5831P]$$

where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.89 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.68 \text{ e } \text{\AA}^{-3}$

Table 1

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

Cu1—O1w	2.066 (4)	Cu1—N1	2.101 (4)
Cu1—O2w	2.044 (4)		
O1w—Cu1—O2w	89.4 (2)	O1w—Cu1—N1 <sup>1</sup>	88.9 (2)
O1w—Cu1—O2w <sup>i</sup>	90.6 (2)	O2w—Cu1—N1	87.3 (2)
O1w—Cu1—N1	91.2 (2)	O2w—Cu1—N1 <sup>1</sup>	92.7 (2)

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

Table 2

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1w—H1w2 $\cdots$ O1 <sup>ii</sup>	0.85	1.94	2.758 (6)	163
O1w—H1w1 $\cdots$ O1 <sup>iii</sup>	0.85	2.04	2.840 (6)	157
O2w—H2w1 $\cdots$ O2 <sup>iv</sup>	0.85	1.94	2.738 (6)	156
O2w—H2w2 $\cdots$ O2 <sup>ii</sup>	0.85	1.93	2.724 (6)	156
C7—H7 $\cdots$ O1 <sup>iii</sup>	0.93	2.49	3.395 (6)	163

Symmetry codes: (ii)  $2 - x, 1 - y, 2 - z$ ; (iii)  $\frac{3}{2} - x, y - \frac{1}{2}, 2 - z$ ; (iv)  $x, y, z - 1$ .

C-bound H atoms were placed at calculated positions in the riding-model approximation (C—H = 0.93  $\text{\AA}$  for aromatic H atoms and C—H = 0.97  $\text{\AA}$  for aliphatic H atoms); water H atoms were placed at chemically sensible positions by using the HYDROGEN option (Nardelli, 1999) in the WinGX suite (Farrugia, 1999), and were refined with distance restraints of O—H = 0.85 (1)  $\text{\AA}$  and H $\cdots$ H = 1.39 (1)  $\text{\AA}$ . For all H atoms, the  $U_{\text{iso}}$  values were set at  $1.2U_{\text{eq}}$  of the parent atom. The structure solution was carried out using atomic

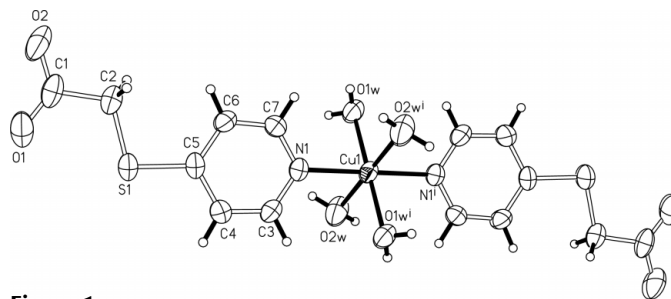


Figure 1

ORTEP (Johnson, 1976) plot of (I), with displacement ellipsoids drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radii.

coordinates taken from the isostructural Ni analog (Zhang *et al.*, 2004a).

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

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