

Diaquabis[(pyrimidin-2-ylsulfanyl)acetato]copper(II)  
dihydrateHong-Qing Hao<sup>a</sup> and Hui  
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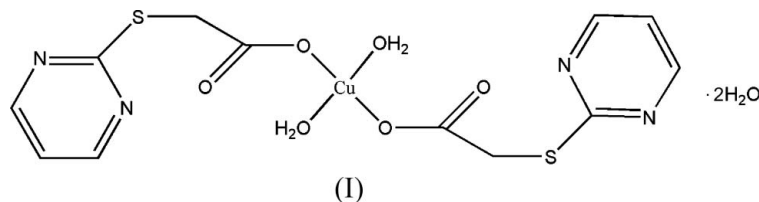
## Key indicators

Single-crystal X-ray study  
 $T = 273\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.007\text{ \AA}$   
 $R$  factor = 0.054  
 $wR$  factor = 0.125  
Data-to-parameter ratio = 14.4For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

In the title compound,  $[\text{Cu}(\text{C}_6\text{H}_5\text{N}_2\text{O}_2\text{S})_2(\text{H}_2\text{O})_2] \cdot 2\text{H}_2\text{O}$ , the Cu atom lies on an inversion centre in a distorted square coordination geometry that consists of two O atoms of two (pyrimidin-2-ylsulfanyl)acetate ligands [ $\text{Cu}-\text{O} = 1.953(2)\text{ \AA}$ ] and two O atoms of two water molecules [ $\text{Cu}-\text{O} = 1.942(3)\text{ \AA}$ ].

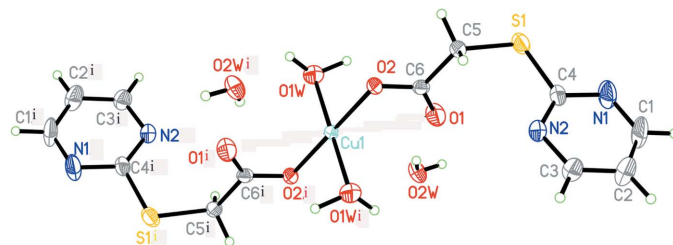
## Comment

Following our studies of complexes of 2-pyrimidylthioacetic acid (Ng *et al.*, 1993; Ma *et al.*, 2004; Hao *et al.*, 2005), we report the structure of the centrosymmetric title compound, (I). The four-coordinate Cu atom is in a square coordination geometry that is made up of two O atoms of two carboxylate groups and two O atoms of two water molecules (Fig. 1). Hydrogen bonds connect the molecules and the solvent water molecules into a three-dimensional network structure.



## Experimental

Cupric nitrate (120.8 mg, 0.5 mmol) was dissolved in water (10 ml). Aqueous ammonium hydroxide (6 M) was added until the solution turned blue. 2-Pyrimidylthioacetic acid (170.2 mg, 1 mmol) was suspended in a small volume of water–ethanol (1:1 *v/v*); aqueous ammonium hydroxide (6 M) was added until the compound dissolved completely. The two solutions were then mixed. After three weeks, dark-blue crystals were obtained in 65% yield. Analysis found: C 30.41, H 3.83, N 11.82%; calculated for  $\text{C}_{12}\text{H}_{18}\text{CuN}_4\text{O}_8\text{S}_2$ : C 30.20, H 3.91, N 11.78%. IR ( $\text{cm}^{-1}$ ): 3423 ( $\nu_{\text{OH}}$  for  $\text{H}_2\text{O}$ ), 1605, 1384 ( $\nu_{\text{as}}$  and  $\nu_{\text{s}}$  for  $\text{COO}^-$ ), 1551, 1309, 1280.



**Figure 1**  
ORTEP (Johnson, 1976) plot of (I). Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (i)  $1 - x, 1 - y, 1 - z$ .]

Crystal data

[Cu(C<sub>6</sub>H<sub>5</sub>N<sub>2</sub>O<sub>2</sub>S)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>].2H<sub>2</sub>O  
*M<sub>r</sub>* = 473.96  
 Monoclinic, *P*2<sub>1</sub>/*c*  
*a* = 17.160 (5) Å  
*b* = 5.1577 (16) Å  
*c* = 10.568 (3) Å  
 $\beta$  = 99.942 (5)°  
*V* = 921.3 (5) Å<sup>3</sup>  
*Z* = 2

*D<sub>x</sub>* = 1.709 Mg m<sup>-3</sup>  
 Mo *K*α radiation  
 Cell parameters from 3246 reflections  
 $\theta$  = 3.6–26.9°  
 $\mu$  = 1.46 mm<sup>-1</sup>  
*T* = 273 (2) K  
 Plate, blue  
 0.27 × 0.16 × 0.07 mm

Data collection

Bruker APEX 2000 area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
*T<sub>min</sub>* = 0.694, *T<sub>max</sub>* = 0.905  
 9709 measured reflections

2009 independent reflections  
 1874 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.056  
 $\theta_{\text{max}}$  = 27.0°  
*h* = -21 → 21  
*k* = -6 → 6  
*l* = -13 → 13

Refinement

Refinement on *F*<sup>2</sup>  
*R* [*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.054  
*wR* (*F*<sup>2</sup>) = 0.125  
*S* = 1.16  
 2009 reflections  
 140 parameters  
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0443P)^2 + 1.6524P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.54 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.66 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

Cu1—O1W	1.942 (3)	O2—C6	1.252 (4)
Cu1—O2	1.953 (2)	O1—C6	1.202 (4)
O1W—Cu1—O2	89.34 (12)	O1—C6—O2	124.4 (3)
O1W <sup>i</sup> —Cu1—O2	90.66 (12)		

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

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>
O2W—H2WA···O1	0.85 (1)	1.86 (2)	2.695 (4)	169 (5)

The water H atoms were located in difference Fourier maps and were refined with distance restraints of O—H = 0.85 (1) Å and H···H = 1.39 (1) Å [*U<sub>iso</sub>*(H) = 0.85 Å<sup>2</sup>]. The aromatic and aliphatic H atoms were placed at calculated positions (C—H = 0.93 and 0.97 Å) and refined using the riding-model approximation, with *U<sub>iso</sub>*(H) = 1.2*U<sub>eq</sub>*(C).

Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 2001); 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); software used to prepare material for publication: SHELXL97.

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References

- Bruker (2001). SAINT and SMART. Bruker AXS Inc., Madison, Wisconsin, USA.  
 Hao, H.-Q., Zhang, H., Chen, J.-G. & Ng, S. W. (2005). *Acta Cryst.* **E61**, m1960–m1962.  
 Johnson, C. K. (1976). ORTEPII. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.  
 Ma, C.-L., Han, Y.-F. & Zhang, R.-F. (2004). *J. Organomet. Chem.* **689**, 1675–1683.  
 Ng, S. W., Das, V. G. K., Yip, W.-H. & Mak, T. C. W. (1993). *J. Crystallogr. Spectrosc. Res.* **23**, 441–444.  
 Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.  
 Sheldrick, G. M. (1997). SHELXS97 and SHELXL97. University of Göttingen, Germany.