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Key indicators

Single-crystal X-ray study
 T = 273 K
 Mean $\sigma(\text{C}-\text{C}) = 0.007 \text{ \AA}$
 R factor = 0.054
 wR factor = 0.125
 Data-to-parameter ratio = 14.4

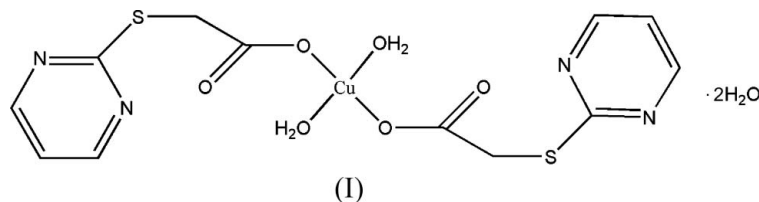
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

Diaquabis[(pyrimidin-2-ylsulfanyl)acetato]copper(II) dihydrate

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 (cm^{-1}): 3423 (ν_{OH} for H_2O), 1605, 1384 (ν_{as} and ν_{s} for COO^-), 1551, 1309, 1280.

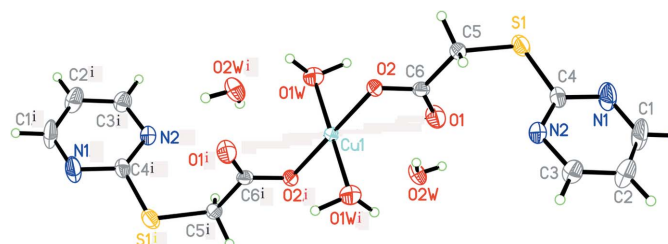


Figure 1
 ORTEP (Johnson, 1976) plot of (I). Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (i) 1 - x, 1 - y, 1 - z.]

Received 28 November 2005
 Accepted 1 December 2005
 Online 7 December 2005

Crystal data

[Cu(C₆H₅N₂O₂S)₂(H₂O)₂].2H₂O
M_r = 473.96
 Monoclinic, *P*2₁/*c*
a = 17.160 (5) Å
b = 5.1577 (16) Å
c = 10.568 (3) Å
 β = 99.942 (5)°
V = 921.3 (5) Å³
Z = 2

Data collection

Bruker APEX 2000 area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
*T*_{min} = 0.694, *T*_{max} = 0.905
 9709 measured reflections

Refinement

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

D_x = 1.709 Mg m⁻³
 Mo *K* α radiation
 Cell parameters from 3246 reflections
 θ = 3.6–26.9°
 μ = 1.46 mm⁻¹
T = 273 (2) K
 Plate, blue
 0.27 × 0.16 × 0.07 mm

2009 independent reflections
 1874 reflections with *I* > 2 σ (*I*)
*R*_{int} = 0.056
 θ _{max} = 27.0°
h = -21 → 21
k = -6 → 6
l = -13 → 13

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

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 ⁱ —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*_{iso}(H) = 0.85 Å²]. 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*_{iso}(H) = 1.2*U*_{eq}(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.

The authors thank the National Science Foundation of China (20171037 and 20373056) and the Fujian Province Science Foundation of China (2002F016 and C0020001).

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