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Key indicators

Single-crystal X-ray study
 T = 571 K
 Mean $\sigma(\text{C}-\text{C}) = 0.006 \text{ \AA}$
 R factor = 0.060
 wR factor = 0.145
 Data-to-parameter ratio = 15.1

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

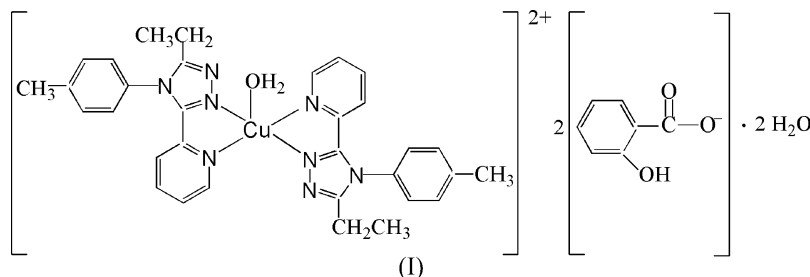
**Aquabis[3-ethyl-4-(4-methylphenyl)-5-(2-pyridyl)-
 4H-1,2,4-triazole- $\kappa^2\text{N},\text{N}'$]copper(II) disalicylate
 dihydrate**

In the title complex, $[\text{Cu}(\text{C}_{16}\text{H}_{16}\text{N}_4)_2(\text{H}_2\text{O})](\text{C}_7\text{H}_5\text{O}_3)_2 \cdot 2\text{H}_2\text{O}$, the Cu^{II} atom is in a slightly distorted square-pyramidal coordination geometry. In the crystal structure, intermolecular $\text{O}-\text{H} \cdots \text{O}$ hydrogen bonds form centrosymmetric clusters.

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Comment

The coordination chemistry of 1,2,4-triazole derivatives has received considerable attention in recent years (Bencini *et al.*, 1987; Koningsbruggen *et al.*, 1995; Moliner *et al.*, 1998, 2001; Klingele & Brooker, 2003). Some spin-crossover complexes of 1,2,4-triazoles with iron(II) salts have been reported, which could be used as molecular-based memory devices, displays and optical switches (Garcia *et al.*, 1997; Kahn & Martinez, 1998). We report here the crystal structure of the title compound, (I).



The molecular structure of (I) is shown in Fig. 1. The Cu^{II} atom is coordinated by two bis-chelating 3-ethyl-4-(*p*-methylphenyl)-5-(2-pyridyl)-1,2,4-triazole ligands and one water molecule in a slightly distorted square-pyramidal coordination geometry having a $\text{CuN}_2\text{N}'_2\text{O}$ centre. In the crystal structure, intermolecular $\text{O}-\text{H} \cdots \text{O}$ hydrogen bonds (Table 2) link all the components of the asymmetric unit and form centrosymmetric clusters.

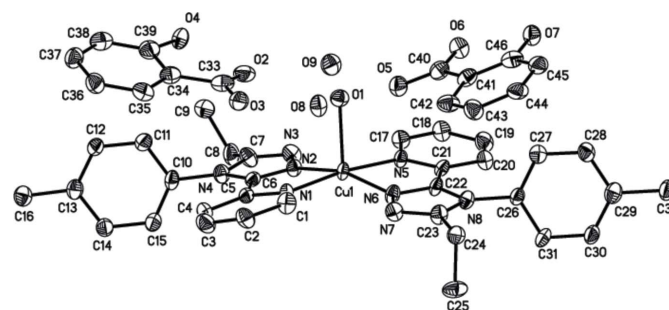


Figure 1
 The asymmetric unit of the title compound with atomic labelling. Displacement ellipsoids are shown at 30% probability level. H atoms are not shown.

Experimental

A solution of 3-ethyl-4-(*p*-methylphenyl)-5-(2-pyridyl)-1,2,4-triazole (1.06 g, 4.0 mmol) in 15 ml of ethanol was added to a solution of copper(II) disalicylate (0.68 g, 2.0 mmol) in 15 ml of water at room temperature, and stirred for 5 min, then filtered; the filtrate was left to stand at room temperature. Single crystals suitable for X-ray diffraction were obtained by slow evaporation of an ethanol–water solution (1:1 *v/v*) at room temperature for several days.

Crystal data

[Cu(C ₁₆ H ₁₆ N ₄) ₂ (H ₂ O)]· (C ₇ H ₅ O ₃) ₂ ·2H ₂ O	$\gamma = 92.669 (14)^\circ$
$M_r = 920.46$	$V = 2225 (3) \text{ \AA}^3$
Triclinic, $P\bar{1}$	$Z = 2$
$a = 10.076 (9) \text{ \AA}$	$D_x = 1.374 \text{ Mg m}^{-3}$
$b = 12.845 (11) \text{ \AA}$	Mo $K\alpha$ radiation
$c = 18.337 (16) \text{ \AA}$	$\mu = 0.56 \text{ mm}^{-1}$
$\alpha = 106.716 (11)^\circ$	$T = 571 (2) \text{ K}$
$\beta = 100.195 (12)^\circ$	Block, blue
	$0.28 \times 0.24 \times 0.22 \text{ mm}$

Data collection

Bruker SMART APEX CCD diffractometer	20846 measured reflections
φ and ω scans	8763 independent reflections
Absorption correction: multi-scan (SADABS; Bruker, 2000)	7180 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.860$, $T_{\max} = 0.887$	$R_{\text{int}} = 0.037$
	$\theta_{\max} = 26.0^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.07P)^2 + 1.99P]$
$R[F^2 > 2\sigma(F^2)] = 0.060$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.145$	$(\Delta/\sigma)_{\max} < 0.001$
$S = 1.01$	$\Delta\rho_{\max} = 0.29 \text{ e \AA}^{-3}$
8763 reflections	$\Delta\rho_{\min} = -0.51 \text{ e \AA}^{-3}$
581 parameters	
H-atom parameters constrained	

Table 1

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

Cu1–N6	1.970 (3)	Cu1–N5	2.042 (3)
Cu1–N2	1.984 (3)	Cu1–O1	2.186 (3)
Cu1–N1	2.011 (3)		
N6–Cu1–N2	162.39 (12)	N1–Cu1–N5	172.20 (12)
N6–Cu1–N1	98.66 (12)	N6–Cu1–O1	98.82 (12)
N2–Cu1–N1	80.05 (12)	N2–Cu1–O1	98.79 (12)
N6–Cu1–N5	79.92 (12)	N1–Cu1–O1	94.73 (12)
N2–Cu1–N5	98.96 (12)	N5–Cu1–O1	93.07 (12)

Table 2

Hydrogen-bond geometry (\AA , $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1–H1C \cdots O5	0.85	1.98	2.675 (4)	139
O1–H1A \cdots O2	0.82	2.01	2.799 (4)	161
O4–H4A \cdots O2	0.82	1.55	2.301 (4)	152
O7–H7 \cdots O6	0.82	1.73	2.470 (4)	148
O8–H8A \cdots O5	0.85	2.00	2.808 (4)	157
O8–H8B \cdots O3	0.85	2.29	2.753 (4)	114
O9–H9F \cdots O8	0.85	2.13	2.976 (4)	180
O9–H9E \cdots O8 ⁱ	0.85	2.33	3.015 (4)	139

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

All H atoms were located in a difference Fourier map and allowed to ride on their parent atoms at distances of 0.93 (C–H aromatic), 0.96 (C–H methyl), 0.97 (C–H methylene), 0.82 (O–H phenol) and 0.85 \AA (O–H water), and with $U_{\text{iso}}(\text{H})$ values of 1.2–1.5 times U_{eq} of the parent atoms.

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

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