

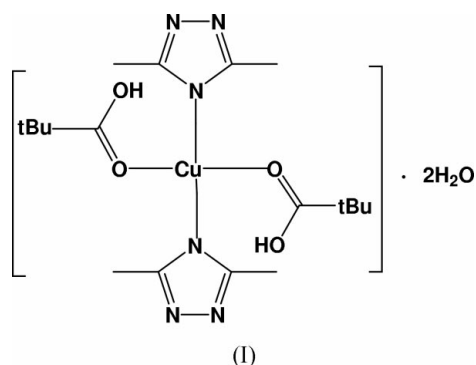
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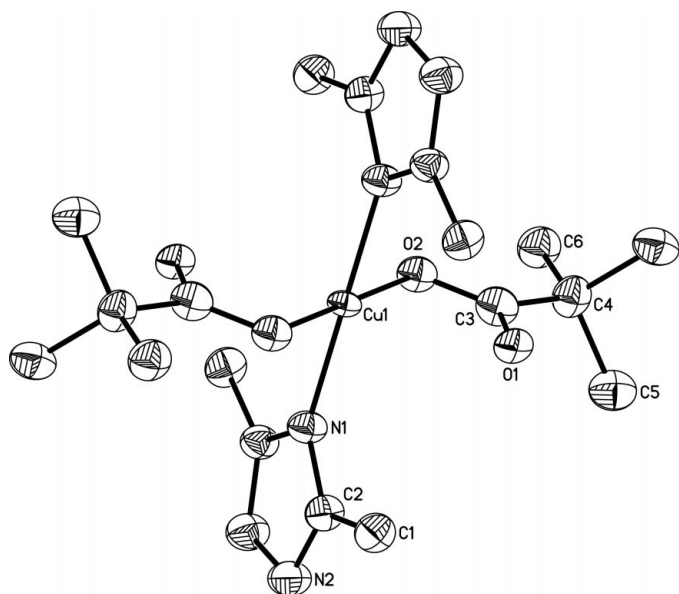
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## Key indicators

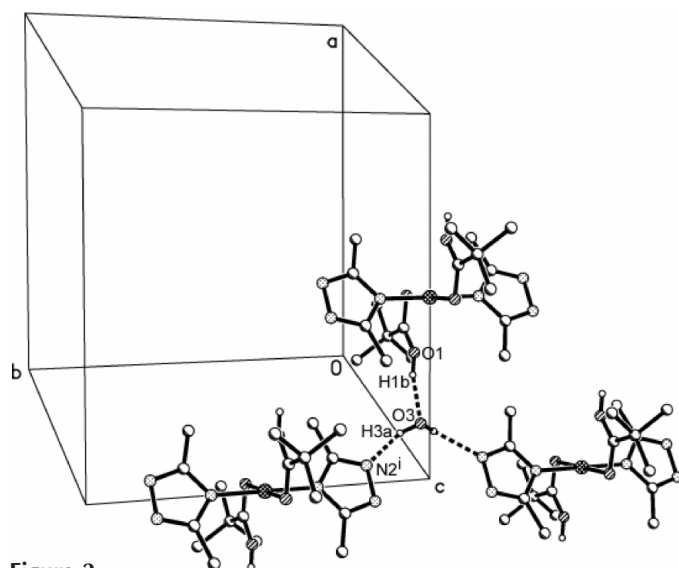
Single-crystal X-ray study  
 $T = 293\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.008\text{ \AA}$   
 $R$  factor = 0.062  
 $wR$  factor = 0.164  
Data-to-parameter ratio = 15.6For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.Bis(3,5-dimethyl-1,2,4-triazolato- $\kappa N^4$ )bis(pivalic  
acid- $\kappa O$ )copper(II) dihydrateThe molecule of the title complex,  $[\text{Cu}(\text{C}_4\text{H}_6\text{N}_3)_2(\text{C}_5\text{H}_9\text{O}_2)_2] \cdot 2\text{H}_2\text{O}$ , is situated about a site of symmetry  $2/m$  and shows a *trans*- $\text{N}_2\text{O}_2$  square-planar coordination geometry for the  $\text{Cu}^{\text{II}}$  centre. The crystal structure exhibits a two-dimensional layer arrangement mediated by intermolecular hydrogen bonds.Received 8 October 2004  
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## Comment

Molecular materials exhibiting interesting magnetic and luminescent properties have received increasing attention in recent years (Kahn *et al.*, 1992; Kahn, 1993; Haasnoot, 2000; Thompson, 2002). 1,2,4-Triazole and its derivatives are able to provide several bridging coordination modes to link metal(II) ions, an important consideration for molecular materials. Indeed, many structures of coordination complexes have been reported, showing a variety of coordination modes (Haasnoot, 2000). Rare examples of structures containing the bridging 3,5-dimethyl-1,2,4-triazole ligand include  $N^1, N^2$  bridging (Yi *et al.*, 2004) and  $N^1, N^2, N^4$  bridging (Drew *et al.*, 1985; Zhang *et al.*, 2004). Here, we report the title copper(II) complex, (I), with the 3,5-dimethyl-1,2,4-triazole ligand exhibiting a monodentate  $N^4$  coordination mode.The molecule of (I) is disposed about a site of symmetry  $2/m$  (Fig. 1 and Table 1). The  $\text{Cu}^{\text{II}}$  atom is coordinated by two  $N^4$  atoms from two 3,5-dimethyl-1,2,4-triazole anions in a *trans* configuration. The  $\text{Cu}-N^4$  bond distances [mean  $1.994(5)\text{ \AA}$ ] are in the range of those reported for *catena*-[[ $\mu_3$ -3,5-dimethyl-1,2,4-triazolato- $\kappa^3 N, N', N''$ ]]copper(I) [ $1.963(1)$ – $2.016(1)\text{ \AA}$ ; Zhang *et al.*, 2004]. The two remaining coordination sites in the square-planar geometry are occupied by O atoms from two pivalic acid molecules.The crystal structure of (I) features intermolecular hydrogen bonds, as shown in Fig. 2; geometric details are given in Table 2. The hydroxyl group of (I) forms a hydrogen bond with the O atom of the solvent water molecule ( $\text{O1}-\text{H1B} \cdots \text{O3}$ ). The water molecule, in turn, links two N2 atoms, so that a two-dimensional layer structure results.



**Figure 1**  
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms have been omitted for clarity.



**Figure 2**  
The two-dimensional layer structure of (I) [symmetry code: (i)  $\frac{1}{2} - x, \frac{1}{2} - y, 2 - z$ ]. Dashed lines indicate hydrogen bonds.

### Experimental

3,5-Dimethyl-1,2,4-triazole (0.068 g, 0.7 mmol) was added to an ethanol solution (10 ml) of  $[\text{Cu}(\text{Me}_3\text{CCOO})_2]_2$  (0.15 g, 0.28 mmol) with stirring. The resulting solution was stirred at 276 K for 24 h and then filtered. Uncharacterized blue compounds, which formed on slow evaporation of the mother liquor, were filtered off several times, before red crystals of (I) suitable for X-ray diffraction analysis were obtained from the mother liquor (18% yield). Analysis calculated for  $\text{C}_{18}\text{H}_{36}\text{Cu}_1\text{N}_6\text{O}_6$ : C 43.58, H 7.32, N 16.94%; found: C 43.83, H 7.61, N 16.74%; IR (KBr,  $\nu$ ,  $\text{cm}^{-1}$ ): 3375 (*br*), 3053 (*w*), 2966 (*m*), 2935 (*w*), 2720 (*w*), 1596 (*m*), 1553 (*vs*), 1484 (*m*), 1439 (*w*), 1418 (*s*), 1378 (*m*),

1364 (*m*), 1322 (*w*), 1225 (*m*), 1146 (*w*), 1087 (*w*), 1051 (*w*), 902 (*w*), 754 (*w*), 619 (*m*).

### Crystal data

$[\text{Cu}(\text{C}_4\text{H}_6\text{N}_3)_2(\text{C}_5\text{H}_{10}\text{O}_2)_2] \cdot 2\text{H}_2\text{O}$   
 $M_r = 496.07$   
 Monoclinic,  $C2/m$   
 $a = 13.270$  (3) Å  
 $b = 12.861$  (3) Å  
 $c = 8.770$  (2) Å  
 $\beta = 115.791$  (4)°  
 $V = 1347.6$  (5) Å<sup>3</sup>  
 $Z = 2$

$D_x = 1.222$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 Cell parameters from 709 reflections  
 $\theta = 2.9\text{--}22.9^\circ$   
 $\mu = 0.85$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
 Block, red  
 $0.33 \times 0.28 \times 0.23$  mm

### Data collection

Bruker SMART APEX CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Bruker, 2000)  
 $T_{\text{min}} = 0.767$ ,  $T_{\text{max}} = 0.829$   
 3525 measured reflections

1311 independent reflections  
 1141 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.053$   
 $\theta_{\text{max}} = 25.5^\circ$   
 $h = -16 \rightarrow 15$   
 $k = -15 \rightarrow 15$   
 $l = -10 \rightarrow 9$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.062$   
 $wR(F^2) = 0.164$   
 $S = 1.09$   
 1311 reflections  
 84 parameters  
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.09P)^2 + 1.95P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.38$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.50$  e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

|              |           |                             |            |
|--------------|-----------|-----------------------------|------------|
| Cu1—O2       | 1.974 (4) | C3—O2                       | 1.253 (8)  |
| Cu1—N1       | 1.994 (5) | C3—C4                       | 1.480 (7)  |
| C1—C2        | 1.488 (6) | C4—C5                       | 1.501 (7)  |
| C2—N2        | 1.306 (6) | C4—C6                       | 1.503 (10) |
| C2—N1        | 1.337 (5) | N2—N2 <sup>i</sup>          | 1.399 (8)  |
| C3—O1        | 1.251 (7) |                             |            |
| O1—C3—O2     | 120.7 (5) | Cu1—N1—C2                   | 127.6 (3)  |
| O1—C3—C4     | 120.8 (6) | Cu1—O2—C3                   | 103.3 (3)  |
| O1—C3—C4—C6  | 180       | C1—C2—N1—Cu1                | 1.1 (6)    |
| O2—C3—C4—C6  | 0         | O2—Cu1—N1—C2                | 120.2 (3)  |
| N2—C2—N1—Cu1 | 179.6 (3) | O2 <sup>ii</sup> —Cu1—N1—C2 | -59.8 (3)  |

Symmetry codes: (i)  $1 - x, y, 2 - z$ ; (ii)  $1 - x, -y, 2 - z$ .

**Table 2**

Hydrogen-bonding geometry (Å, °).

| $D\text{—}H \cdots A$     | $D\text{—}H$ | $H \cdots A$ | $D \cdots A$ | $D\text{—}H \cdots A$ |
|---------------------------|--------------|--------------|--------------|-----------------------|
| O1—H1B <sup>i</sup> ···O3 | 0.85         | 1.86         | 2.637 (6)    | 151                   |
| O3—H3A···N2 <sup>i</sup>  | 0.85         | 2.07         | 2.748 (5)    | 137                   |

Symmetry code: (i)  $\frac{1}{2} - x, \frac{1}{2} - y, 2 - z$ .

Atoms H1B and H3A were found in a difference Fourier map and not refined. All other H atoms were positioned geometrically and refined in the riding-model approximation, with  $C\text{—}H = 0.96$  Å and  $U_{\text{iso}}(H) = 1.2$  (1.5 for methyl H) times  $U_{\text{eq}}(\text{parent atom})$ .

Data collection: SMART (Bruker, 2000); cell refinement: SMART; data reduction: SAINT (Bruker, 2000); 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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