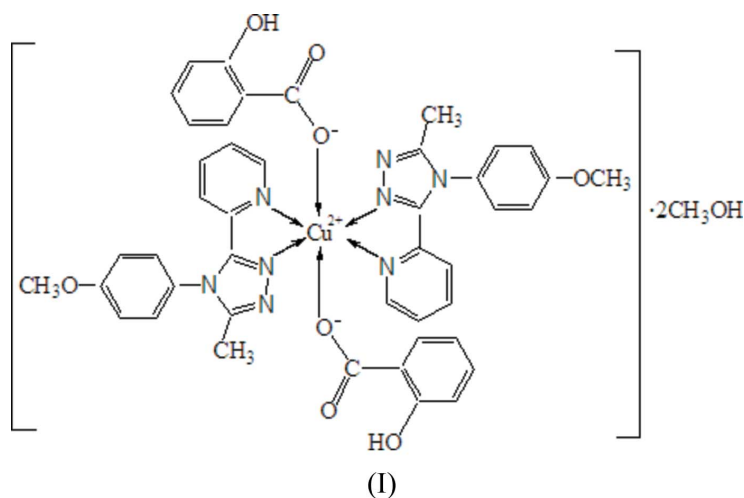


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## Key indicators

Single-crystal X-ray study  
 $T = 293\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.005\text{ \AA}$   
 $R$  factor = 0.058  
 $wR$  factor = 0.129  
Data-to-parameter ratio = 14.3For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.Bis[4-(4-methoxyphenyl)-3-methyl-5-(2-pyridyl)-4H-  
1,2,4-triazole- $\kappa\text{N}^1$ ]bis(salicylato- $\kappa\text{O}$ )copper(II)  
methanol disolvateIn the title complex,  $[\text{Cu}(\text{C}_7\text{H}_5\text{O}_3)_2(\text{C}_{15}\text{H}_{14}\text{N}_4\text{O})_2] \cdot 2\text{CH}_3\text{OH}$ , the  $\text{Cu}^{\text{II}}$  cation is located on a centre of inversion and exists in a distorted octahedral geometry defined by a  $\text{CuN}_2\text{N}'_2\text{O}_2$  donor set.Received 23 December 2005  
Accepted 16 January 2006

## Comment

The coordination chemistry of substituted 1,2,4-triazoles has received considerable attention in recent years (Bencini *et al.*, 1987; Koningsbruggen *et al.*, 1997; Moliner *et al.*, 1998, 2001; Klingele & Brooker, 2003). This arises, in part, because the ligand donor ability is optimal to give  $\text{Fe}^{\text{II}}$  spin-crossover complexes, which could be used as molecular-based memory devices, displays and optical switches (Garcia *et al.*, 1997; Kahn & Martinez, 1998). Recently, we have prepared some new substituted 1,2,4-triazole derivatives (Wang *et al.*, 2005; Liu *et al.*, 2005) and their transition metal complexes. Here, we report the crystal structure analysis of the title complex, (I).The crystal structure of (I) (Fig. 1 and Table 1) contains centrosymmetric  $\text{Cu}^{\text{II}}$  complexes in which individual Cu centres exist in a  $\text{CuN}_2\text{N}'_2\text{O}_2$  donor set that defines a distorted octahedral geometry. From symmetry, the four N atoms coordinate in a plane around the Cu atom. The O atoms derived from the two carboxylate groups interact more weakly in the axial positions; the  $\text{Cu1}-\text{O1}$  distance is  $2.442(2)\text{ \AA}$ .

The N1 atom of the 1,2,4-triazole ring and the carboxylate atom O1 each form a hydrogen bond with the OH atom of the solvent methanol molecule, indicating that this H atom is bifurcated; details are presented in Table 2.

Experimental

The title complex was synthesized by the reaction of 3-methyl-4-(*p*-methoxyphenyl)-5-(2-pyridyl)-1,2,4-triazole (1.20 g, 3.0 mmol) with copper(II) disalicylate (0.51 g, 1.5 mmol) dissolved in methanol (20 ml) at room temperature. Single crystals of (I) suitable for X-ray diffraction were obtained by evaporation of the methanol solution at room temperature.

Crystal data

[Cu(C<sub>7</sub>H<sub>5</sub>O<sub>3</sub>)<sub>2</sub>(C<sub>15</sub>H<sub>14</sub>N<sub>4</sub>O)<sub>2</sub>]<sub>2</sub>·2CH<sub>4</sub>O  
*M<sub>r</sub>* = 934.45  
 Monoclinic, *P*2<sub>1</sub>/*n*  
*a* = 8.643 (3) Å  
*b* = 14.638 (2) Å  
*c* = 17.715 (3) Å  
 $\beta$  = 100.579 (5)°  
*V* = 2203.3 (9) Å<sup>3</sup>  
*Z* = 2  
*D<sub>x</sub>* = 1.409 Mg m<sup>-3</sup>  
 Mo *K*α radiation  
 Cell parameters from 895 reflections  
 $\theta$  = 2.7–25.6°  
 $\mu$  = 0.56 mm<sup>-1</sup>  
*T* = 293 (2) K  
 Block, blue  
 0.33 × 0.24 × 0.22 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Bruker, 2000)  
*T<sub>min</sub>* = 0.849, *T<sub>max</sub>* = 0.881  
 11519 measured reflections  
 4265 independent reflections  
 2913 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.055  
 $\theta_{max}$  = 26.0°  
*h* = -10 → 10  
*k* = -18 → 15  
*l* = -18 → 21

Refinement

Refinement on *F*<sup>2</sup>  
*R* [*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.058  
*wR* (*F*<sup>2</sup>) = 0.129  
*S* = 1.03  
 4265 reflections  
 298 parameters  
 H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0614P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{max} < 0.001$   
 $\Delta\rho_{max} = 0.42 \text{ e } \text{Å}^{-3}$   
 $\Delta\rho_{min} = -0.32 \text{ e } \text{Å}^{-3}$

Table 1

Selected geometric parameters (Å, °).

Cu1—O1	2.442 (2)	O2—C22	1.249 (4)
Cu1—N1	1.993 (2)	O3—C17	1.339 (4)
Cu1—N4	2.032 (2)	C17—O3	1.339 (4)
O1—C22	1.246 (4)	C22—O2	1.249 (4)
O1—Cu1—N1	94.14 (9)	O1—C22—O2	123.6 (3)
O1—Cu1—N4	90.56 (9)	O1—C22—C16	118.3 (3)
N1—Cu1—N4	79.87 (10)	O2—C22—C16	118.2 (3)

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>
O5—H5D...O1 <sup>i</sup>	0.89	2.29	2.792 (3)	116
O5—H5D...N1 <sup>ii</sup>	0.89	2.47	3.302 (4)	156

Symmetry codes: (i) -*x* + 1, -*y* + 1, -*z* + 1; (ii) *x*, *y*, *z* - 1.

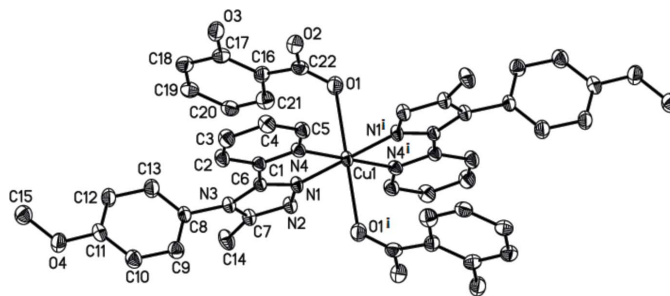


Figure 1

The molecular structure of the cation in (I), showing the atomic labelling. Displacement ellipsoids are shown at the 50% probability level. H atoms have been omitted for clarity. Unlabelled atoms and those with symmetry code (i) are at (1 - *x*, 1 - *y*, 2 - *z*).

All H atoms were allowed to ride on their parent atoms at distances of 0.93 (aromatic H), 0.96 (methyl H), 0.89 (O—H methanol) and 0.96 Å (O—H phenol), and with *U<sub>iso</sub>*(H) values of 1.2*U<sub>eq</sub>*(parent atom) for aromatic H and methanol O—H, and 1.5*U<sub>eq</sub>*(parent atom) for methyl H and phenol O—H.

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.

The authors are grateful to the Department of Chemistry and Chemical Engineering, Southeast University, for financial assistance through project No. 913-9207041142.

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