

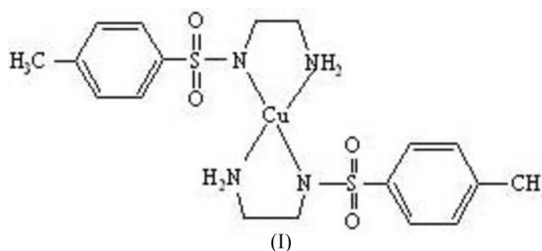
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## Key indicators

Single-crystal X-ray study  
 $T = 296$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å  
 $R$  factor = 0.037  
 $wR$  factor = 0.115  
Data-to-parameter ratio = 15.1For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.Bis[*N*-(2-aminoethyl)-4-methylbenzene-  
sulfonamidato]copper(II)The title compound,  $[\text{Cu}(\text{C}_9\text{H}_{13}\text{N}_2\text{O}_2\text{S})_2]$ , is a centrosymmetric neutral complex with the  $\text{Cu}^{\text{II}}$  atom showing slightly distorted square-planar  $\text{CuN}_4$  geometry. The crystal packing is consolidated by intramolecular  $\text{N}-\text{H}\cdots\text{O}$  and intermolecular  $\text{C}-\text{H}\cdots\pi$  interactions.Received 1 November 2006  
Accepted 3 November 2006

## Comment

Although the substitution of the amide proton by a metal ion is not an easy process (Antolini *et al.*, 1985), in the case of a sulfonamide group the acidity of the H atom is increased and its replacement is easier (Otter *et al.*, 1998; Sanchez-Piso *et al.*, 2002). This process led to the title compound, (I) (Fig. 1), which exists as a neutral complex.

The  $\text{Cu}^{\text{II}}$  atom in (I) (site symmetry  $\bar{1}$ ) is chelated by two ligands, which use their amide and amine N atoms to bond to the metal (Table 1). A square-planar  $\text{CuN}_4$  geometry arises, the  $\text{N1}\cdots\text{N2}$  and  $\text{N1}\cdots\text{N2}^i$  separations being 2.631 (4) and 3.023 (4) Å, respectively. The  $\text{Cu1}-\text{N1}$  distance is significantly longer than  $\text{Cu1}-\text{N2}$  distance, suggesting that the amine N atom is a slightly better donor than the amide N atom. The bond-valence sum for the Cu centre is calculated to be 2.02, which is very close to the expected value of 2 (Thorp, 1992). This suggests that the two very long  $\text{Cu}\cdots\text{O1}$  contacts of 2.699 (2) Å linking the Cu atom to sulfonamide O atoms of neighbouring molecules should not be regarded as bonds.

An intramolecular  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bond helps to stabilize the molecular conformation (Table 2). The crystal structure may be further stabilized by two weak  $\text{C}-\text{H}\cdots\pi$  interactions.

## Experimental

The *N*-(2-aminoethyl)-4-methylbenzenesulfonamide ligand (*L*) was synthesized according to a literature method (Barros & Sineriz, 2000). An ethanol solution (10 ml) of  $\text{Cu}(\text{CH}_3\text{COO})_2\cdot\text{H}_2\text{O}$  (0.19 g, 1 mmol) was added to a solution of *L* (0.214 g, 1 mmol) in ethanol (20 ml) with stirring for 1 h. The resulting blue solution was filtered, the filtrate allowed to stand and blue block-shaped crystals of (I) were obtained by slow evaporation after two weeks.

Crystal data

[Cu(C<sub>9</sub>H<sub>13</sub>N<sub>2</sub>O<sub>2</sub>S)<sub>2</sub>]  
*M<sub>r</sub>* = 490.09  
 Triclinic, *P* $\bar{1}$   
*a* = 5.6497 (6) Å  
*b* = 7.8410 (9) Å  
*c* = 13.2882 (15) Å  
 $\alpha$  = 73.020 (1)°  
 $\beta$  = 84.913 (1)°  
 $\gamma$  = 69.454 (1)°

*V* = 527.12 (10) Å<sup>3</sup>  
*Z* = 1  
*D<sub>x</sub>* = 1.544 Mg m<sup>-3</sup>  
 Mo *K*α radiation  
 $\mu$  = 1.27 mm<sup>-1</sup>  
*T* = 296 (2) K  
 Block, blue  
 0.39 × 0.30 × 0.20 mm

Data collection

Bruker SMART CCD  
 diffractometer  
 $\omega$  scans  
 Absorption correction: multi-scan  
 (SADABS; Bruker, 2001)  
*T<sub>min</sub>* = 0.641, *T<sub>max</sub>* = 0.785

2651 measured reflections  
 1848 independent reflections  
 1715 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.014  
 $\theta_{max}$  = 25.1°

Refinement

Refinement on *F*<sup>2</sup>  
*R* [*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.037  
*wR* (*F*<sup>2</sup>) = 0.115  
*S* = 1.00  
 1848 reflections  
 122 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0885P)^2 + 0.2074P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{max} < 0.001$   
 $\Delta\rho_{max} = 0.54 \text{ e \AA}^{-3}$   
 $\Delta\rho_{min} = -0.32 \text{ e \AA}^{-3}$   
 Extinction correction: SHELXL97  
 Extinction coefficient: 0.044 (7)

Table 1

Selected bond lengths (Å).

Cu1—N2	1.983 (2)	Cu1—N1	2.024 (2)
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Table 2

Hydrogen-bond geometry (Å, °).

C<sub>g</sub> is the centroid of ring C1—C6.

<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>
N2—H2B...O2 <sup>i</sup>	0.90	2.10	2.849 (4)	140
C7—H7B...C <sub>g</sub> <sup>ii</sup>	0.93	3.13	3.989 (3)	154
C15—H15B...C <sub>g</sub> <sup>iii</sup>	0.97	3.01	3.741 (4)	161

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

The H atoms were located in difference maps, relocated in idealized positions (C—H = 0.93–0.97 Å and N—H = 0.90 Å) and refined as riding, with *U*<sub>iso</sub>(H) = 1.2*U*<sub>eq</sub>(C,N).

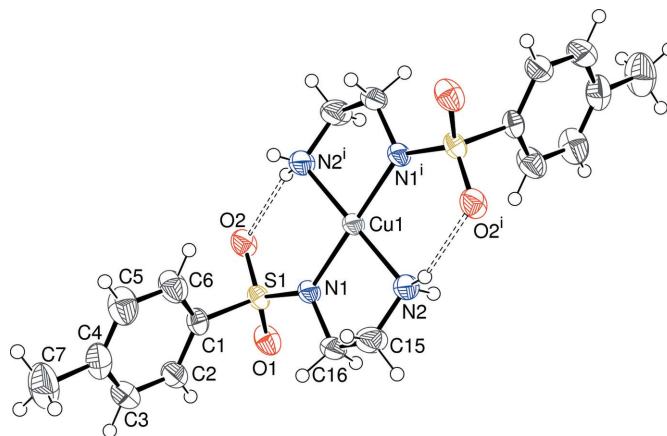


Figure 1

View of the molecular structure of (I), showing 50% probability displacement ellipsoids (arbitrary spheres for the H atoms). Hydrogen bonds are shown as dashed lines. [Symmetry code: (i) 1 - *x*, -*y*, 1 - *z*.]

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: SHELXTL (Bruker, 2001); software used to prepare material for publication: SHELXTL.

Financial support from the National Natural Science Foundation of China (No. 20471035) is acknowledged.

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