

G. M. Golzar Hossain,\* Afroza Banu and A. J. Amoroso

School of Chemistry, Cardiff University, Main Building, Cardiff CF10 3AT, Wales

Correspondence e-mail: acsbd@yahoo.com

#### Key indicators

Single-crystal X-ray study

$T = 150$  K

Mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å

$R$  factor = 0.055

$wR$  factor = 0.144

Data-to-parameter ratio = 16.8

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

## *trans*-Bis(ethylenediamine)bis(sulfadiazinato)-copper(II)

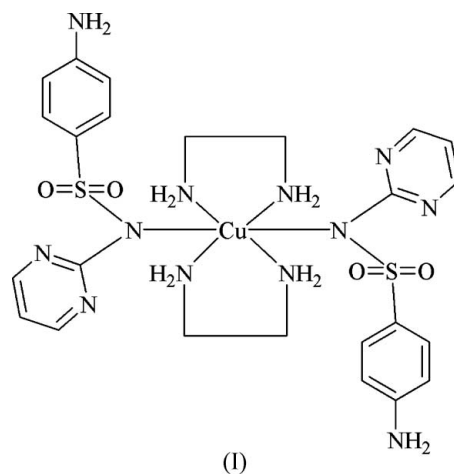
The structure of the title compound, *trans*-[Cu(C<sub>2</sub>H<sub>8</sub>N<sub>2</sub>)<sub>2</sub>-(C<sub>10</sub>H<sub>9</sub>N<sub>4</sub>O<sub>2</sub>S)<sub>2</sub>], consists of neutral molecules. The Cu<sup>2+</sup> ion occupies an inversion centre and exhibits an elongated distorted octahedral geometry, with two monodentate sulfadiazinate (sdz) anions and two bidentate ethylenediamine ligands. Both sdz ligands are *N*-coordinated *via* an N atom of the sulfonamide group. The crystal structure is stabilized by hydrogen bonds and weak van der Waals interactions.

Received 15 September 2006

Accepted 22 September 2006

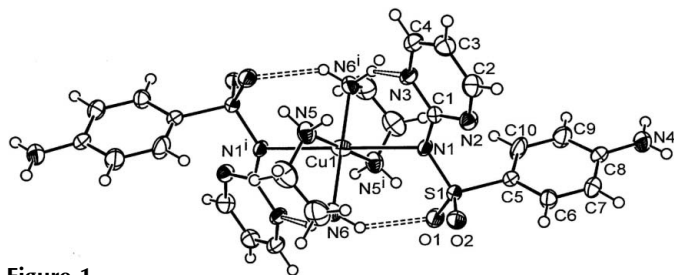
#### Comment

In the structure of the title compound, (I), [Cu(sdz)<sub>2</sub>(en)<sub>2</sub>], the Cu<sup>II</sup> ion occupies an inversion centre and is octahedrally coordinated by two en and two sdz ligands, forming a CuN<sub>6</sub> coordination environment. The en molecules act as bidentate ligands, forming two five-membered chelate rings with a *trans* arrangement. The structure has a Jahn–Teller-distorted octahedral geometry around the Cu<sup>II</sup> atom with four N atoms of the two chelating ethylenediamine molecules and two sulfonamide N atoms from sulfadiazine molecules completing the coordination of the elongated octahedral structure.

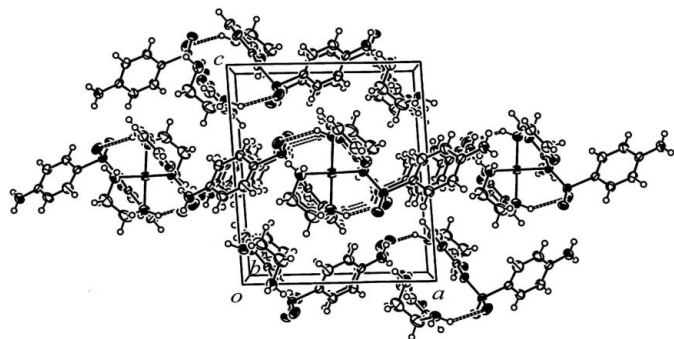


The two Cu–N<sub>en</sub> bond distances are almost equivalent, but significantly shorter than the Cu–N<sub>sdz</sub> bond distances, resulting in the formation of a distorted octahedral geometry elongated along the Cu–N<sub>sdz</sub> bonds. Thus, the en N atoms form the equatorial plane of the coordination octahedron, while the sulfonamide N atoms of sdz occupy the axial positions.

The Cu1–N1 bond distances of 2.672 (2) Å are elongated as a result of the Jahn–Teller effect. The bond lengths within the sulfadiazine and ethylenediamine are as expected. The Cu–N distances of 2.005 (3) and 2.013 (3) Å, involving the


**Figure 1**

The molecular structure, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are omitted for clarity. Symmetry code as in Table 1. Dashed lines indicate hydrogen bonds.


**Figure 2**

The molecular packing of (I) viewed along the *b* axis. Dashed lines indicate the hydrogen-bonding interactions.

ethylenediamine molecules, are comparable to the corresponding values 1.997 (3) and 2.001 (3) Å (Lokaj *et al.*, 1991), 2.033 (3) and 2.042 (3) Å (Anaconda *et al.*, 2002), 1.996 (2) and 2.022 (3) Å (Kovbasyuk *et al.*, 1997), 2.007 (3)–2.024 (3) Å (Kovbasyuk *et al.*, 1997), 2.016 (2) and 2.019 (2) Å (Fun *et al.*, 2002), and 2.007 (3) and 2.010 (3) Å (Kazak *et al.*, 2004). The S1–O bond distances of 1.458 (3) and 1.449 (3) Å are longer than the corresponding bonds in the pure sulfadiazine with values of 1.429 (2) and 1.437 (2) Å.

The crystal structure of the complex exhibits numerous hydrogen bonds (Table 2). The amino H atoms form intramolecular hydrogen bonds with the sulfonyl O atoms, as illustrated in Fig. 1. The amine H atoms of the en ligands and terminal amino H are also involved in intermolecular hydrogen bonding with the sulfonyl O atoms of neighbouring sdz ligands (Fig. 2).

## Experimental

The sodium salt of sulfadiazine (Nasdz) (0.545 g, 2 mmol) was dissolved in 50 ml of hot methanol and a methanol solution (10 ml) of  $\text{CuCl}_2 \cdot 2\text{H}_2\text{O}$  (0.171 g, 1 mmol) was added slowly with constant stirring on a hot-plate at 333 K; a red precipitate was formed and the mixture was stirred for 6 h. The precipitate was filtered off and dried over silica gel. The precipitate was dissolved in a 1:10 mixture of ethylenediamine/water (10 ml), stirred for 30 minutes. The solution was then filtered and left for crystallization; a week later, blue block

crystals were obtained, which were filtered off and dried over silica gel.

## Crystal data

$[\text{Cu}(\text{C}_2\text{H}_8\text{N}_2)_2(\text{C}_{10}\text{H}_9\text{N}_4\text{O}_2\text{S})_2]$   
 $M_r = 682.29$   
 Monoclinic,  $P2_1/n$   
 $a = 10.8610$  (5) Å  
 $b = 10.6329$  (4) Å  
 $c = 12.5227$  (6) Å  
 $\beta = 93.302$  (2)°  
 $V = 1443.77$  (11) Å<sup>3</sup>

$Z = 2$   
 $D_x = 1.569$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 $\mu = 0.96$  mm<sup>-1</sup>  
 $T = 150$  (2) K  
 Block, blue  
 $0.15 \times 0.12 \times 0.10$  mm

## Data collection

Nonius KappaCCD diffractometer  
 $\omega$  scans  
 Absorption correction: multi-scan (Blessing, 1995)  
 $T_{\min} = 0.870$ ,  $T_{\max} = 0.910$

9385 measured reflections  
 3290 independent reflections  
 2428 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.089$   
 $\theta_{\max} = 27.5^\circ$

## Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.055$   
 $wR(F^2) = 0.144$   
 $S = 1.03$   
 3290 reflections  
 196 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0579P)^2 + 1.6363P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.77$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.50$  e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

Cu1–N1	2.672 (2)	Cu1–N6	2.005 (3)
Cu1–N5	2.013 (3)		
N1 <sup>i</sup> –Cu1–N1	180	N1–Cu1–N6	89.68 (10)
N5 <sup>i</sup> –Cu1–N5	180	N5 <sup>i</sup> –Cu1–N6	95.10 (12)
N6 <sup>i</sup> –Cu1–N6	180	N5–Cu1–N6	84.90 (12)
N1–Cu1–N5	94.80 (10)	N1 <sup>i</sup> –Cu1–N5	85.20 (10)
N1 <sup>i</sup> –Cu1–N6	90.32 (10)		

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>
N6–H6B...O1	0.92	2.29	3.068 (4)	142
N6–H6A...N3 <sup>i</sup>	0.92	2.25	3.021 (4)	141
N5–H5B...O1 <sup>i</sup>	0.92	2.15	2.958 (4)	146

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

H atoms were placed in calculated positions ( $\text{C}–\text{H} = 0.95$  and  $0.99$  Å;  $\text{N}–\text{H} = 0.88$  and  $0.92$  Å, respectively, for H atoms on amino N4 (sulfadiazine), and N5 and N6 (ethylenediamine) atoms) and refined using a riding model. H atoms were given isotropic displacement parameters equal to 1.2 times  $U_{\text{eq}}$  of their parent atoms.

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); soft-

ware used to prepare material for publication: *WinGX* (Farrugia, 1999).

The authors acknowledge the School of Chemistry, Cardiff University.

## References

- Anacona, J. R., Ramos, N., Delgado, G. D. D. & Roque, E. M. (2002). *J. Coord. Chem.* **55**, 901–908.
- Blessing, R. H. (1995). *Acta Cryst.* **A51**, 33–38.
- Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
- Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
- Fun, H.-K., Hao, Q.-L., Wu, J., Yang, X.-J., Lu, L.-D., Wang, X., Chantrapromma, S., Razak, I. A. & Usman, A. (2002). *Acta Cryst.* **C58**, m87–m88.
- Hoof, R. W. W. (1998). *COLLECT*. Bruker AXS Inc., Delft, The Netherlands.
- Kazak, C., Yilmaz, V. T. & Yazicilar, T. K. (2004). *Acta Cryst.* **E60**, m593–m595.
- Kovbasyuk, L. A., Frisky, I. O., Kokozay, V. N. & Iskenderov, T. S. (1997). *Polyhedron*, **16**, 1723–172.
- Lokaj, J., Gyerová, K., Sopková, A., Sivý, J., Kettman, V. & Vrabel, V. (1991). *Acta Cryst.* **C47**, 2447–2448.
- Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.