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## Key indicators

 Single-crystal X-ray study  
 T = 150 K  
 Mean  $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$   
 R factor = 0.043  
 wR factor = 0.112  
 Data-to-parameter ratio = 17.4

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

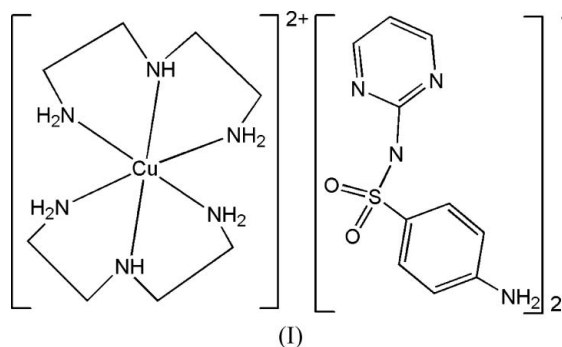
 Bis(diethylenetriamine- $\kappa^3\text{N}$ )copper(II)  
 bis(sulfadiazinate)

 In the title compound,  $[\text{Cu}(\text{C}_4\text{H}_{13}\text{N}_3)_2](\text{C}_{10}\text{H}_9\text{N}_4\text{O}_2\text{S})_2$ , the Cu atom (site symmetry  $\bar{1}$ ) displays a Jahn–Teller distorted octahedral  $\text{CuN}_6$  geometry arising from the two tridentate diethylenetriamine ligands. The cation and anion interact by way of  $\text{N}-\text{H}\cdots\text{N}$  and  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds.

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## Comment

 We have attempted to show the coordination behaviour of sulfadiazine with the copper(II) ion in the presence of diethylenetriamine. In the title complex, (I), the diethylenetriamine molecule coordinates directly with the Cu atom and the sulfadiazine molecule acts as counter-ion. The crystal structure of (I) contains  $[\text{Cu}(\text{dien})_2]^{2+}$  cations and  $\text{sdz}^-$  counter-ions (dien = diethylenetriamine and  $\text{sdzH}$  = sulfadiazine), forming a salt.

 The  $\text{Cu}^{\text{II}}$  centre (site symmetry  $\bar{1}$ ) is octahedrally coordinated by two tridentate dien molecules, with the  $\text{Cu}-\text{N}$  bond distances (Table 1) showing a typical Jahn–Teller distortion (Ye *et al.*, 1998). The central N atom of the ligand displays the shortest  $\text{Cu}-\text{N}$  bond. The *cis*  $\text{N}-\text{Cu}-\text{N}$  angles vary from  $80.49(9)$  to  $99.51(9)^\circ$ . The dihedral angle between the aromatic rings of the anion is  $71.10(14)^\circ$ .

 The cation and anion interact by way of  $\text{N}-\text{H}\cdots\text{N}$  and  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds (Table 2), resulting in a three-dimensional framework (Fig. 2). A weak  $\text{N}-\text{H}\cdots\text{N}$  bond between the anions also occurs. Compound (I) is the first copper complex containing sulfadiazine acting as a counter-ion.

## Experimental

 The sodium salt of sulfadiazine (Nasdz, 5.446 g, 2 mmol) was dissolved in hot methanol (50 ml) and a methanol solution (10 ml) of  $\text{CuCl}_2\cdot 2\text{H}_2\text{O}$  (1.705 g, 1 mmol) was added slowly with constant stirring on a hot plate. A red precipitate was formed and the mixture was

stirred for a further 6 h. The precipitate was filtered off and dried over silica gel; it was then dissolved in dimethylformamide solution (50 ml), diethylenetriamine (5 ml) was added and the mixture stirred for 30 min. A week later, blue block-shaped crystals of (I) were filtered off and dried over silica gel.

## Crystal data

$[\text{Cu}(\text{C}_4\text{H}_{13}\text{N}_3)_2](\text{C}_{10}\text{H}_9\text{N}_4\text{O}_2\text{S})_2$	$V = 1701.26 (8) \text{ \AA}^3$
$M_r = 768.43$	$Z = 2$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 14.5949 (3) \text{ \AA}$	$\mu = 0.82 \text{ mm}^{-1}$
$b = 7.8231 (2) \text{ \AA}$	$T = 150 (2) \text{ K}$
$c = 15.9672 (5) \text{ \AA}$	$0.18 \times 0.15 \times 0.12 \text{ mm}$
$\beta = 111.065 (1)^\circ$	

## Data collection

Nonius KappaCCD diffractometer	12097 measured reflections
Absorption correction: multi-scan (SORTAV; Blessing, 1995)	3882 independent reflections
$T_{\min} = 0.866$ , $T_{\max} = 0.908$	2736 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.061$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.043$	223 parameters
$wR(F^2) = 0.112$	H-atom parameters constrained
$S = 1.04$	$\Delta\rho_{\max} = 0.36 \text{ e \AA}^{-3}$
3882 reflections	$\Delta\rho_{\min} = -0.61 \text{ e \AA}^{-3}$

**Table 1**

Selected bond lengths ( $\text{\AA}$ ).

Cu1—N2	2.030 (2)	Cu1—N1	2.339 (3)
Cu1—N3	2.116 (3)		

**Table 2**

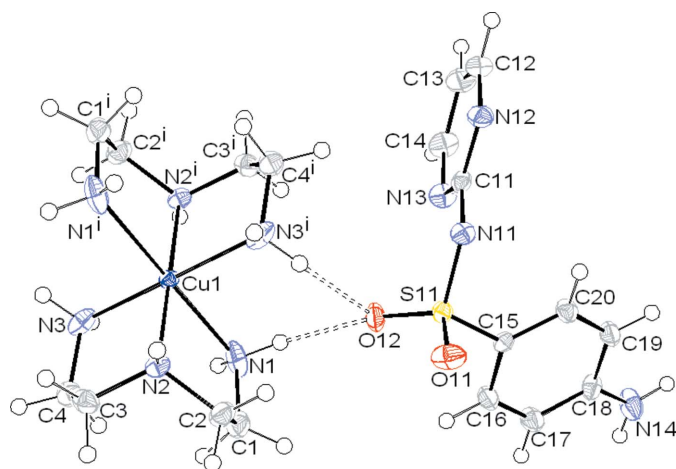
Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1B $\cdots$ O12	0.92	2.06	2.887 (3)	149
N1—H1A $\cdots$ N11 <sup>i</sup>	0.92	2.24	3.121 (3)	161
N2—H2 $\cdots$ N12 <sup>ii</sup>	0.93	2.14	3.068 (3)	174
N3—H3B $\cdots$ N11 <sup>i</sup>	0.92	2.44	3.283 (3)	152
N3—H3A $\cdots$ O12 <sup>iii</sup>	0.92	2.20	3.071 (3)	157
N14—H14A $\cdots$ N13 <sup>iv</sup>	0.88	2.47	3.161 (3)	136

Symmetry codes: (i)  $x, y - 1, z$ ; (ii)  $-x, -y + 1, -z$ ; (iii)  $-x, -y, -z$ ; (iv)  $-x + 1, y + \frac{1}{2}, -z + \frac{1}{2}$ .

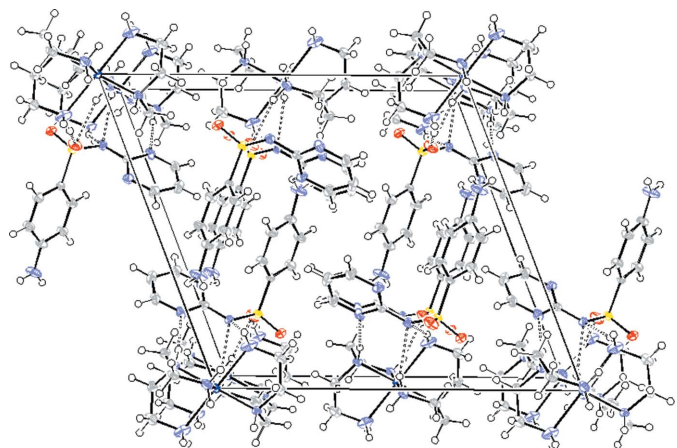
The H atoms were positioned geometrically ( $C-H = 0.95-0.99$  and  $N-H = 0.88-0.93 \text{ \AA}$ ) and refined as riding, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C,N})$ .

Data collection: COLLECT (Nonius, 2000); 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); software used to prepare material for publication: WinGX (Farrugia, 1999).



**Figure 1**

View of the molecular structure of (I), showing 50% displacement ellipsoids (arbitrary spheres for the H atoms) [symmetry code: (i)  $-x, -y, -z$ ]. Hydrogen bonds are indicated by dashed lines.



**Figure 2**

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

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