Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

Bis(4-aminobenzenesulfonato-κN)diaquabis(dimethylformamide-κO)copper(II)

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Received 28 March 2007
Accepted 4 April 2007

In the title compound, $[Cu(C_6H_6NO_3S)_2(C_3H_7NO)_2(H_2O)_2]$, the Cu^{II} atom lies on an inversion centre and is six-coordinate, with a distorted octahedral coordination geometry. It is coordinated by the amine N atoms of two 4-aminobenzenesulfonate anions, the O atoms of two dimethylformamide molecules and two water molecules. Each pair of equivalent ligands is mutually *trans*. N—H···O and O—H···O hydrogen-bonding interactions generate a three-dimensional architecture.

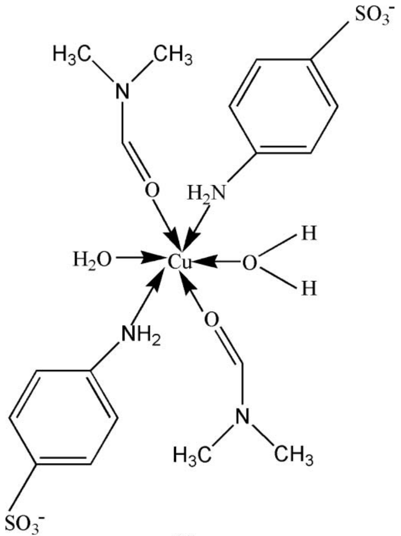
Key indicators

Single-crystal X-ray study
T = 291 K
Mean σ(C–C) = 0.002 Å
R factor = 0.025
wR factor = 0.074
Data-to-parameter ratio = 14.0

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

Comment

Currently, complexes with multidentate ligands coordinated to transition metals are of great interest, due to their use in constructing two- and three-dimensional polymers, with functional properties, that can be used as catalysts (Han *et al.*, 2006; Baca *et al.*, 2006), optical materials (Evans & Lin, 2001) or gas adsorbents (Kitagawa *et al.*, 2004). Sulfanilic acid, SAA, is a versatile ligand that can coordinate to metals in a variety of modes with donor atoms from both the amine and sulfonate groups (Starynowicz, 1992; Gunderman *et al.*, 1996; Huang *et al.*, 2004). In addition, it can act as a hydrogen-bond acceptor and donor (Wang *et al.*, 2002). We report here the structure of the title complex, (I) (Fig. 1).



(I)

The Cu^{II} atom of (I) lies on an inversion centre and is coordinated by the amine N atoms of two SAA^- ligands, the O atoms of two dimethylformamide molecules and two water molecules. The inversion symmetry means that each pair of equivalent ligands is mutually *trans*.

In the crystal structure of (I), O—H···O, O—H···S and N—H···O hydrogen bonds involving the three sulfonate O atoms, the amine N atom of the SAA$^-$ ligands and the water molecules form an extensive three-dimensional network (Table 1, Fig. 2).

Experimental

Sulfanilic acid (0.5 mmol, 0.086 g) was dissolved in water and dimethylformamide (12 ml, 5:1 *v*/*v*). To this solution, $CuCl_2 \cdot 2H_2O$ (0.5 mmol, 0.085 g) was added; the resulting mixture was stirred and refluxed at 353 K for 5 h, and the solution was then filtered. Blue block-like crystals of (I) were obtained from the filtrate after several days at room temperature.

Crystal data

$[Cu(C_6H_6NO_3S)_2(C_3H_7NO)_2(H_2O)_2]$
$M_r = 590.12$
Monoclinic, $P2_1/n$
$a = 7.178$ (1) Å
$b = 11.8969$ (16) Å
$c = 14.649$ (2) Å
$\beta = 100.973$ (1)°
$V = 1228.1$ (3) Å^3
$Z = 2$
Mo $K\alpha$ radiation
$\mu = 1.12$ mm^{-1}
$T = 291$ (2) K
0.49 × 0.46 × 0.36 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
$T_{min} = 0.610$, $T_{max} = 0.689$
7724 measured reflections
2287 independent reflections
2151 reflections with $I > 2\sigma(I)$
$R_{int} = 0.016$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.025$
$wR(F^2) = 0.074$
$S = 1.03$
2287 reflections
163 parameters
H-atom parameters constrained
$\Delta\rho_{max} = 0.37$ e Å^{-3}
$\Delta\rho_{min} = -0.41$ e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H1*W*···O5^{i}	0.83	2.11	2.927 (2)	171
O2—H1*W*···S1^{i}	0.83	3.00	3.7372 (14)	150
O2—H2*W*···O4^{ii}	0.84	2.09	2.9215 (19)	172
O2—H2*W*···S1^{ii}	0.84	3.00	3.7672 (14)	154
N1—H1*A*···O3^{ii}	0.90	2.10	2.9991 (19)	173
N1—H1*B*···O3^{iii}	0.90	2.19	3.0421 (18)	158

Symmetry codes: (i) $x-\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$; (ii) $x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$; (iii) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$.

Water H atoms were located in a difference Fourier map and refined as riding. All other H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$ for aromatic H, C—H = 0.96 Å and $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl H, and N—H = 0.90 Å and $U_{iso}(H) = 1.2U_{eq}(N)$ for N-bound H atoms.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); 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, 2004); software used to prepare material for publication: *SHELXTL*.

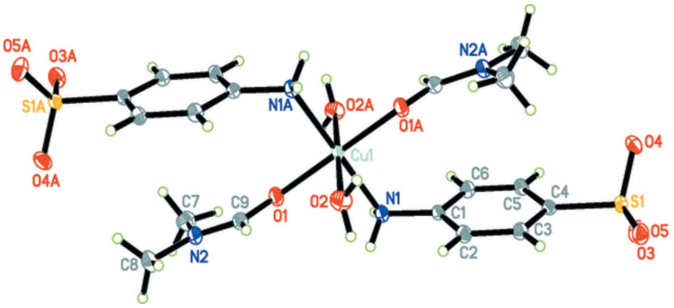


Figure 1
The molecular structure of compound (I). Displacement ellipsoids are drawn at the 30% probability level. Atoms labelled A and unlabelled atoms are related to the atoms of the asymmetric unit by the symmetry operation ($-x$, $-y$, $-z$).

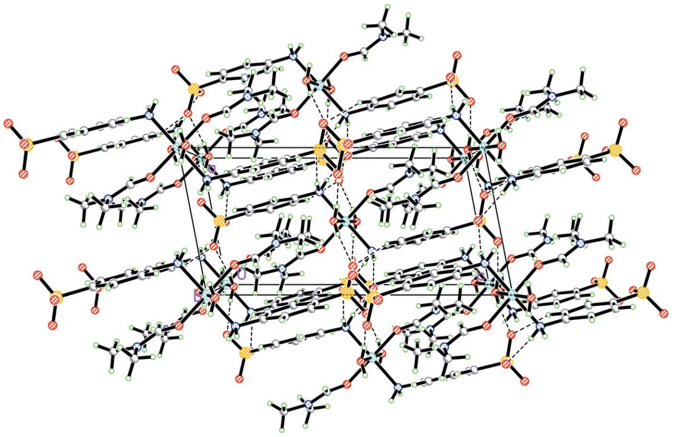


Figure 2
The packing of (I), with hydrogen bonds shown as dashed lines.

This work was supported by the National Natural Science Foundation of China (Nos. 20471026 and 20331010) and the Natural Science Foundation of Henan Province (No. 0311021200).

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Acta Cryst. (2007). E**63**, m1354–m1355 Du *et al.* • $[Cu(C_6H_6NO_3S)_2(C_3H_7NO)_2(H_2O)_2]$ **m1355**