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Key indicators

Single-crystal X-ray study
 $T = 299$ K
Mean $\sigma(\text{C}-\text{C}) = 0.006$ Å
 R factor = 0.071
 wR factor = 0.202
Data-to-parameter ratio = 12.7For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Bis[4-nitro-*N*-(quinolin-8-yl)benzenesulfon-
amidato- κ^2N,N']copper(II)

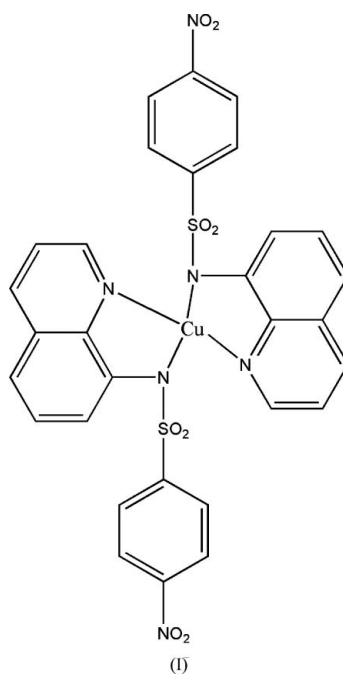
The asymmetric unit of the title compound, $[\text{Cu}(\text{C}_{15}\text{H}_{10}\text{N}_3\text{O}_4\text{S})_2]$, contains one half-molecule. The other half of the complex molecule is related by a C_2 axis running through the Cu atom. The Cu atom is four-coordinated by two quinoline N and two sulfonamide N atoms. In the crystal structure, the molecules are linked through intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds.

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Comment

Copper complexes based on sulfonamides have been investigated as potential reagents for the cleavage of nucleic acids (Macías *et al.*, 2003). Moreover, organic copper complexes based on quinoline rings can potentially and selectively inhibit the chymotrypsin-like activity of the proteasome (Daniel *et al.*, 2004). In the light of this interest, we report here the structure of the title compound, (I). As in related structure reported by Macías *et al.* (2002), in (I), the Cu atom is four-coordinated by the two quinoline N and the two sulfonamide N atoms. A C_2 axis runs through the Cu atom. The Cu—N bonds are slightly longer to the quinoline N atom [1.996 (3) Å] than to the sulfonamide N atom [1.943 (3) Å]. Both bond lengths lie in the usual range. Selected bond distances and angles around the central Cu atom are given in Table 1.



The crystal packing is stabilized by three intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds, which build a three-dimensional network, as shown in Fig. 2 and detailed in Table 2.

Experimental

Compound (I) was prepared according to a literature procedure (Macías *et al.*, 2002). Single crystals of (I) suitable for X-ray data collection appeared after a few days from a methanol solution.

Crystal data

[Cu(C₁₅H₁₀N₃O₄S)₂]

M_r = 720.18

Monoclinic, *C*2/*c*

a = 14.101 (2) Å

b = 16.823 (2) Å

c = 13.172 (2) Å

β = 102.35 (1)°

V = 3052.4 (7) Å³

Z = 4

D_x = 1.567 Mg m⁻³

Cu Kα radiation

Cell parameters from 25 reflections

θ = 4.1–22.8°

μ = 2.83 mm⁻¹

T = 299 (2) K

Prism, dark green

0.38 × 0.13 × 0.10 mm

Data collection

Nonius CAD-4 diffractometer

ω/2θ scans

Absorption correction: ψ scan

(North *et al.*, 1968)

T_{min} = 0.556, *T_{max}* = 0.789

5582 measured reflections

2720 independent reflections

2074 reflections with *I* > 2σ(*I*)

R_{int} = 0.108

θ_{max} = 67.0°

h = -16 → 16

k = -20 → 20

l = -15 → 0

3 standard reflections

frequency: 120 min

intensity decay: 5.0%

Refinement

Refinement on *F*²

R [*F*² > 2σ(*F*²)] = 0.071

wR (*F*²) = 0.202

S = 1.06

2720 reflections

214 parameters

H-atom parameters constrained

w = 1/[σ²(*F_o*²) + (0.1447*P*)²]

where *P* = (*F_o*² + 2*F_c*²)/3

(Δ/σ)_{max} < 0.001

Δρ_{max} = 1.00 e Å⁻³

Δρ_{min} = -1.58 e Å⁻³

Extinction correction: *SHELXL97*

Extinction coefficient: 0.0019 (3)

Table 1

Selected geometric parameters (Å, °).

N1—Cu1	1.943 (3)	Cu1—N1 ⁱ	1.943 (3)
N2—Cu1	1.996 (3)	Cu1—N2 ⁱ	1.996 (3)
N1—Cu1—N1 ⁱ	162.1 (2)	N1—Cu1—N2 ⁱ	82.95 (14)
N1—Cu1—N2	103.79 (14)	N2—Cu1—N2 ⁱ	136.37 (19)

Symmetry code: (i) -*x*, *y*, -*z* + ½

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> — <i>H</i> ... <i>A</i>	<i>D</i> — <i>H</i>	<i>H</i> ... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> — <i>H</i> ... <i>A</i>
C3—H3...O1 ⁱⁱ	0.93	2.50	3.354 (5)	153
C11—H11...O3 ⁱⁱⁱ	0.93	2.40	3.271 (6)	156
C15—H15...O1 ⁱ	0.93	2.54	3.335 (5)	144

Symmetry codes: (i) -*x*, *y*, -*z* + ½; (ii) -*x* - ½, -*y* + ½, -*z*; (iii) *x*, -*y* + 1, *z* - ½

The H atoms were positioned with idealized geometry, with C—H = 0.93 Å, and were refined as riding with fixed isotropic displacement parameters set to 1.2 times *U_{eq}* of the parent atom. The residual electron-density peaks were located in the region of the Cu atom. The highest peak and deepest hole are 1.14 and 1.12 Å, respectively, from Cu.

Data collection: *CAD-4/PC* (Nonius, 1996); cell refinement: *CAD-4/PC*; data reduction: *REDU4* (Stoe & Cie, 1987); program(s) used to

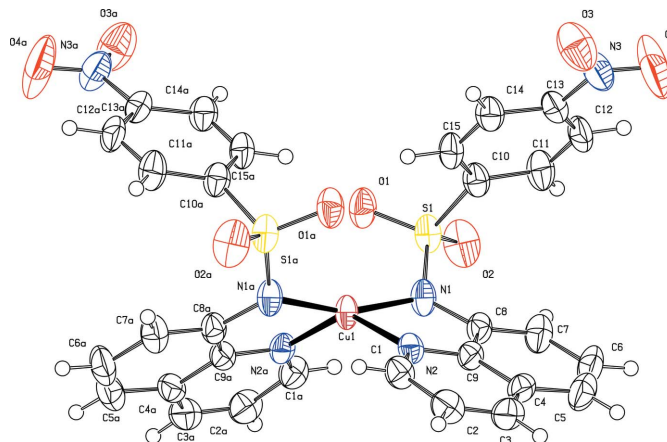


Figure 1

The molecular structure of (I), showing the atom labeling and displacement ellipsoids drawn at the 50% probability level. [Symmetry code: (a) -*x*, *y*, ½ - *z*.]

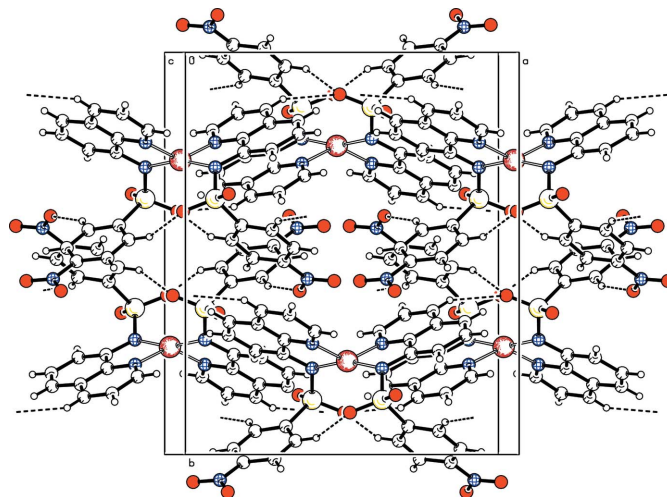


Figure 2

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

solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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