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Bis[2,4,6-triisopropyl-*N*-(quinolin-8-yl)benzenesulfonamidato-κ^2N,N']copper(II)

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Key indicators

Single-crystal X-ray study
T = 299 K
Mean σ(C–C) = 0.004 Å
R factor = 0.043
wR factor = 0.126
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.

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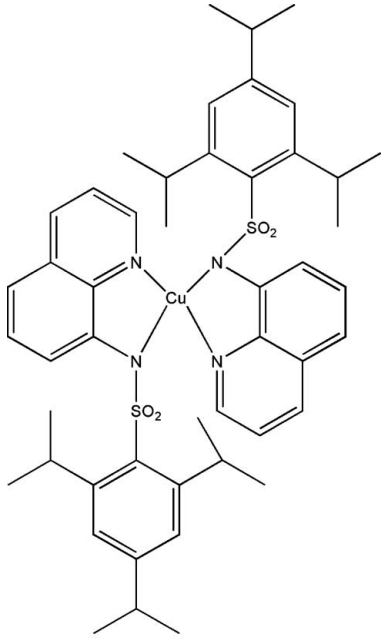
The molecule of the title complex, $[Cu(C_{24}H_{29}N_2O_2S)_2]$, occupies a special position on a twofold axis. The Cu atom has a severely distorted tetrahedral environment formed by two quinoline and two sulfonamide N atoms of two chelate quinolinyl-benzenesulfonamide ligands..

Comment

Copper complexes are known to be promising reagents for the cleavage of nucleic acids (Macías *et al.*, 2003). Organic copper complexes based on a quinoline ring system have also been investigated as potential and selective proteasome inhibitors in human cancer cells (Daniel *et al.*, 2004). In the light of this interest, we report here the structure of the title compound, (I).



(I)

In the molecule of (I), the Cu atom (Fig. 1) occupies a special position on a twofold axis. It has a severely distorted tetrahedral coordination, formed by two quinolinyl and two sulfonamide N atoms of the two bidentate chelate ligands. The Cu1—N1 bond involving quinoline atom N1 is significantly longer than the Cu1—N2 bond involving sulfonamide (Table 1). The N1—Cu1—N2 bite angle in the five-membered chelate ring is considerably narrower than the ideal tetrahedral value, whereas the N2—Cu1—N2^{i} angle [symmetry code (i): $1-x, y, \frac{3}{2}-z$] is much wider than one would expect to see in a tetrahedron. The other bond angles at atom Cu1,

N1—Cu1—N1^{i} and N1—Cu1—N2^{i}, are closer to the tetrahedral value.

Experimental

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

Crystal data

$[Cu(C_{24}H_{29}N_2O_2S)_2]$	D_x = 1.318 Mg m^{-3}
M_r = 882.64	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 3257 reflections
a = 24.513 (2) Å	θ = 2.1–21.0°
b = 9.4679 (7) Å	μ = 0.63 mm^{-1}
c = 19.600 (1) Å	T = 299 (2) K
β = 102.140 (6)°	Prism, black
V = 4447.2 (5) Å^3	0.32 × 0.30 × 0.22 mm
Z = 4	

Data collection

Oxford Diffraction Xcalibur diffractometer with a Sapphire CCD detector.	15625 measured reflections
	4493 independent reflections
	3310 reflections with $I > 2\sigma(I)$
ω and φ scans	R_{int} = 0.061
Absorption correction: analytical (*CrysAlis RED*; Oxford Diffraction, 2004)	θ_{max} = 26.4°
	$h = -30 \rightarrow 29$
	$k = -11 \rightarrow 11$
T_{min} = 0.788, T_{max} = 0.893	$l = -23 \rightarrow 23$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.043	$w = 1/[\sigma^2(F_o^2) + (0.0752P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.126	$(\Delta/\sigma)_{max}$ = 0.002
S = 1.02	$\Delta\rho_{max}$ = 0.68 e Å^{-3}
4493 reflections	$\Delta\rho_{min}$ = −0.32 e Å^{-3}
267 parameters	

Table 1
Selected geometric parameters (Å, °).

N1—Cu1	2.0248 (19)	N2—Cu1	1.9265 (19)
N2^{i}—Cu1—N2	163.83 (11)	N2—Cu1—N1	82.25 (8)
N2—Cu1—N1^{i}	105.39 (8)	N1^{i}—Cu1—N1	124.65 (12)

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

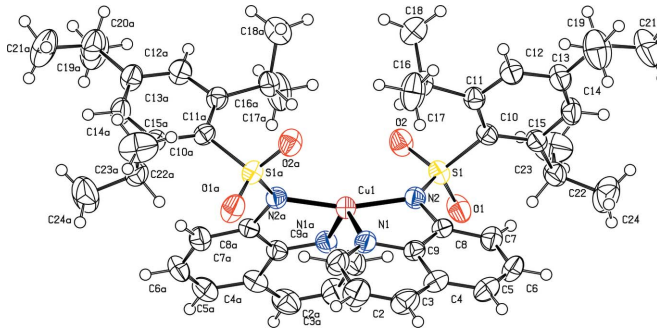


Figure 1
Molecular structure of (I), showing the atom labeling and displacement ellipsoids drawn at the 50% probability level. [Symmetry code: (a) $1-x$, y, $\frac{3}{2}-z$.]

H atoms were positioned geometrically and included in the refinement in the riding-model approximation, with C—H = 0.93 Å (aromatic), 0.96 Å (methyl), 0.98 Å (methine) and with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2004); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2004); data reduction: *CrysAlis RED*; program(s) used to 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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