

catena-Poly[[*(2,2'*-biquinoline- κ^2N,N')copper(I)]- μ -isothiocyanato- $\kappa^2N:S$]Rui Zhou^a and Seik Weng Ng^{b*}^aDepartment of Chemistry, Medical College, Shantou University, Shantou, Guangdong 515041, People's Republic of China, and^bDepartment of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia

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Key indicators

Single-crystal X-ray study

 $T = 295\text{ K}$ Mean $\sigma(\text{C}-\text{C}) = 0.003\text{ \AA}$ R factor = 0.030 wR factor = 0.085

Data-to-parameter ratio = 16.0

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

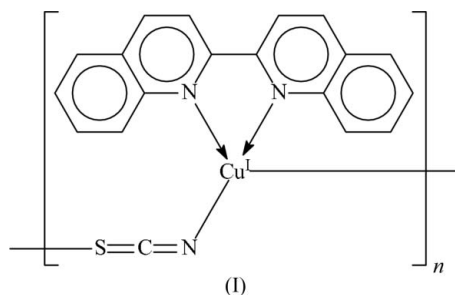
The isothiocyanate ligand in the title compound, $[\text{Cu}(\text{NCS})(\text{C}_{18}\text{H}_{12}\text{N}_2)]_n$, links adjacent tetrahedral Cu^{I} atoms into a zigzag chain; the Cu lies on a mirror plane that bisects the chelating biquinoline ligand.

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Comment

The crystal structures of a number of copper isothiocyanate complexes of 2,2'-bipyridine have been reported, *e.g.* bis(2,2'-bipyridine)(isothiocyanato)copper(II) thiocyanate (Kabesova *et al.* 1993), *catena*-(2,2'-bipyridine)sesqui(μ_2 -thiocyanato)-hemiisocyanatocopper(II) (Ferlay *et al.*, 1999), (2,2'-bipyridine)bis- μ_2 -isothiocyanatocopper(II) (Diaz *et al.*, 1999; Madalan *et al.*, 2002; Parker *et al.*, 1994) and *catena*-(5,5'-dimethyl-2,2'-bipyridine)- μ -isothiocyanatocopper(II) (Albada *et al.*, 2004). The 2,2'-biquinoline heterocycle is an analog of 2,2'-bipyridine and, although the synthesis of the compound has been known for a long time (Crowne & Breckenridge, 1954), it is not widely used in the formation of coordination complexes. The only known crystal structure of a copper complex is that of tetrahedral bis(2,2'-biquinoline)copper(I) tetrafluoroborate, which has been reported recently (Ali *et al.*, 2006).



The reaction of this *N*-heterocycle with copper(I) thiocyanate affords a monochelated compound, (I), in which the isothiocyanate functions as a bridging unit (Fig. 1); the mode of bridging gives rise to a zigzag chain that propagates along the *c* axis of the orthorhombic unit cell. The Cu^{I} center, which lies on a special position of site symmetry *m*, exhibits a distorted tetrahedral coordination. The bite angle of the heterocycle is similar to those found in the 2,2'-bipyridine adducts. The *N*-heterocycle straddles a mirror plane that relates the two quinoline units; the two ring systems are twisted by $10.1(1)^\circ$ with respect to each other.

Experimental

A mixture of copper(I) thiocyanate (0.121 g, 1.0 mmol), sodium thiocyanate (0.081 g, 1.0 mmol), 2,2'-biquinoline (0.256 g, 1.0 mmol),

water (5.0 ml) and acetonitrile (5 ml) was sealed in a 25 ml Teflon-lined stainless steel Parr bomb. The bomb was heated in an oven to 433 K for 72 h, and was then cooled to room temperature at a rate of 5 K h⁻¹. Brown, almost black, crystals were obtained in about 50% yield. Elemental analysis calculated for C₁₉H₁₂CuN₃S: C 60.38, H 3.20, N 11.12%; found C 60.25, H 3.15, N 11.23%.

Crystal data

[Cu(NCS)(C₁₈H₁₂N₂)]
M_r = 377.92
 Orthorhombic, *Pnma*
a = 9.0249 (6) Å
b = 15.855 (1) Å
c = 10.8836 (7) Å
V = 1557.4 (2) Å³
Z = 4
D_x = 1.612 Mg m⁻³
 Mo Kα radiation
 μ = 1.54 mm⁻¹
T = 295 (2) K
 Column, black
 0.16 × 0.14 × 0.10 mm

Data collection

Bruker APEX area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
T_{min} = 0.663, *T_{max}* = 0.862
 7944 measured reflections
 1844 independent reflections
 1606 reflections with *I* > 2σ(*I*)
R_{int} = 0.021
 θ_{max} = 27.5°

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.030
wR (*F*²) = 0.085
S = 1.07
 1844 reflections
 115 parameters
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0486P)^2 + 0.4432P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 (Δσ)_{max} = 0.001
 Δρ_{max} = 0.41 e Å⁻³
 Δρ_{min} = -0.17 e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Cu1—N1	2.107 (1)	Cu1—N2 ⁱⁱ	1.931 (2)
Cu1—N1 ⁱ	2.107 (1)	Cu1—S1	2.286 (1)
N1—Cu1—N1 ⁱ	77.79 (8)	N1 ⁱ —Cu1—N2 ⁱⁱ	112.21 (6)
N1—Cu1—N2 ⁱⁱ	112.21 (6)	N2 ⁱⁱ —Cu1—S1	123.28 (7)
N1—Cu1—S1	111.19 (4)	N1 ⁱ —Cu1—S1	111.19 (4)

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

H atoms were placed in calculated positions [C—H = 0.93 Å and *U*_{iso}(H) = 1.2*U*_{eq}(C)] and were included in the refinement in the riding-model approximation.

Data collection: SMART (Bruker, 2003); cell refinement: SAINT (Bruker, 2003); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics:

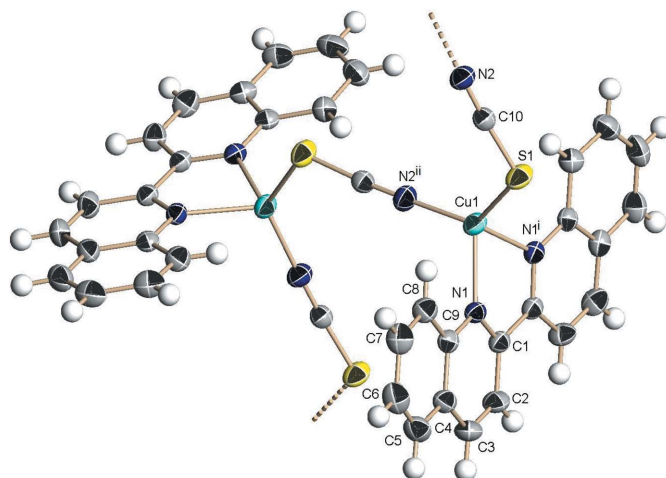


Figure 1

Plot illustrating the coordination environment of the Cu atom in (I). Displacement ellipsoids are plotted at the 50% probability level. [Symmetry codes: (i) *x*, $\frac{3}{2}$ - *y*, *z*; (ii) *x* - $\frac{1}{2}$, *y*, $\frac{3}{2}$ - *z*.]

ORTEP II (Johnson, 1976); software used to prepare material for publication: SHELXL97.

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