Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

Bis(isothiocyanato-κN)bis[8-(methoxycarbonylmethoxy)quinoline-κN]copper(II)

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Received 4 October 2004
Accepted 11 October 2004
Online 22 October 2004

In the title mononuclear complex, $[Cu(NSC)_2(C_{13}H_{11}NO_3)_2]$, the isothiocyanate ions and 8-(methoxycarbonylmethoxy)quinoline molecules act as monodentate ligands. The ligand geometry about the Cu centre, which lies on a twofold rotation axis, can be described as square-planar or grossly distorted octahedral, formed by two N atoms of the isothiocyanate ions, two quinoline N atoms and two methoxy O atoms of the 8-(methoxycarbonylmethoxy)quinoline ligands. The N—Cu—N *cis* angles around the Cu atom vary from 88.38 (12) to 94.27 (15)° and the Cu—N bond distances are 1.950 (2) and 2.024 (2) Å.

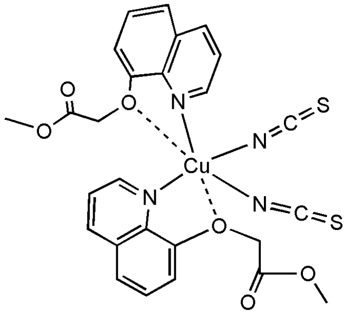
Key indicators

Single-crystal X-ray study
T = 193 K
Mean σ(C–C) = 0.005 Å
R factor = 0.055
wR factor = 0.101
Data-to-parameter ratio = 17.2

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

Comment

Derivatives of quinoline are well-known ligands in transition metal coordination compounds (Ghedini *et al.*, 2002; Inomata *et al.*, 1999; Jotterand *et al.*, 2001; Sivakolunthu *et al.*, 1998). Such compounds are being increasingly studied in modelling biological systems, one target being the metal binding site of copper metalloenzymes (Sorrel, 1989). In the light of this interest, we have prepared the biologically relevant ligand 8-(methoxycarbonylmethoxy)quinoline and its title copper complex, (I).



(I)

As shown in Fig. 1, (I) is mononuclear. Each Cu^{II} centre has a slightly distorted square geometry (Table 1) comprising of two isothiocyanate N atoms and two quinoline N atoms of the 8-(methoxycarbonylmethoxy)quinoline ligands. The coordination plane is defined by N1, N2, N2^{i} and N1^{i} [symmetry code: (i) $1 - x, y, \frac{1}{2} - z$]. Atoms N1, N2, N2^{i} and N1^{i} show deviations of 0.3295 (1), −0.3248 (1), 0.3248 (1) and −0.3295 (1)°, respectively, from the least-squares mean plane, and the Cu centre is constrained to lie in the plane by symmetry. The N—Cu—N angles vary from 88.38 (12) to 94.27 (15)°. The Cu—N$_q$ (q = quinoline) bond length of

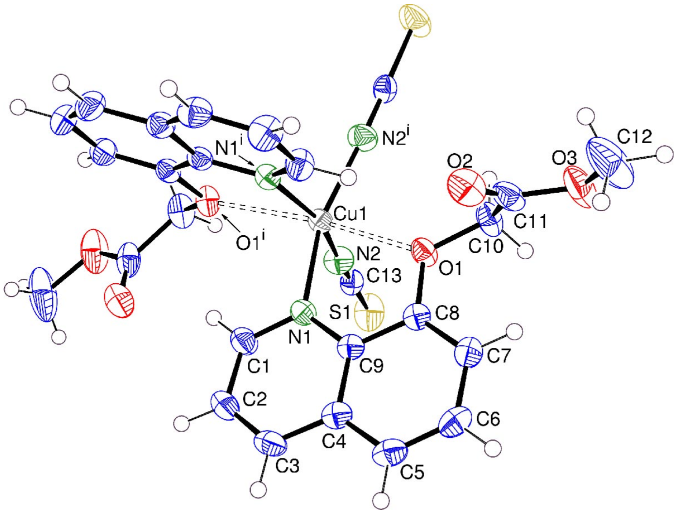


Figure 1
View of (I), shown with 30% probability displacement ellipsoids and small spheres for H atoms [symmetry code: (i) $1 - x, y, \frac{1}{2} - z$]. The long Cu1$\cdots$O1 interactions are indicated by dashed lines.

2.024 (2) Å is somewhat longer than the Cu—N_{NSC} bond length of 1.950 (2) Å, although both distances fall within the expected range of distances for Cu—N bonds (Breneman & Parker, 1993; Kožišek & Kabešová, 1990). The NSC groups in (I) are almost linear [179.0 (3)°], and slight bending is observed in the Cu—N—C linkage [177.1 (2)°]. The mean planes of the two quinoline moieties form a dihedral angle of 86.5 (1)°. There is a also pair of O atoms, O1 and O1^{i}, each some 2.4708 (19) Å from Cu1. If these are considered to be chemically significant interactions, a grossly distorted octahedral coordination about Cu1 results (Fig. 1).

The molecular packing in (I) is influenced by intermolecular π–π interactions which exist between the parallel quinoline rings of neighbouring complex molecules, with a separation of approximately 3.56 Å.

Experimental

Solid KSCN (19.4 mg, 2 mmol) was added slowly with continuous stirring to a solution of $Cu(ClO_4)_4 \cdot 6H_2O$ (57 mg, 1 mmol) in distilled water (5 ml). 8-(Methoxycarbonylmethoxy)quinoline (21.8 mg, 1 mmol) was dissolved in methanol (20 ml) and the two solutions were mixed and stirred for 5 h. The resulting solution was filtered. Pale green square-prismatic crystals suitable for X-ray diffraction analysis were obtained by slow evaporation of the resulting solution at room temperature. Analysis found: C 50.12, H 3.57, N 9.09%; calculated for $C_{26}H_{22}CuN_4O_6S_2$: C 50.85, H 3.61, N 9.12%

Crystal data

$[Cu(NSC)_2(C_{13}H_{11}NO_3)_2]$
$M_r = 614.14$
Monoclinic, $C2/c$
$a = 16.921$ (4) Å
$b = 10.073$ (2) Å
$c = 17.590$ (5) Å
$\beta = 115.647$ (4)°
$V = 2702.6$ (11) Å^3
$Z = 4$

$D_x = 1.509$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5205 reflections
$\theta = 3.0$–27.5°
$\mu = 1.01$ mm^{-1}
$T = 193$ (2) K
Block, green
0.38 × 0.24 × 0.10 mm

Data collection

Rigaku Mercury diffractometer
ω scans
Absorption correction: multi-scan (Jacobson, 1998)
$T_{min} = 0.700$, $T_{max} = 0.906$
14799 measured reflections
3086 independent reflections

2849 reflections with $I > 2\sigma(I)$
$R_{int} = 0.042$
$\theta_{max} = 27.5°$
$h = -21 \rightarrow 17$
$k = -13 \rightarrow 13$
$l = -20 \rightarrow 22$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.055$
$wR(F^2) = 0.101$
$S = 1.22$
3086 reflections
179 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0246P)^2 + 6.2754P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.42$ e Å^{-3}
$\Delta\rho_{min} = -0.43$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N2	1.950 (2)	Cu1—O1	2.4708 (19)
Cu1—N1	2.024 (2)		
N2^{i}—Cu1—N2	94.27 (15)	N2—Cu1—O1	101.17 (9)
N2—Cu1—N1	91.79 (10)	N1—Cu1—O1	72.38 (7)
N2—Cu1—N1^{i}	160.81 (9)	N2—Cu1—O1^{i}	88.58 (9)
N1—Cu1—N1^{i}	88.38 (12)	N1—Cu1—O1^{i}	97.17 (8)

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

H atoms were included in calculated positions and refined as riding, with C—H distances of 0.93 (aromatic), 0.99 (ethyl) and 0.98 Å (methyl), and with U_{iso}(aromatic and ethyl) = $1.2U_{eq}$(C) and U_{iso}(methyl) = $1.5U_{eq}$(C).

Data collection: *CrystalClear* (Molecular Structure Corporation, 2000; Rigaku Corporation, 1999); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Rigaku/MSC, 2003); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

The work was supported by the Natural Science Foundation of the University of Jiangsu Province (No. 03KJD150203) and the Science Foundation of the University of Science and Technology of Suzhou.

References

Breneman, G. L. & Parker, O. J. (1993). Polyhedron, **12**, 891–895.
Bruker (1998). *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Ghedini, M., Deda, M. L., Aiello, I. & Annarita Grisolia, A. (2002). *J. Chem. Soc. Dalton Trans.* pp. 3406–3409.
Inomata, Y., Haneda, T. & Howell, F. S. (1999). *J. Inorg. Biochem.* **76**, 13–17.
Jacobson, R. (1998). Private communication to Rigaku Corporation, Tokyo, Japan.
Jotterand, N., Pearce, D. A. & Imperiali, B. (2001). *J. Org. Chem.* **66**, 3224–3228.
Kožíšková. Z., Kožišek, J. & Kabešová, M. (1990). *Polyhedron*, **9**, 1029–1034.
Molecular Structure Corporation (2000). *CrystalClear*. MSC, 9009 New Trails Drive, The Woodlands, TX 77381–5209, USA.
Rigaku/MSC (2003). *CrystalStructure*. Version 3.5.1. Rigaku/MSC, 9009 New Trails Drive, The Woodlands, TX 77381–5209, USA.
Rigaku (1999). *CrystalClear*. Rigaku Corporation, 3-9-12 Akishima, Tokyo 196–8666, Japan.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Sivakolunthu, S., Saroja, B. & Sivasubramanian, S. (1998). *Indian J. Chem. Sect. A*, **37**, 357–360.
Sorrel, T. N. (1989). *Tetrahedron*, **45**, 3–68.