Acta Crystallographica Section C
Crystal Structure
Communications
ISSN 0108-2701

1,2-Bis(8-quinolylthiomethyl)benzene

Liao Sen *et al.*

Electronic paper

Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

1,2-Bis(8-quinolylthiomethyl)benzene

Liao Sen,[a] Cheng-Yong Su,[a]* Ze-Fu Zhang,[b] Han-Qin Liu[a] and Hai-Liang Zhu[a]

[a]School of Chemistry and Chemical Engineering, Zhongshan University, Guangzhou 510275, People's Republic of China, and [b]Laboratory of Solid Lubrication, Lanzhou Institute of Chemical Physics, Academy of Chinese Sciences, Lanzhou 730000, People's Republic of China
Correspondence e-mail: cesscy@zsu.edu.cn

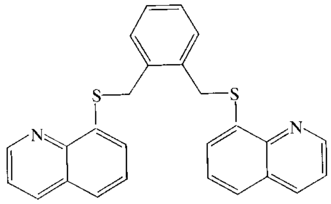
Received 13 June 2000
Accepted 26 June 2000

Data validation number: IUC0000170

The title potentially tetradentate *N*,*S*,*S*,*N*-donor ligand, $C_{26}H_{20}N_2S_2$, has been structurally characterized. The two S atoms adopt a *trans* conformation, lying above and below the benzene ring. The two quinoline rings are planar, with one parallel to the benzene ring and the other nearly perpendicular to it.

Comment

Among the tasks of bioinorganic chemistry, structural and functional modelling of the properties of biocomplexes has a special position. It is well known that in 'blue' or type I copper proteins, the Cu^{II} atom is coordinated by two histidine imidazole N atoms, a cysteine thiolate S atom and a methionine thioether S atom in a distorted tetrahedral geometry (Colman *et al.*, 1978). Biomodelling with the help of copper(II) coordination compounds with sulfur-containing ligands is used at present to explain the structural details of the coordination unit of copper of type I for their low *A* value in ESR spectra, abnormally high intensity absorption bands at *ca* 600 nm and the positive values of the redox potentials (Colman *et al.*, 1978). So far, no models have been obtained having these three properties simultaneously. In particular, the binding of thiolate groups to copper(II) is hard to achieve in low-molecular-weight compounds, the end product being an often insoluble, polymeric copper(I) compound and disulfide (Hughey *et al.*, 1979). So, in some literature, such models are tried with ligands containing thioether groups (Amundsen *et al.*, 1977; Addison *et al.*, 1984; Sakaguchi & Addison, 1979; Dockal *et al.*, 1976; Ritmeijer *et al.*, 1982; Pavlishchuk *et al.*, 1988). We are interested in models of blue copper proteins with low-molecular-weight complexes and report here the crystal structure of a model ligand, namely 1,2-bis(8-quinolylthiomethyl)benzene [or α,α′-bis(8-sulfanylquinoline)-*o*-xylene], (I).


(I)

The C—N and C—S distances show no remakable features, with C—N distances in the range 1.315 (4)–1.374 (3) Å, and C—S distances in the ranges 1.774 (3)–1.757 (3) Å and 1.817 (3)—1.819 (3) Å. The C atoms in the shorter C—S bonds belong to the quinoline moieties and the C atoms in the longer C—S bonds belong to the methylene groups. The C11—C10—S1 angle [107.03 (17)°] is almost the same as C16—C17—S2 [107.78 (18)°], but the two dihedral angles between the two quinoline moieties and the *o*-xylene moiety are obviously not the same. This suggests that the two quinoline moieties can rotate freely about the two C atoms of the methylene groups even though the bridge between the two quinoline moieties is rigid. So, it is possible to form a distorted tetrahedral geometry which is necessary to model blue copper proteins when the ligand coordinates with Cu^{II} ions.

Experimental

To a hot ethanol (60 ml) solution of 8-mercaptoquinoline sodium salt (3.684 g, 10 mmol) was added under nitrogen a solution of α,α′-dibromo-*o*-xylene (2.64 g, 10 mmol) in acetone (30 ml) with stirring. The mixture was reluxed under nitrogen for 6 h. After cooling to room temperaure, the mixture was cooled in a refrigerator to give a white precipitate. The precipitate was extracted with chloroform (15 ml). The white crystals were obtained when acetonitile (2 ml) was added carefuly to a chloroform (2 ml) solution of α,α′-bis(8-sulfanylquinoline)-*o*-xylene (0.085 g, 0.2 mmol), which was then left to stand at room temperature for 2 d; yield 67%. Analysis found: C 73.59, H 4.69, N 6.60%; calculated for $C_{26}H_{20}N_2S_2$: C 73.55, H 4.75, N 6.60%.

Crystal data

$C_{26}H_{20}N_2S_2$
$M_r = 424.56$
Triclinic, $P\bar{1}$
$a = 9.230$ (8) Å
$b = 10.907$ (6) Å
$c = 12.056$ (12) Å
$\alpha = 112.68$ (6)°
$\beta = 95.20$ (7)°
$\gamma = 106.05$ (6)°
$V = 1049.2$ (15) Å^3
$Z = 2$
$D_x = 1.344$ Mg m^{-3}
Mo *K*α radiation
Cell parameters from 26 reflections
$\theta = 6$–14°
$\mu = 0.270$ mm^{-1}
$T = 293$ (2) K
Block, colourless
0.54 × 0.35 × 0.24 mm

Data collection

Siemens *R*3*m* diffractometer
ω scans
Absorption correction: empirical (North *et al.*, 1968)
$T_{\min} = 0.869$, $T_{\max} = 0.918$
3961 measured reflections
3949 independent reflections
2680 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.040$
$\theta_{\max} = 26°$
$h = 0 \rightarrow 10$
$k = -13 \rightarrow 12$
$l = -14 \rightarrow 14$
3 standard reflections every 97 reflections intensity decay: 3%

e348 Liao Sen *et al.* • $C_{26}H_{20}N_2S_2$ *Acta Cryst.* (2000). C**56**, e348–e349

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0432P)^2 + 0.2725P]$
$R[F^2 > 2\sigma(F^2)] = 0.046$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.111$	$(\Delta/\sigma)_{\max} = 0.001$
$S = 1.030$	$\Delta\rho_{\max} = 0.18$ e Å^{-3}
3949 reflections	$\Delta\rho_{\min} = -0.17$ e Å^{-3}
271 parameters	
H-atom parameters constrained	

Data collection: *XSCANS* (Siemens, 1996); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); software used to prepare material for publication: *SHELXTL*.

This work has been supported by NSF of China and NSF of Guangdong Province.

References

Addison, A. W., Rao, T. N. & Sinn, E. (1984). *Inorg. Chem.* **23**, 1957–1967.

Amundsen, A. R., Whelan, J. & Bosnich, B. (1977). *J. Am. Chem. Soc.* **99**, 6730–6739.

Colman, P. M., Freeman, H. C., Guss, J. M., Murata, M., Norris, V. A., Ramshaw, J. A. M. & Venkatappa, M. P. (1978). *Nature* (*London*), **272**, 319–324.

Dockal, E. R., Jones, T. E., Sokol, W. F., Engerer, R. J., Rorabacher, D. B. & Ochrymowycz, L. A. (1976). *J. Am. Chem. Soc.* **98**, 4322–4324.

Hughey, J. L., Fawcett, T. G., Rudich, S. M., Lalancette, R. A., Potenza, J. A. & Schugar, H. J. (1979). *J. Am. Chem. Soc.* **101**, 2617–2623.

North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.

Pavlishchuk, V. V., Strizhak, P. E. & Yatsimirskii, K. B. (1988). *Inorg. Chim. Acta*, **151**, 133–137.

Ritmeijer, F. J., Birker, P. J. M. W. L., Gorter, S. & Reedijk, J. (1982). *J. Chem. Soc. Dalton Trans.* pp. 1191–1198.

Sakaguchi, U. & Addison, A. W. (1979). *J. Chem. Soc. Dalton Trans.* pp. 600–608.

Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.

Sheldrick, G. M. (1997). *SHELXL*97, University of Göttingen, Germany.

Siemens (1996). *XSCANS*. Version 2.2. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.