Acta Crystallographica Section E
Structure Reports Online

ISSN 1600-5368

1,4-Bis(2-pyridylsulfanyl)butane

Ya-Bo Xie[a]* and Jian-Rong Li[b]

[a]College of Environmental and Energy Engineering, Beijing University of Technology, Beijing 100022, People's Republic of China, and [b]Department of Chemistry, Nankai University, Tianjin 300071, People's Republic of China

Correspondence e-mail: xieyabo@bjut.edu.cn

Key indicators

Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.006 Å
R factor = 0.049
wR factor = 0.080
Data-to-parameter ratio = 15.5

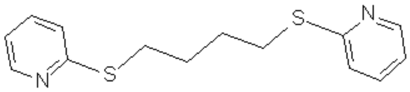
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The crystal structure of the title compound, $C_{14}H_{16}N_2S_2$, adopts an *anti* conformation based on the two pyridine rings with respect to the central alkyl chain. The two terminal pyridine rings are almost parallel to each other, with a dihedral angle of 18.1 (4)°.

Received 25 October 2004
Accepted 26 October 2004
Online 13 November 2004

Comment

There has been significant current interest in the rational design and synthesis of new discrete or polymeric metal-organic coordination architectures for their potential use as functional materials (Goodgame *et al.*, 2002; Hamblin *et al.*, 2002). The generation of coordination architectures depends mainly on the combination of two factors, the coordination geometry of metal ions and the nature of the ligands (Sun *et al.*, 2002). Therefore, the use of well designed ligands to control the assembly of supramolecular architectures has become a popular and rapidly growing discipline (Bu *et al.*, 2001). Recently, increasing attention has been paid to the use of flexible bridging units in the construction of supramolecular architectures (Bu *et al.*, 2002; Cai *et al.*, 2001), and this approach is attractive because the flexibility and conformational freedom of such ligands offer the possibility for the construction of unprecedented frameworks with tailored properties and functions. As part of our investigation on flexible ligands and their complexes, the structure of a flexible dithioether ligand, namely 1,4-bis(2-pyridylsulfanyl)butane, (I), is reported here.



(I)

The molecular structure of (I) is shown in Fig. 1. The skeleton of the central alkyl chain is extended, and all C atoms of the alkyl chain and two terminal S atoms are almost coplanar, the C6—C7—C8—C9 torsion angle being 178.3 (4)°. The two terminal pyridine rings are located on opposite sides

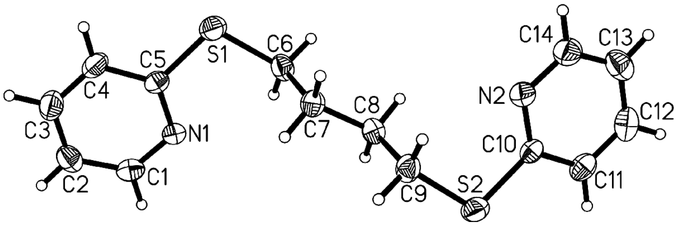


Figure 1
The molecular structure of the title compound, shown with 30% probability displacement ellipsoids.

doi: 10.1107/S1600536804027230

of the C6/C7/C8/C9 plane, and the dihedral angles between the terminal pyridine rings and the C6/C7/C8/C9 plane are 87.7 (5)° (plane N1/C1–C5) and 76.4 (5)° (plane N2/C10–C14). The terminal pyridine rings are almost parallel to one another, with a dihedral angle of 18.1 (4)°.

Experimental

1,4-Bis(2-pyridylsulfanyl)butane was prepared according to the method of Hartley *et al.* (1979) (yield: 84%). IR (KBr, cm^{-1}): 1578 (*s*), 1554 (*s*), 1455 (*s*), 1413 (*s*), 1309 (*w*), 1284 (*w*), 1146 (*m*), 1124 (*s*), 1042 (*w*), 984 (*m*), 761 (*s*), 731 (*w*), 711 (*w*); ^{1}H NMR (CDCl$_3$): δ 1.88 (*p*, 4H, J = 7.2 Hz, C–CH$_2$CH$_2$–C), 3.21 (*t*, 4H, J = 7.2 Hz, —SCH$_2$—), 6.94–6.98 (*m*, 2H, py-3), 7.14–7.17 (*m*, 2H, py-5), 7.43–7.49 (*m*, 2H, py-4), 8.40, 8.42 (*d*, 2H, py-6); analysis calculated for $C_{14}H_{16}N_2S_2$: C 60.83, H 5.83, N 10.13%; found: C 60.61, H 5.75, N 10.19%. Yellow single crystals of (I) were obtained by recrystallization from ethanol.

Crystal data

$C_{14}H_{16}N_2S_2$
M_r = 276.41
Monoclinic, $P2_1/c$
a = 10.979 (5) Å
b = 11.480 (5) Å
c = 11.694 (6) Å
β = 103.508 (8)°
V = 1433.2 (12) Å^3
Z = 4

D_x = 1.281 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 870 reflections
θ = 2.5–18.3°
μ = 0.36 mm^{-1}
T = 273 (2) K
Block, colorless
0.25 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996; Blessing, 1995)
$T_{\min}$ = 0.916, $T_{\max}$ = 0.932
5737 measured reflections

2526 independent reflections
1168 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.089
$\theta_{\max}$ = 25.0°
$h = -12 \rightarrow 13$
$k = -10 \rightarrow 13$
$l = -11 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.080
S = 1.05
2526 reflections
163 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.01P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max}$ = 0.002
$\Delta\rho_{\max}$ = 0.18 e Å^{-3}
$\Delta\rho_{\min}$ = −0.20 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—C5	1.758 (3)	S2—C9	1.800 (3)
S1—C6	1.806 (3)	S2—C10	1.754 (3)
C5—S1—C6	103.1 (2)	C1—N1—C5	116.5 (3)
C9—S2—C10	103.9 (2)	C10—N2—C14	116.7 (3)

The H atoms were included in calculated positions and treated as riding atoms; C—H = 0.93 or 0.97 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; 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 authors thank Beijing University of Technology and Nankai University, for supporting this work.

References

Bu, X. H., Chen, W., Du, M., Biradha, K., Wang, W. Z. & Zhang, R. H. (2002). *Inorg. Chem.* **41**, 437–439.

Bu, X. H., Chen, W., Lu, S. L., Zhang, R. H., Liao, D. Z., Bu, W. M., Shionoya, M., Brisse, F. & Ribas, J. (2001). *Angew. Chem. Int. Ed.* **40**, 3201–3203.

Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.

Bruker (1998). *SMART*, *SAINT* and *SHELXTL* (Version 5.16). Bruker AXS Inc., Madison, Wisconsin, USA.

Cai, Y. P., Zhang, H. X., Xu, A. W., Su, C. Y., Chen, C. L., Liu, H. Q., Zhang, L. & Kang, B. S. (2001). *J. Chem. Soc. Dalton Trans.* pp. 2429–2434.

Goodgame, D. M. L., Grachvogel, D. A. & Williams, D. J. (2002). *J. Chem. Soc. Dalton Trans.* pp. 2259–2260.

Hamblin, J., Childs, L. J., Alcock, N. W. & Hannon, M. J. (2002). *J. Chem. Soc. Dalton Trans.* pp. 164–169.

Hartley, F. R., Murray, S. G., Levason, W., Soutter, H. E. & McAuliffe, C. A. (1979). *Inorg. Chim. Acta*, **35**, 265–277.

Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.

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

Sun, W. Y., Kusukawa, T. & Fujita, M. (2002). *J. Am. Chem. Soc.* **124**, 11570–11571.