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# 1,2-Bis[4-(2-pyridyl)pyrimidin-2-ylsulfanyl]ethane

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**Key indicators**

Single-crystal X-ray study
*T* = 294 K
Mean σ(C–C) = 0.005 Å
*R* factor = 0.064
*wR* factor = 0.205
Data-to-parameter ratio = 13.4

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



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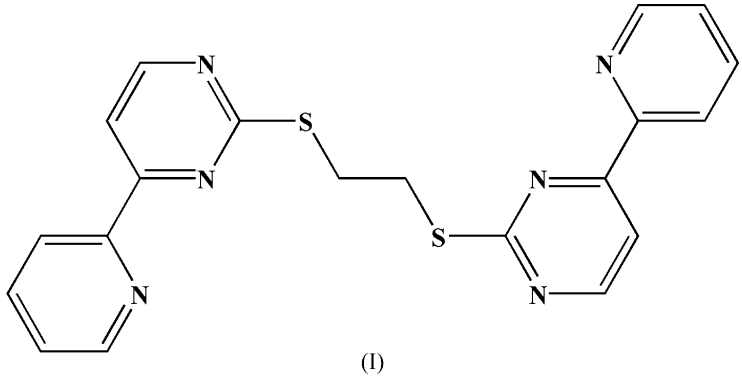
The title compound, $C_{20}H_{16}N_6S_2$, was obtained by the reaction of 1,2-dibromoethane and the potassium salt of 4-(2-pyridyl)-pyrimidine-2-thione in EtOH. The molecule has an inversion centre, with the two 4-(2-pyridyl)pyrimidin-2-yl fragments parallel.

## Comment

The design and syntheses of flexible multi-thioether ligands bearing N-atom donors have attracted much attention due to their diverse coordination capabilities and the important properties of their metal complexes (Caradoc-Davies & Hanton, 2001; Hartshorn & Steel, 1998; Hong *et al.*, 2000). Recently, we synthesized a new dithioether ligand bearing N-atom donors, (I). We here report the crystal structure of this ligand.



(I)

As shown in Fig. 1, the molecule of (I) has an inversion centre at the mid-point of the central C—C bond, with the two 4-(2-pyridyl)pyrimidin-2-yl fragments parallel. The C9—S1 [1.770 (4) Å] and C10—S1 [1.802 (4) Å] bonds and the C9—S1—C10 [103.45 (16)°] and S1—C10—C10$^{i}$ [112.6 (3)°] angles [symmetry code: (i) $-x, 2-y, 2-z$] are all in normal ranges, and are comparable with the corresponding values in other compounds (Allen *et al.*, 1987; Casabó *et al.*, 1995). The dihedral angle between rings *A* (N1/C1–C5) and *B* (N2/N3/C6–C9) is 3.42 (4)°.

## Experimental

The title compound was prepared according to a literature method (Mikhailov *et al.*, 1984). 1,2-Dibromoethane (10 mmol, 0.87 ml, 99%) was dded dropwise to a hot solution (about 323 K) of the potassium salt of 4-(2-pyridyl)pyrimidine-2-thione (Wang & Schwabacher, 1999; 4.55 g, 20 mmol) in ethanol (30 ml), and the mixture was further stirred at 323 K for 6 h. After cooling, water (30 ml) was added to the mixture and it was allowed to stand for 5 h. The yellow precipitate

was filtered off, washed with ethanol and water, and then recrystallized from a mixture of chloroform and methanol (1:1), which gave single crystals suitable for X-ray diffraction analysis (yield: 6.47 g, 80%).

*Crystal data*

| | |
|---|---|
| $C_{20}H_{16}N_6S_2$ | $Z = 2$ |
| $M_r = 404.53$ | $D_x = 1.431$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation |
| $a = 9.307$ (2) Å | $\mu = 0.30$ mm$^{-1}$ |
| $b = 11.672$ (3) Å | $T = 294$ (2) K |
| $c = 8.7531$ (19) Å | Block, yellow |
| $\beta = 99.221$ (4)° | 0.24 × 0.22 × 0.16 mm |
| $V = 938.5$ (4) Å$^3$ | |

*Data collection*

| | |
|---|---|
| Bruker APEX-II CCD area-detector diffractometer | 4756 measured reflections<br>1706 independent reflections |
| $\varphi$ and $\omega$ scans | 1337 reflections with $I > 2\sigma(I)$ |
| Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) | $R_{int} = 0.028$ |
| $T_{min} = 0.931$, $T_{max} = 0.953$ | $\theta_{max} = 25.3°$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | $w = 1/[\sigma^2(F_o^2) + (0.1197P)^2 + 0.8118P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $R[F^2 > 2\sigma(F^2)] = 0.064$ | $(\Delta/\sigma)_{max} < 0.001$ |
| $wR(F^2) = 0.205$ | $\Delta\rho_{max} = 0.70$ e Å$^{-3}$ |
| $S = 1.08$ | $\Delta\rho_{min} = -0.62$ e Å$^{-3}$ |
| 1706 reflections | |
| 127 parameters | |
| H-atom parameters constrained | |

H atoms were positioned geometrically, with C—H = 0.93 and 0.97 Å for aromatic and methylene H atoms, respectively, and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

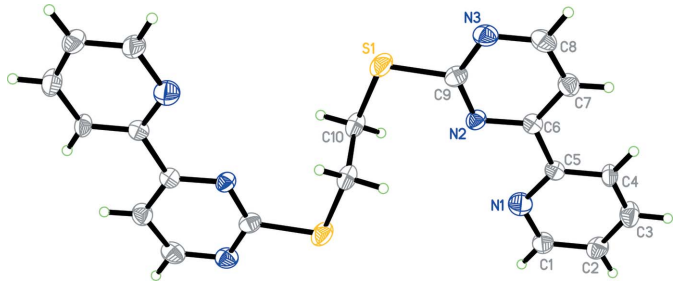



**Figure 1**
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Unlabelled atoms are related to labelled atoms by $-x, 2-y, 2-z$.

## References


Bruker (1998). *SMART* and *SAINT*. Versions 5.051. Bruker AXS Inc., Madison, Wisconsin, USA.

Caradoc-Davies, P. L. & Hanton, L. R. (2001). *Chem. Commun.* pp. 1098–1099.

Casabó, J., Flor, T., Hill, M. N. S., Jenkins, H. A., Lockhart, J. C., Loeb, S. J., Romero, I. & Teixidor, F. (1995). *Inorg. Chem.* **34**, 5410–5415.

Hartshorn, C. M. & Steel, P. J. (1998). *J. Chem. Soc. Dalton Trans.* pp. 3935–3940.

Hong, M. C., Su, W. P., Cao, R., Fujita, M. & Lu, J. X. (2000). *Chem. Eur. J.* **6**, 427–431.

Mikhailov, A. S., Pashkurov, N. G., Reznik, V. S. & Podzigun, G. I. (1984). *Izv. Akad. Nauk SSSR [Khim.]*, pp. 1396–1402. (In Russian.)

Orpen, A. G., Brammer, L., Allen, F. H., Kennard, O., Watson, D. G. & Taylor, R. (1989). *Dalton Trans.* S1–S83.

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

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

Wang, F. & Schwabacher, A. W. (1999). *Tetrahedron Lett.* **40**, 4779–4782.