Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1,4-Bis(2-mercaptobenzothiazolyl)butane

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.042
wR factor = 0.081
Data-to-parameter ratio = 14.3

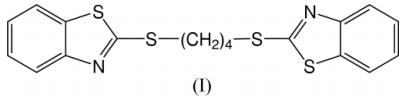
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 3 March 2003
Accepted 7 March 2003
Online 14 March 2003

The molecular structure of the title compound, $C_{18}H_{16}N_2S_4$, has a center of symmetry. All the C and S atoms in the central alkyl chain are coplanar, and this plane is almost perpendicular to the benzothiazolyl rings. The molecules are linked together by intermolecular S···S interactions to form a one-dimensional chain.

Comment

One of the reasons for the recent intensive interest in the design of flexible multidentate ligands is to develop a new family of microporous, helicate materials, and other coordination polymers with unusual porous structures (Cai *et al.*, 2001; Albada *et al.*, 2000; Zhang *et al.*, 2002). Moreover, the flexibility and conformational freedom of such ligands offer the possibility of generating unique frameworks with useful properties (Bu *et al.*, 2001; Hou *et al.*, 2002). As part of our systematic investigation of the coordination chemistry of flexible ligands, we report here the synthesis and crystal structure of the title compound, (I).



(I)

The title molecule has a center of symmetry at the midpoint of the central C—C bond (Fig. 1). The C1—C2 and C1—C1^{i} bond lengths are all close to the standard value for a single-bond length (see Table 1). All the C and S atoms between the two benzothiazolyl rings are coplanar; this plane is almost perpendicular to the planes of the benzothiazolyl rings, which are parallel to each other. The S—C bond distances are in the range 1.727 (2)–1.809 (3) Å, which are similar to those of S—C bonds in the analogous compound 1,5-bis(benzothiazolyl)-3-thiapentane (Grapperhaus *et al.*, 2002); the C atom in the longest C—S bond belongs to the methylene group. The molecules are linked together by an intermolecular S2···S2($-x$, $-y$, $1-z$) interaction of 3.485 (2) Å to form a one-dimensional chain.

Experimental

The title compound, (I), was prepared from 2-mercaptobenzothiazole and 1,4-dibromobutane in 56% yield, using a similar method to that reported by Chen *et al.* (2003). Crystals of (I) suitable for X-ray analysis were grown from a chloroform solution. Calculated (%) for $C_{18}H_{16}N_2S_4$: C 55.64, H 4.15, N 7.21; found (%): C 55.48, H 4.10, N 7.18.

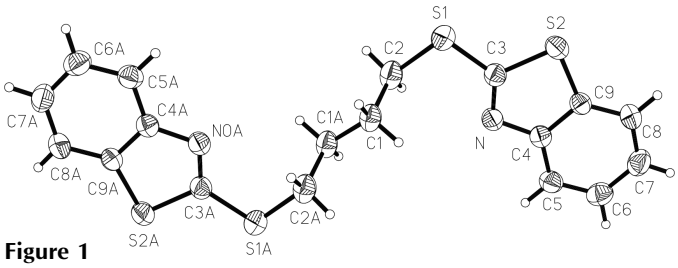


Figure 1
A view of the molecular structure of (I). Displacement ellipsoids are drawn at the 50% probability level. The subscript 'A' corresponds to symmetry code (i) in Table 1.

Crystal data

$C_{18}H_{16}N_2S_4$
$M_r = 388.57$
Monoclinic, $P2_1/c$
$a = 10.9072\ (18)$ Å
$b = 4.9003\ (8)$ Å
$c = 16.767\ (3)$ Å
$\beta = 104.868\ (3)^\circ$
$V = 866.2\ (2)$ Å^3
$Z = 2$
$D_x = 1.49$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 887 reflections
$\theta = 5.5$–46.2°
$\mu = 0.55$ mm^{-1}
$T = 293\ (2)$ K
Block, colourless
0.25 × 0.20 × 0.06 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: none
5025 measured reflections
2020 independent reflections
1248 reflections with $I > 2\sigma(I)$
$R_{int} = 0.050$
$\theta_{max} = 28.3^\circ$
$h = -14 \rightarrow 14$
$k = -6 \rightarrow 6$
$l = -17 \rightarrow 22$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.081$
$S = 0.84$
2020 reflections
141 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0257P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.34$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ e Å^{-3}

Table 1
Selected geometric parameters (Å).

S1—C3	1.747 (2)	S2—C3	1.754 (2)
S1—C2	1.809 (3)	C2—C1	1.510 (3)
S2—C9	1.727 (2)	C1—C1^{i}	1.522 (5)

Symmetry code: (i) $1-x, 1-y, 1-z$.

All H atoms were located from difference syntheses and refined isotropically. The C—H distances are in the range 0.89 (2)–0.98 (2) Å.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1999); 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*.

This work is supported by the National Natural Science Foundation of China and the Natural Science Foundation of Guangdong Province

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