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1,2-Bis(benzothiazol-2-ylsulfanyl)ethane

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.039
wR factor = 0.094
Data-to-parameter ratio = 14.0

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

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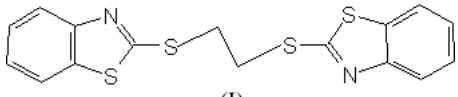
The title compound, $C_{16}H_{12}N_2S_4$, was synthesized by reaction of 1,2-dibromoethane with the sodium salt of 2-mercaptobenzothiazole. The molecule has an approximate inversion centre, with two benzothiazole fragments having an antiparallel orientation, their least-squares planes forming a dihedral angle of 4.12 (12)°. The central four-atom S—C—C—S link is almost planar, its plane being approximately orthogonal to the benzothiazole planes [dihedral angles 84.98 (14) and 84.13 (15)°]. Intermolecular S···S interactions [3.657 (3) Å] link the molecules in the crystal structure into infinite chains stretching along the [10$\bar{1}$] direction.

Comment

Numerous flexible or rigid multi-thioether ligands containing N-heterocyclic entities have been synthesized and studied. They attract substantial attention due to their diverse coordination capabilities and the important properties of their metal complexes (Bu *et al.*, 2002; Hong *et al.*, 2000; Alcock *et al.*, 1978). In addition, studies of the S-containing compounds have also been carried out with the goal of designing an improved optical sensor for the Ag^I ion (Lerchi *et al.*, 1996). As a continuation of our systematic studies of the coordination chemistry of various multi-thioether ligands and the architecture of their polymeric metal complexes, a dithioether ligand with 'terminal' benzothiazole groups, namely 1,2-bis(benzothiazol-2-ylsulfanyl)ethane, (I), has been synthesized.



(I)

As shown in Fig. 1, the molecule of (I) has an approximate inversion centre, with two benzothiazole rings having an antiparallel orientation, the dihedral angle formed by their mean planes being 4.12 (12)°. The central four-atom S—C—C—S link is planar to within 0.01 Å and almost orthogonal to the benzothiazole mean planes, the dihedral angles being 84.98 (14) and 84.13 (15)° for the S1- and S4-containing benzothiazole systems, respectively.

Intermolecular S1···S4^{i} interactions [3.657 (3) Å; symmetry code (i): $\frac{1}{2}+x, \frac{1}{2}-y, -\frac{1}{2}+z$] link the molecules in the crystal structure into infinite chains stretching along the [10$\bar{1}$] direction. In addition, π–π-stacking interactions between the benzothiazole fragments of neighbouring molecules are observed; the average separation is 3.895 Å.

Experimental

The title compound has been synthesized by the reaction of 1,2-dibromoethane and the sodium salt of 2-mercaptobenzothiazole in

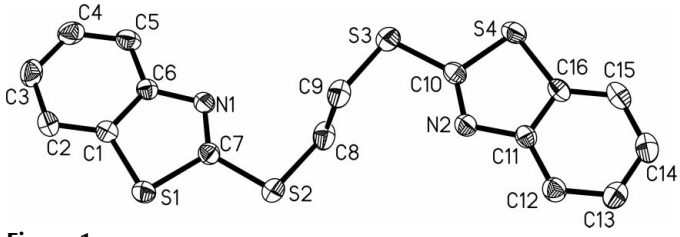


Figure 1
View of the title compound, with displacement ellipsoids at the 30% probability level. H atoms have been omitted.

EtOH at 353 K, as described by Liu *et al.* (2001) (yield: 80%, m.p.: 411–413 K). Yellow single crystals of the title compound were obtained by recrystallization from chloroform.

Crystal data

$C_{16}H_{12}N_2S_4$	D_x = 1.514 Mg m^{-3}
M_r = 360.53	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 719 reflections
a = 11.534 (4) Å	θ = 3.7–25.6°
b = 10.719 (4) Å	μ = 0.60 mm^{-1}
c = 14.006 (5) Å	T = 293 (2) K
β = 114.029 (5)°	Needle, yellow
V = 1581.5 (10) Å^3	0.30 × 0.25 × 0.20 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	2791 independent reflections
	1833 reflections with $I > 2\sigma(I)$
φ and ω scans	R_{int} = 0.037
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	θ_{max} = 25.0°
	$h = -13 \rightarrow 13$
T_{min} = 0.841, T_{max} = 0.890	$k = -12 \rightarrow 6$
6363 measured reflections	$l = -15 \rightarrow 16$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0413P)^2 + 0.2548P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.039	
$wR(F^2)$ = 0.094	
S = 1.00	$(\Delta/\sigma)_{max} < 0.001$
2791 reflections	$\Delta\rho_{max}$ = 0.27 e Å^{-3}
199 parameters	$\Delta\rho_{min}$ = −0.21 e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

S1—C1	1.738 (3)	S4—C10	1.755 (3)
S1—C7	1.754 (3)	S4—C16	1.730 (3)
S2—C7	1.742 (3)	N1—C6	1.390 (3)
S2—C8	1.821 (3)	N1—C7	1.294 (3)
S3—C9	1.827 (3)	N2—C10	1.284 (3)
S3—C10	1.743 (3)	N2—C11	1.391 (3)
C7—S2—C8	100.64 (14)	C10—S3—C9	100.98 (14)

H atoms were added theoretically, riding on their attached atoms and were refined with fixed displacement parameters.

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

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