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

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.031
wR factor = 0.086
Data-to-parameter ratio = 16.2

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

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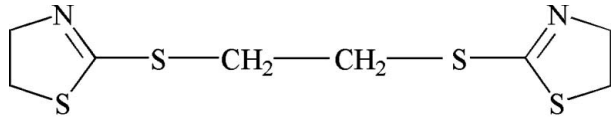
The title compound, $C_8H_{12}N_2S_4$, was synthesized by the reaction of 1,2-dibromoethane and thiazoline-2-thione. The molecule contains a centre of inversion at the mid-point of the central C—C bond.

Comment

As a type of ditopic ligand, dithioethers can be used as bridging ligands in the construction of coordination polymers with soft metal ions. *N*-Heterocylic units have been synthesized and investigated (Sharma *et al.*, 1999; Constable *et al.*, 2002; Bu *et al.*, 2003; Hong *et al.*, 2000). Thiazoline derivatives possess diverse acaricide properties. Now a new thiazoline derivative, 1,2-bis(2-thiazolin-2-ylsulfanyl)ethane, (I), has been synthesized and the results are presented here.



(I)

In the molecular structure of (I), there is an inversion centre at the mid-point of the central C—C bond. Atom C3 has a distorted trigonal geometry, with the N1—C3—S2 [125.56 (17)°] and S2—C3—S1 [115.59 (12)°] angles deviating significantly from the ideal sp^2-hybridized value.

The Csp^2—S bond distances are significantly shorter than the Csp^3—S bond distances (Table 1). These values are comparable with those reported in the literature (Wang *et al.*, 2004; Wang, Zhao & Zhang, 2005; Wang, Zhao, Zheng & Duan, 2005).

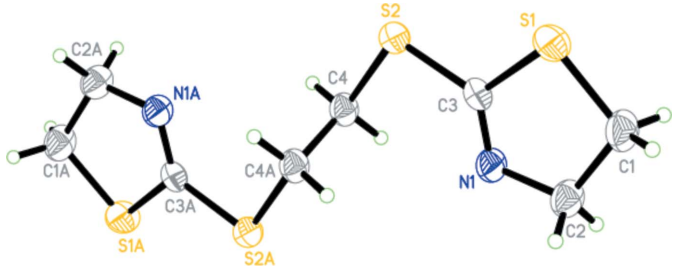


Figure 1
View of the molecule of (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. Atoms with suffix A are generated by the symmetry code $(-x+1, -y, -z+1)$.

Experimental

A solution of 1,2-dibromoethane (1.32 g, 5 mmol) in ethanol (10 ml) was added dropwise to a mixture of thiazoline-2-thione (1.31 g, 11 mmol), KOH (0.62 g, 11 mmol) and ethanol (5 ml). The reaction mixture was then stirred for 60 h at room temperature. The precipitate was filtered off, washed with water and recrystallized from water (yield 47%, m.p. 398–399 K). Analysis calculated for $C_8H_{12}N_2S_4$: C 35.85, H 4.71, N 8.24%; found: C 38.89, H 4.76, N 8.16%. Crystals of (I) suitable for single-crystal X-ray analysis were grown by slow evaporation of a chloroform–ethanol (1:3 *v*/*v*) solution.

Crystal data

$C_8H_{12}N_2S_4$
M_r = 264.44
Monoclinic, $P2_1/c$
a = 5.8169 (13) Å
b = 10.001 (2) Å
c = 10.216 (2) Å
β = 95.187 (4)°
V = 591.9 (2) Å^3
Z = 2
D_x = 1.484 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.77 mm^{-1}
T = 293 (2) K
Block, colourless
0.24 × 0.20 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.769, T_{max} = 1.000
(expected range = 0.680–0.885)
2909 measured reflections
1038 independent reflections
856 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.086
S = 1.05
1038 reflections
64 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0429P)^2 + 0.2261P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S2—C3	1.753 (2)	S1—C1	1.807 (3)
S2—C4	1.819 (2)	N1—C3	1.260 (3)
S1—C3	1.771 (2)	N1—C2	1.467 (3)
C3—S2—C4	100.68 (11)	N1—C2—C1	111.1 (2)
C3—S1—C1	89.01 (11)	N1—C3—S2	125.56 (17)
C3—N1—C2	111.51 (19)	N1—C3—S1	118.85 (17)
C2—C1—S1	105.99 (16)	S2—C3—S1	115.59 (12)

All H atoms were positioned geometrically and refined as riding (C—H = 0.97 Å), with $U_{iso}(H) = 1.2U_{eq}(C)$.

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

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