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2,2′-(*m*-Phenylenedimethylenedithio)-bis(1,3-thiazoline)

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.039
wR factor = 0.129
Data-to-parameter ratio = 15.4

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

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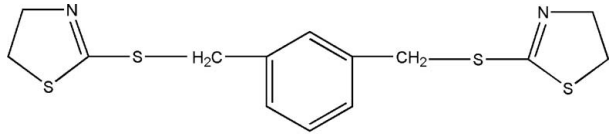
The title compound, $C_{14}H_{16}N_2S_4$, was synthesized by the reaction of 1,3-dibromomethylbenzene and thiazoline-2-thione. The molecule is located on a crystallographic twofold rotation axis.

Comment

Dithioethers are often used as bridging ligands in the construction of coordination polymers with soft metal ions. Flexible or rigid chain-linked dithioethers containing *N*-heterocyclic units have been synthesized and investigated (Constable *et al.*, 2002; Hong *et al.*, 2000). Thiazoline derivatives possess acaricide properties. In order to study the properties of these compounds, we have synthesized several new thiazoline derivatives, and we present here the crystal structure of the title compound, (I).



(I)

A crystallographic twofold rotation axis passes through C7 and C8. The improper torsion angle of the two C—S bonds [S2—C4···C4*A*—S2*A*] is 102.13 (15)°, forcing the two thiazoline rings to extend in opposite directions to minimize the steric hindrance. The dihedral angle between the planes of C3—C4—S2(*A*) and C3*A*—C4*A*—S2*A*(*B*) is 69.7 (2)°. Atom C3 has a distorted trigonal geometry, with the N1—C3—S2 [126.8 (2)°] and S1—C3—S2 [114.56 (16)°] angles deviating significantly from the ideal sp^2 hybridized value.

The Csp^2—S bond distances are significantly shorter than the Csp^3—S bonds (Table 1). These latter values are comparable with those in the literature (Wang *et al.*, 2004, 2005).

Experimental

A solution of 1,3-dibromomethylbenzene (1.32 g, 5 mmol) in ethanol (5 ml) was added dropwise to a mixture of thiazoline-2-thione (1.31 g, 11 mmol), KOH (0.615 g, 11 mmol) and ethanol (5 ml). The reaction mixture was then stirred for 48 h at room temperature. The precipitate was then filtered off, washed with water and recrystallized from ethanol–water (1:4) (yield 62%; m.p. 335–336 K). Analysis, calculated for $C_{14}H_{16}N_2S_4$: C 49.21, H 4.71, N 8.24%; found: C 49.17, H 4.69, N 8.28%. Crystals of (I) suitable for single-crystal X-ray analysis were grown by slow evaporation of an acetone–water (3:1 *v*/*v*) solution.

Crystal data

$C_{14}H_{16}N_2S_4$
M_r = 340.53
Monoclinic, $C2/c$
a = 24.47 (2) Å
b = 7.195 (6) Å
c = 9.097 (8) Å
β = 91.61 (3)°
V = 1601 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.58 mm^{-1}
T = 294 (2) K
0.20 × 0.18 × 0.14 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.658, T_{max} = 1.000
(expected range = 0.606–0.921)
3865 measured reflections
1420 independent reflections
1024 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.129
S = 1.11
1420 reflections
92 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S2—C3	1.748 (3)	S2—C4	1.820 (3)
C3—S2—C4	102.13 (15)	S2—C3—S1	114.56 (16)
N1—C3—S2	126.8 (2)		

All H atoms were positioned geometrically and refined as riding, with C—H = 0.93–0.97 Å, and allowed to ride on their parent atoms, 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*.

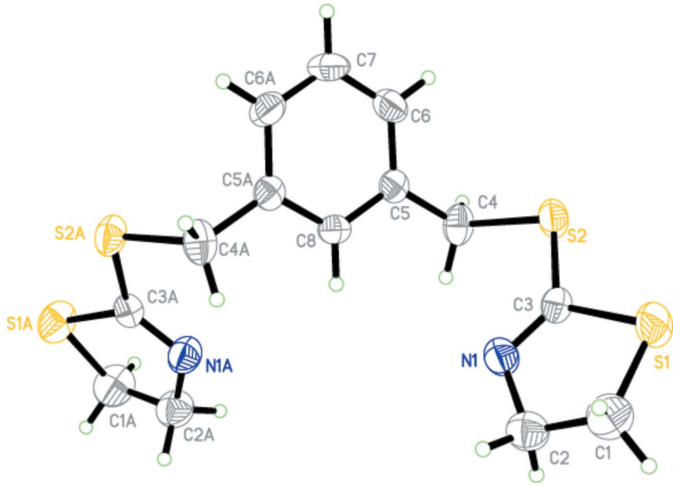


Figure 1
The molecular structuure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (A) $1-x, y, \frac{3}{2}-z$.]

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