

2,4,6-Trimethyl-1,3,5-tris(2-thiazolin-2-yl-sulfanylmethyl)benzene

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Key indicators

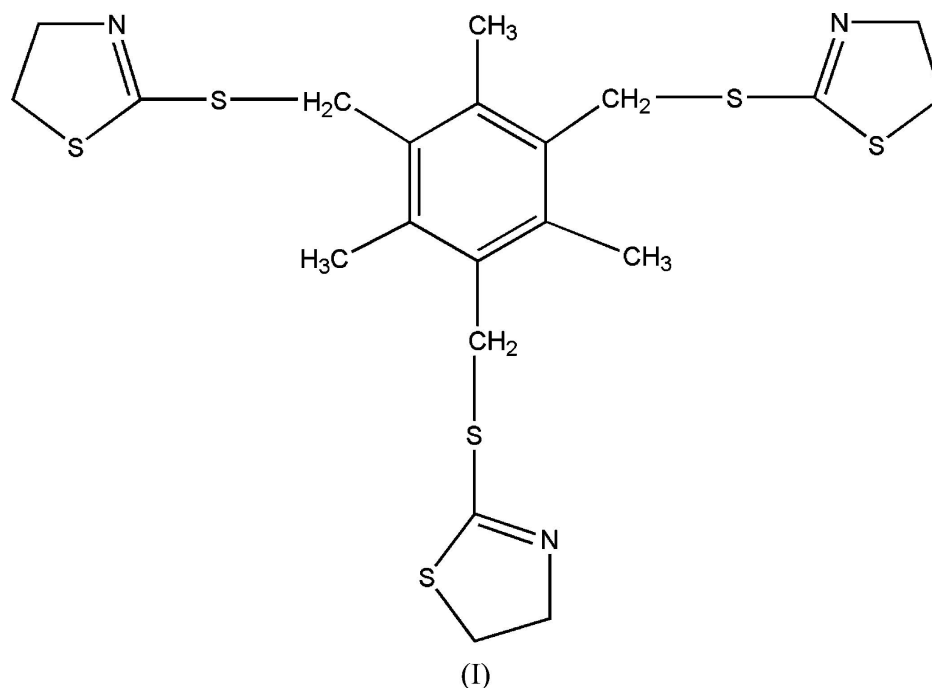
Single-crystal X-ray study
 $T = 294$ K
Mean $\sigma(\text{C}-\text{C}) = 0.005$ Å
 R factor = 0.044
 wR factor = 0.131
Data-to-parameter ratio = 15.8For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

The title compound, $\text{C}_{21}\text{H}_{27}\text{N}_3\text{S}_6$, was synthesized by the reaction of 2,4,6-trimethyl-1,3,5-tris(bromomethyl)benzene and thiazoline-2-thione. In the molecule, two thiazoline rings are located on one side of the central benzene plane, while the third thiazoline ring is located on the other side of the central benzene plane.

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Comment

A large number of flexible or rigid chain-linked dithioether ligands containing *N*-heterocyclic units have been synthesized and investigated due to their diverse coordination capabilities and the important properties of their metal complexes (Zheng *et al.*, 2003; Bu *et al.*, 2002; Hong *et al.*, 2000). Thiazoline derivatives exhibit various acaricide properties. Recently, we synthesized a new thiazoline derivative, namely, 2,4,6-trimethyl-1,3,5-tris(thiazoline-2-ylsulfanylmethyl)benzene, (I), the structure of which is reported here.



In the molecular structure of (I), there are three thiazoline rings *A* (atoms C8–C10/ N1/S1), *B* (C13–C15/N2/S4) and *C* (C18–C20/N3/S6). Rings *B* and *C* are located on one side of the central benzene ring while *A* is located on the opposite side. Atom C9 deviates by 0.273 (8) Å from the plane of the remaining four atoms in *A*. Atom C18 attached to the sulfanyl group has a distorted trigonal geometry, the N3–C18–S5

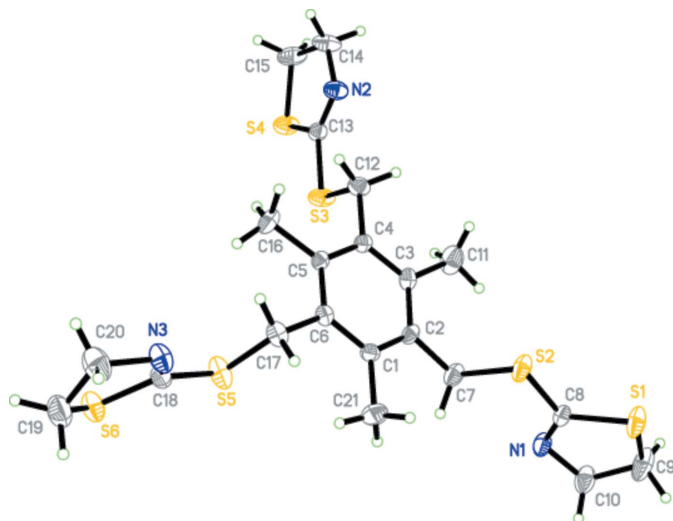


Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

[125.9 (3)°] and S5—C18—S6 [115.8 (2)°] angles deviating significantly from the ideal sp^2 -hybridized values.

As a result of π - π conjugation, the Csp^2 -S bonds (S2—C8, S3—C13 and S5—C18) are significantly shorter than the Csp^3 -S bonds (S2—C7, S3—C12 and S5—C17) (Table 1). The average lengths of the Csp^2 -S and Csp^3 -S bonds are 1.759 (7) and 1.820 (6) Å, respectively. These bond lengths are in good agreement with the values of 1.726 (2)/1.800 (3) and 1.720 (8)/1.811 (2) Å for the corresponding bonds reported by Wang *et al.* (2004) and Wang *et al.* (2005).

Experimental

A solution of 2,4,6-trimethyl-1,3,5-tris(bromomethyl)benzene (2.00 g, 5 mmol) in ethanol (10 ml) was added dropwise to a mixture of thiazoline-2-thione (1.79 g, 15 mmol), KOH (0.84 g, 15 mmol) and ethanol (10 ml). The reaction mixture was then stirred for 24 h at room temperature. The precipitate was filtered off, washed with water and recrystallized from water (yield 70%, m.p. 421–422 K). Analysis calculated for $C_{21}H_{27}N_3S_6$: C 49.12, H 5.26, N 8.19%; found: C 49.14, H 5.31, N 8.23%. Crystals of (I) suitable for single-crystal X-ray analysis were grown by slow evaporation of a solution in chloroform and ethanol (1:3 v/v).

Crystal data

$C_{21}H_{27}N_3S_6$	$Z = 8$
$M_r = 513.82$	$D_x = 1.390 \text{ Mg m}^{-3}$
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
$a = 19.834 (4) \text{ \AA}$	$\mu = 0.57 \text{ mm}^{-1}$
$b = 14.899 (3) \text{ \AA}$	$T = 294 (2) \text{ K}$
$c = 16.797 (3) \text{ \AA}$	Block, colourless
$\beta = 98.381 (3)^\circ$	$0.18 \times 0.14 \times 0.10 \text{ mm}$
$V = 4910.5 (15) \text{ \AA}^3$	

Data collection

Bruker SMART CCD area-detector diffractometer	12381 measured reflections
φ and ω scans	4341 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	2688 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.617$, $T_{\max} = 1.000$ (expected range = 0.583–0.944)	$R_{\text{int}} = 0.050$ $\theta_{\text{max}} = 25.0^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0638P)^2 + 0.8708P]$
$R[F^2 > 2\sigma(F^2)] = 0.044$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.131$	$(\Delta/\sigma)_{\text{max}} = 0.004$
$S = 1.03$	$\Delta\rho_{\text{max}} = 0.32 \text{ e \AA}^{-3}$
4341 reflections	$\Delta\rho_{\text{min}} = -0.25 \text{ e \AA}^{-3}$
274 parameters	
H-atom parameters constrained	

Table 1

Selected geometric parameters (Å, °).

S1—C9	1.787 (4)	S3—C13	1.753 (3)
S2—C8	1.745 (3)	S4—C15	1.784 (4)
S2—C7	1.812 (3)	S5—C18	1.730 (4)
N3—C18—S5	125.9 (3)	S5—C18—S6	115.8 (2)

All H atoms were positioned geometrically and refined as riding (C—H = 0.96 and 0.97 Å). For the CH₂ groups, $U_{\text{iso}}(\text{H})$ values were set equal to $1.2U_{\text{eq}}(\text{carrier atom})$ and for the methyl groups they were set equal to $1.5U_{\text{eq}}(\text{carrier atom})$.

Data collection: SMART (Bruker, 1997); cell refinement: SAINT (Bruker, 1997); 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, 1997); software used to prepare material for publication: SHELXTL.

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