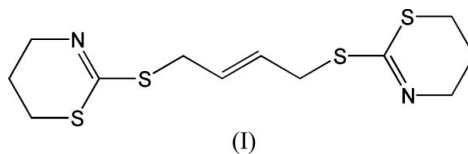


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## Key indicators

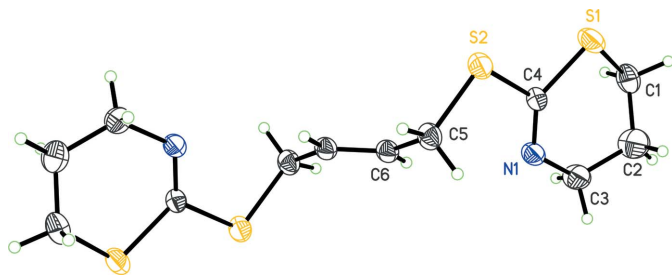
Single-crystal X-ray study  
 $T = 294$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.006$  Å  
 $R$  factor = 0.050  
 $wR$  factor = 0.144  
Data-to-parameter ratio = 19.0For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.*trans*-2,2'-[(2-Butene-1,4-diyl)dithio]bis(4,5-  
dihydro-1,3-thiazine)The title compound,  $\text{C}_{12}\text{H}_{18}\text{N}_2\text{S}_4$ , was synthesized by the reaction of *trans*-1,4-dibromo-2-butene and 1,3-thiazine-2-thione. The molecule contains a centre of inversion at the mid-point of the central double bond and the thiazine rings have an envelope conformation.Received 18 August 2006  
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## Comment

As a type of ditopic ligand, dithioethers can be used as bridging ligands in the building of coordination polymers with soft metal ions. *N*-Heterocyclic units have been synthesized and investigated (Sharma *et al.*, 1999; Constable *et al.*, 2002; Bu *et al.*, 2003; Hong *et al.*, 2000). Thiazine derivatives possess acaricide properties. In order to study the properties of these compounds, we have synthesized several new thiazine derivatives, and we present here the crystal structure of one of them, (I).In the molecular structure of (I) (Fig. 1), there is an inversion centre at the mid-point of the central  $\text{C6}=\text{C6}^i$  bond [symmetry code: (i)  $-x, 1 - y, -z$ ]. The thiazine ring has an envelope conformation, with atom C2 deviating by 0.559 (9) Å from the plane of the remaining five ring atoms. As a result of the centrosymmetric character of (I), the two thiazine rings point in opposite directions, reducing potential steric hindrance. Atom C4 has a distorted trigonal geometry, with the  $\text{N1}-\text{C4}-\text{S1}$  and  $\text{S1}-\text{C4}-\text{S2}$  angles (Table 1) deviating significantly from the ideal geometry for an  $sp^2$ -hybridized C atom.The  $\text{C}=\text{C}$  bond distance of 1.318 (6) Å of the butene group is shorter than the value of 1.34 Å expected for a normal  $\text{C}=\text{C}$  bond (Lide, 1992–1993). The butenediyl group is planar. The  $\text{C}sp^2-\text{S}$  bonds distance are significantly shorter than the  $\text{C}sp^3-\text{S}$  bonds (Table 1), as expected, and are comparable with those found in the literature (*e.g.* Wang *et al.*, 2004, 2005).As shown in Fig. 2, intermolecular  $\text{S}\cdots\text{S}$  interactions [3.587 (3) Å] link the molecules of (I) into a two-dimensional network.

## Experimental

A solution of *trans*-1,4-dibromo-2-butene (1.07 g, 5 mmol) in ethanol (5 ml) was added dropwise to a mixture of 1,3-thiazine-2-thione (1.46 g, 11 mmol), KOH (0.615 g, 11 mmol) and ethanol (5 ml). The


**Figure 1**

The molecular structure of (I), showing the atom-labelling scheme for the asymmetric unit. Non-labelled atoms are generated through symmetry code  $(-x, 1-y, -z)$ . Displacement ellipsoids are drawn at the 30% probability level.

reaction mixture was then stirred for 24 h at 298 K. The precipitate was then filtered off, washed with water and recrystallized from ethanol and water (1:1 v/v) (yield 44%, m.p. 357–358 K). Analysis found: C 45.17, H 5.62, N 8.83%; calculated for  $C_{12}H_{18}N_2S_4$ : C 45.25, H 5.70, N 8.79%. Crystals of (I) suitable for single-crystal X-ray analysis were grown by slow evaporation of an acetone–dichloromethane (3:1) solution.

#### Crystal data

$C_{12}H_{18}N_2S_4$	$Z = 2$
$M_r = 318.52$	$D_x = 1.374 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 8.282(5) \text{ \AA}$	$\mu = 0.60 \text{ mm}^{-1}$
$b = 10.578(6) \text{ \AA}$	$T = 294(2) \text{ K}$
$c = 9.625(6) \text{ \AA}$	Block, colourless
$\beta = 114.100(8)^\circ$	$0.26 \times 0.20 \times 0.16 \text{ mm}$
$V = 769.7(8) \text{ \AA}^3$	

#### Data collection

Bruker SMART CCD area-detector diffractometer	4202 measured reflections
$\varphi$ and $\omega$ scans	1567 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	1102 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.726$ , $T_{\max} = 0.910$	$R_{\text{int}} = 0.033$
	$\theta_{\text{max}} = 26.4^\circ$

#### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0586P)^2 + 0.568P]$
$R[F^2 > 2\sigma(F^2)] = 0.050$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.144$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.06$	$\Delta\rho_{\text{max}} = 0.97 \text{ e \AA}^{-3}$
1567 reflections	$\Delta\rho_{\text{min}} = -0.48 \text{ e \AA}^{-3}$
82 parameters	
H-atom parameters constrained	

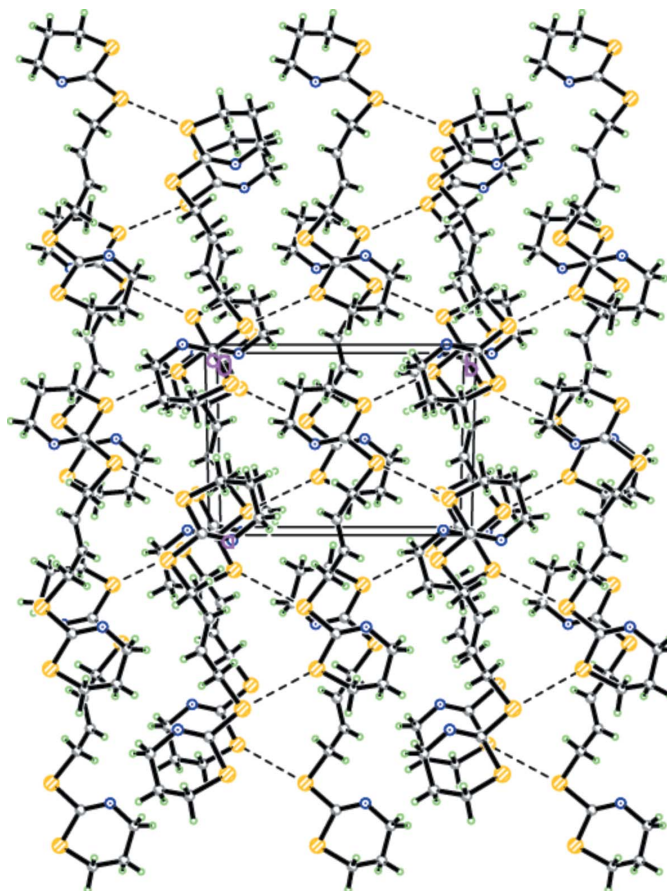
**Table 1**

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

S1–C4	1.771 (3)	N1–C4	1.252 (4)
S1–C1	1.793 (4)	N1–C3	1.463 (4)
S2–C4	1.768 (3)	C6–C6 <sup>i</sup>	1.318 (6)
S2–C5	1.819 (3)		
N1–C4–S1	129.3 (3)	S1–C4–S2	108.36 (18)

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

All H atoms were positioned geometrically and refined as riding on their parent atoms, with C–H = 0.93 ( $C_{sp^2}$ –H6) and 0.97  $\text{\AA}$  (methylene  $CH_2$ ), and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .


**Figure 2**

A packing diagram for (I). The dashed lines indicate S...S short contacts between neighbouring molecules.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINTE* (Bruker, 1997); data reduction: *SAINTE*; 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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