

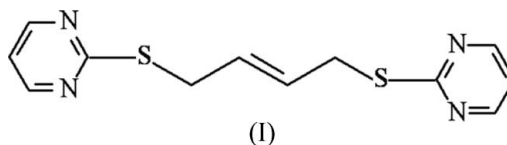
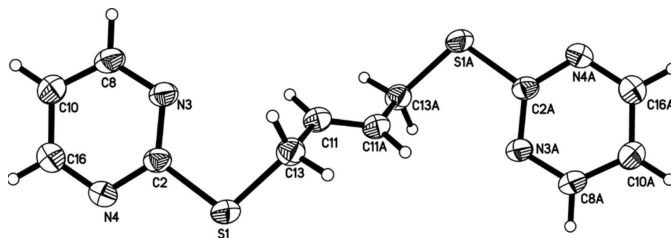
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Key indicators

Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.007$ Å
 R factor = 0.094
 wR factor = 0.255
Data-to-parameter ratio = 17.0For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.*trans*-1,4-Bis(pyrimidin-2-ylsulfanyl)but-2-eneThe title compound, $\text{C}_{12}\text{H}_{12}\text{N}_4\text{S}_2$, adopts a *trans* configuration about the central $\text{C}=\text{C}$ double bond. There is a centre of inversion at the mid-point of the $\text{C}=\text{C}$ bond. The dihedral angle between each pyrimidine ring and the butenyl backbone chain is $62.6(3)^\circ$.

Comment

A large number of complexes of dithioether ligands containing *N*-heterocyclic systems have been synthesized and investigated because of their interesting structures and the properties of their metal complexes (Hong *et al.*, 2000). With this background, we are attempting to obtain a series of analogous compounds as block units for the construction of coordination polymers. In the present paper, we report the crystal structure of *trans*-1,4-bis(pyrimidin-2-ylsulfanyl)but-2-ene, (I), the result of a recent synthesis.As shown in Fig. 1, compound (I) adopts a *trans* configuration about the central $\text{C}=\text{C}$ double bond. The conformation is *anti*, with a centre of inversion at the mid-point of the $\text{C}=\text{C}$ bond. The butenyl spacer unit, C13/C11/C11A/C13A [symmetry code: (A) $-x, 1 - y, 1 - z$], is essentially planar, excluding H atoms, and each pyrimidine ring is inclined to the plane by $62.6(3)^\circ$. Each S atom deviates from the plane by $1.480(7)$ Å, with an $\text{S1}\cdots\text{S1A}$ distance of $6.484(3)$ Å. The $\text{S}-\text{C}$ bond distances and $\text{C}-\text{S}-\text{C}$ angles are comparable with those observed in the analogous compound, 1,2-(pyrimidin-2-ylsulfanyl)butene (Zhang *et al.*, 2005). The ligand also adopts the *anti* conformation in the crystal structure of a silver(I) nitrate complex (Zheng *et al.*, 2005). On the other hand, it adopts both *anti* and *gauche* conformations in a silver(I) perchlorate complex (Zheng *et al.*, 2005).**Figure 1**
ORTEP (Johnson, 1976) view of (I), showing atomic displacement ellipsoids at the 30% probability level. [Symmetry code: (A) $-x, 1 - y, 1 - z$.]

Experimental

Thiophenol (4.0 ml, 0.04 mol) and KOH (2.24 g, 0.04 mol) were stirred in 30 ml ethanol at reflux over a period of an hour. *meso*-1,2,3,4-Tetrabromobutane (3.73 g, 0.01 mol) in 10 ml THF was then added dropwise. A white precipitate appeared. After stirring under reflux for 3 h, the mixture was cooled to room temperature and the precipitate was filtered off. The filtrate was evaporated to dryness under vacuum, the residue taken up in the minimum amount of ethanol, filtered and the title compound allowed to crystallize at 273 K. Yellow single crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of a chloroform solution at room temperature.

Crystal data

$C_{12}H_{12}N_4S_2$	$D_x = 1.404 \text{ Mg m}^{-3}$
$M_r = 276.38$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 6221 reflections
$a = 7.7711 (16) \text{ \AA}$	$\theta = 3.2\text{--}27.5^\circ$
$b = 9.7259 (19) \text{ \AA}$	$\mu = 0.39 \text{ mm}^{-1}$
$c = 9.825 (4) \text{ \AA}$	$T = 293 (2) \text{ K}$
$\beta = 118.29 (2)^\circ$	Needle, yellow
$V = 653.9 (3) \text{ \AA}^3$	$0.52 \times 0.16 \times 0.05 \text{ mm}$
$Z = 2$	

Data collection

Rigaku R-AXIS RAPID IP area-detector diffractometer	1495 independent reflections
ω scans	935 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$R_{\text{int}} = 0.081$
$T_{\text{min}} = 0.820$, $T_{\text{max}} = 0.979$	$\theta_{\text{max}} = 27.5^\circ$
6221 measured reflections	$h = -10 \rightarrow 10$
	$k = -12 \rightarrow 12$
	$l = -12 \rightarrow 12$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.094$	$w = 1/[\sigma^2(F_o^2) + (0.1509P)^2]$
$wR(F^2) = 0.255$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{\text{max}} = 0.008$
1495 reflections	$\Delta\rho_{\text{max}} = 0.66 \text{ e \AA}^{-3}$
88 parameters	$\Delta\rho_{\text{min}} = -0.26 \text{ e \AA}^{-3}$

Table 1

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

S1–C2	1.752 (4)	S1–C13	1.804 (4)
C2–S1–C13	102.5 (2)		

All H atoms were positioned geometrically, with $Csp^2-H = 0.93 \text{ \AA}$ and $Csp^3-H = 0.97 \text{ \AA}$, and were constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The large values of R and wR may be due to the poor quality of the crystal.

Data collection: *RAPID-AUTO* (Rigaku/MSC, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *CrystalStructure* (Rigaku/MSC, 2004).

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