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# 5,5′-[(*p*-Phenylenedimethylene)dithio]-bis(1-phenyl-1*H*-1,2,3,4-tetrazole)

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**Key indicators**

Single-crystal X-ray study
*T* = 293 K
Mean σ(C–C) = 0.005 Å
*R* factor = 0.040
*wR* factor = 0.129
Data-to-parameter ratio = 13.6

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

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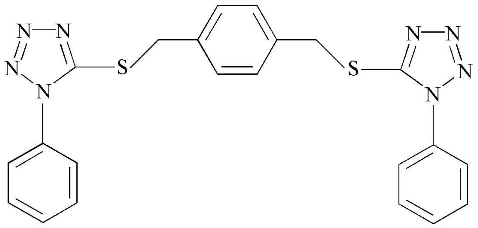
The title compound, $C_{22}H_{18}N_8S_2$, was synthesized by the reaction of α,α′-dibromo-*p*-xylene and 1-phenyl-5-thio-1,2,3,4-tetrazole. In the molecule, the two tetrazole rings are almost parallel, making a dihedral angle of 9.8 (3)°. The two terminal phenyl rings attached to the tetrazole rings are perpendicular to the central benzene ring.

## Comment

Dithioethers are often used as bridging ligands in the construction of coordination polymers with soft metal ions. Flexible and rigid chain-linked dithioethers containing *N*-heterocyclic groups have been synthesized and investigated (Constable *et al.*, 2002; Hong *et al.*, 2000). Some of the tetrazole derivatives possess diverse pharmacological properties (July *et al.*, 1968; 1982). However, the crystal structures of only a few complexes of monosubstituted tetrazole derivatives have been reported to date (Lyakhov *et al.*, 2003). The title compound, (I), has been synthesized by the reaction of α,α′-dibromo-*p*-xylene and 1-phenyl-5-thio-1,2,3,4-tetrazole. We present its crystal structure here.



(I)

In (I) (Fig. 1), the two tetrazole rings are almost parallel, with a dihedral angle of 9.8 (3)° between them. Interestingly, the two terminal phenyl rings, C1–C6 (*A*) and C17–C22 (*B*), attached to these tetrazole rings make a dihedral angle of 29.7 (3)°. Rings *A* and *B* are essentially perpendicular to the central benzene ring C9–C14, making dihedral angles of 97.3 (3) and 94.8 (3)°, respectively, with the latter. Atoms C7 and C16 in the tetrazole moieties each have distorted trigonal geometry, with the N—C—N and N—C—S angles (Table 1) deviating significantly from the ideal $sp^2$ hybridized values. The average lengths of the S—C$sp^3$ and S—C$sp^2$ bonds [1.800 (3) and 1.720 (8) Å, respectively] are close to the values of 1.811 (2) and 1.726 (2) Å reported in the literature (Wang *et al.*, 2004).

In the crystal structure of (I), there are no short intermolecular contacts.

An isomer of (I) is reported in the preceding paper (Luo *et al.*, 2005).

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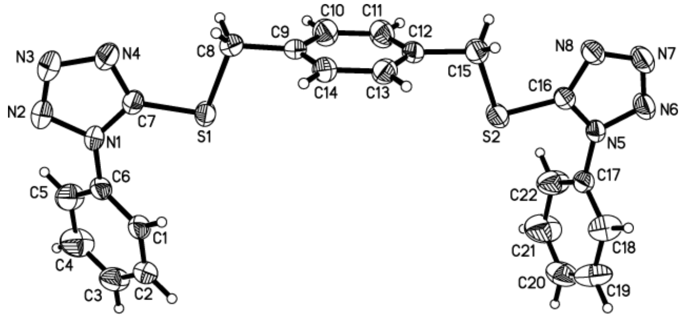

**Figure 1**
A view of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

## Experimental

A solution of $\alpha,\alpha'$-dibromo-*p*-xylene (1.07 g, 5 mmol) in ethanol (10 ml) was added dropwise to a mixture of 1-phenyl-5-thio-1,2,3,4-tetrazole (1.96 g, 11 mmol), KOH (0.615 g, 11 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 ethanol (yield 70%; m.p. 460–461 K). Spectroscopic analysis: IR (KBr, $\nu$, cm$^{-1}$): 3062, 2363, 1594, 1500, 1460, 1382, 1274, 1235, 763, 693; $^1$H NMR (CDCl$_3$, $\delta$, p.p.m.): 4.57 (4H, *s*), 7.37 (4H, *s*), 7.48–7.53 (10H, *m*). Analysis calculated for $C_{22}H_{18}N_8S_2$: C 57.64, H 3.93, N 24.45%; found: C 57.59, H 4.01, N 24.36%. Crystals of (I) suitable for single-crystal X-ray analysis were grown by slow evaporation of a solution in acetonitrile.

### *Crystal data*

$C_{22}H_{18}N_8S_2$
$M_r$ = 458.58
Monoclinic, $P2_1/c$
$a$ = 10.114 (15) Å
$b$ = 10.537 (15) Å
$c$ = 20.92 (3) Å
$\beta$ = 95.56 (3)°
$V$ = 2219 (6) Å$^3$
$Z$ = 4
$D_x$ = 1.373 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 955 reflections
$\theta$ = 2.9–25.8°
$\mu$ = 0.27 mm$^{-1}$
$T$ = 293 (2) K
Prism, colourless
0.30 × 0.28 × 0.24 mm

### *Data collection*

Bruker SMART CCD area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min}$ = 0.923, $T_{\max}$ = 0.938
11 289 measured reflections
3916 independent reflections
2692 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.030
$\theta_{\max}$ = 25.0°
$h = -12 \rightarrow 11$
$k = -12 \rightarrow 12$
$l = -13 \rightarrow 24$

### *Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.129
$S$ = 1.06
3916 reflections
289 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0619P)^2 + 0.5887P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max}$ = 0.20 e Å$^{-3}$
$\Delta\rho_{\min}$ = −0.21 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| S1—C7 | 1.719 (3) | S2—C16 | 1.721 (3) |
| S1—C8 | 1.797 (3) | S2—C15 | 1.803 (3) |
| | | | |
| N4—C7—N1 | 109.2 (2) | N8—C16—N5 | 109.0 (2) |
| N4—C7—S1 | 126.3 (2) | N8—C16—S2 | 128.0 (2) |

All H atoms were positioned geometrically and refined as riding (C—H = 0.93–0.97 Å), with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(parent).

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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