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1,3-Bis(1-phenyl-1*H*-tetrazole-5-ylsulfanyl)-propane

Peng Lei, Wei Wang,* Qing-Shan Yang and De-Qian Shi

School of Chemical Engineering, University of Science and Technology Liaoning, Anshan 114002, People's Republic of China

Correspondence e-mail: wangweitfj@gmail.com

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Key indicators

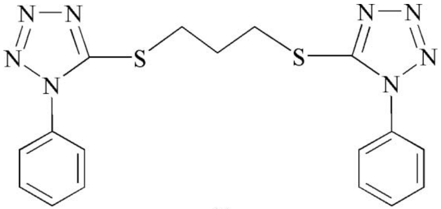
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.050
wR factor = 0.131
Data-to-parameter ratio = 18.3

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

In the title compound, $C_{17}H_{16}N_8S_2$, the terminal ring systems extend in opposite directions to minimize steric hindrance.

Comment

To date, 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 (Heuvel *et al.*, 1983; Bu *et al.*, 2002). Earlier studies reported that several tetrazole derivatives possess diverse pharmacological properties (Juby *et al.*, 1968, 1982). However, crystallographic studies of only a few complexes of mono-substituted tetrazole derivaties have been reported (Lyakhov *et al.*, 2003). We have reported some tetrazole derivatives using rigid chains as linkers, such as 1,2-phenylene, 1,4-phenylene (Luo *et al.*, 2005; Wang *et al.*, 2005). We have now synthesized a new tetrazole derivative, namely 1,3-bis(1-phenyl-1*H*-tetrazole-5-ylsulfanyl)propane, (I), using flexible 1,3-dipropyl as linker. We present its crystal structure here.



(I)

In the molecule of (I), the two terminal phenyl rings make a dihedral angle of 50.0 (1)°. The dihedral angles between the phenyl ring C1–C6 and the corresponding tetrazole ring (C7,N1–N4) is 68.8 (1) [54.8 (1)° between C12–C17 and C11,N5–N8]. The pseudo-torsion angle of the two C—S bonds (C7—S1···S2—C11) is 124.4 (3)°, showing that the terminal ring systems extend in opposite directions to minimize steric hindrance.

The π–π conjugation of atom S1 with the tetrazole ring affects the C7—S1 bond distance [1.737 (2) Å] which is shorter than C8—S1 [1.814 (2) Å]. This effect is also observed for S2 and in other tetrazole-thio derivatives reported in the literature (Wang *et al.*, 2004, 2005).

Experimental

A solution of 1,3-dibromopropane (1.01 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

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precipitate was filtered off, washed with water and recrystallized from ethanol (yield 70%). Crystals of (I) suitable for single-crystal X-ray analysis were grown by slow evaporation of a solution in chloroform.

Crystal data

$C_{17}H_{16}N_8S_2$
$M_r = 396.5$
Monoclinic, $P2_1/n$
$a = 16.774$ (3) Å
$b = 6.5029$ (13) Å
$c = 18.691$ (4) Å
$\beta = 112.24$ (3)°
$V = 1887.1$ (8) Å^3
$Z = 4$
$D_x = 1.396$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.30$ mm^{-1}
$T = 293$ (2) K
Block, colourless
0.14 × 0.12 × 0.10 mm

Data collection

Rigaku Saturn 70 diffractometer
ω scans
Absorption correction: multi-scan (*REQAB*; Jacobson, 1998) $T_{\min} = 0.959$, $T_{\max} = 0.970$
14105 measured reflections
4478 independent reflections
3342 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.048$
$\theta_{\max} = 27.9$°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.050$
$wR(F^2) = 0.131$
$S = 1.10$
4478 reflections
245 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0652P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.002$
$\Delta\rho_{\max} = 0.24$ e Å^{-3}
$\Delta\rho_{\min} = -0.30$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0165 (19)

Table 1
Selected geometric parameters (Å, °).

S1—C7	1.737 (2)	S2—C11	1.731 (2)
S1—C8	1.814 (2)	S2—C10	1.8094 (19)
N4—C7—N1	108.23 (17)	N5—C11—N8	108.76 (18)
N4—C7—S1	128.68 (15)	N5—C11—S2	129.12 (15)

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

Data collection: *CrystalClear* (Molecular Structure Corporation & Rigaku, 1999); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Rigaku/MSC, 2005); 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*.

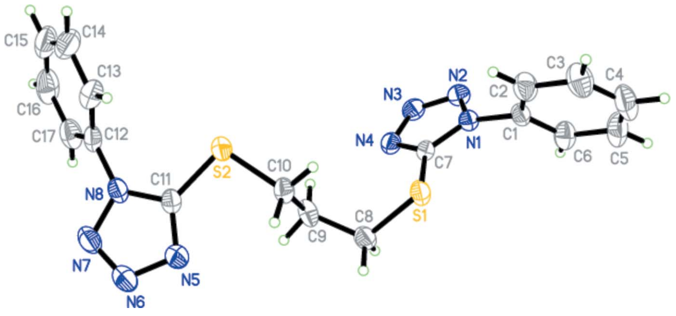

Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

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