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2,3-Bis[(1-phenyl-1*H*-tetrazol-5-ylsulfanyl)-methyl]quinoxaline

Wei Wang,[a]* Ning-Ning Pan[a] and Bing Zhao[b]

[a]School of Chemical Engineering, Anshan University of Science and Technology, Anshan 114002, People's Republic of China, and [b]School of Chemical Engineering and Technology, Tianjin University, Tianjin 300072, People's Republic of China

Correspondence e-mail: tju_chemistry@yahoo.com.cn

Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.044
wR factor = 0.133
Data-to-parameter ratio = 14.9

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

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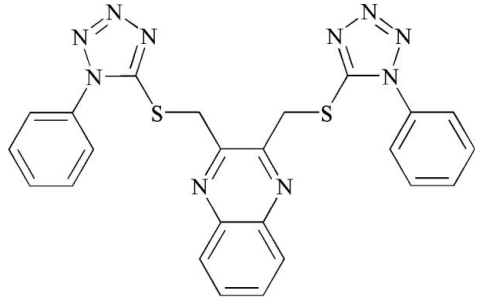
The title compound, $C_{24}H_{18}N_{10}S_2$, crystallizes with two independent molecules in the asymmetric unit. The two terminal (1-phenyltetrazol-5-yl)sulfanyl groups adopt a *trans* configuration with respect to the central quinoxaline ring system in both independent molecules.

Comment

To date, a large number of flexible or rigid chain-linked dithioether ligands containing *N*-heterocyclic groups 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). Earlier studies reported that several tetrazole derivatives possess varied pharmacological properties (Juby *et al.*, 1968, 1982). A new tetrazole derivative, the title compound, (I), has been synthesized and its crystal structure is presented here.



(I)

The asymmetric unit of compound (I) contains two independent molecules, *A* and *B*. The two terminal (1-phenyl-1,2,3,4-tetrazol-5-yl)sulfanyl groups adopt a *trans* configuration with respect to the central quinoxaline ring system in both molecules *A* and *B* (Fig. 1). In molecule *A*, the planar quinoxaline ring system makes dihedral angles of 11.5 (3) and 8.8 (3)° with the two tetrazolyl rings, indicating that the three groups are approximately coplanar. A similar result is also observed in molecule *B*. In molecule *A*, the two terminal phenyl rings make a dihedral angle of 39.5 (3)°, while in molecule, *B*, the dihedral angle is 19.2 (2)°.

Due to π–π conjugation, the Csp^2—S bonds, *i.e.* S1—C1, S2—C18, S3—C25 and S4—C42, are significantly shorter than the Csp^3—S bonds, *i.e.* S1—C8, S2—C17, S3—C32 and S4—C41 (Table 1). The average lengths of the Csp^2—S and Csp^3—S bonds are 1.732 (3) and 1.807 (3) Å, respectively, which are comparable with those reported in the literature (Wang *et al.*, 2004, 2005).

Experimental

A solution of 2,3-bis(bromomethyl)quinoxaline (1.58 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 (0.62 g, 11 mmol) and ethanol (5 ml). The reaction mixture was then stirred for 24 h at room temperature. The precipitate which formed was filtered off, washed with water and recrystallized from ethanol (yield 70%, m.p. 446–447 K). Analysis, calculated for $C_{24}H_{18}N_{10}S_2$: C 56.45, H 3.55, N 27.43%; found: C 56.41, H 3.60, N 27.37%. Crystals of (I) suitable for single-crystal X-ray analysis were grown by slow evaporation of a solution in chloroform.

Crystal data

$C_{24}H_{18}N_{10}S_2$
M_r = 510.62
Triclinic, $P\overline{1}$
a = 6.3813 (18) Å
b = 16.758 (5) Å
c = 22.214 (6) Å
α = 96.538 (5)°
β = 92.822 (4)°
γ = 95.274 (5)°
V = 2345.8 (12) Å^3
Z = 4
D_x = 1.446 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.26 mm^{-1}
T = 294 (2) K
Block, colourless
0.32 × 0.20 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.910, T_{max} = 0.969
13253 measured reflections
9645 independent reflections
4834 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 26.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.133
S = 0.99
9645 reflections
649 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0533P)^2 + 0.326P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—C1	1.731 (3)	S3—C25	1.726 (3)
S1—C8	1.810 (3)	S3—C32	1.810 (3)
S2—C18	1.736 (3)	S4—C42	1.736 (3)
S2—C17	1.807 (3)	S4—C41	1.801 (3)
N4—C1—N1	108.4 (2)	N14—C25—N11	108.7 (2)
N4—C1—S1	126.8 (2)	N14—C25—S3	125.8 (2)
N10—C18—N7	108.7 (2)	N20—C42—N17	109.0 (2)
N10—C18—S2	126.9 (2)	N20—C42—S4	126.8 (2)

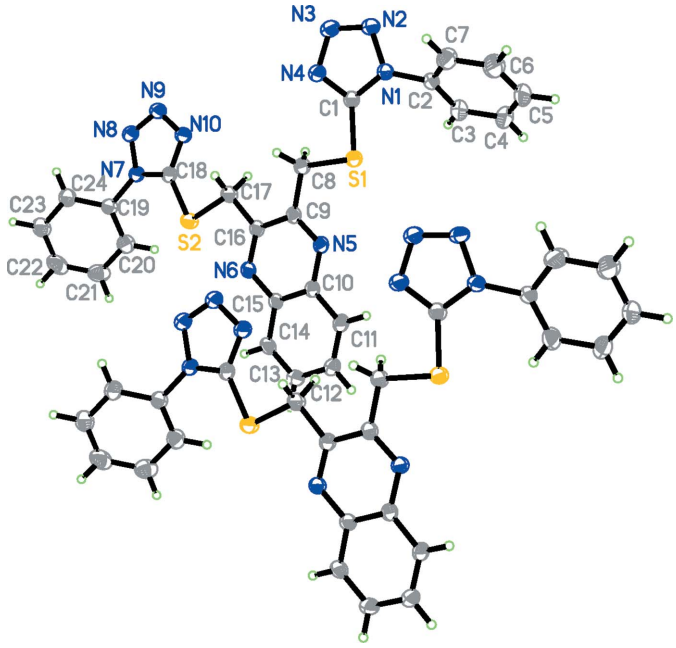


Figure 1
The asymmetric unit of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

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

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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