

1,2-Bis(1-phenyl-1*H*-tetrazol-5-ylsulfanyl)ethaneWei Wang,^{a,b} Hui-Min Liu,^a Yan Zheng^{a*} and Wen-Qin Zhang^a^aDepartment of Chemistry, Tianjin University, Tianjin 300072, People's Republic of China, and ^bDepartment of Chemical Engineering, Anshan University of Science and Technology, Anshan 114002, People's Republic of ChinaCorrespondence e-mail:
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Key indicators

Single-crystal X-ray study
T = 293 K
Mean $\sigma(\text{C}-\text{C}) = 0.003 \text{ \AA}$
R factor = 0.037
wR factor = 0.093
Data-to-parameter ratio = 15.2For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.The title compound, $\text{C}_{16}\text{H}_{14}\text{N}_8\text{S}_2$, contains a centre of inversion. The mean planes of the phenyl and 1*H*-tetrazol-5-ylsulfanyl moieties make a dihedral angle of $45.8(3)^\circ$.

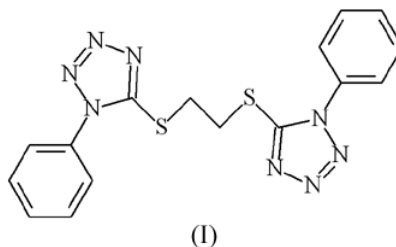
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Comment

As a type of ditopic ligand, dithioethers can be used as bridging ligands in the construction of coordination polymers with soft metal ions. A series of flexible or rigid chain-linked dithioethers containing *N*-heterocyclic moieties have been synthesized and investigated (Sharma *et al.*, 1999; Constable *et al.*, 2002; Bu *et al.*, 2003; Hong *et al.*, 2000; Zheng *et al.*, 2003). Earlier studies have shown that several tetrazole derivatives possess diverse pharmacological properties (Juby *et al.*, 1968, 1982), but only a few metal complexes of monosubstituted tetrazole derivatives are known (van den Heuvel *et al.*, 1983; Lyakhov *et al.*, 2003). We report here the synthesis and structure of a new tetrazole dithioether, namely 1,2-bis(1-phenyl-1*H*-tetrazol-5-ylsulfanyl)ethane, (I).



In (I), there is an inversion centre at the midpoint of the C8—C8' bond [symmetry code: (i) $1 - x, -y, -z$]. The mean planes of the phenyl and the 1*H*-tetrazol-5-ylsulfanyl moieties make a dihedral angle of $45.8(3)^\circ$.

In (I), the $\text{Csp}^2\text{-S}$ bond distance (C1—S1) is significantly shorter than that of $\text{Csp}^3\text{-S}$ (C8—S1) because of $p-\pi$ conjugation, as is observed in other dithioethers (Zhang *et al.*, 2003; Zheng & Liu, 2003).

Experimental

A solution of 0.94 g (5 mmol) of 1,2-dibromoethane in 10 ml of ethanol was added dropwise to a mixture of 1.96 g (11 mmol) of 1-phenyl-5-thio-1,2,3,4-tetrazole, 0.615 g (11 mmol) of KOH and 10 ml of ethanol. 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: 62%; m.p. 432–433 K). IR (KBr, ν , cm^{-1}): 3070 (*w*), 3021 (*w*), 2361 (*s*), 1596 (*m*); 1499 (*vs*), 1465 (*w*), 1418 (*m*), 1385 (*s*), 1315 (*s*), 1276 (*m*), 1249 (*s*), 1140 (*w*), 1088 (*m*), 1014 (*m*), 981 (*m*), 758 (*s*), 695 (*s*). $^1\text{H NMR}$ (CDCl_3): δ 3.88 (*s*, 4 H),

7.54 (s, 10 H); ^{13}C NMR (CDCl_3): δ 32.30, 123.73, 129.90, 130.31, 133.45, 153.41. Analysis calculated for $\text{C}_{16}\text{H}_{14}\text{N}_8\text{S}_2$: C 50.2, H 3.7, N 29.3%; found: C 49.9, H 3.8, N 29.5%. Crystals suitable for single-crystal X-ray analysis were obtained by recrystallization from acetonitrile solution.

Crystal data

$\text{C}_{16}\text{H}_{14}\text{N}_8\text{S}_2$
 $M_r = 382.47$
 Monoclinic, $P2_1/c$
 $a = 9.333$ (3) Å
 $b = 13.456$ (4) Å
 $c = 7.181$ (2) Å
 $\beta = 103.55$ (1)°
 $V = 876.7$ (5) Å³
 $Z = 2$

$D_x = 1.449$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 744 reflections
 $\theta = 2.7\text{--}25.2^\circ$
 $\mu = 0.32$ mm⁻¹
 $T = 293$ (2) K
 Block, colourless
 $0.22 \times 0.18 \times 0.14$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1997)
 $T_{\min} = 0.930$, $T_{\max} = 0.956$
 4942 measured reflections

1793 independent reflections
 1199 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.037$
 $\theta_{\text{max}} = 26.5^\circ$
 $h = -11 \rightarrow 8$
 $k = -16 \rightarrow 16$
 $l = -8 \rightarrow 8$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.037$
 $wR(F^2) = 0.093$
 $S = 1.01$
 1793 reflections
 118 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0438P)^2 + 0.0706P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.17$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.20$ e Å⁻³

All H atoms were treated as riding, with C—H distances of 0.93 (aromatic) and 0.97 Å (CH₂), and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

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.

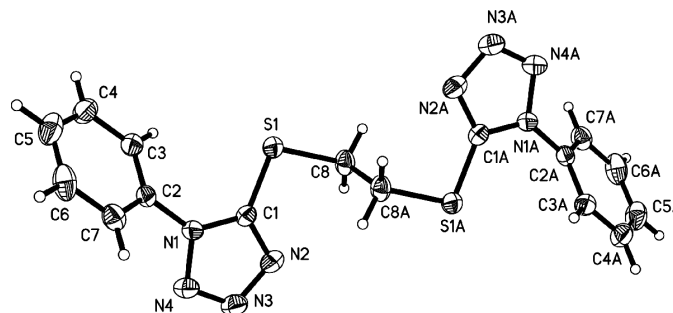


Figure 1 View of the title compound, with the atom-labelling scheme and displacement ellipsoids drawn at the 30% probability level.

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