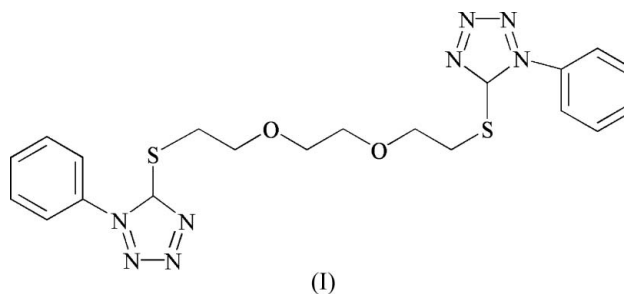


Bis[2-(1-phenyl-1*H*-tetrazol-5-ylsulfanyl)-ethoxy] etherWei Wang,^{a*} Bing Zhao,^b
Peng-Wu Zheng^c and
Xue-Min Duan^c^aSchool of Chemical Engineering, Anshan University of Science and Technology, Anshan 114002, People's Republic of China, ^bSchool of Chemical Engineering and Technology, Tianjin University, Tianjin 300072, People's Republic of China, and ^cSchool of Pharmaceuticals and Biotechnology, Jiangxi Science and Technology Normal University, Nanchang 330013, People's Republic of ChinaCorrespondence e-mail:
wangweitf@yahoo.com.cn

Key indicators

Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å
 R factor = 0.044
 wR factor = 0.128
Data-to-parameter ratio = 16.2For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.The title compound, $\text{C}_{20}\text{H}_{22}\text{N}_8\text{O}_2\text{S}_2$, contains a center of inversion at the mid-point of the central C—C bond. The mean planes of the phenyl and the 1*H*-tetrazol-5-ylsulfanyl rings make a dihedral angle of $53.95(16)^\circ$.

Comment

Dithioethers are often used as bridging ligands in the construction of coordination polymers with soft metal ions and a series of flexible or rigid chain-linked dithioethers containing *N*-heterocyclic groups have been synthesized and investigated (Constable *et al.*, 2002; Hong *et al.*, 2000). Earlier studies have reported that several tetrazole derivatives possess diverse pharmacological properties (Juby *et al.*, 1968, 1982). We have reported some tetrazole derivatives using flexible and rigid chains as linkers; these include 1,2-diethyl (Wang, Liu, Zheng & Zhang, 2004), 1,4-dibutyl (Wang, Liu & Zhang, 2004) and 1,2-phenylene (Luo, *et al.*, 2005), 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 bis[2-(1-phenyl-1*H*-tetrazol-5-ylsulfanyl)ethoxy] ether, (I).In the molecular structure of (I), there is an inversion center at the mid-point of the C1—C1A bond (Fig. 1) [symmetry code: (A) $-x, 1 - y, 1 - z$]. The bond distance C1—C1A of $1.493(6)$ Å confirms its single-bond character. The dihedral angle between the phenyl ring and the attached tetrazolyl ring is $53.95(16)^\circ$. As is usual for substituted 1*H*-tetrazoles (Wang, Zhao & Zhang, 2005; Wang, Zhao, Zheng & Duan, 2005), atom C4 has a distorted trigonal geometry, with the N1—C4—N4 [$109.4(2)^\circ$] and N1—C4—S1 [$127.5(2)^\circ$] angles deviating significantly from the ideal sp^2 -hybridized values. Due to the π - π conjugation, the Csp^2 -S bonds [C4—S1 = $1.742(3)$ Å] are significantly shorter than the Csp^3 -S bonds [C3—S1 = $1.813(2)$ Å]. These values compare with the values of $1.726(2)$, $1.720(8)$, $1.800(3)$ and $1.811(2)$ Å reported in the literature (Wang, Liu & Zhang, 2004; Wang, Zhao & Zhang, 2005; Wang, Zhao, Zheng & Duan, 2005).

Experimental

A solution of 1-bromo-2-[2-(2-bromoethoxy)ethoxy]ethane (1.38 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 65%, m.p. 397–398 K). IR (KBr, ν cm⁻¹): 3428, 2870, 2362, 1594, 1497, 1472, 1383, 1244, 1118, 762, 697; ¹H NMR (CDCl₃): δ 3.57 (4H, t), 3.62 (4H, s), 3.85 (4H, t), 7.50–7.56 (10H, m). Analysis calculated for C₂₂H₁₈N₈O₈S₂: C 51.06, H 4.68, N 23.83%; found: C 51.22, H 4.53, N 23.67%. Crystals suitable for single-crystal X-ray analysis were grown by slow evaporation of a solution in acetonitrile.

Crystal data

C ₂₀ H ₂₂ N ₈ O ₂ S ₂	Mo K α radiation
<i>M_r</i> = 470.60	Cell parameters from 2662 reflections
Orthorhombic, <i>Pbca</i>	θ = 2.6–25.2°
<i>a</i> = 14.929 (5) Å	μ = 0.27 mm ⁻¹
<i>b</i> = 8.2223 (16) Å	<i>T</i> = 293 (2) K
<i>c</i> = 18.737 (6) Å	Block, colorless
<i>V</i> = 2300.0 (12) Å ³	0.24 × 0.20 × 0.10 mm
<i>Z</i> = 4	
<i>D_x</i> = 1.359 Mg m ⁻³	

Data collection

Bruker SMART CCD area-detector diffractometer	2356 independent reflections
φ and ω scans	1429 reflections with <i>I</i> > 2 σ (<i>I</i>)
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	<i>R</i> _{int} = 0.070
<i>T</i> _{min} = 0.938, <i>T</i> _{max} = 0.974	θ_{\max} = 26.4°
12227 measured reflections	<i>h</i> = -13 → 18
	<i>k</i> = -10 → 9
	<i>l</i> = -21 → 23

Refinement

Refinement on <i>F</i> ²	$w = 1/[\sigma^2(F_o^2) + (0.0575P)^2 + 0.95P]$
$R[F^2 > 2\sigma(F^2)] = 0.044$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.128$	$(\Delta/\sigma)_{\max} < 0.001$
<i>S</i> = 1.01	$\Delta\rho_{\max} = 0.21 \text{ e \AA}^{-3}$
2356 reflections	$\Delta\rho_{\min} = -0.28 \text{ e \AA}^{-3}$
145 parameters	
H-atom parameters constrained	

Table 1

Selected geometric parameters (Å, °).

S1–C4	1.742 (3)	S1–C3	1.813 (2)
N1–C4–N4	109.4 (2)	N1–C4–S1	127.5 (2)

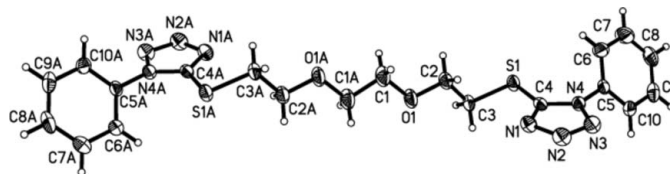


Figure 1

View of the molecule of (I) showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (A) $-x, 1 - y, 1 - z$].

All H atoms were positioned geometrically and refined as riding, with *Csp*³–H = 0.97 Å and *Csp*²–H = 0.93 Å, and *U*_{iso}(H) = 1.2*U*_{eq}(parent atom).

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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