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1,3,5-Tris(1-phenyl-1*H*-tetrazol-5-ylsulfanylmethyl)benzene

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.005 Å
R factor = 0.044
wR factor = 0.094
Data-to-parameter ratio = 13.3

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

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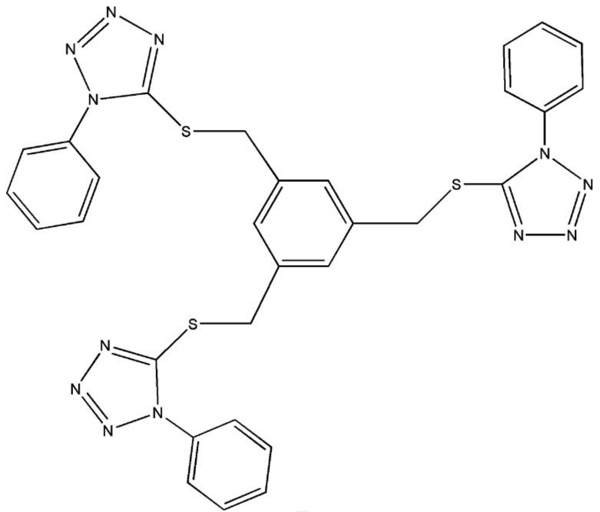
All three phenyltetrazole substituents in the molecule of the title compound, $C_{30}H_{24}N_{12}S_3$, are located on one side of the central benzene plane. The planes of the terminal phenyl groups are roughly orthogonal to the plane of the central benzene ring; the dihedral angles are 73.0 (2), 76.1 (2) and 89.3 (2)°. The tetrazole planes form dihedral angles of 49.1 (2), 54.1 (2) and 36.8 (2)° with the planes of the attached phenyl rings.

Comment

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 papers pointed out that several tetrazole derivatives exhibit various pharmacological properties (Juby *et al.*, 1968; Juby *et al.*, 1982). However, X-ray structural studies of only a few complexes of monosubstituted tetrazole derivatives have been reported (van den Heuvel *et al.*, 1983; Lyakhov *et al.*, 2003). Recently, we synthesized a new tetrazole derivative, namely 1,3,5-tris(1-phenyl-1*H*-tetrazole-5-ylsulfanylmethyl)-benzene, (I), the structure of which is reported here.



(I)

All three 1-phenyl-1*H*-tetrazole-5-thio-methyl substituents in the molecule of (I) are located on the same side of the plane of the central benzene ring. The terminal phenyl ring planes [C9–C14 (*A*), C17–C22 (*B*) and C25–C30 (*C*)] are roughly orthogonal to the plane of the central benzene ring; the corresponding dihedral angles are 73.0 (2), 76.1 (2) and

89.3 (2)°, respectively. The dihedral angles formed by the planes of the terminal phenyl rings and the attached tetrazole planes are 49.1 (2), 54.1 (2) and 36.8 (2)°, respectively.

As a result of π–π conjugation, the Csp^2—S bonds S1—C8, S2—C16 and S3—C24 are significantly shorter than the Csp^3—S bonds S1—C7, S2—C15 and S3—C23. The average lengths of the Csp^2—S and Csp^3—S bonds are 1.729 (3) and 1.821 (3) Å, respectively. These bond lengths are in good agreement with the values of 1.726 (2)/1.800 (3) and 1.720 (8)/1.811 (2) Å for the corresponding bonds reported by Wang *et al.* (2004) and Wang *et al.* (2005).

Experimental

A solution of 1,3,5-tris(bromomethyl)benzene (1.78 g, 5 mmol) in ethanol (10 ml) was added dropwise to a mixture of 1-phenyl-5-thio-1,2,3,4-tetrazole (2.67 g, 15 mmol), KOH (0.84 g, 15 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. 425–426 K). IR (KBr, ν cm^{-1}): 3068, 1592, 1498, 1456, 1410, 1382, 1276, 1072, 1012, 754, 684; ^{1}H NMR (CDCl$_3$, δ, p.p.m.): 4.55 (*s*, 2H), 7.46 (*s*, 1H), 7.50–7.54 (*m*, 5H). Analysis calculated for $C_{30}H_{24}N_{12}S_3$: C 55.54, H 3.73, N 25.91%; found: C 55.42, H 3.77, N 25.87%. Crystals of (I) suitable for single-crystal X-ray analysis were grown by slow evaporation of a solution in chloroform.

Crystal data

$C_{30}H_{24}N_{12}S_3$
M_r = 648.82
Triclinic, $P\bar{1}$
a = 10.0160 (19) Å
b = 11.323 (2) Å
c = 15.379 (3) Å
α = 68.488 (3)°
β = 71.162 (3)°
γ = 84.523 (3)°
V = 1535.2 (5) Å^3
Z = 2
D_x = 1.404 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2083 reflections
θ = 2.3–22.5°
μ = 0.28 mm^{-1}
T = 294 (2) K
Block, colourless
0.28 × 0.24 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min}$ = 0.925, $T_{\max}$ = 0.972
7852 measured reflections
5403 independent reflections
3377 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.026
$\theta_{\max}$ = 25.0°
$h = -11 \rightarrow 11$
$k = -11 \rightarrow 13$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.094
S = 1.07
5403 reflections
406 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.028P)^2 + 0.2486P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max}$ = 0.005
$\Delta\rho_{\max}$ = 0.25 e Å^{-3}
$\Delta\rho_{\min}$ = −0.25 e Å^{-3}

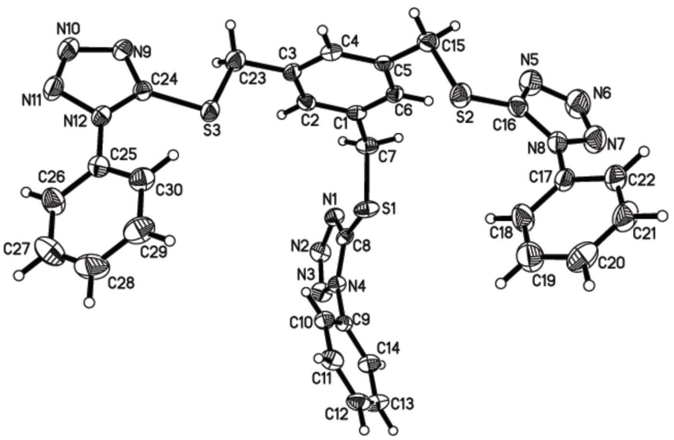


Figure 1
View of the molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level.

Table 1
Selected bond lengths (Å).

S1—C8	1.727 (3)	S2—C15	1.826 (3)
S1—C7	1.815 (3)	S3—C24	1.733 (3)
S2—C16	1.726 (3)	S3—C23	1.822 (3)

All H atoms were positioned geometrically (C—H = 0.93–0.97 Å) and allowed to ride on their parent atoms, with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(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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