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1,6-Bis(1-methyl-1*H*-tetrazol-5-ylsulfanyl)hexane

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.041
wR factor = 0.119
Data-to-parameter ratio = 10.7

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

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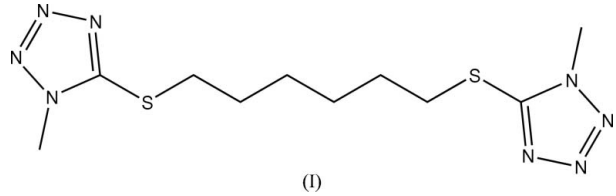
The molecule of the title compound, $C_{10}H_{18}N_8S_2$, lies on a twofold rotation axis. Methyl C atoms contact N atoms of adjacent molecules through C—H···N hydrogen bonds [3.445 (3) Å] in a molecular layer. In addition, the layers are linked by weak S···S interactions [3.636 (3) Å].

Comment

In current coordination and supramolecular chemistry, the rational design of coordination architectures represents one of the most exciting and rapidly developing fields, owing to their potential as functional materials (Braga *et al.*, 1998). The title compound, (I), is a derivative of tetrazole. Tetrazole compounds have a wide range of pharmaceutical applications, where they act as stimulants or sedatives on the central nervous system (Gilchrist, 1992). Many of them are found to possess antihypertensive (Segarra *et al.*, 1998), antifungal (Upadhayaya *et al.*, 2004) or anti-emetic (Armour *et al.*, 1996) activities.



(I)

In the crystal structure of (I), the molecule lies on a crystallographic twofold rotation axis. The C1–N1, N1—N2 and N3—N4 distances (Table 1) are slightly longer than the corresponding distances in 1,2-di(1,2,3,4-tetrazol-2-yl)ethane [1.328 (2), 1.333 (2) and 1.326 (2) Å, respectively; Bronisz, 2002], while the N4—C1 and N2—N3 distances are slightly shorter than the corresponding distances in the same compound [1.340 (2) and 1.323 (2) Å, respectively]. The C1—

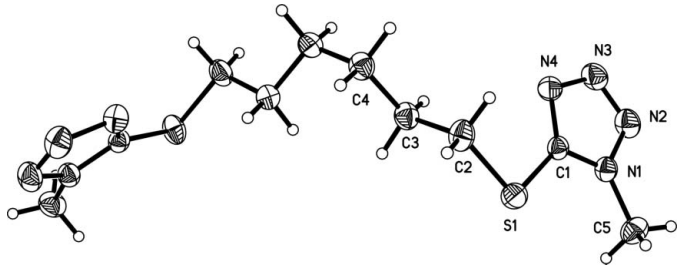


Figure 1
A view of compound (I), showing the atom-numbering scheme and with displacement ellipsoids at the 30% probability level. Unlabelled atoms are related to labelled atoms by the symmetry code $(-x, y, -\frac{1}{2} - z)$.

N1—N2, N2—N3—N4, N1—N2—N3, N3—N4—C1 and N1—C1—N4 bond angles are 108.55 (19), 111.62 (18), 105.87 (19), 104.98 (18) and 108.98 (19)°, respectively, while the corresponding angles in 1,2-di(1,2,3,4-tetrazol-2-yl)ethane are 101.40 (8), 105.96 (8), 113.95 (8), 105.90 (8) and 112.79 (9)° (Bronisz, 2002). The C1—S1 and C2—S1 distances and the C1—S1—C2 angle agree well with the corresponding distances [1.743 (3) and 1.812 (3) Å, respectively,] and angle [102.13 (12)°] in 2,2′-[1,4-phenylenebis(methylenethio)]dithiazole (Zhang *et al.*, 2003). The N2—N1—C1—S1 torsion angle is −179.93 (15)°, S1—C1—N4—N3 is 179.72 (16)° and C1—S1—C2—C3 is 79.9 (2)°. The dihedral angle between the planes of atoms C1/N1–N4 and C1*A*/N1*A*–N4*A* [symmetry code: (*A*) $-x, y, -\frac{1}{2}-z$] is 74.0 (18)°.

The C atoms of the methyl groups contact the N atoms of an adjacent molecule through C—H···N hydrogen bonds [3.445 (3) Å] in a molecular layer. In addition, the layers are linked by a weak S—S interaction [3.636 (3) Å].

Experimental

Sodium hydroxide (1.7 g, 0.043 mol) was added to 5-mercapto-1-methyltetrazole (5 g, 0.043 mol) in dry dimethylsulfoxide (35 ml). The reaction mixture was stirred at 363 K for 1 h. 1,6-Dichlorohexane (3.1 ml, 0.0215 mol) was then added to the solution dropwise with the formation of a grey suspension. The suspension was stirred for 4 h, cooled to room temperature and filtered. The solvent was removed completely under reduced pressure. The residue was recrystallized from ethanol to give a white crystalline product (3.84 g; m.p. 353–354 K). Single crystals of (I) suitable for X-ray diffraction analysis were isolated after a week from a solution in acetone. Spectroscopic analysis: ^{1}H NMR (300 MHz, $CDCl_3$, δ, p.p.m.): 1.44 (4H, *tt*), 1.77 (4H, *tt*), 3.27 (4H, *t*), 3.84 (6H, *s*); analysis calculated for $C_{10}H_{18}N_8S_2$: C 38.20, H 5.77, N 35.64%; found: C 38.25, H 5.55, N 35.75%.

Crystal data

$C_{10}H_{18}N_8S_2$
M_r = 314.44
Monoclinic, $C2/c$
a = 18.485 (8) Å
b = 9.818 (4) Å
c = 9.632 (4) Å
β = 118.286 (5)°
V = 1539.2 (11) Å^3
Z = 4
D_x = 1.357 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1851 reflections
θ = 2.4–26.6°
μ = 0.35 mm^{-1}
T = 293 (2) K
Block, colourless
0.53 × 0.46 × 0.41 mm

Data collection

Bruker SMART area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.836, T_{max} = 0.870
3923 measured reflections
1357 independent reflections
1077 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 25.0°
$h = -21 \rightarrow 21$
$k = -11 \rightarrow 11$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.119
S = 1.00
1357 reflections
127 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0736P)^2 + 0.7751P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

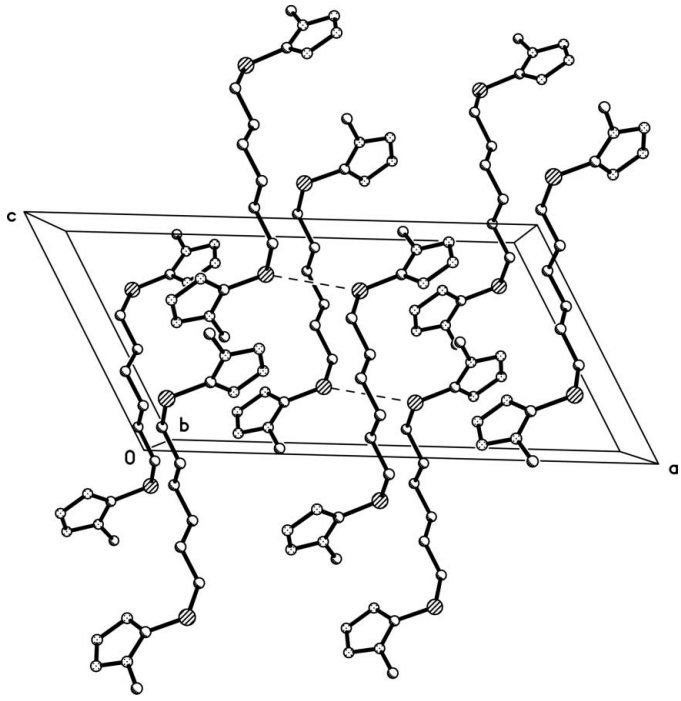


Figure 2
The molecular packing of (I), viewed along the *b* axis. Contacts between S atoms are indicated by dashed lines. H atoms have been omitted for clarity.

Table 1
Selected geometric parameters (Å, °).

N1—C1	1.332 (3)	N4—C1	1.321 (3)
N1—N2	1.350 (3)	S1—C1	1.731 (2)
N1—C5	1.461 (3)	S1—C2	1.811 (3)
N2—N3	1.289 (3)	C2—C3	1.520 (4)
N3—N4	1.359 (3)	C3—C4	1.519 (3)
C1—N1—N2	108.55 (19)	C1—S1—C2	100.25 (12)
C1—N1—C5	129.7 (2)	N4—C1—N1	108.98 (19)
N2—N1—C5	121.7 (2)	N4—C1—S1	128.66 (17)
N3—N2—N1	105.87 (19)	N1—C1—S1	122.36 (16)
N2—N3—N4	111.62 (18)	C3—C2—S1	114.11 (18)
C1—N4—N3	104.98 (18)	C4—C3—C2	111.6 (2)

All H atoms were located in a difference Fourier map and refined isotropically [C—H distances are in the range 0.90 (5)–1.01 (3) Å

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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