Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis[4-(2-isopropyl-2*H*-tetrazol-5-yl)-phenyl]dimethylsilane

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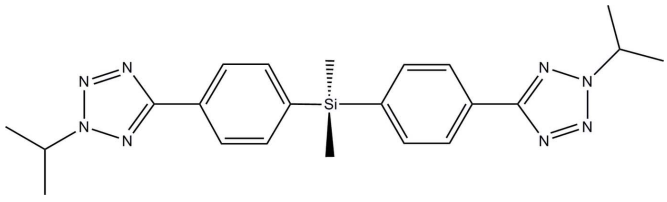
Received 8 December 2010; accepted 5 January 2011

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.088; wR factor = 0.207; data-to-parameter ratio = 18.1.

The title compound, $C_{22}H_{28}N_8Si$, has crystallographic 2 symmetry with the Si atom located on a twofold rotation axis. The tetrazole ring is oriented at a dihedral angle of 5.32 (18)° with respect to the benzene ring. A C—H$\cdots\pi$ interaction occurs between adjacent molecules in the crystal structure.

Related literature

For applications of tetrazole compounds, see: Bhandari *et al.* (2000). For the synthesis of tetrazole derivatives, see: Demko & Sharpless (2001).



Experimental

Crystal data

$C_{22}H_{28}N_8Si$
M_r = 432.61
Orthorhombic, *Pbcn*
a = 7.2722 (14) Å
b = 11.536 (2) Å
c = 28.444 (6) Å
V = 2386.2 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 298 K
0.46 × 0.37 × 0.07 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.945, T_{max} = 0.991
12923 measured reflections
2613 independent reflections
1827 reflections with $I > 2\sigma(I)$
R_{int} = 0.049

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.088
$wR(F^2)$ = 0.207
S = 1.14
2613 reflections
144 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

Cg is the centroid of the tetrazole ring.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C9—H9*B*$\cdots Cg^{i}$	0.96	2.86	3.738 (5)	152

Symmetry code: (i) $-x+1, -y+1, -z+1$.

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

The authors thank the Testing Centre of Shandong Normal University for the diffraction measurements and are grateful for financial support from the National Natural Science Foundation of China (No. 20874057) and the Key Natural Science Foundation of Shandong Province of China (No. Z2007B02).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5118).

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supporting information

Acta Cryst. (2011). E**67**, o368 [doi:10.1107/S160053681100033X]

Bis[4-(2-isopropyl-2*H*-tetrazol-5-yl)phenyl]dimethylsilane

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S1. Comment

Due to the application of tetrazoles in coordination chemistry, medicinal chemistry and material science (Bhandari *et al.*, 2000), series of organic compounds with tetrazole group have been synthesized through different methods. Since a safe, convenient and envrironmentally friendly procedure for the synthesis of 5-substituted 1*H*-tetrazoles in water was reported by Demko and Sharpless (2001), synthesis of such compounds has been developed rapidly. However, due to the difficult in synthesis, tetrazole functional silane was never reported to our best knowledge. Here, we reported the synthesis and crystal structure of the title compound(I), namely, bis(4-(2-isopropyl-2*H*-tetrazol- 5-yl)phenyl)dimethylsilane.

The molecular structure of (I) is shown in Fig. 1. Bond lengths and angles in (I) are normal. The phenyl and tetrazole rings are not coplanar, and the two rings twisted to each other at a dihedral angle of 5.32 (18)°. The crystal packing is stablized by C—H···π interaction (Table 1).

S2. Experimental

Tert-butyl lithium (4 mmol) in 3.08 ml n-pentane solution and 5-(4-bromophenyl)-2-isopropyl-2*H*-tetrazole (0.54 g, 2 mmol) were reacted at 195 K in 20 ml e ther. To the resulted solution was added dimethyldichlorosilane (0.13 g, 1 mmol), the solution was warmed slowly to room temperature and stirred overnight. Then the solution was filtered. The volatiles were removed from the resulting filtrate by vacuum distillation. The residue was purified by column chromatography using ethyl acetate/n-hexane as eluent to afford the pure compound. Single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation methanol solvent.

S3. Refinement

The H atoms were positioned geometrically and refined using a riding model with C—H = 0.93–0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for methyl and 1.2U_{eq}(C) for the others.

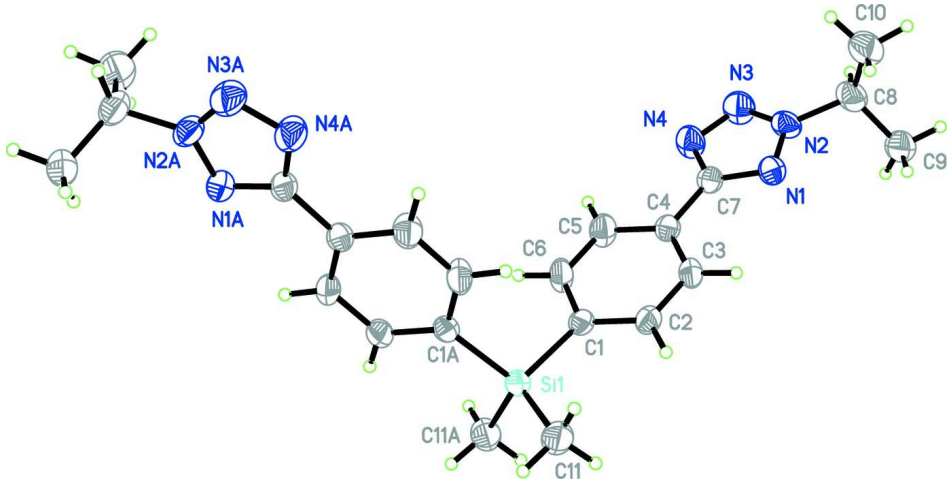

Figure 1

The molecular structure of (I), with atom labels and 30% probability displacement ellipsoids.

Bis[4-(2-isopropyl-2*H*-tetrazol-5-yl)phenyl]dimethylsilane

Crystal data

$C_{22}H_{28}N_8Si$
$M_r = 432.61$
Orthorhombic, *Pbcn*
Hall symbol: -P 2n 2ab
$a = 7.2722\ (14)$ Å
$b = 11.536\ (2)$ Å
$c = 28.444\ (6)$ Å
$V = 2386.2\ (8)$ Å^3
$Z = 4$
$F(000) = 920$
$D_x = 1.204$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1662 reflections
$\theta = 2.9$–$20.6°$
$\mu = 0.12$ mm^{-1}
$T = 298$ K
Plate, colourless
0.46 × 0.37 × 0.07 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
$T_{min} = 0.945$, $T_{max} = 0.991$
12923 measured reflections
2613 independent reflections
1827 reflections with $I > 2\sigma(I)$
$R_{int} = 0.049$
$\theta_{max} = 27.0°$, $\theta_{min} = 1.4°$
$h = -9\rightarrow9$
$k = -14\rightarrow10$
$l = -36\rightarrow36$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.088$
$wR(F^2) = 0.207$
$S = 1.14$
2613 reflections
144 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0693P)^2 + 1.6746P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.32$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Si1	0.0000	0.80602 (11)	0.2500	0.0536 (4)
N1	0.5087 (4)	0.4553 (2)	0.40351 (9)	0.0610 (8)
N2	0.5050 (4)	0.3688 (2)	0.43454 (10)	0.0634 (8)
N3	0.3420 (5)	0.3270 (3)	0.44279 (12)	0.0804 (10)
N4	0.2291 (4)	0.3870 (3)	0.41648 (11)	0.0748 (9)
C1	0.1069 (4)	0.7079 (3)	0.29478 (10)	0.0473 (7)
C2	0.2904 (5)	0.7098 (3)	0.30746 (12)	0.0600 (9)
H2	0.3668	0.7655	0.2942	0.072*
C3	0.3639 (5)	0.6321 (3)	0.33902 (12)	0.0604 (9)
H3	0.4883	0.6361	0.3465	0.072*
C4	0.2560 (4)	0.5490 (3)	0.35956 (10)	0.0489 (8)
C5	0.0720 (5)	0.5455 (3)	0.34793 (12)	0.0679 (10)
H5	−0.0042	0.4903	0.3617	0.082*
C6	0.0004 (5)	0.6231 (3)	0.31617 (12)	0.0663 (10)
H6	−0.1239	0.6186	0.3087	0.080*
C7	0.3320 (5)	0.4640 (3)	0.39285 (10)	0.0512 (8)
C8	0.6736 (6)	0.3243 (3)	0.45759 (14)	0.0759 (11)
H8	0.6317	0.2726	0.4828	0.091*
C9	0.7768 (6)	0.4185 (4)	0.48099 (16)	0.0952 (15)
H9A	0.8732	0.3859	0.4999	0.143*
H9B	0.6949	0.4622	0.5007	0.143*
H9C	0.8292	0.4687	0.4576	0.143*
C10	0.7788 (6)	0.2512 (4)	0.42484 (17)	0.1005 (15)
H10A	0.6997	0.1925	0.4120	0.151*
H10B	0.8788	0.2151	0.4413	0.151*
H10C	0.8264	0.2982	0.3998	0.151*
C11	0.1814 (6)	0.8966 (3)	0.22270 (15)	0.0823 (13)
H11A	0.2715	0.8474	0.2082	0.123*
H11B	0.2394	0.9431	0.2464	0.123*
H11C	0.1273	0.9461	0.1994	0.123*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Si1	0.0603 (8)	0.0454 (7)	0.0552 (7)	0.000	−0.0171 (6)	0.000
N1	0.0659 (18)	0.0600 (18)	0.0569 (16)	0.0010 (15)	−0.0129 (14)	0.0044 (14)
N2	0.081 (2)	0.0553 (17)	0.0538 (16)	0.0102 (16)	−0.0108 (16)	0.0096 (13)
N3	0.084 (2)	0.080 (2)	0.078 (2)	−0.009 (2)	−0.0036 (19)	0.0279 (18)
N4	0.073 (2)	0.080 (2)	0.071 (2)	−0.0060 (17)	−0.0105 (17)	0.0253 (18)

C1	0.0533 (18)	0.0454 (17)	0.0431 (15)	−0.0011 (14)	−0.0056 (14)	−0.0048 (14)
C2	0.055 (2)	0.054 (2)	0.071 (2)	−0.0136 (16)	−0.0133 (17)	0.0106 (17)
C3	0.0481 (19)	0.063 (2)	0.070 (2)	−0.0021 (17)	−0.0174 (16)	0.0072 (18)
C4	0.0549 (18)	0.0506 (18)	0.0413 (15)	−0.0002 (14)	−0.0045 (14)	−0.0031 (14)
C5	0.058 (2)	0.079 (3)	0.066 (2)	−0.0155 (18)	−0.0068 (18)	0.021 (2)
C6	0.0496 (19)	0.084 (3)	0.065 (2)	−0.0095 (19)	−0.0155 (17)	0.0157 (19)
C7	0.061 (2)	0.0526 (19)	0.0403 (15)	0.0018 (15)	−0.0083 (15)	−0.0028 (15)
C8	0.090 (3)	0.071 (3)	0.067 (2)	0.014 (2)	−0.018 (2)	0.012 (2)
C9	0.105 (3)	0.078 (3)	0.103 (3)	0.013 (3)	−0.047 (3)	−0.014 (3)
C10	0.089 (3)	0.094 (3)	0.119 (4)	0.026 (3)	−0.008 (3)	−0.022 (3)
C11	0.088 (3)	0.073 (3)	0.085 (3)	−0.024 (2)	−0.025 (2)	0.028 (2)

Geometric parameters (Å, º)

Si1—C11	1.853 (4)	C4—C7	1.471 (4)
Si1—C11^{i}	1.853 (4)	C5—C6	1.374 (5)
Si1—C1^{i}	1.873 (3)	C5—H5	0.9300
Si1—C1	1.873 (3)	C6—H6	0.9300
N1—C7	1.324 (4)	C8—C10	1.471 (6)
N1—N2	1.332 (4)	C8—C9	1.479 (5)
N2—N3	1.301 (4)	C8—H8	0.9800
N2—C8	1.483 (4)	C9—H9A	0.9600
N3—N4	1.309 (4)	C9—H9B	0.9600
N4—C7	1.342 (4)	C9—H9C	0.9600
C1—C2	1.382 (4)	C10—H10A	0.9600
C1—C6	1.388 (4)	C10—H10B	0.9600
C2—C3	1.377 (4)	C10—H10C	0.9600
C2—H2	0.9300	C11—H11A	0.9600
C3—C4	1.370 (4)	C11—H11B	0.9600
C3—H3	0.9300	C11—H11C	0.9600
C4—C5	1.379 (4)		
C11—Si1—C11^{i}	111.4 (3)	C1—C6—H6	118.8
C11—Si1—C1^{i}	110.56 (16)	N1—C7—N4	112.1 (3)
C11^{i}—Si1—C1^{i}	109.28 (16)	N1—C7—C4	124.2 (3)
C11—Si1—C1	109.28 (16)	N4—C7—C4	123.6 (3)
C11^{i}—Si1—C1	110.56 (16)	C10—C8—C9	116.3 (4)
C1^{i}—Si1—C1	105.63 (19)	C10—C8—N2	110.4 (3)
C7—N1—N2	100.9 (3)	C9—C8—N2	111.3 (3)
N3—N2—N1	114.6 (3)	C10—C8—H8	106.0
N3—N2—C8	123.1 (3)	C9—C8—H8	106.0
N1—N2—C8	122.4 (3)	N2—C8—H8	106.0
N2—N3—N4	105.8 (3)	C8—C9—H9A	109.5
N3—N4—C7	106.6 (3)	C8—C9—H9B	109.5
C2—C1—C6	115.8 (3)	H9A—C9—H9B	109.5
C2—C1—Si1	124.7 (2)	C8—C9—H9C	109.5
C6—C1—Si1	119.5 (2)	H9A—C9—H9C	109.5
C3—C2—C1	122.4 (3)	H9B—C9—H9C	109.5

C3—C2—H2	118.8	C8—C10—H10A	109.5
C1—C2—H2	118.8	C8—C10—H10B	109.5
C4—C3—C2	120.7 (3)	H10A—C10—H10B	109.5
C4—C3—H3	119.6	C8—C10—H10C	109.5
C2—C3—H3	119.6	H10A—C10—H10C	109.5
C3—C4—C5	118.3 (3)	H10B—C10—H10C	109.5
C3—C4—C7	121.7 (3)	Si1—C11—H11A	109.5
C5—C4—C7	120.0 (3)	Si1—C11—H11B	109.5
C6—C5—C4	120.4 (3)	H11A—C11—H11B	109.5
C6—C5—H5	119.8	Si1—C11—H11C	109.5
C4—C5—H5	119.8	H11A—C11—H11C	109.5
C5—C6—C1	122.4 (3)	H11B—C11—H11C	109.5
C5—C6—H6	118.8		

C7—N1—N2—N3	−0.1 (4)	C7—C4—C5—C6	−178.7 (3)
C7—N1—N2—C8	179.8 (3)	C4—C5—C6—C1	−0.5 (6)
N1—N2—N3—N4	0.0 (4)	C2—C1—C6—C5	−0.1 (5)
C8—N2—N3—N4	−180.0 (3)	Si1—C1—C6—C5	177.4 (3)
N2—N3—N4—C7	0.2 (4)	N2—N1—C7—N4	0.2 (4)
C11—Si1—C1—C2	4.3 (3)	N2—N1—C7—C4	179.4 (3)
C11^{i}—Si1—C1—C2	−118.6 (3)	N3—N4—C7—N1	−0.3 (4)
C1^{i}—Si1—C1—C2	123.2 (3)	N3—N4—C7—C4	−179.4 (3)
C11—Si1—C1—C6	−173.0 (3)	C3—C4—C7—N1	−4.4 (5)
C11^{i}—Si1—C1—C6	64.1 (3)	C5—C4—C7—N1	174.9 (3)
C1^{i}—Si1—C1—C6	−54.0 (2)	C3—C4—C7—N4	174.7 (3)
C6—C1—C2—C3	0.5 (5)	C5—C4—C7—N4	−6.0 (5)
Si1—C1—C2—C3	−176.9 (3)	N3—N2—C8—C10	103.6 (4)
C1—C2—C3—C4	−0.3 (5)	N1—N2—C8—C10	−76.3 (5)
C2—C3—C4—C5	−0.2 (5)	N3—N2—C8—C9	−125.6 (4)
C2—C3—C4—C7	179.1 (3)	N1—N2—C8—C9	54.4 (5)
C3—C4—C5—C6	0.6 (5)		

Symmetry code: (i) −*x*, *y*, −*z*+1/2.

Hydrogen-bond geometry (Å, º)

Cg is the centroid of the tetrazole ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9*B*···*Cg*^{ii}	0.96	2.86	3.738 (5)	152

Symmetry code: (ii) −*x*+1, −*y*+1, −*z*+1.