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2,6-Bis(trimethylsilylethynyl)dithieno[3,2-*b*:2′,3′-*d*]thiophene

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Key indicators

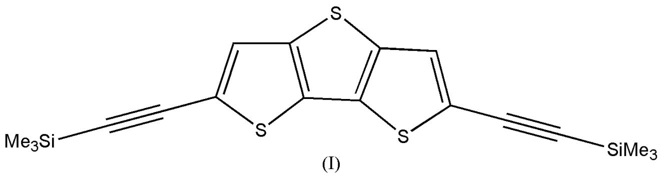
Single-crystal synchrotron study
T = 150 K
Mean σ(C–C) = 0.005 Å
Disorder in main residue
R factor = 0.055
wR factor = 0.114
Data-to-parameter ratio = 13.7

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

The title compound, $C_{18}H_{20}S_3Si_2$, is a precursor in the formation of platinum and gold di-yne complexes and poly-yne polymers. These materials are of interest because of the π-conjugation that extends through the fused oligothienyl linker unit along the rigid backbone of the polymer. In the structure of the title compound, the oligothienyl group is planar and the trimethylsilylalkyne groups are essentially linear.

Comment

The title compound, 2,6-bis(trimethylsilylethynyl)dithieno[3,2-*b*:2′,3′-*d*]thiophene, (I), is a trimethylsilyl-protected di-yne. It is a precursor in the formation of the following series of compounds: the terminal di-yne, H—C≡C—*R*—C≡C—H, the dinuclear platinum(II) di-yne, [(Ph)(PEt$_3$)$_2$Pt—C≡C—*R*—C≡C—Pt(PEt$_3$)$_2$(Ph)], and the platinum(II) poly-yne, *trans*-[(^{n}Bu$_3$P)$_2$Pt—C≡C—*R*—C≡C—]$_\infty$ (*R* = thieno[3,2-*b*]thiophene-2,5-diyl). Rigid-rod platinum(II) poly-ynes with the general formula *trans*-[(^{n}Bu$_3$P)$_2$Pt—C≡C—*R*—C≡C—]$_\infty$ (*R* = conjugated aromatic/heteroaromatic linker group) are considered to be good model systems to study the triplet excited state in polymers and provide important information on the photophysical processes that occur within them (Khan, Al-Mandhary, Al-Suti, Hisham *et al.*, 2002; Khan, Al-Mandhary, Al-Suti, Feeder *et al.*, 2002; Khan *et al.*, 2003). The incorporation of heavy transition metals, such as platinum, at regular intervals along the rigid polymer backbone introduces a large component of spin-orbit coupling that allows emission from the triplet excited state of the system *via* spin cross-over processes (Wittmann *et al.*, 1994; Beljonne *et al.*, 1996; Younus *et al.*, 1998; Chawdhury *et al.*, 1999). The novel photophysics of the platinum(II) poly-ynes leads to materials that are useful for applications in modern opto-electronic devices such as light-emitting diodes (LEDs), lasers, photocells and field-effect transistors (FETs) (Wilson *et al.*, 2000; Wilson, Chawdhury *et al.*, 2001; Wilson, Dhoot *et al.*, 2001).



(I)

The title compound, (I), crystallizes in the monoclinic space group $P2_1/n$, with one molecule in the asymmetric unit, so that there is no crystallographically imposed symmetry (Fig. 1). The central dithieno[3,2-*b*:2′,3′-*d*]thiophene group is essentially planar and the bond parameters associated with this group are similar to those found in other materials containing this thiophene ring system (Li *et al.*, 1998; Osterod *et al.*, 2001; Frey *et al.*, 2002). The bond parameters for the acetylene groups and the trimethylsilyl ligands are similar to those observed in related compounds (Khan, Ahrens *et al.*, 2002; Khan *et al.*, 2004).

There are a number of significant intermolecular interactions within the crystal structure. All three of the unique S atoms show contacts to symmetry-related S atoms: S1···S2 (related by the symmetry operation $x - 1, y, z$) at a distance of 3.338 (2) Å; S2···S1 (related by $1 + x, y, z$) at a distance of 3.338 Å; S2···S2 (related by $2 + x, -y, -z$) at a distance of 3.545 (2) Å; the S3···S2 (related by $x - 1, y, z$) distance is 3.404 (2) Å, which is the shortest. There is also an indication of the presence of π-stacking between pairs of adjacent dithieno[3,2-*b*:2′,3′-*d*]thiophene ring systems, with centroid–centroid separations between the five-membered S1-containing ring and the S3-containing ring, related by the symmetry operation $1 - x, -y, -z$, of 4.328 (5) Å, and the S2-containing ring and its symmetry-related partner (again by $1 - x, -y, -z$) with a distance of 4.539 (5) Å.

Experimental

5,5′-Dibromodithieno[3,2-*b*:2′,3′-*d*]thiophene (2.0 g, 5.64 mmol), trimethylsilylethyne (1.46 g, 14.9 mmol) and $^i\mathrm{Pr_2NH}$–THF (70 ml, 1:1 *v*/*v*) were mixed with catalytic amounts of CuI (20 mg), $\mathrm{Pd(OAc)_2}$ (20 mg) and $\mathrm{PPh_3}$ (60 mg). The crude product was worked up to yield a dark-brown residue, which was then applied to a silica column in hexane and eluted with the same solvent. The title compound was obtained as a colourless crystalline solid in 78% isolated yield (1.72 g).

Crystal data

$\mathrm{C_{18}H_{20}S_3Si_2}$
$M_r = 388.7$
Monoclinic, $P2_1/n$
$a = 6.191$ (2) Å
$b = 28.671$ (9) Å
$c = 12.066$ (4) Å
$\beta = 92.51$ (2)°
$V = 2139.7$ (13) Å^3
$Z = 4$
$D_x = 1.207$ Mg m^{-3}

Synchrotron radiation, $\lambda = 0.6887$ Å
Cell parameters from 11495 reflections
$\theta = 3.2$–29.4°
$\mu = 0.46$ mm^{-1}
$T = 150$ (2) K
Plate, yellow
0.07 × 0.05 × 0.01 mm

Data collection

Bruker AXS SMART 1K CCD diffractometer
Thin-slice ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{\min} = 0.969$, $T_{\max} = 0.996$
11094 measured reflections

3062 independent reflections
2494 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.063$
$\theta_{\max} = 22.5°$
$h = -6 \rightarrow 6$
$k = -28 \rightarrow 31$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.055$
$wR(F^2) = 0.114$
$S = 1.17$
3062 reflections
224 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0415P)^2 + 1.5269P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.40$ e Å^{-3}
$\Delta\rho_{\min} = -0.33$ e Å^{-3}

The crystal, a small thin plate, did not diffract significantly beyond 45° in 2θ and the final refinement $\theta_{\max}$ was limited to 22.5°. One of the methyl groups associated with Si1 showed positional disorder over two sites, C13 and C13*A*. These two atoms, and their associated H atoms, were refined with occupancies fixed at 50% each. All the aromatic and methyl H atoms were constrained as riding atoms, fixed to the parent atoms with distances of 0.95 and 0.98 Å, respectively, and U(H) = 1.2 (aromatic H atoms) and 1.5 (methyl H atoms) times $U_{\rm eq}$(parent atom).

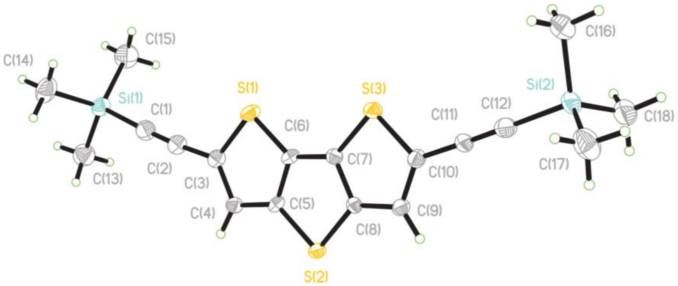


Figure 1
View of (I) (50% probability displacement ellipsoids). The disordered methyl group is not shown for clarity.

Data collection: *SMART* (Bruker, 1998); cell refinement: *LSCELL* (Clegg, 1997); data reduction: *SAINT* (Bruker, 2000); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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supporting information

Acta Cryst. (2004). E**60**, o1226–o1228 [https://doi.org/10.1107/S1600536804014369]

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$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.055$
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$S = 1.17$
3062 reflections
224 parameters
105 restraints
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0415P)^2 + 1.5269P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.40$ e Å^{-3}
$\Delta\rho_{min} = -0.33$ 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 (Å^2)

	x	*y*	*z*	$U_{iso}*/U_{eq}$	Occ. (<1)
Si1	0.24574 (18)	−0.09576 (4)	−0.49942 (9)	0.0297 (3)	
Si2	0.37743 (19)	0.27129 (4)	0.36288 (10)	0.0331 (3)	

S1	0.31917 (14)	0.03319 (4)	−0.17119 (8)	0.0260 (3)	
S2	0.91465 (14)	0.05896 (3)	−0.00764 (8)	0.0225 (2)	
S3	0.34385 (14)	0.12945 (3)	0.05801 (8)	0.0246 (3)	
C1	0.3626 (7)	−0.06041 (15)	−0.3841 (3)	0.0324 (10)	
C2	0.4347 (6)	−0.03567 (14)	−0.3110 (3)	0.0265 (9)	
C3	0.5055 (6)	−0.00484 (13)	−0.2261 (3)	0.0233 (8)	
C4	0.7105 (6)	0.00053 (13)	−0.1775 (3)	0.0217 (8)	
H4	0.8334	−0.0171	−0.1966	0.026*	
C5	0.7125 (5)	0.03560 (13)	−0.0962 (3)	0.0189 (8)	
C6	0.5143 (5)	0.05650 (13)	−0.0822 (3)	0.0210 (8)	
C7	0.5230 (5)	0.09124 (13)	0.0006 (3)	0.0193 (8)	
C8	0.7281 (5)	0.09704 (12)	0.0481 (3)	0.0178 (8)	
C9	0.7440 (6)	0.13197 (13)	0.1298 (3)	0.0216 (8)	
H9	0.8742	0.14	0.1699	0.026*	
C10	0.5506 (6)	0.15279 (13)	0.1443 (3)	0.0236 (8)	
C11	0.4998 (6)	0.19001 (14)	0.2161 (3)	0.0262 (9)	
C12	0.4528 (6)	0.22214 (15)	0.2739 (3)	0.0330 (10)	
C13	0.477 (2)	−0.1223 (5)	−0.5695 (11)	0.044 (4)	0.5
H13A	0.555	−0.0981	−0.6087	0.066*	0.5
H13B	0.4234	−0.1459	−0.6227	0.066*	0.5
H13C	0.5754	−0.1371	−0.514	0.066*	0.5
C13A	0.4674 (17)	−0.1115 (4)	−0.5939 (10)	0.034 (3)	0.5
H13D	0.5474	−0.0833	−0.6127	0.05*	0.5
H13E	0.4045	−0.1256	−0.6618	0.05*	0.5
H13F	0.566	−0.1337	−0.5564	0.05*	0.5
C14	0.0943 (8)	−0.14495 (17)	−0.4427 (4)	0.0459 (12)	
H14A	0.1906	−0.1633	−0.3931	0.069*	
H14B	0.0382	−0.1647	−0.5036	0.069*	
H14C	−0.0264	−0.133	−0.4012	0.069*	
C15	0.0619 (8)	−0.05777 (18)	−0.5829 (4)	0.0483 (12)	
H15A	−0.0592	−0.0483	−0.5383	0.072*	
H15B	0.0066	−0.0748	−0.6486	0.072*	
H15C	0.1406	−0.03	−0.6061	0.072*	
C16	0.0780 (8)	0.27513 (18)	0.3558 (5)	0.0570 (14)	
H16A	0.0266	0.2793	0.2785	0.085*	
H16B	0.0322	0.3018	0.3999	0.085*	
H16C	0.017	0.2464	0.3853	0.085*	
C17	0.4837 (9)	0.25928 (18)	0.5056 (4)	0.0493 (13)	
H17A	0.4196	0.2304	0.5325	0.074*	
H17B	0.4466	0.2852	0.5542	0.074*	
H17C	0.6412	0.2559	0.5057	0.074*	
C18	0.4935 (8)	0.32505 (16)	0.3055 (4)	0.0456 (12)	
H18A	0.6516	0.3229	0.3095	0.068*	
H18B	0.4479	0.352	0.3486	0.068*	
H18C	0.4425	0.3287	0.228	0.068*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Si1	0.0310 (6)	0.0330 (7)	0.0245 (6)	−0.0033 (5)	−0.0053 (4)	−0.0055 (5)
Si2	0.0334 (6)	0.0312 (7)	0.0345 (6)	0.0074 (5)	−0.0008 (5)	−0.0133 (5)
S1	0.0186 (5)	0.0339 (6)	0.0252 (5)	−0.0026 (4)	−0.0018 (4)	−0.0084 (4)
S2	0.0171 (5)	0.0247 (5)	0.0253 (5)	0.0022 (4)	−0.0023 (4)	−0.0076 (4)
S3	0.0176 (5)	0.0276 (5)	0.0287 (5)	0.0025 (4)	0.0010 (4)	−0.0077 (4)
C1	0.035 (2)	0.032 (2)	0.029 (2)	0.0014 (19)	−0.0036 (18)	−0.0013 (19)
C2	0.030 (2)	0.030 (2)	0.0194 (19)	−0.0008 (18)	0.0001 (16)	−0.0008 (18)
C3	0.025 (2)	0.026 (2)	0.0192 (18)	−0.0020 (16)	−0.0006 (15)	0.0003 (16)
C4	0.0213 (19)	0.022 (2)	0.0218 (19)	0.0002 (15)	−0.0006 (15)	0.0009 (16)
C5	0.0170 (18)	0.022 (2)	0.0175 (17)	−0.0057 (15)	−0.0009 (14)	0.0004 (15)
C6	0.0153 (18)	0.025 (2)	0.0222 (19)	−0.0041 (15)	−0.0008 (14)	0.0000 (16)
C7	0.0179 (18)	0.020 (2)	0.0205 (18)	0.0003 (15)	0.0018 (14)	0.0024 (15)
C8	0.0190 (18)	0.0165 (19)	0.0181 (17)	0.0008 (15)	0.0029 (14)	0.0004 (15)
C9	0.0186 (18)	0.024 (2)	0.0218 (19)	0.0000 (16)	−0.0002 (14)	−0.0028 (16)
C10	0.0222 (19)	0.025 (2)	0.0241 (19)	−0.0023 (16)	0.0017 (15)	−0.0039 (17)
C11	0.023 (2)	0.025 (2)	0.031 (2)	0.0036 (17)	−0.0011 (16)	−0.0075 (18)
C12	0.026 (2)	0.038 (3)	0.035 (2)	0.0035 (19)	−0.0024 (17)	−0.009 (2)
C13	0.044 (4)	0.044 (4)	0.044 (4)	0.0003 (10)	0.0021 (10)	−0.0003 (10)
C13A	0.034 (3)	0.034 (3)	0.033 (3)	0.0000 (10)	0.0017 (10)	−0.0003 (10)
C14	0.053 (3)	0.044 (3)	0.039 (3)	−0.013 (2)	−0.012 (2)	0.000 (2)
C15	0.055 (3)	0.051 (3)	0.037 (3)	−0.001 (2)	−0.015 (2)	0.005 (2)
C16	0.038 (3)	0.049 (3)	0.085 (4)	0.007 (2)	0.010 (3)	−0.025 (3)
C17	0.066 (3)	0.044 (3)	0.038 (3)	0.012 (3)	0.003 (2)	−0.007 (2)
C18	0.048 (3)	0.040 (3)	0.048 (3)	0.008 (2)	−0.006 (2)	−0.011 (2)

Geometric parameters (Å, º)

Si1—C14	1.842 (5)	C9—H9	0.95
Si1—C15	1.843 (5)	C10—C11	1.418 (5)
Si1—C1	1.843 (4)	C11—C12	1.199 (5)
Si1—C13	1.859 (12)	C13—H13A	0.98
Si1—C13A	1.877 (10)	C13—H13B	0.98
Si2—C12	1.844 (4)	C13—H13C	0.98
Si2—C18	1.848 (5)	C13A—H13D	0.98
Si2—C17	1.848 (5)	C13A—H13E	0.98
Si2—C16	1.855 (5)	C13A—H13F	0.98
S1—C6	1.716 (4)	C14—H14A	0.98
S1—C3	1.739 (4)	C14—H14B	0.98
S2—C5	1.744 (4)	C14—H14C	0.98
S2—C8	1.745 (3)	C15—H15A	0.98
S3—C7	1.725 (3)	C15—H15B	0.98
S3—C10	1.747 (4)	C15—H15C	0.98
C1—C2	1.203 (6)	C16—H16A	0.98
C2—C3	1.408 (5)	C16—H16B	0.98
C3—C4	1.383 (5)	C16—H16C	0.98

C4—C5	1.405 (5)	C17—H17A	0.98
C4—H4	0.95	C17—H17B	0.98
C5—C6	1.382 (5)	C17—H17C	0.98
C6—C7	1.410 (5)	C18—H18A	0.98
C7—C8	1.380 (5)	C18—H18B	0.98
C8—C9	1.406 (5)	C18—H18C	0.98
C9—C10	1.356 (5)		

C14—Si1—C15	110.1 (2)	C9—C10—S3	112.5 (3)
C14—Si1—C1	109.3 (2)	C11—C10—S3	118.4 (3)
C15—Si1—C1	107.5 (2)	C12—C11—C10	177.8 (4)
C14—Si1—C13	105.7 (5)	C11—C12—Si2	179.4 (4)
C15—Si1—C13	117.6 (5)	Si1—C13—H13A	109.5
C1—Si1—C13	106.5 (4)	Si1—C13—H13B	109.5
C14—Si1—C13A	116.1 (4)	Si1—C13—H13C	109.5
C15—Si1—C13A	105.1 (4)	Si1—C13A—H13D	109.5
C1—Si1—C13A	108.5 (4)	Si1—C13A—H13E	109.5
C13—Si1—C13A	13.2 (5)	H13D—C13A—H13E	109.5
C12—Si2—C18	107.9 (2)	Si1—C13A—H13F	109.5
C12—Si2—C17	108.1 (2)	H13D—C13A—H13F	109.5
C18—Si2—C17	112.1 (2)	H13E—C13A—H13F	109.5
C12—Si2—C16	107.2 (2)	Si1—C14—H14A	109.5
C18—Si2—C16	109.7 (2)	Si1—C14—H14B	109.5
C17—Si2—C16	111.6 (3)	H14A—C14—H14B	109.5
C6—S1—C3	91.27 (18)	Si1—C14—H14C	109.5
C5—S2—C8	90.39 (17)	H14A—C14—H14C	109.5
C7—S3—C10	90.89 (17)	H14B—C14—H14C	109.5
C2—C1—Si1	177.2 (4)	Si1—C15—H15A	109.5
C1—C2—C3	175.9 (4)	Si1—C15—H15B	109.5
C4—C3—C2	128.9 (3)	H15A—C15—H15B	109.5
C4—C3—S1	112.4 (3)	Si1—C15—H15C	109.5
C2—C3—S1	118.7 (3)	H15A—C15—H15C	109.5
C3—C4—C5	110.8 (3)	H15B—C15—H15C	109.5
C3—C4—H4	124.6	Si2—C16—H16A	109.5
C5—C4—H4	124.6	Si2—C16—H16B	109.5
C6—C5—C4	114.5 (3)	H16A—C16—H16B	109.5
C6—C5—S2	112.1 (3)	Si2—C16—H16C	109.5
C4—C5—S2	133.4 (3)	H16A—C16—H16C	109.5
C5—C6—C7	112.7 (3)	H16B—C16—H16C	109.5
C5—C6—S1	111.0 (3)	Si2—C17—H17A	109.5
C7—C6—S1	136.3 (3)	Si2—C17—H17B	109.5
C8—C7—C6	112.7 (3)	H17A—C17—H17B	109.5
C8—C7—S3	110.7 (3)	Si2—C17—H17C	109.5
C6—C7—S3	136.7 (3)	H17A—C17—H17C	109.5
C7—C8—C9	114.3 (3)	H17B—C17—H17C	109.5
C7—C8—S2	112.2 (3)	Si2—C18—H18A	109.5
C9—C8—S2	133.5 (3)	Si2—C18—H18B	109.5
C10—C9—C8	111.6 (3)	H18A—C18—H18B	109.5

C10—C9—H9	124.2	Si2—C18—H18C	109.5
C8—C9—H9	124.2	H18A—C18—H18C	109.5
C9—C10—C11	129.1 (4)	H18B—C18—H18C	109.5