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Diethyl 2,5-bis(triisopropylsilylethynyl)-terephthalate

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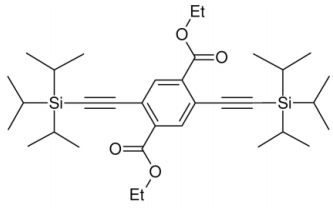
In the crystal structure of the title compound, $C_{34}H_{54}O_4Si_2$, at 180 K, the molecules lie on inversion centres.



(I)

Experimental

The title compound was prepared according to a procedure similar to that for the related compound diethyl 2,5-bis(1-decynyl)-terephthalate (Zhang *et al.*, 2000). Crystals suitable for X-ray analysis were prepared by slow evaporation of a dichloromethane solution.

Crystal data

$C_{34}H_{54}O_4Si_2$
M_r = 582.95
Triclinic, $P\overline{1}$
a = 7.6344 (4) Å
b = 7.7017 (4) Å
c = 16.2680 (9) Å
α = 89.224 (2)°
β = 77.873 (2)°
γ = 69.352 (1)°
V = 873.19 (8) Å^3
Z = 1
D_x = 1.109 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5107 reflections
θ = 2.6–30.5°
μ = 0.14 mm^{-1}
T = 180 (2) K
Block, colourless
0.35 × 0.20 × 0.20 mm

Data collection

Bruker–Nonius X8APEX-II CCD diffractometer
Thin-slice ω and φ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.800, T_{max} = 0.974
11772 measured reflections
5139 independent reflections
4112 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 30.5°
$h = -10 \rightarrow 10$
$k = -10 \rightarrow 10$
$l = -20 \rightarrow 23$

Key indicators

Single-crystal X-ray study
T = 180 K
Mean σ(C–C) = 0.002 Å
R factor = 0.045
wR factor = 0.134
Data-to-parameter ratio = 27.3

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

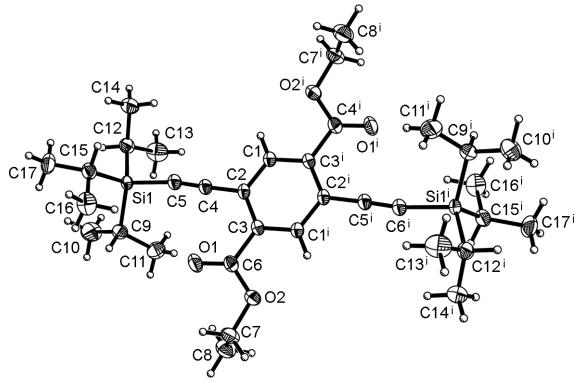


Figure 1
The molecular unit of (I), showing displacement ellipsoids at the 50% probability level for non-H atoms. H atoms are shown as spheres of arbitrary radius. [Symmetry code (i): $1-x, 1-y, 1-z$.]

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0768P)^2 + 0.1418P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.045$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.134$	$\Delta\rho_{max} = 0.47$ e Å^{-3}
$S = 1.07$	$\Delta\rho_{min} = -0.23$ e Å^{-3}
5139 reflections	
188 parameters	
H-atom parameters constrained	

H atoms bound to C atoms were positioned geometrically and allowed to ride during subsequent refinement with C—H = 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C) for the H atom bound to C1; C—H = 0.99 Å and U_{iso}(H) = 1.2U_{eq}(C) for H atoms bound to C7; C—H = 1.00 Å and U_{iso}(H) = 1.2U_{eq}(C) for H atoms bound to C9, C12 and C15; C—H = 0.98 Å and U_{iso}(H) = 1.5U_{eq}(C) for H atoms of the methyl groups. The methyl groups were allowed to rotate about their local threefold axes.

Data collection: *APEX*2 (Bruker–Nonius, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

The structure is the first to be produced from a new Bruker–Nonius X8APEX-II system. We are grateful to the Danish Natural Science Research Council (SNF) and Calsbergfondet for providing the funds to purchase this equipment.

References

Bruker (2003). *SAINT*. Version 7.06a. Bruker AXS Inc., Madison, Wisconsin, USA.

Bruker–Nonius (2003). *APEX*2. Version 1.0–8. Bruker–Nonius BV, Delft, The Netherlands.

Sheldrick, G. M. (2003). *SADABS*. Version 2.10. Bruker AXS Inc., Madison, Wisconsin, USA.

Sheldrick, G. M. (2000). *SHELXTL*. Version 6.10. Bruker AXS Inc., Madison, Wisconsin, USA.

Zhang, Q., Shi, C., Zhang, H.-R. & Wang, K. K. (2000). *J. Org. Chem.* **65**, 7977–7983.