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[(2*R*,5*S*)-2,5-Bis(4-nitrophenyl)perhydrofuro-[2,3-*b*]furan-3-yl]triisopropylsilane

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In the title compound, $C_{27}H_{36}N_2O_6Si$, the angle between the two least-squares planes of the nitrophenyl groups is 34.65 (9)°. Owing to the presence of an approximate non-crystallographic mirror plane, the title compound is an example of an achiral molecule crystallizing in a chiral space group.

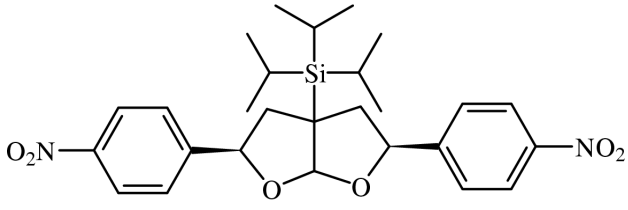
Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.003 Å
R factor = 0.034
wR factor = 0.081
Data-to-parameter ratio = 14.1

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

Comment

The title compound, (I), was prepared as part of an ongoing study into the Lewis-acid-mediated additions of silylated methylenecyclopropanes to aldehydes. It is an example of an achiral molecule crystallizing in a chiral space group and the angle between the two least-squares planes of the nitrophenyl groups is 34.65 (9)°.



(I)

Experimental

The synthesis of the title compound was carried out by the $BF_3{\cdot}Et_2O$-mediated addition of triisopropyl(2-methylidenecyclopropyl)silane to 4-nitrobenzaldehyde in dichloromethane in 29% yield.

Crystal data

$C_{27}H_{36}N_2O_6Si$
M_r = 512.67
Orthorhombic, $P2_12_12_1$
a = 11.4829 (3) Å
b = 14.5419 (3) Å
c = 15.7595 (4) Å
V = 2631.57 (11) Å^3
Z = 4
D_x = 1.294 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4610 reflections
θ = 2.9–25.0°
μ = 0.13 mm^{-1}
T = 120 (2) K
Block, colourless
0.20 × 0.15 × 0.10 mm

Data collection

Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1997)
T_{min} = 0.974, T_{max} = 0.987
14158 measured reflections
4610 independent reflections
4150 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
θ_{max} = 25.0°
$h = -13 \rightarrow 13$
$k = -17 \rightarrow 17$
$l = -18 \rightarrow 18$

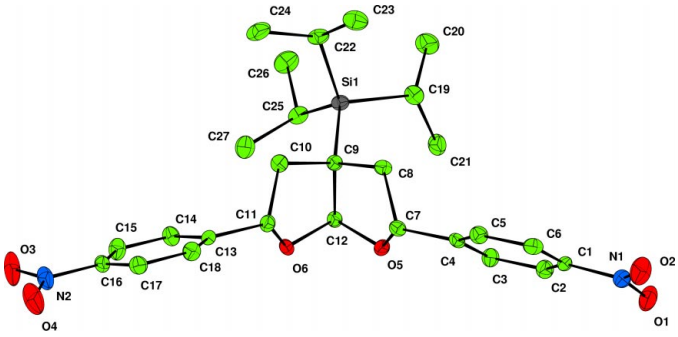


Figure 1
The molecular structure of (I) (30% probability displacement ellipsoids).

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.081$
$S = 1.08$
4610 reflections
326 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0435P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.011$
$\Delta\rho_{max} = 0.28$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0054 (9)
Absolute structure: Flack (1983), 1974 Friedel pairs
Flack parameter = −0.04 (11)

Data collection: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Hooft, 1998); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO*, *COLLECT* and *maXus* (Mackay *et al.*, 1998); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *CAMERON* (Watkin, *et al.*, 1993); software used to prepare material for publication: *WinGX* (Farrugia, 1998).

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