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Triisopropyl[5-(4-nitrophenyl)tetrahydrofuran-3-ylidenemethyl]silane

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Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.009 Å
R factor = 0.082
wR factor = 0.254
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.

In the title compound, $C_{20}H_{31}NO_3Si$, the nitrophenyl groups of adjacent molecules overlap to form π–π-stacked pairs.

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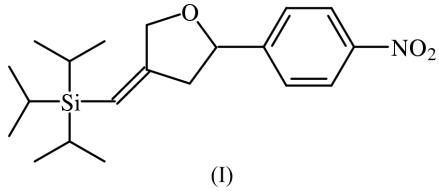
Comment

The title compound, (I), was prepared as part of an ongoing study into the Lewis-acid-mediated additions of silylated methylenecyclopropanes to aldehydes. The nitrophenyl groups of adjacent molecules overlap to form π–π-stacked pairs.



(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 44% yield.

Crystal data

$C_{20}H_{31}NO_3Si$
M_r = 361.55
Monoclinic, $C2/c$
a = 14.6339 (3) Å
b = 7.7463 (1) Å
c = 35.8752 (7) Å
β = 91.066 (3)°
V = 4066.06 (13) Å^3
Z = 8
D_x = 1.181 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3107 reflections
θ = 3.0–25.0°
μ = 0.13 mm^{-1}
T = 120 (2) K
Needle, colourless
0.15 × 0.07 × 0.06 mm

Data collection

Nonius KappaCCD area-detector diffractometer
Φ and ω scans to fill asymmetric unit
Absorption correction: multi-scan (*SORTAV*; Blessing, 1997)
T_{min} = 0.980, T_{max} = 0.992
6912 measured reflections
3107 independent reflections
1445 reflections with $I > 2\sigma(I)$
R_{int} = 0.103
θ_{max} = 25.0°
$h = -17 \rightarrow 17$
$k = -8 \rightarrow 8$
$l = -42 \rightarrow 42$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.082
$wR(F^2)$ = 0.254
S = 0.97
3107 reflections
226 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.13P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.73 e Å^{-3}
$\Delta\rho_{min}$ = −0.58 e Å^{-3}

The fraction of unique reflections measured out to θ_{max} (25°) is relatively low (0.86), which may be partly due to the weakly

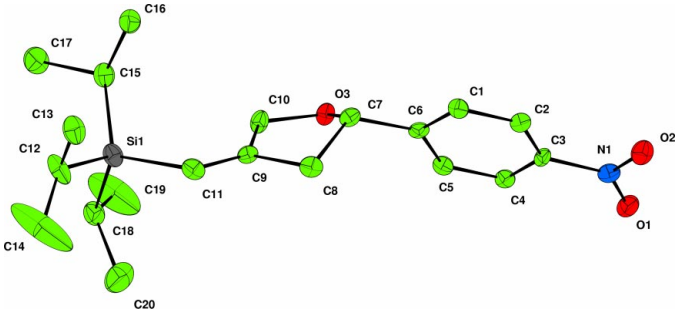


Figure 1
The molecular structure of (I) (30% probability displacement ellipsoids).

diffracting nature of the crystal. The probability displacement ellipsoids of C14 and C19 were found to be prolate. Splitting the sites was tried without success, leading to the conclusion that the atoms are affected by dynamic disorder.

Data collection: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Hooft, 1998); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO*, *COLLECT* (Hooft, 1998) 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).

References

Blessing, R. H. (1997). *J. Appl. Cryst.* **30**, 421–426.
Farrugia, L. J. (1998). *WinGX*. University of Glasgow, Scotland.
Hooft, R. (1998). *COLLECT*. Data Collection Software. Nonius BV, The Netherlands.
Mackay, S., Gilmore, C. J., Edwards, C., Tremayne, M., Stewart, N. & Shankland, K. (1998). *maXus*. University of Glasgow, Scotland.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter and R. M. Sweet, pp. 307–326. London: Academic Press.
Sheldrick, G. M. (1997). *SHELXL*97 and *SHELXS*97. University of Göttingen, Germany.
Watkin, D. M., Pearce, L. & Prout, C. K. (1993). *CAMERON*. Chemical Crystallography Laboratory, University of Oxford, England.