organic papers

Jian-Zhong Liu, Raj K. Dhar, Frank R. Fronczek, Peter W. Rabideau‡ and Steven F. Watkins*

Department of Chemistry, Louisiana State University, Baton Rouge, LA 70803-1804, USA

‡ Current address: Department of Chemistry, Mississippi State University, MS 39762, USA

Correspondence e-mail: swatkins@lsu.edu

Key indicators

Single-crystal X-ray study
$T = 110$ K
Mean σ(C–C) = 0.002 Å
R factor = 0.051
wR factor = 0.149
Data-to-parameter ratio = 25.9

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

9,9-Dibenzyl-10-trimethylsilyl-9,10-dihydro-anthracene

The title compound, $C_{31}H_{32}Si$ or $(C_6H_5CH_2)_2C_{14}H_9Si(CH_3)_3$, has a concave dihydroanthracene unit. The central ring adopts a half-chair conformation and the two benzene rings are tilted by 14.40 (7)° with respect to one another. The trimethylsilyl group is substituted in the axial position of the half-chair.

Comment

In the solid state at room temperature, 9,10-dihydro-anthracene (DHA) is V-shaped (Herbstein *et al.*, 1986; Reboul *et al.*, 1987), with an average angle between the planes of 36.4 (2)°; an *MM2* model calculation yields 37.8°. The central ring adopts a boat conformation. Acyclic substitution at C9 and C10 results in five structural classes, with characteristic changes in conformation and dimensions. The title compound, (I), belongs to the class of trisubstituted DHA analogs, of which three previous structures have been reported. Two of these (Masnovi & Kochi, 1985; Dhar *et al.*, 1992) adopt the V-boat shape of DHA, while in the other (Dhar *et al.*, 1992), the central ring displays a highly flattened chair conformation.

(I)
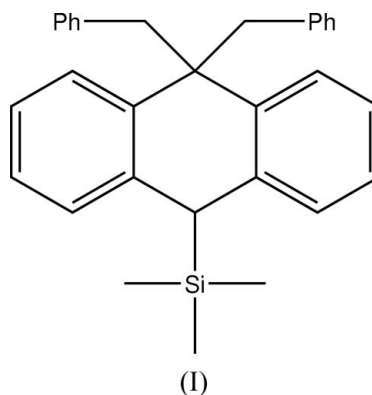
The DHA core of (I) adopts a shape in which the central ring has a half-chair conformation; five of the C atoms of the central ring define a mean plane [r.m.s. deviation 0.011 (1) Å], while the sixth (C10) lies 0.202 (2) Å above this plane, the dihedral angle between the three-atom and five-atom planes being 14.71 (5)°. The two benzene rings are tilted by 7.62 (7) and 7.13 (6)° with respect to the half-chair plane, and by 14.40 (7)° with respect to one another.

Experimental

The preparation of (I) has been detailed by Dhar *et al.* (1992). Crystals suitable for X-ray diffraction were obtained by recrystallization from methanol–diethyl ether.

Crystal data

$C_{31}H_{32}Si$
$M_r = 432.66$
Monoclinic, $P2_1/c$
$a = 10.1218\ (15)$ Å
$b = 13.583\ (2)$ Å
$c = 18.622\ (3)$ Å
$\beta = 103.072\ (6)°$
$V = 2493.9\ (7)$ Å^3

$Z = 4$
$D_x = 1.152$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.11$ mm^{-1}
$T = 110\ (2)$ K
Prism, colorless
$0.43 \times 0.35 \times 0.25$ mm

Data collection

Nonius KappaCCD diffractometer (with an Oxford Cryosystems Cryostream cooler)
ω scans
Absorption correction: multi-scan (*SCALEPACK*; Otwinowski & Minor, 1997)
$T_{min} = 0.954$, $T_{max} = 0.973$
13967 measured reflections
7551 independent reflections
5890 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 30.4°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.149$
$S = 1.02$
7551 reflections
292 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0776P)^2 + 0.757P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.34$ e Å^{-3}
$\Delta\rho_{min} = -0.42$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Si1—C29	1.8553 (17)	Si1—C31	1.8718 (19)
Si1—C30	1.870 (2)	Si1—C10	1.9394 (14)
C10—C14—C13—C9	−12.39 (18)	C14—C10—C11—C12	−16.30 (17)
C11—C10—C14—C13	18.64 (17)	C14—C13—C9—C12	2.32 (16)
C13—C9—C12—C11	−0.04 (16)	C9—C12—C11—C10	7.75 (19)

All H atoms were placed in idealized positions (C—H = 0.95–1.00 Å) and were treated as riding, with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}$(methyl C). A torsional parameter was refined for each methyl group.

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics:
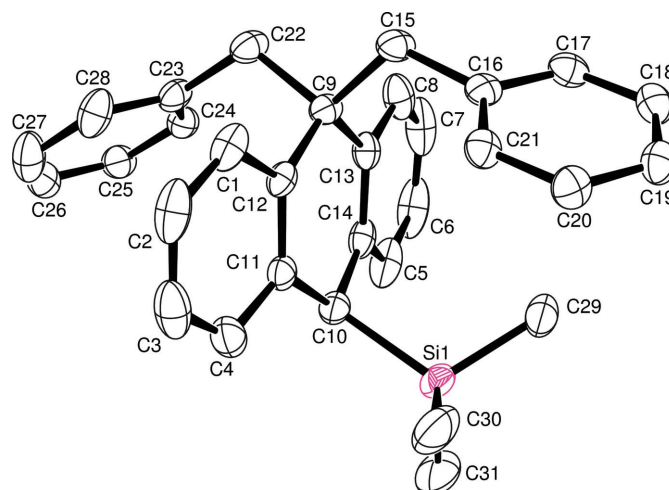

Figure 1
View of (I), showing 50% probability displacement ellipsoids. H atoms have been omitted.

ORTEP-3 for Windows (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

References

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