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Triphenylmethylium tetrakis[4-(*p*-*tert*-butyldimethylsilyl)-2,3,5,6-tetrafluorophenyl]borate

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.017 Å
R factor = 0.079
wR factor = 0.273
Data-to-parameter ratio = 19.5

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

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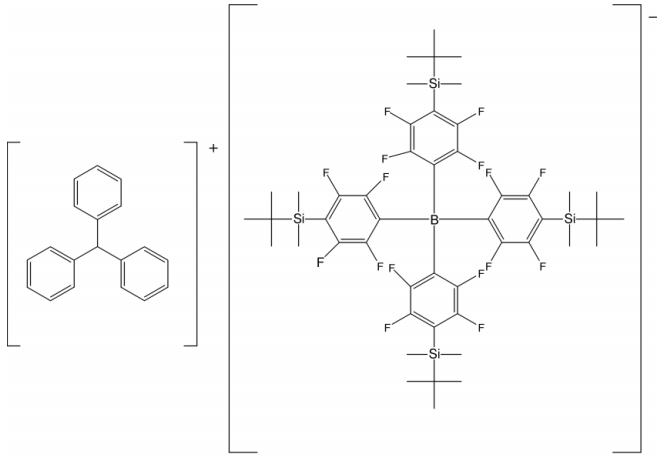
The title compound, $C_{19}H_{15}^{+}\cdot C_{48}H_{60}BF_{16}Si_4^{-}$, consists of discrete cations and anions. There are two ions of each kind in the asymmetric unit.

Comment

The title compound, (I), consists of discrete cations and anions. There are two ions of each kind in the asymmetric unit. The central atoms of the trityl cations exhibit a trigonal planar geometry. The dihedral angles between the plane formed by the central C atom and its three adjacent atoms and the phenyl rings are 29.7 (6), 31.2 (5) and 37.2 (3)° for C1, and 28.5 (6), 30.6 (5) and 38.4 (3)° for C2.



(I)

Experimental

The title compound was synthesized according to a literature procedure (Jia *et al.*, 1997). Comparison of ^{1}H, ^{13}C and ^{19}F NMR data with literature specifications (Jia *et al.*, 1997) confirmed the identity of the synthesized material. Yellow crystals suitable for X-ray analysis were grown during four weeks from a pentane solution under solvothermal conditions. Analytical data: ^{29}Si NMR, 49.6 MHz, CD_2Cl_2, 330 K, ($\delta(H_3C)_2SiHCl$): 11.1) δ 5.6.

Crystal data

$C_{19}H_{15}^{+}\cdot C_{48}H_{60}BF_{16}Si_4^{-}$
M_r = 1307.44
Monoclinic, $P2_1/c$
a = 22.064 (2) Å
b = 33.477 (3) Å
c = 22.730 (2) Å
β = 93.689 (8)°
V = 16754 (3) Å^3
Z = 8
D_x = 1.037 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 23 765 reflections
θ = 1.4–22.4°
μ = 0.14 mm^{-1}
T = 173 (2) K
Plate, orange
0.28 × 0.22 × 0.03 mm

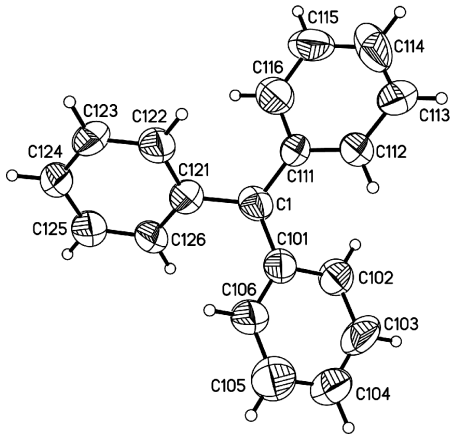


Figure 1
Perspective view of cation 1 of the title compound with the atom numbering; displacement ellipsoids are drawn at the 50% probability level.

Data collection

Stoe IPDS-II two-circle diffractometer
ω scans
Absorption correction: multi-scan (*MULABS*; Spek, 1990; Blessing, 1995)
T_{min} = 0.952, T_{max} = 0.990
142 757 measured reflections
30 915 independent reflections
3913 reflections with $I > 2\sigma(I)$
R_{int} = 0.182
θ_{max} = 25.5°
$h = -26 \rightarrow 26$
$k = -40 \rightarrow 40$
$l = -27 \rightarrow 27$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.079
$wR(F^2)$ = 0.273
S = 0.84
30 915 reflections
1585 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1144P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.78 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

H atoms were refined with fixed individual displacement parameters [U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C_{methyl})], using a riding model with C—H = 0.95 Å or methyl C—H = 0.98 Å. The percentage of observed data was only 13% of the unique data available to a θ_{max} of 25.1°. Inclusion of such a high percentage of essentially unobserved data into the structure refinement restricts the precision of the results. The intensities of the data, in general being weak, lead to the high value for R_{int} of 0.18.

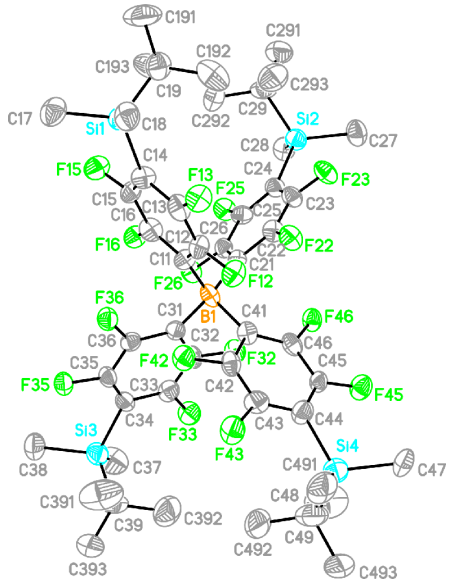


Figure 2
Perspective view of anion 1 of the title compound with the atom numbering; displacement ellipsoids are drawn at the 30% probability level.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL*97.

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