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Thallium tetrakis(pentafluorophenyl)borate

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Key indicators

Single-crystal X-ray study
T = 123 K
Mean σ(C–C) = 0.009 Å
Disorder in solvent or counterion
R factor = 0.040
wR factor = 0.087
Data-to-parameter ratio = 11.7

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

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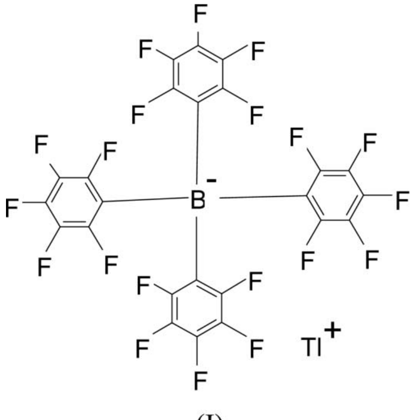
The crystal structure of thallium perfluorotetraphenylborate, $Tl^+ \cdot B(C_6F_5)_4^-$, consists of discrete partial occupancy Tl cations lying on threefold rotation axes, surrounded by perfluorotetraphenylborate anions, with Tl···F interactions in the range 2.942 (4)–3.663 (4) Å.

Comment

There has been increased interest in the synthesis and chemistry of weakly coordinating anions due to their importance in catalysis, electrochemistry, and in the generation of reactive cationic complexes and ionic liquids (Krossing & Raabe, 2004). Recently developed anions that show weak nucleophilicity are $B(C_6F_5)_4^-$, $MeB(C_6F_5)_3^-$, $B[3,5\text{-}C_6H_3(CF_3)_2]_4^-$ (Strauss, 1993; Piers & Chivers, 1997), and the carborane $CB_{11}H_{12}^-$ and its derivatives (Reed, 1998). Of these, $B(C_6F_5)_4^-$, first prepared as a lithium salt (Massey & Park, 1986), is of particular interest, due to its high stability and ready availability. Alberti & Porschke (2004) have recently published a variation to this anion, that is the thallium salt $TlB(C_6F_5)_4^-$. We have been using this salt to generate reactive boron cations and found that X-ray quality crystals could be grown from a CH_2Cl_2/hexane mixture at room temperature. We present here the structure of thallium perfluorotetraphenylborate, (I).



(I)

In the crystal structure of (I) (Fig. 1), discrete Tl cations lie on threefold rotation axes. The partial occupancy of 0.25 for the Tl cation is required by the 1:1 cation–anion stoichiometry. The cations are surrounded by perfluorotetraphenylborate anions, with short Tl···F1 interactions of 2.942 (4) Å; the rest of the Tl···F distances are in the range 3.195 (4)–3.663 (4) Å, showing weak interactions (Fig. 2). Similar Tl···F interactions have been reported in the structure of thallium tetrakis[3,5-

bis(trifluoromethyl)phenyl]borate (Hughes *et al.*, 1997). The geometry around the B atom is distorted tetrahedral, with two C—B—C angles of 101.6 (4)° and the others with a value of 113.6 (2)°. The remaining dimensions in the anion are normal with mean B—C, C—C and C—F distances of 1.656 (6), 1.380 (10) and 1.351 (14) Å, respectively.

Experimental

The synthesis of the title compound was performed according to the procedure described in the literature by Alberti & Pörschke (2004). Single crystals for this study were grown by slow diffusion of *n*-hexane into a dichloromethane solution of thallium perfluorotetraphenylborate.

Crystal data

$Tl^+\cdot C_{24}BF_{20}^-$
$M_r = 883.42$
Cubic, $I\bar{4}3d$
$a = 19.095$ (12) Å
$V = 6962$ (8) Å^3
$Z = 12$
$D_x = 2.528$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2240 reflections
$\theta = 4.0$–$27.5°$
$\mu = 7.14$ mm^{-1}
$T = 123$ (2) K
Plate, colorless
0.10 × 0.08 × 0.05 mm

Data collection

Nonius KappaCCD diffractometer
ω and φ scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1997)
$T_{min} = 0.523$, $T_{max} = 0.703$
2240 measured reflections
1236 independent reflections
949 reflections with $I > 2\sigma(I)$
$R_{int} = 0.051$
$\theta_{max} = 27.5°$
$h = -24 \rightarrow 24$
$k = -17 \rightarrow 17$
$l = -17 \rightarrow 17$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.087$
$S = 1.03$
1236 reflections
106 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0365P)^2 + 3.02P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.65$ e Å^{-3}
$\Delta\rho_{min} = -0.69$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.00038 (5)
Absolute structure: Flack (1983), 504 Friedel pairs
Flack parameter: 0.007 (13)

Table 1
Selected geometric parameters (Å, °).

F1—C2	1.364 (7)	C2—C3	1.394 (9)
F2—C3	1.338 (7)	C3—C4	1.363 (9)
F3—C4	1.353 (7)	C4—C5	1.378 (9)
F4—C5	1.333 (6)	C5—C6	1.381 (9)
F5—C6	1.368 (7)	B1—C1^{i}	1.655 (6)
C1—C6	1.375 (8)	B1—C1^{ii}	1.655 (6)
C1—C2	1.386 (8)	B1—C1^{iii}	1.656 (6)
C1—B1	1.656 (6)		
C1^{i}—B1—C1^{ii}	101.6 (4)	C1^{i}—B1—C1	113.6 (2)

Symmetry codes: (i) $z-\frac{1}{4}, -y+\frac{1}{4}, -x+\frac{3}{4}$; (ii) $-z+\frac{3}{4}, -y+\frac{1}{4}, x+\frac{1}{4}$; (iii) $-x+\frac{1}{2}, y, -z+1$.

The final difference map was free of any chemically significant features.

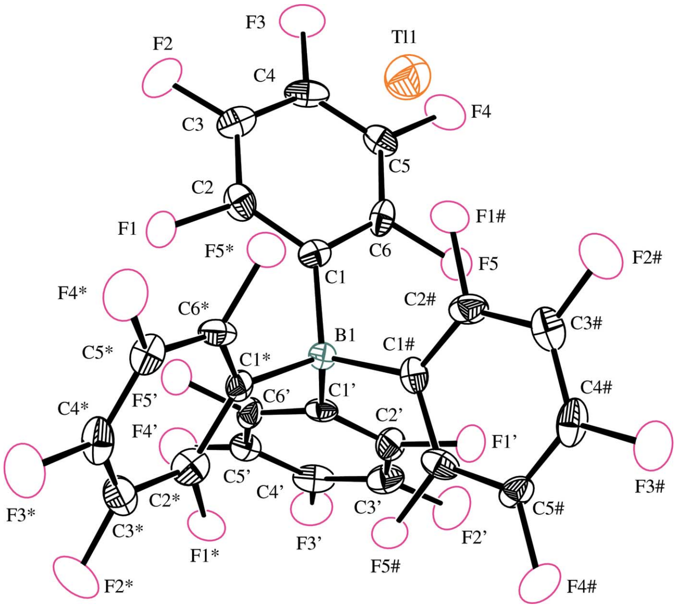


Figure 1
ORTEPII (Johnson, 1976) drawing of (I), with displacement ellipsoids plotted at the 50% probability level. [Symmetry codes: (*) $z-\frac{1}{4}, \frac{1}{4}-y, \frac{3}{4}-x$; (') $\frac{1}{2}-x, y, 1-z$; (#) $\frac{3}{4}-z, \frac{1}{4}-y, \frac{1}{4}+x$.]

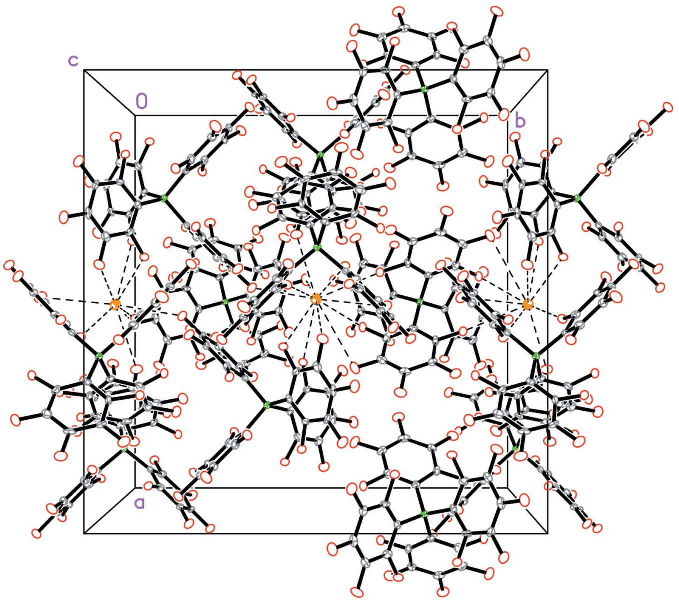


Figure 2
The unit-cell packing diagram of (I), viewed down the *c* axis.

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SAPI* (Fan, 1991); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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m1802 Parvez *et al.* • $Tl^+\cdot C_{24}BF_{20}^-$ *Acta Cryst.* (2005). E**61**, m1801–m1803

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