Exploring the fate of the tris(pentafluorophenyl)borane radical anion in weakly coordinating solvents

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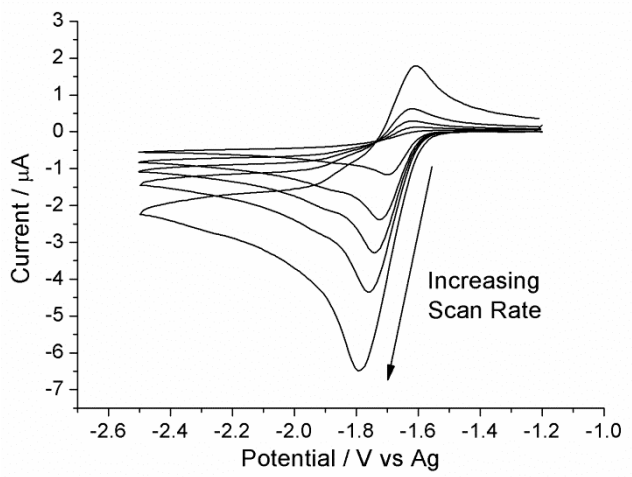
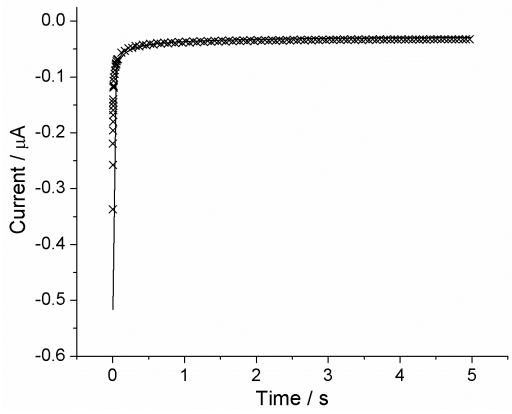
Supporting Information

Cyclic Voltammetry



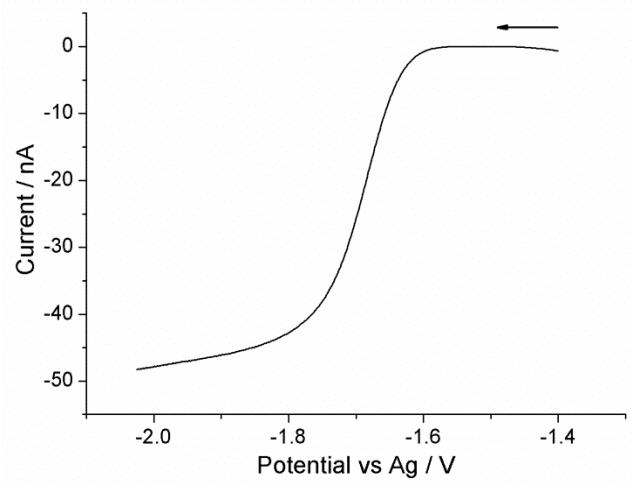
SI 1 Overlaid cyclic voltammograms of $B(C_6F_5)_3$ in CH_2Cl_2 (5 mM, 0.05 M $[^nBu_4N][B(C_6F_5)_4]$) recorded at scan rates of 50-5000 mV s^{-1} at a Pt macrodisk working electrode and ambient temperature.

Chronoamperometry



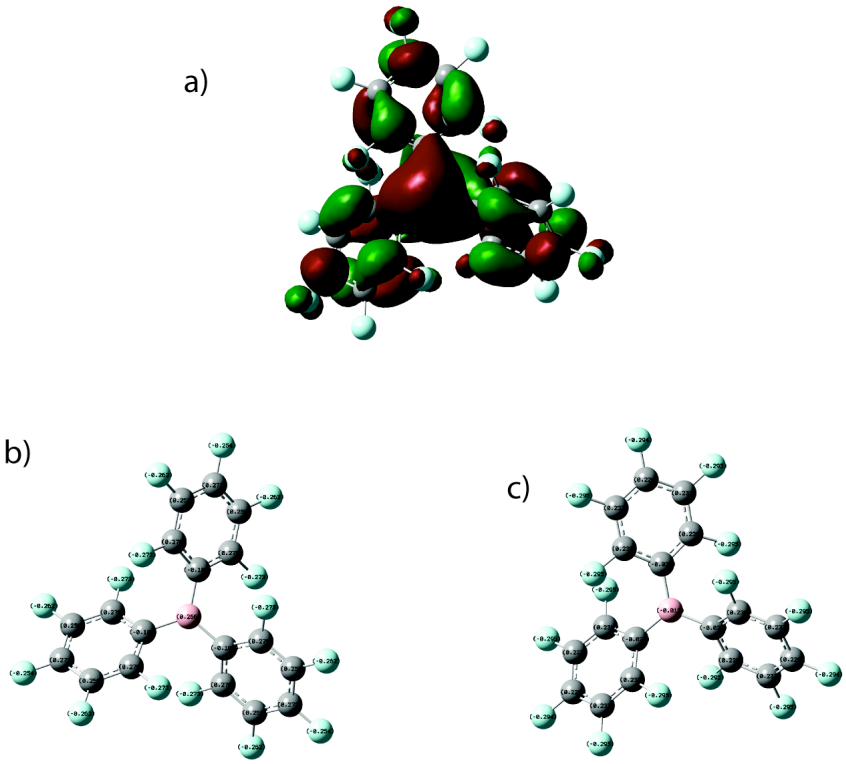
SI 2 Experimental chronoamperogram (crosses) and Shoup–Szabo best fit (solid line) for the reduction of $B(C_6F_5)_3$ in DFB (5 mM, 0.05 M $[^nBu_4N][B(C_6F_5)_4]$) at a 30 μm radius Pt microdisk.

Linear Sweep Voltammetry



SI 3 Linear sweep voltammogram for the one-electron reduction of $B(C_6F_5)_3$ in CH_2Cl_2 (4.8 mM, 0.05 M [^{n}Bu$_4$N][$B(C_6F_5)_4$]) recorded at a scan rate of 5 mV s^{-1} at a 31 μm Pt microdisk working electrode.

DFT calculations



SI 4 DFT calculations using the spin–unrestricted B3LYP 6-311+G(d,p) basis set for: **a)** the SOMO of the $B(C_6F_5)_3\bullet^-$ radical anion; Charge density distribution based on Mulliken electron population analysis for **b)** $B(C_6F_5)$ and **c)** $B(C_6F_5)_3\bullet^-$ radical anion.