Migratory insertion of $[B(C_6F_5)_2]$ into C-H bonds: CO promoted transfer of the boryl fragment

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Supporting information (2 pages)

Photolysis of 2: identification of [η^5-$C_5H_4B(C_6F_5)_2F$]$Fe(CO)_3$ (3)

Prolonged photolysis of solutions of **2** in benzene-d_6 leads to the formation of a mixture of **2** and **3**, as judged by ^{1}H and ^{11}B NMR. Although isolation of bulk samples of **3** free from **2** by fractional crystallization proved impossible, single crystals of **3** suitable for X-ray crystallography could be separated manually and spectroscopic (NMR, IR) data for **3** deduced from the mixture.

Spectroscopic data for **3**: ^{1}H NMR (300 MHz, C_6D_6) δ 3.52, 4.85 [m, both 2H, C_5H_4]. ^{11}B NMR (96 MHz, C_6D_6) δ –2.2 [d, $^1J_{BF}$ = 66 Hz]. ^{19}F NMR (283 MHz, C_6D_6) δ –132.6 [d, $^3J_{FF}$ = 20.8 Hz, ortho-CF], -158.4 [t, $^3J_{FF}$ = 20.8 Hz, para-CF], -162.1 [m, meta-CF], -188.7 [b, BF]. IR (KBr, cm^{-1}) ν(CO) 2110 st, 2063 m sh, 2049 st.