Electronic Supplementary Information

for

Highly Fluorinated Hydrotris(indazolyl)borate Calcium Complexes: Structure and Reactivity Heavily Depend on the Ligand Electronic Properties

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Content

19F NMR spectrum of [Ca(F12-Tp4Bo,3Ph)2] (1)
Series of 19F NMR spectra of [(F12-Tp4Bo,3Ph)CaI(THF)] (2)
19F NMR spectrum of [Ca(THF)6][F12-Tp4Bo,3Ph]2 (3)
ORTEP drawing of [Ca(THF)6][F12-Tp4Bo,3Ph]2 (3)
Figure S1: $^{19}$F NMR spectrum of $[\text{Ca(F}_{12}\text{-Tp}^{(4\text{Bo},3\text{Ph})^2})_2]$ (1) in acetone-$d_6$ highlighting the 2:1 ratio for each type of fluorine.
Figure S2a: $^{19}$F NMR spectrum of [(F$_{12}$-Tp$^{4Bo,3Ph}$)Ca(THF)] (2) in THF: crude reaction mixture after elimination of TII affording an equilibrating mixture of (F$_{12}$-Tp$^{4Bo,3Ph}$)Ca(THF)$_x$ species.
Figure S2b: $^{19}$F NMR spectrum of [(F$_{12}$-Tp$^{4Bo,3Ph}$)Ca(THF)] (2) in a THF-acetone-$d_6$ mixture. Same sample as Figure S2a with a more concentrated THF solution. Further concentration yields the spectrum in Figure S2c.
Figure S2c: $^{19}$F NMR spectrum of (acetone-$d_6$) [(F$_{12}$-Tp$^{4B0,3Ph}$)CaI(THF)] (2). Same sample as Figure S2a and S2b after complete removing of THF showing the presence of 2 (from irreversible Schlenk equilibrium), 1 and indazole (IndH).
Figure S3: $^{19}$F NMR spectra of $[\text{Ca(THF)}_6][\text{F}_{21}-\text{Tp}^{4\text{Bo},3\text{CF}_3}]_2$ (3), $\text{Na[F}_{21}-\text{Tp}^{4\text{Bo},3\text{CF}_3}]$ and $\text{Tl[F}_{21}-\text{Tp}^{4\text{Bo},3\text{CF}_3}]$ in acetone-$d_6$. 
Figure S4. ORTEP drawing of $[\text{Ca(THF)}_6][\text{F}_{21}\text{-Tp}^{\text{aBo,CF}}]_2$ (3).