

Hexaethyl-2,4-dicarba-*nido*-hexaborane(8), Deprotonation and Complexation Studied by NMR Spectroscopy and Density Functional Theory (DFT) Calculations

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Deprotonation of hexaethyl-2,4-dicarba-*nido*-borane(8) **2** leads first to the hexaethyl-2,4-dicarba-*nido*-borate(1^-) **3**, and further deprotonation, using BuLi/KO^tBu, gives the hexaethyl-2,4-dicarba-*nido*-hexaborate(2^-) **4**. The reaction of **3** with FeCl₂ affords the *commo*-ferracarborane [Fe(Et₆-2,4-C₂B₄H)₂] **5**, and the analogous reaction of **4** leads to the anionic sandwich complex [Fe(Et₆-2,4-C₂B₄)₂]²⁻ **6** which can be protonated to give **5**. The complex **5** contains two hydrido ligands, each bridging the iron and two boron atoms. Reactions were monitored and the products were characterised by ¹¹B NMR spectroscopy in solution. The geometries of the carboranes, the borates (all unsubstituted and permethyl-substituted) and the iron complexes (all unsubstituted) were optimised by DFT methods [B3LYP/6-311+G(d,p) or B3LYP/6-31+G(d)], and the relevant NMR data [chemical shifts $\delta^{11}\text{B}$, $\delta^{13}\text{C}$, $\delta^{57}\text{Fe}$, and coupling constants $^1J(^{13}\text{C}, ^1\text{H})$, $^1J(^{11}\text{B}, ^1\text{H})$, $^1J(^{57}\text{Fe}, ^1\text{H})$, $^1J(^{57}\text{Fe}, ^{11}\text{B})$] were calculated at the same level of theory.

Key words: Carboranes, Iron Complexes, NMR, MO Calculations