Supplementary Material

Experimental assessment of the relative affinity of benzene and ferrocene towards the Li^+ cation.

Linda Kaufmann, Hannes Vitze, Michael Bolte, Hans-Wolfram Lerner and Matthias Wagner*

Figure 1S

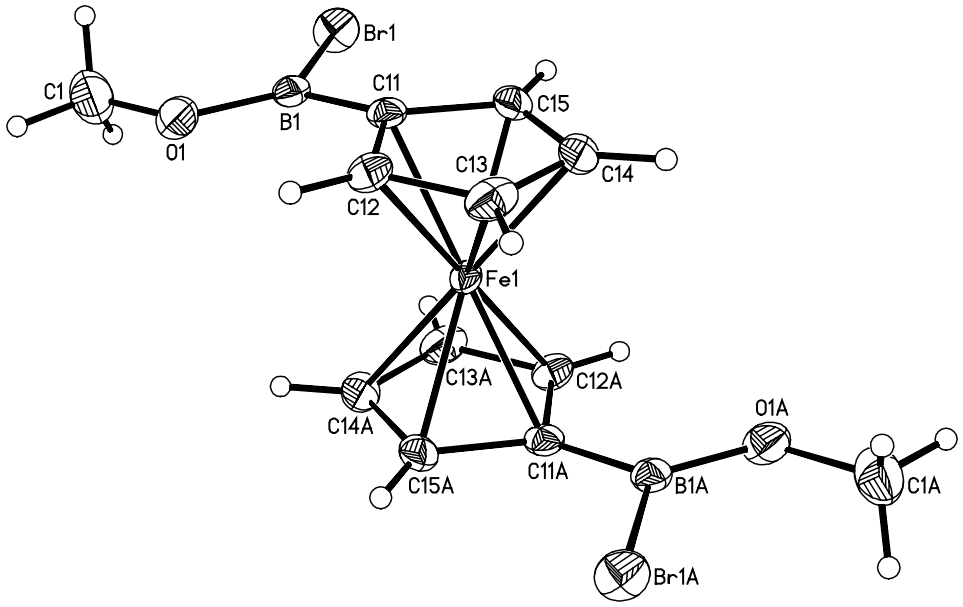

Figure 1S. Structure of **7** in the crystal; H atoms omitted for clarity. Selected bond lengths (Å), bond angles (deg), and torsion angles (deg): B(1)-O(1) = 1.367(4)**,** B(1)-C(11) = 1.533(4), B(1)-Br(1) = 1.967(3), COG(Cp)-C(11)-B(1) = 171.7; O(1)-B(1)-C(11) = 121.8(3), O(1)-B(1)-Br(1) = 119.7(2), C(11)-B(1)-Br(1) = 118.5(2); O(1)-B(1)-C(11)-C(12) = 3.2(4), Br(1)-B(1)-C(11)-C15) = -7.7(4), C(1)-O(1)-B(1)-C(11) = 177.2(3).

Description of the molecular structure of 7 in the solid state: Compound **7** adopts a centrosymmetric conformation in the crystal lattice. Each boron atom possesses a trigonal planar configuration (sum of angles around B(1) = 360°) and is slightly bent out of the plane of the cyclopentadienyl ring towards the central iron atom (COG(Cp)-C(11)-B(1) = 171.7°). Both torsion angles O(1)-B(1)-C(11)-C(12) and Br(1)-B(1)-C(11)-C15) are close to 0° so that an interaction of the π electron system of the cyclopentadienyl ring with the empty p-orbital of the boron atom is possible.