Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information

for the paper

Ferrocenyl(trihydro)borates: Building Blocks for the Synthesis of Heterooligonuclear Metallocene Complexes

Adelina Reichert, Michael Bolte, Hans-Wolfram Lerner and Matthias Wagner

X-ray crystal structure analyses of compounds 2 and 5

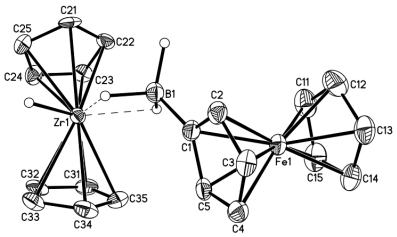

Figure 1S: Molecular structure of **2** in the solid state. Hydrogen atoms except on boron and zirconium have been omitted for clarity; displacement ellipsoids are drawn at the 50% probability level. Selected bond lengths (Å), atom···atom distance (Å), bond angle (°), and dihedral angles (°): B(1)−C(1) 1.593(8), Zr(1)−H(1) 1.64(5), Zr(1)···B(1) 2.588(5); B(1)···Zr(1)−H(1) 94(2); Cp(C(1))//B(1)Zr(1)H(1) 71(1), Cp(C(21))//Cp(C(31)) 48.3(2).

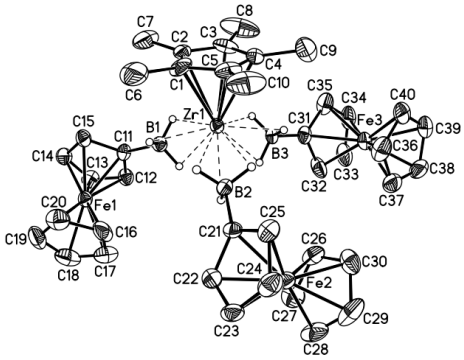

Figure 2S: Molecular structure of **5** in the solid state. Hydrogen atoms except on boron have been omitted for clarity; displacement ellipsoids are drawn at the 50% probability level. Selected bond lengths (Å), atom···atom distances (Å), and bond angles (°): B(1)−C(11) 1.573(12), B(2)−C(21) 1.583(10), B(3)−C(31) 1.577(9), Zr(1)···B(1) 2.380(9), Zr(1)···B(2) 2.363(7), Zr(1)···B(3) 2.384(6); B(1)···Zr(1)···B(2) 103.7(3), B(1)···Zr(1)···B(3) 103.8(3), B(2)···Zr(1)···B(3) 103.0(3).

Table 1S: Crystallographic Data for **2** and **5**

	2	**5**
formula	$C_{20}H_{23}BFeZr$	$C_{40}H_{51}B_3Fe_3Zr$
fw	421.26	823.01
colour, shape	orange, needle	orange, needle
temp (K)	173(2)	173(2)
cryst. syst.	monoclinic	monoclinic
space group	$P2_1/c$	$P2_1/n$
a (Å)	7.8828(5)	7.7895(7)
b (Å)	12.3274(8)	23.3720(19)
c (Å)	17.7040(12)	20.470(2)
α (°)	90	90
β (°)	95.903(6)	90.081(8)
γ (°)	90	90
V (Å^3)	1711.25(19)	3726.7(6)
Z	4	4
$D_{calcd.}$ (g cm^{-3})	1.635	1.467
F(000)	856	1696
μ (mm^{-1})	1.452	1.444
cryst. size (mm^3)	0.21 × 0.09 × 0.09	0.27 × 0.13 × 0.12
reflections collected	14384	21865
indep. reflns (R_{int})	3212 (0.1123)	6621 (0.1558)
data/restraints/params	3212/0/224	6621/6/432
GOOF on F^2	0.885	0.866
*R*1, w*R*2 ($I > 2\sigma(I)$)	0.0419, 0.0770	0.0598, 0.1134
*R*1, w*R*2 (all data)	0.0775, 0.0851	0.1281, 0.1328
Largest diff peak and hole (eÅ^{-3})	0.812 and −0.977	0.752 and −0.883