Electronic Supplementary Information for Dalton Transactions

Electronic Communication in Oligonuclear Ferrocene Complexes with Anionic Four-Coordinate Boron Bridges

Linda Kaufmann, Jens-Michael Breunig, Hannes Vitze, Frauke Schödel, Israel Nowik, Markus Pichlmaier, Michael Bolte, Hans-Wolfram Lerner, Rainer F. Winter, Rolfe H. Herber and Matthias Wagner*

Supplementary Material

Synthesis of 5

A solution of $MeOSiMe_3$ (0.36 g, 3.47 mmol) in toluene (8 mL) was added dropwise with stirring at -78 °C to a solution of $BrBPh_2$ (0.85 g, 3.47 mmol) in toluene (12 mL). The reaction mixture was slowly warmed to r. t. and stirred overnight. All volatiles were removed from the reaction mixture in vacuo and the crude oily product was extracted into hexane. Yield of **5**: 0.48 g (71 %).

All NMR data were consistent with the values for $MeOBPh_2$ reported in the following reference: P. J. Domaille, J. D. Druliner, L. W. Gosser, J. M. Read, Jr., E. R. Schmelzer and W. R. Stevens, *J. Org. Chem.*, 1985, **50**, 189.

Crystal Structure Analysis of 7

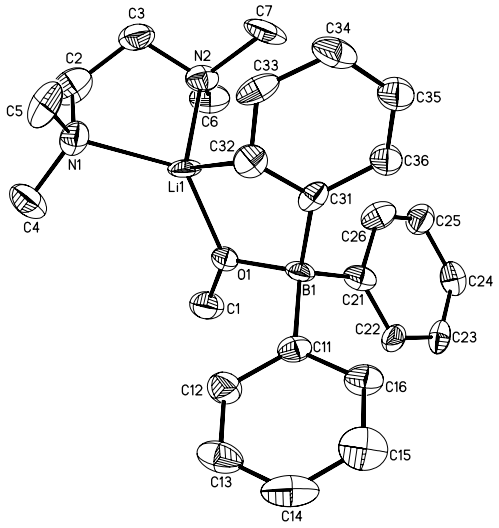

Figure 1S: Structure of **7** in the crystal. Displacement ellipsoids are drawn at the 50 % probability level. H atoms omitted for clarity. Selected bond lengths (Å), and bond angles (°): B(1)-O(1) = 1.553(16), B(1)-C(11) = 1.688(16), B(1)-C(21) = 1.594(18), B(1)-C(31) = 1.662(17); C(11)-B(1)-C(21) = 113.0(10), C(11)-B(1)-C(31) = 107.0(9), C(21)-B(1)-C(31) = 112.5(9), O(1)-B(1)-C(11) = 108.0(9), O(1)-B(1)-C(21) = 111.3(10), O(1)-B(1)-C(31) = 104.4(9).

Table 1S: Crystallographic Data of **7**.

compound	**7**
formula	$C_{25}H_{34}BLiN_2O$
fw	396.29
colour, shape	colourless, plate
temperature (K)	173(2)
crystal system	monoclinic
space group	$P2_1/n$
a (Å)	11.551(4)
b (Å)	13.504(5)
c (Å)	16.349(4)
α (°)	90
β (°)	98.36(2)
γ (°)	90
V (Å^3)	2523.1(14)
Z	4
$D_{calcd.}$ (g cm^{-3})	1.043
F(000)	856
μ (mm^{-1})	0.062
crystal size (mm^3)	$0.16 \times 0.09 \times 0.04$
no. of rflns collected	14212
no. of indep rflns (R_{int})	4444 (0.2274)
data / restraints / parameters	4444 / 0 / 272
GOOF on F^2	0.989
$R1$, $wR2$ ($I>2\sigma(I)$)	0.1613, 0.2526
$R1$, $wR2$ (all data)	0.4022, 0.3728
largest diff peak and hole (eÅ^{-3})	0.227, -0.260

Figure 2S: Spectroscopic changes upon the first a), second (b) and third (c) oxidation of Li[**10**] in an OTTLE cell (0.2 M $[NBu_4][PF_6]$; 1,2-$C_2H_4Cl_2$).