"High-spin and low-spin iron(II) complexes with facially coordinated borohydride ligands" Mehn, M.P.; Brown, S.D.; Paine, T.K.; Brennessel, W. W.; Cramer, C.J.; Peters, J.C.; Que, L., Jr.
Supporting Information

Table S1 Bond Lengths and Angles

	1	**2**	$LFe(H_3BH_3)FeL$[a]	$L_3Fe(H_3BH_3)FeL_3$[b]	$LNiH_3BH$[c]
Fe-B2	2.084(4)	1.855(2)	1.9122(11)	1.903(3), 1.913(3)	2.048(5)
Fe-H3(H47)	1.99(2)	1.57(2)	1.58(8)	1.54(2), 1.523(19)	1.89(3)
(Fe-H48)		1.62(2)	1.39(8)	1.547(18), 1.530(19)	1.89(3)
(Fe-H49)		1.61(2)	1.32(10)	1.500(19), 1.54(2)	1.94(4)
B2-H3 (H47)	1.16(2)	1.20(2)	1.46(8)	1.482(19), 1.492(19)	1.12(3)
(B2-H48)		1.18(2)	1.43(8)	1.558(19), 1.59(2)	1.19(3)
(B2-H49)		1.26(2)	1.32(10)	1.53(2), 1.501(19)	1.19(5)
B2-H2(H46)	0.98(5)	1.07(2)			0.85(6)
Fe-N11 (P1)	2.106(1)	2.2119(4)	2.187(2)	2.2367(8), 2.2328(7)	1.995(3)
(Fe-P2)		2.2088(4)	2.185(2)	2.2192(6), 2.2462(7)	1.998(3)
(Fe-P3)		2.1977(4)	2.181(2)	2.2264(6), 2.2374(8)	2.009(3)
B2-Fe-N11 (P1)	126.10(4)	124.24(5)	126.51(7)	124.44(9), 116.53(8)	123.54(16)
(B2-Fe-P2)		126.54(5)	122.89(7)	114.37(8), 113.32(8)	123.19(17)
(B2-Fe-P3)		124.50(5)	123.67(7)	116.41(8), 118.12(8)	127.37(16)
N11-Fe-N11	88.81(5)				
P1-Fe-P2		92.06(2)	89.96(8)	97.90(3), 105.45(3)	90.92(11)
P2-Fe-P3		89.03(2)	92.98(8)	100.77(3), 98.99(3)	90.64(11)
P3-Fe-P1		89.53(2)	90.90(8)	98.92(3), 102.18(3)	90.75(11)
B2-Fe-H3 (H47)	33.1(7)	39.9(7)	48(3)	49.7(7), 49.9(7)	32.9(10)
(B2-Fe-H48)		39.0(5)	48(3)	52.5(7), 53.6(8)	34.9(10)
(B2-Fe-H49)		41.9(6)	44(4)	52.0(8), 50.1(7)	34.5(13)
Fe-B2-H3(H47)	69(1)	57.2(8)	54(3)	52.2(8), 51.4(8)	65.9(17)
(Fe-B2-H48)		59.5(7)	46(3)	51.9(7), 50.8(7)	65.4(16)
(Fe-B2-H49)		58.7(7)	44(5)	50.4(8), 52.0(8)	68(2)
Fe-B2-H2 (H46)	180.000(3)	178.6(9)	180.00(10)	176.63(16)	167(4)
H3-B2-H2	111(1)				
(H46-B2-H47)		124(1)			106(3)
(H46-B2-H48)		121(1)			102(3)
(H46-B2-H49)		120(1)			124(5)

[a]Ref 9a [b] Ref 9b [c] Ref 7 All previously published numbers are directly from cif files. Numbering changes for each complex.