Supporting Information for:

Ferrocene- like iron bis(dicarbollide), $[3\text{-Fe}^{III}\text{-}(1,2\text{-}C_2B_9H_{11})_2]^-$. The first experimental and theoretical refinement of a paramagnetic ^{11}B NMR spectrum

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Table S1: Contraction schemes for the used basis sets, in the [primitive|contracted] notation.

def-TZVP:
C: [11s6p1d|5s3p1d]
B: [11s6p1d|5s3p1d]
H: [5s1p|3s1p]

HII:
C: [9s5p1d|5s4p1d]
B: [9s5p1d|5s4p1d]
H: [5s1p|3s1p]

HIII+d1:
C: [12s8p2d|8s7p2d]
B: [11s7p2d|7s6p2d]
H: [7s2p|5s2p]

Stuttgart ECP valence basis:
Fe: [8s7p6d|6s5p3d]

Munzarová-Kaupp NMR:
Fe: [16s12p7d|10s8p5d]

Table S2: Geometry of compound **1**, optimised at BP86/TZVP(ECP) level, in Ångstroms.
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Fe	0.00000	0.00000	0.00063
B	1.56857	1.57264	0.00575
B	1.52807	0.50535	1.43153
B	1.52680	0.51513	-1.42736
C	1.54459	-1.08479	0.81149
C	1.54396	-1.07912	-0.81803
B	3.00906	-1.51839	-0.00558
B	3.01800	-0.47853	-1.43303
B	3.01894	-0.48817	1.42896
B	3.06952	1.21475	-0.89101
B	3.07031	1.20879	0.89779
B	3.97974	-0.04475	-0.00110
H	1.11113	2.68466	0.00976
H	1.05309	0.72377	2.50688
H	1.05076	0.74052	-2.50086
H	1.10766	-1.94276	1.31917
H	1.10678	-1.93361	-1.33131
H	3.32796	-2.66671	-0.00965
H	3.42774	-0.93461	-2.45796
H	3.42997	-0.95093	2.45042
H	3.63181	2.04452	-1.54655
H	3.63354	2.03403	1.55831
H	5.17355	-0.12572	-0.00174
B	-1.56857	-1.57264	0.00588
B	-1.52809	-0.50524	1.43158
B	-1.52677	-0.51523	-1.42730
C	-1.54461	1.08484	0.81143
C	-1.54395	1.07907	-0.81809
B	-3.00906	1.51839	-0.00570
B	-3.01798	0.47842	-1.43308
B	-3.01897	0.48827	1.42891
B	-3.06950	-1.21481	-0.89093
B	-3.07033	-1.20873	0.89787
B	-3.97974	0.04475	-0.00113
H	-1.11113	-2.68466	0.00999
H	-1.05313	-0.72356	2.50695
H	-1.05071	-0.74071	-2.50078
H	-1.10768	1.94284	1.31906
H	-1.10677	1.93353	-1.33143
H	-3.32797	2.66670	-0.00987
H	-3.42770	0.93441	-2.45806
H	-3.43002	0.95112	2.45033
H	-3.63177	-2.04464	-1.54642
H	-3.63357	-2.03392	1.55844
H	-5.17355	0.12571	-0.00181

Experimental peak frequencies, widths and integrals obtained from Varian VNMR software, after applying Lorentzian deconvolution.

Table S3: Estimated linewidths in Hz based on Solomon-Bloembergen equations, similar approximations and equations used as in (Rastrelli & Bagno, *Chem. Eur. J.* 2009, **15**, 7990), ordered from closest to metal centre outward. All values at 293.15 K.

	Contact		Dipolar	Total		Total	Total
Boron #	PBE	PBE0		PBE	PBE0	Exp.[a]	Exp.[b]
8,8′	1960	4435	10	1970	4445	1396.82	693.92
4,7,4′,7′	2647	5130	12	2658	5142	1256.35	829.90
6,6′	7	40	1	8	41	214.36	195.04
5,11,5′,11′	0	3	1	1	3	161.41	195.39
9,12,9′,12′	2	0	1	2	1	141.31	187.25
10,10′	57	67	0	57	67	344.67	254.22

[a] In acetone. [b] In acetonitrile.

Table S4: Experimental linewidths in acetone, ordered by increasing frequency.

t/°C	1	2	3	4	5	6
-40	675.80	327.69	432.31	395.35	1583.55	1382.75
-30	562.20	253.91	333.98	335.70	1491.59	1238.02
-20	604.12	255.33	323.23	318.60	1825.40	1887.10
-10	376.23	174.14	219.61	254.97	1185.33	1032.43
0	450.37	176.65	215.06	253.13	1500.45	1673.13
10	279.41	140.27	165.27	215.76	982.71	909.43
20	344.67	141.31	161.41	214.36	1256.35	1396.82
30	220.04	116.81	129.29	189.29	838.74	767.81
40	272.22	118.18	127.40	188.52	1049.54	1118.48

Table S5: Peak integrals from experimental spectra measured at 20°C.

Assigned Boron #	Frequency/Hz[a]	Frequency/Hz[b]	Integral[a]	Integral[b]
8,8′	-63042.900	-61624.000	16291.53	12607.15
4,7,4′,7′	-54883.700	-53546.700	30258.44	30592.22
6,6′	-4344.770	-4235.680	15533.73	19339.95
5,11,5′,11′	-36.844	-68.930	29488.26	37045.35
9,12,9′,12′	2441.100	2303.160	28681.73	35950.71
10,10′	13784.000	13326.800	15015.14	16792.32

[a] In acetone. [b] In acetonitrile.

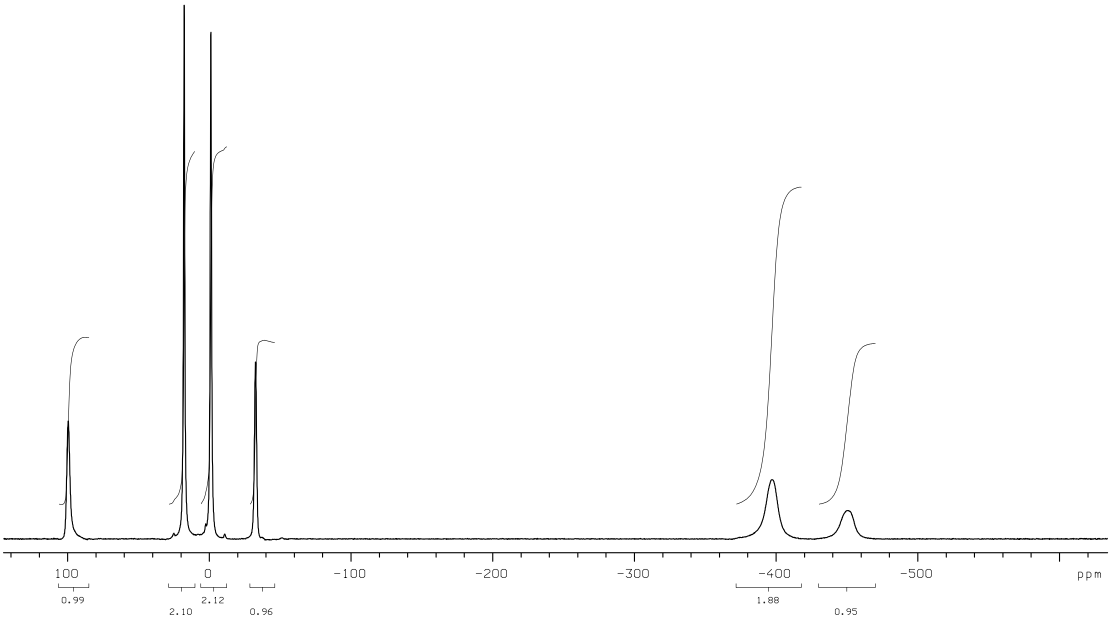

Figure S1: Experimental spectrum of compound **1** in acetone at 40°C, showing peak integrals and their values.

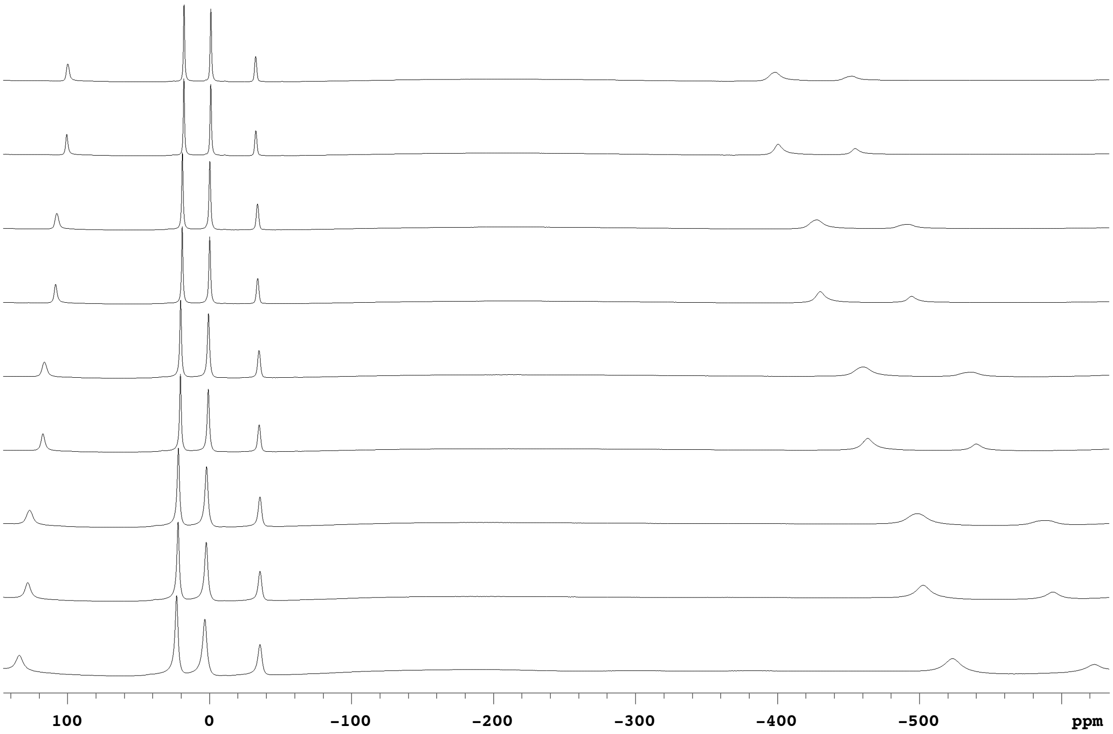

Figure S2: Experimental spectra of compound **1** in acetone, measured at temperatures of -40°C (bottom) to 40°C (top) at 10°C intervals.