Supporting Information

^{11}B Solid-State NMR Interaction Tensors of Linear Two-Coordinate Boron: The Dimesitylborinium Cation

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Table S1. Calculated ^{11}B EFG and magnetic shielding tensors for dimesitylborinium with varying C–B^{+}–C bond angles. B3LYP/6-311++G(d,p).

angle / deg	C_Q(^{11}B) / MHz	η_Q	σ_{iso} / ppm	Ω / ppm	κ
160	-5.84	0.02	8.9	123	0.97
165	-5.87	0.01	9.3	123	0.99
170	-5.89	0.00	9.8	123	1.00
175	-5.91	0.00	11.8	126	1.00
180	-5.91	0.00	12.4	127	1.00

Table S2. Calculated ^{11}B EFG and magnetic shielding tensors for diphenylborinium with varying C–B^{+}–C bond angles. B3LYP/6-311++G(d,p).

angle / deg	C_Q(^{11}B) / MHz	η_Q	σ_{iso} / ppm	Ω / ppm	κ
160	-6.04	0.01	11.4	128	0.97
165	-6.06	0.01	12.7	127	0.98
170	-6.08	0.00	13.6	126	0.99
175	-6.10	0.00	14.1	125	1.00
180	-6.10	0.00	14.3	125	1.00

Table S3. Calculated ^{11}B EFG and magnetic shielding tensors for a borininum ion (R–B^+– R) with changing side groups (R) using a bond angle of 172.1 degrees. B3LYP/6-311++G(d,p).

Side Group (R)	$C_Q(^{11}B)$ / MHz	η_Q	σ_{iso} / ppm	Ω / ppm	κ
H	-8.71	0.00	1.3	291	1.00
Methyl	-7.00	0.00	-27.8	339	0.99
Phenyl	-5.84	0.01	-2.7	147	0.98
Mesityl	-5.65	0.01	-13.6	135	0.99

Table S4. Experimental ^{11}B chemical shift tensor parameters for dimesitylborinium tetrakis(pentafluorophenyl)borate and selected other boron compounds using the Haeberlen convention.[a] See also Table 1 in the main text.

	dimesitylborinium	trimesitylborane	$[Cp^*_2B]^+$	Cp_2^*BMe
δ_{iso} / ppm	91.2	77.4	-41.3	81.9
$\Delta\delta$ / ppm	-126.75	-121.0	-72.64	-136.88
η_δ	0.08	0.00	0.02	0.20

a. In this convention, $\delta_{iso} = (1/3)(\delta_{11} + \delta_{22} + \delta_{33})$; the anisotropy $\Delta\delta = \delta_{zz} - (\delta_{xx} + \delta_{yy})/2$; the asymmetry $\eta_\delta = (\delta_{yy} - \delta_{xx})/(\delta_{zz} - \delta_{iso})$; components are ordered according to $|\delta_{zz} - \delta_{iso}| \geq |\delta_{xx} - \delta_{iso}| \geq |\delta_{yy} - \delta_{iso}|$. See U. Haeberlen, In Advances in Magnetic Resonance; Suppl. 1; J. S. Waugh, Ed.; Academic Press: New York, 1976.