^{11}B NMR chemical shift predictions via Density Functional Theory and Gauge-Including Atomic Orbital approach: Applications to structural elucidations of boron-containing molecules

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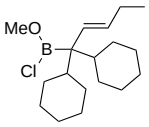
1. Development of the Linear Regression Models

1.1 Molecules included in the dataset

Table S1. The molecules and their experimental NMR chemical shifts in THF.

Molecule#	Structure	Exptl. δ (ppm)[a]
#1	BF_3 • THF	-2.8
#2	BF_3 • Pydine	-0.9
#3	BCl_3 • THF	10.2
#4	BH_3 • THF	-1.1
#5	$LiBH_4$	-42.0
#6	$LiB(NHMe)_4$	0.2
#7		30.5
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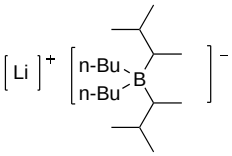
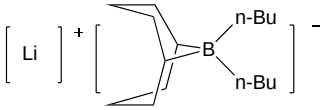
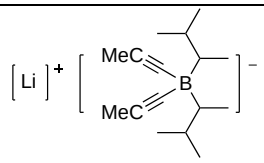
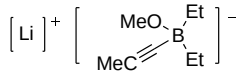
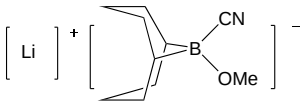
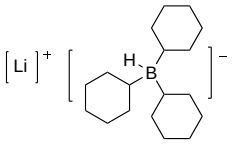
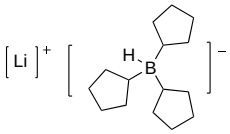
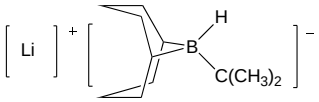
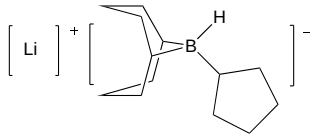
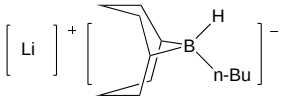
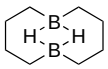
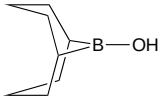
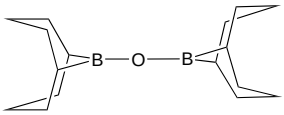
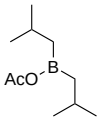
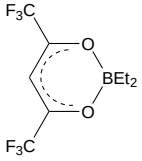
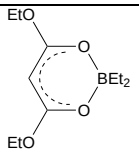
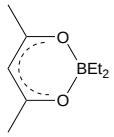
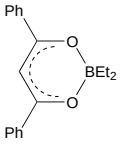
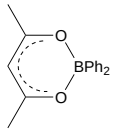
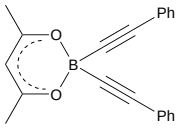
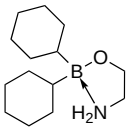
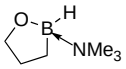
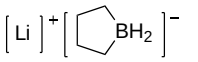
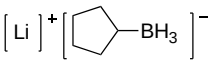
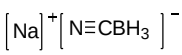
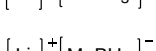
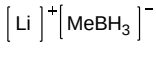
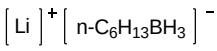
#9		-15.2
#10		-18.5

#11		-18.4
#12		-2.2
#13		-2.8
#14		-6.7
#15		-9.7
#16		-9.0
#17		-9.3
#18		-12.3
#19		28.5
#20		56.6
#21		55.2
#22		57.7
#23		20.3

#24		15.0
#25		14.2
#26		14.5
#27		10.8
#28		-1.2
#29		4.6
#30		5.7
#31		-20.2
#32		-26.3
#33		-44.2
#34		-26.0
#35		-30.9
#36		-28.1

[a]The experimental data were retrieved from the online database compiled by the Cole research group: http://www.chemistry.sdsu.edu/research/BNMR

1.2 The linear correlations between the computed isotropic shielding constants and the experimental chemical shifts

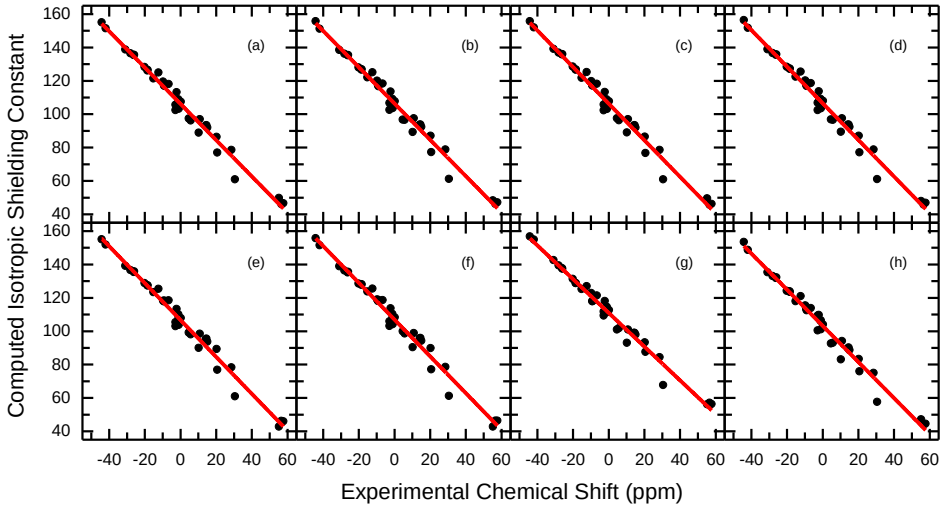


Figure S1. Linear correlation between experimental chemical shifts and calculated shielding constants in THF with the SMD solvent model for NMR calculation. a. Method 1; b. Method 2; c. Method 3; d. Method 4; e. Method 5; f. Method 6; g. Method 7; h. Method 8.

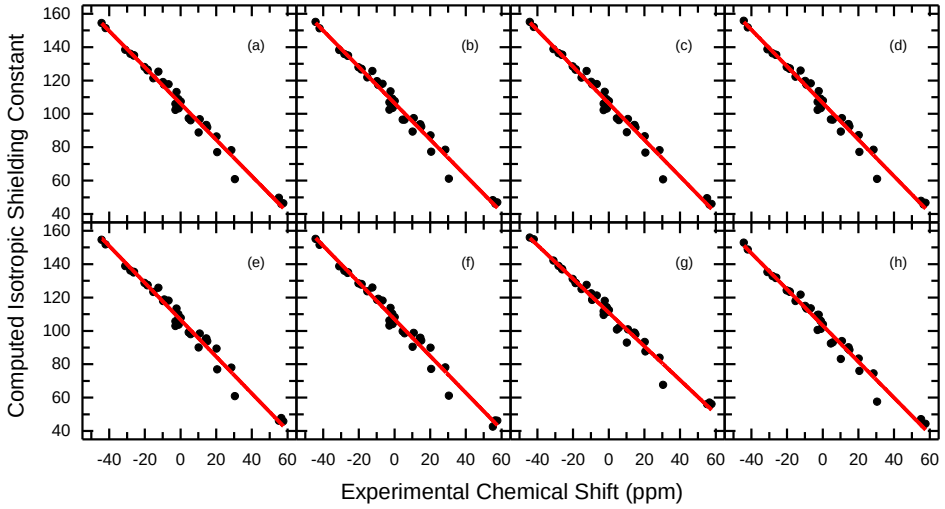


Figure S2. Linear correlation between experimental chemical shifts and calculated shielding constants in THF with the CPCM solvent model for NMR calculation. a. Method 1; b. Method 2; c. Method 3; d. Method 4; e. Method 5; f. Method 6; g. Method 7; h. Method 8.

Table S2. The adopted eight methods for calculating ^{11}B isotropic shielding constants and the fitted empirical scaling parameters (slope and intercept) in THF with both SMD and CPCM models for NMR calculation.

			Scaling Factors (SMD)		Scaling Factors (CPCM)	
	Geo. opt (in vacuo)	NMR (with the solvent model)	Slope	Intercept	Slope	Intercept
1	B3LYP/6-31+G(d,p)	mPW1PW91/6-311+G(2d,p)	-1.0869	106.19	-1.0851	106.02
2	B3LYP/6-311+G(2d,p)	mPW1PW91/6-311+G(2d,p)	-1.0877	106.40	-1.0867	106.25
3	B3LYP/6-31+G(d,p)	PBE0/6-311+G(2d,p)	-1.0959	106.32	-1.0941	106.15

4	B3LYP/6-311+G(2d,p)	PBE0/6-311+G(2d,p)	-1.0967	106.53	-1.0956	106.37
5	M062X/6-31+G(d,p)	mPW1PW91/6-311+G(2d,p)	-1.1050	106.67	-1.0903	106.65
6	M062X/6-311+G(2d,p)	mPW1PW91/6-311+G(2d,p)	-1.1014	106.94	-1.1003	106.79
7	B3LYP/cc-pvdz	B3LYP/cc-pvdz	-1.0104	110.96	-1.0078	110.79
8	B3LYP/cc-pvtz	B3LYP/cc-pvtz	-1.0824	103.20	-1.0823	103.09

1.3 Performances of the linear regression models

Table S3. The performances of the eight fitted empirical scaling factors in **Table S2**.

	Geo. Opt (in vacuo)	NMR (with the solvent model)	R^2 (SMD)[a]	RMSD (SMD)[b]	R^2 (CPCM)[c]	RMSD(CPCM)[d]
1	B3LYP/6-31+G(d,p)	mPW1PW91/6-311+G(2d,p)	0.9812	3.40	0.9813	3.39
2	B3LYP/6-311+G(2d,p)	mPW1PW91/6-311+G(2d,p)	0.9811	3.40	0.9812	3.40
3	B3LYP/6-31+G(d,p)	PBE0/6-311+G(2d,p)	0.9812	3.40	0.9813	3.39
4	B3LYP/6-311+G(2d,p)	PBE0/6-311+G(2d,p)	0.9811	3.41	0.9812	3.40
5	M062X/6-31+G(d,p)	mPW1PW91/6-311+G(2d,p)	0.9807	3.45	0.9803	3.48
6	M062X/6-311+G(2d,p)	mPW1PW91/6-311+G(2d,p)	0.9801	3.50	0.9800	3.50
7	B3LYP/cc-pvdz	B3LYP/cc-pvdz	0.9811	3.41	0.9815	3.37
8	B3LYP/cc-pvtz	B3LYP/cc-pvtz	0.9807	3.45	0.9808	3.44

[a] [c] R^2 is the coefficient of determination for the linear regression for the models with the SMD model (a) and the CPCM model (c), respectively. [b] [d] RMSD is the root mean square deviation for the predicted chemical shifts with respect to their respective experimental values (in ppm).

1.4 Detailed error analyses for the test set for Method 5 with both SMD and CPCM models

Table S4. Errors between experimental and predicted ^{11}B NMR chemical shifts (in ppm) for molecules listed in **Table S1** based on Method 5 using both SMD and CPCM solvent models.

Molecule	Exptl. δ (ppm) in THF	Calculated Isotropic [a]	Pred. δ (ppm) [b]	Pred. [b] - Exptl.	Calculated Isotropic [c]	Pred. δ (ppm) [d]	Pred. [d] - Exptl.
1	-2.8	102.95	3.36	6.16	102.86	3.48	6.28
2	-0.9	103.76	2.63	3.53	103.70	2.71	3.61
3	10.2	90.04	15.05	4.85	90.00	15.27	5.07
4	-1.1	108.14	-1.33	-0.23	107.50	-0.78	0.32
5	-42	151.85	-40.89	1.11	151.80	-41.41	0.59
6	0.2	107.91	-1.12	-1.32	107.80	-1.05	-1.25
7	30.5	60.97	41.36	10.86	60.84	42.01	11.51
8	20.6	76.84	27.00	6.40	76.86	27.32	6.72
9	-15.2	123.36	-15.11	0.09	123.22	-15.20	0.00
10	-18.5	127.41	-18.77	-0.27	127.25	-18.90	-0.40
11	-18.4	127.54	-18.89	-0.49	127.44	-19.07	-0.67
12	-2.2	113.38	-6.07	-3.87	113.26	-6.07	-3.87

13	-2.8	105.33	1.21	4.01	105.57	0.99	3.79
14	-6.7	118.53	-10.73	-4.03	118.07	-10.48	-3.78
15	-9.7	118.26	-10.49	-0.79	117.85	-10.27	-0.57
16	-9	118.29	-10.52	-1.52	118.72	-11.07	-2.07
17	-9.3	117.77	-10.05	-0.75	118.14	-10.53	-1.23
18	-12.3	125.37	-16.92	-4.62	125.74	-17.51	-5.21
19	28.5	78.29	25.68	-2.82	77.88	26.38	-2.12
20	56.6	46.25	54.68	-1.92	47.76	54.01	-2.59
21	55.2	42.83	57.77	2.57	46.09	55.54	0.34
22	57.7	45.95	54.95	-2.75	45.71	55.89	-1.81
23	20.3	89.28	15.74	-4.56	89.30	15.92	-4.38
24	15	93.77	11.68	-3.32	93.66	11.91	-3.09
25	14.2	95.13	10.44	-3.76	94.92	10.75	-3.45
26	14.5	95.56	10.06	-4.44	95.45	10.27	-4.23
27	10.8	98.45	7.44	-3.36	98.31	7.65	-3.15
28	-1.2	110.13	-3.13	-1.93	110.01	-3.08	-1.88
29	4.6	99.19	6.77	2.17	98.98	7.03	2.43
30	5.7	98.08	7.77	2.07	98.01	7.92	2.22
31	-20.2	128.86	-20.08	0.12	128.64	-20.17	0.03
32	-26.3	135.50	-26.09	0.21	134.91	-25.92	0.38
33	-44.2	155.09	-43.82	0.38	154.50	-43.88	0.32
34	-26	135.83	-26.39	-0.39	135.28	-26.26	-0.26
35	-30.9	139.18	-29.42	1.48	138.82	-29.51	1.39
36	-28.1	136.62	-27.10	1.00	136.12	-27.03	1.07
RMSDs [e]				3.45			3.48

[a]The isotropic shielding constants are calculated via Method 5 with the SMD solvent model.
[b]The scaling factors were fitted based on Method 5 (slope: -1.1050, intercept: -106.67).
[c]The isotropic shielding constants are calculated via Method 5 with the CPCM solvent model.
[d]The scaling factors were fitted based on Method 5 (slope: -1.0903, intercept: -106.65).
[e]Root-mean-square deviations.

Table S5. Errors between experimental and predicted ^{11}B NMR chemical shifts (in ppm) for molecules listed in **Table S1** based on Method 7 using both SMD and CPCM solvent models.

Molecule	Exptl. δ (ppm) in THF	Calculated Isotropic [a]	Pred. δ (ppm) [b]	Pred. [b] - Exptl.	Calculated Isotropic [c]	Pred. δ (ppm) [d]	Pred. [d] - Exptl.
1	-2.8	111.67	-0.71	2.09	111.54	-0.75	2.05
2	-0.9	111.34	-0.38	0.52	111.26	-0.46	0.44
3	10.2	93.00	17.78	7.58	92.91	17.74	7.54
4	-1.1	114.70	-3.70	-2.60	114.09	-3.27	-2.17
5	-42	154.95	-43.54	-1.54	154.74	-43.61	-1.61
6	0.2	112.60	-1.62	-1.82	112.44	-1.64	-1.84
7	30.5	67.67	42.84	12.34	67.58	42.88	12.38
8	20.6	87.64	23.08	2.48	87.60	23.01	2.41
9	-15.2	125.18	-14.07	1.13	125.01	-14.11	1.09
10	-18.5	128.77	-17.62	0.88	128.56	-17.63	0.87
11	-18.4	128.84	-17.69	0.71	128.74	-17.81	0.59
12	-2.2	118.04	-7.01	-4.81	117.93	-7.08	-4.88
13	-2.8	109.28	1.66	4.46	109.53	1.25	4.05
14	-6.7	121.37	-10.30	-3.60	121.12	-10.25	-3.55
15	-9.7	122.84	-11.75	-2.05	122.49	-11.61	-1.91
16	-9	117.89	-6.86	2.14	118.93	-8.08	0.92
17	-9.3	117.95	-6.91	2.39	118.49	-7.64	1.66
18	-12.3	126.93	-15.81	-3.51	127.46	-16.55	-4.25
19	28.5	84.40	26.29	-2.21	83.93	26.65	-1.85
20	56.6	57.13	53.28	-3.32	56.98	53.39	-3.21
21	55.2	56.20	54.20	-1.00	56.01	54.36	-0.84
22	57.7	56.38	54.01	-3.69	56.12	54.25	-3.45
23	20.3	93.27	17.51	-2.79	93.27	17.38	-2.92
24	15	97.98	12.85	-2.15	97.87	12.82	-2.18
25	14.2	98.94	11.89	-2.31	98.72	11.97	-2.23
26	14.5	99.01	11.83	-2.67	98.88	11.82	-2.68

27	10.8	100.99	9.87	-0.93	100.80	9.91	-0.89
28	-1.2	114.24	-3.25	-2.05	114.12	-3.31	-2.11
29	4.6	101.03	9.83	5.23	100.78	9.93	5.33
30	5.7	101.84	9.03	3.33	101.73	8.99	3.29
31	-20.2	131.31	-20.14	0.06	131.12	-20.17	0.03
32	-26.3	137.88	-26.64	-0.34	137.21	-26.22	0.08
33	-44.2	156.81	-45.38	-1.18	155.88	-44.74	-0.54
34	-26	137.43	-26.20	-0.20	136.71	-25.72	0.28
35	-30.9	142.62	-31.33	-0.43	142.12	-31.09	-0.19
36	-28.1	139.47	-28.22	-0.12	138.85	-27.84	0.26
RMSDs [e]				3.41			3.37

[a]The isotropic shielding constants are calculated via Method 7 with the SMD solvent model.
[b]The scaling factors were fitted based on Method 5 (slope: -1.0104, intercept: -110.96).
[c]The isotropic shielding constants are calculated via Method 7 with the CPCM solvent model.
[d]The scaling factors were fitted based on Method 5 (slope: -1.0078, intercept: -110.79).
[e]Root-mean-square deviations.

1.5 Effects of the geometries on the single point NMR calculations

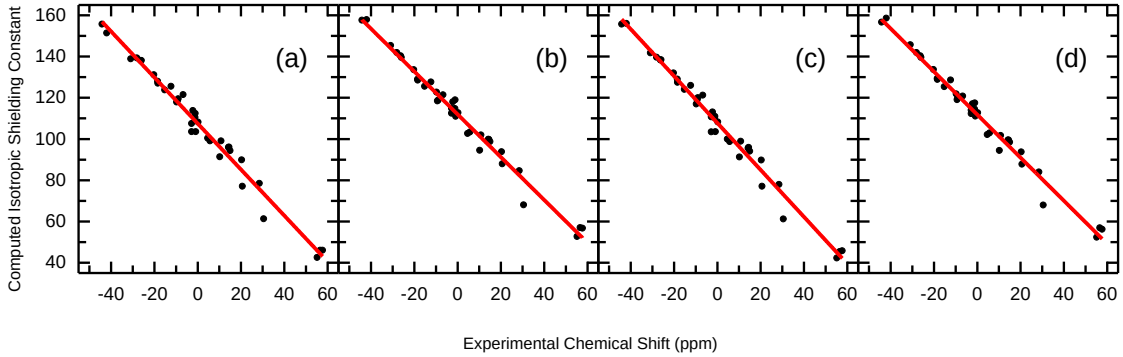


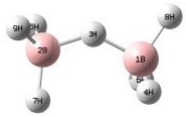
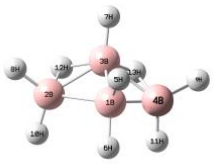
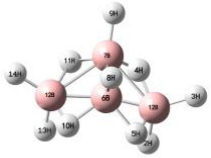
Figure S3. Linear correlation between experimental chemical shifts and calculated shielding constants in THF for a. Method 5 with the SMD solvent model in geometry optimisation step; b. Method 7 with the SMD solvent model in geometry optimisation step; c. Method 5 with the CPCM solvent model in geometry optimisation step; d. Method 7 with the CPCM solvent model in geometry optimisation step.

2. Application of the developed linear regression models

2.1 Boron-hydrogen compounds

Table S6. The boron-hydrogen compounds and their experimental NMR chemical shifts.

Compound	Structure	Exptl. δ (ppm)
BH_3		B-1 = 86 [1]

B_2H_6		B-1,2 = -16.6 [2]
$B_2H_7^-$		B-1,2 = -24.6 [3]
$B_3H_8^-$		B-1,2,3 = -30.4 [4]
$B_4H_9^-$		B-1 = -54.5 B-2,4 = -10.2 B-3 = 0.8 [5]
B_4H_{10}		B-6,7 = -6.9 B-12 = -41.8 [6]
B_5H_9		B-1 = -53.1 B-2-5 = -13.4 [7]
B_5H_{11}		B-1-5 = -55.3 [8]
B_6H_{10}		B-3-6 = 18.6 B-2 = -6.5 B-1 = -51.8 [9]

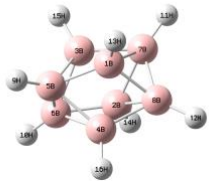
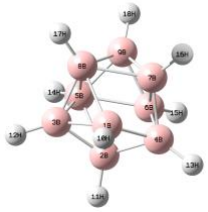
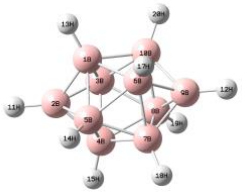
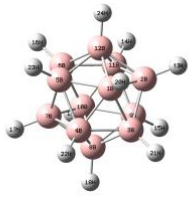
B_6H_{12}		B-1, 4 = 22.6 B-3, 6 = 7.9 [10]
$B_8H_8^{2-}$		B-1-8 = -6.8 [11]
$B_9H_9^{2-}$		B-3,4,9 = -2.9 B- 1,2,5-8 = -20.5 [12]
$B_{10}H_{10}^{2-}$		B-1,3-8,10: δ^a = -30.9 B- 2,9: δ^b = 0.9 [12]
$B_{10}H_{14}$		B-5,6 = 13.5 B-1,10 = 10.7 B-3,4,8,9 = 1.6 B-2,7= -35.2 [13]
$B_{11}H_{11}^{2-}$		B-1-11 = -16.9 [14]
$B_{12}H_{12}^{2-}$		B-1-12 = -15.6 [12]

Table S7. The differences between the predicted and experimental ^{11}B chemical shifts for boron-hydrogen compounds based on Method 5 with both the SMD and CPCM models.

	Boron-hydrogen compounds	Position	Exptl. Value (ppm)	Linear scaled. value [a] (ppm)	Scaled-Exptl. [a] (ppm)	Linear scaled. value [b] (ppm)	Scaled-Exptl. [b] (ppm)
1	BH_3	B-1	86.0	84.22	-1.78	85.34	-0.66
2	B_2H_6	B-1,2	16.6	17.84	1.24	18.06	1.46
3	$B_2H_7^-$	B-1,2	-24.6	-24.51	0.09	-24.86	-0.26
4	$B_3H_8^-$	B-1,2,3	-30.4	-10.92, -43.05	3.41 [c,γ]	-11.08, -43.65	3.03 [γ]
5	$B_4H_9^-$	B-1	-54.5	-54.41	0.09	-55.16	-0.66
		B-2,4	-10.2	-11.65	-1.45	-11.83	-1.63
		B-3	0.8	0.06	-0.74	0.05	-0.75
6	B_4H_{10}	B-6,7	-6.9	-6.85	0.05	-6.97	-0.07
		B-12	-41.8	-40.18	1.62	-40.74	1.06
7	B_5H_9	B-1	-13.4	-14.17	-0.77	-14.38	-0.98
		B-2-5	-53.1	-50.65	2.45	-51.35	1.75
8	B_5H_{11}	B-1-5	-55.3	-51.38	3.92	-52.09	3.21
9	B_6H_{10}	B-3-6	18.6	14.77	-3.83	14.95	-3.65
		B-2	-6.5	-8.23	-1.73	-8.36	-1.86
		B-1	-51.8	-48.95	2.85	-49.63	2.17
10	B_6H_{12}	B-1,4	22.6	22.56	-0.04	22.85	0.25
		B-3,6	7.9	11.04	3.14	11.17	3.27
11	$B_8H_8^{2-}$	B-1-8	-6.8	-1.55	5.25	-1.59	5.21
12	$B_9H_9^{2-}$	B-3,4,9	-2.9	-3.60	-0.70	-3.67	-0.77
		B-1,2,5-8	-20.5	-21.98	-1.48	-22.30	-1.80
13	$B_{10}H_{10}^{2-}$	B-1,3-8,10	-30.9	-28.38	2.52	-28.78	2.12
		B-2,9	0.9	-2.47	-3.37	-2.52	-3.42
14	$B_{10}H_{14}$	B-5,6	13.5	12.66	-0.84	12.81	-0.69
		B-1,10	10.7	8.18	-2.52	8.27	-2.43
		B-3,4,8,9	1.6	0.65	-0.95	0.64	-0.96
		B-2,7	-35.2	-33.14	2.06	-33.60	1.60
15	$B_{11}H_{11}^{2-}$	B-1-11	-16.9	-17.10	-0.20	-17.35	-0.45
16	$B_{12}H_{12}^{2-}$	B-1-12	-15.6	-13.82	1.78	-14.03	1.57

[a] [b] The predicted chemical shifts by Method 5 with scaling factors of SMD and CPCM sets, respectively.
[c] For $B_3H_8^-$ we got two different chemical shifts for boron atoms, and use the averaged value to compare with exptl. value.

Table S8. The differences between the predicted and experimental ^{11}B chemical shifts for boron-hydrogen compounds based on Method 7 with both the SMD and CPCM sets.

	Boron-hydrogen compounds	Position	Exptl. Value (ppm)	Linear scaled. value [a] (ppm)	Scaled-Exptl. [a] (ppm)	Linear scaled. value [b] (ppm)	Scaled-Exptl. [b] (ppm)
1	BH_3	B-1	86.0	83.16	-2.84	83.20	-2.80
2	B_2H_6	B-1,2	16.6	15.98	-0.62	15.85	-0.75
3	$B_2H_7^-$	B-1,2	-24.6	-23.48	1.12	-23.71	0.89
4	$B_3H_8^-$	B-1,2,3	-30.4	-11.34, -44.97	2.24 [γ,c]	-11.54, -45.25	2.00 [γ]
5	$B_4H_9^-$	B-1	-54.5	-56.46	-1.96	-56.77	-2.27
		B-2,4	-10.2	-12.72	-2.52	-12.92	-2.72
		B-3	0.8	-1.41	-2.21	-1.58	-2.38
6	B_4H_{10}	B-6,7	-6.9	-7.51	-0.61	-7.70	-0.80
		B-12	-41.8	-42.75	-0.95	-43.03	-1.23
7	B_5H_9	B-1	-13.4	-15.47	-2.07	-15.68	-2.28
		B-2-5	-53.1	-55.75	-2.65	-56.06	-2.96
8	B_5H_{11}	B-1-5	-55.3	-53.43	1.87	-53.74	1.56
9	B_6H_{10}	B-3-6	18.6	14.98	-3.62	14.85	-3.75
		B-2	-6.5	-11.13	-4.63	-11.33	-4.83
		B-1	-51.8	-51.64	0.16	-51.94	-0.14
10	B_6H_{12}	B-1,4	22.6	20.43	-2.17	20.32	-2.28
		B-3,6	7.9	10.15	2.25	10.01	2.11
11	$B_8H_8^{2-}$	B-1-8	-6.8	-3.60	3.20	-3.78	3.02
12	$B_9H_9^{2-}$	B-3,4,9	-2.9	-6.40	-3.50	-6.59	-3.69
		B-1,2,5-8	-20.5	-22.22	-1.72	-22.45	-1.95

13	$B_{10}H_{10}^{2-}$	B-1,3-8,10	-30.9	-28.85	2.05	-29.10	1.80
		B-2,9	0.9	-3.18	-4.08	-3.36	-4.26
14	$B_{10}H_{14}$	B-5,6	13.5	12.20	-1.30	12.06	-1.44
		B-1,10	10.7	7.62	-3.08	7.47	-3.23
		B-3,4,8,9	1.6	0.42	-1.18	0.25	-1.35
		B-2,7	-35.2	-34.95	0.25	-35.21	-0.01
15	$B_{11}H_{11}^{2-}$	B-1-11	-16.9	-17.63	-0.73	-17.85	-0.95
16	$B_{12}H_{12}^{2-}$	B-1-12	-15.6	-14.62	0.98	-14.83	0.77

[a] [b]The predicted chemical shifts by Method 7 with scaling factors of SMD and CPCM sets, respectively.
[c] For $B_3H_8^-$, we got two different chemical shifts for boron atoms, and use the averaged value to compare with exptl. value.

2.2 Other Boron containing compounds

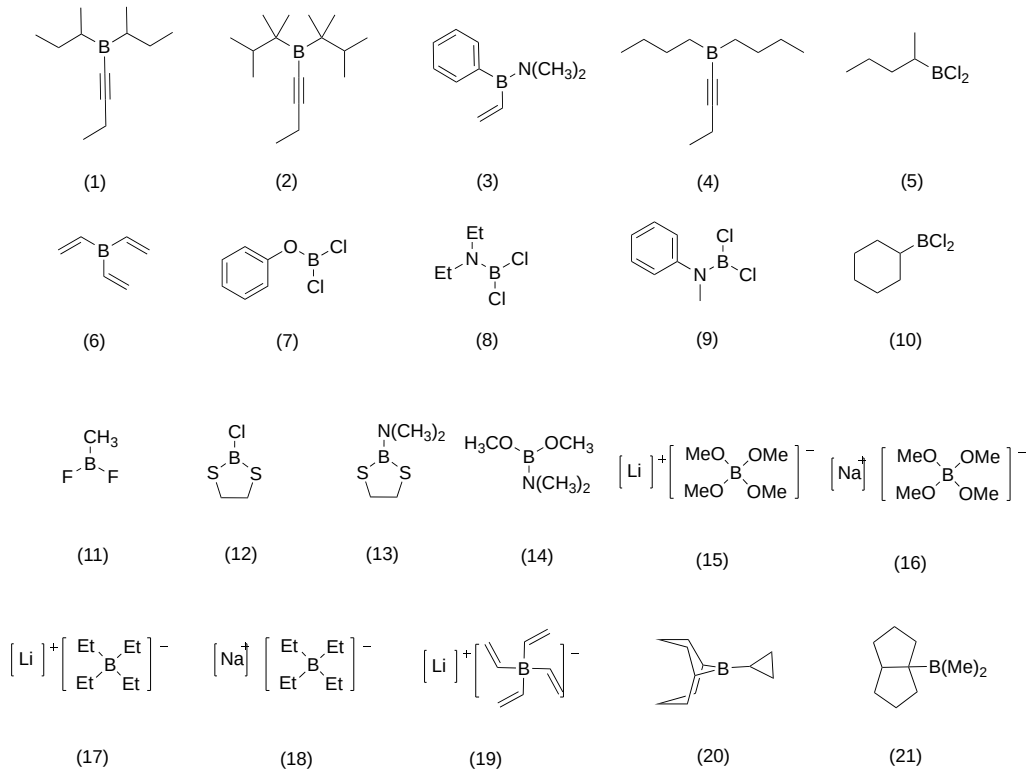


Figure S4. Other boron containing molecules. The experimental data were retrieved from the online database compiled by the Cole research group: http://www.chemistry.sdsu.edu/research/BNMR

Table S9. The differences between the predicted and experimental ^{11}B chemical shifts for boron containing molecules listed in Figure S4 based on Method 5 with both the SMD and CPCM sets.

	Exptl.	Exptl. Value (ppm)	Linear scaled. value [a] (ppm)	Scaled-Exptl. [a] (ppm)	Linear scaled. value [b] (ppm)	Scaled-Exptl. [b] (ppm)
1	in THF	72.2	67.32	-4.88	68.22	-3.98
2	in THF	81.1	76.99	-4.11	78.67	-2.43
3	neat	40.0	37.88	-2.12	38.38	-1.62
4	neat	72.0	66.94	-5.06	67.82	-4.18
5	neat	65.3	61.98	-3.32	62.80	-2.50
6	neat	55.2	51.21	-3.99	51.88	-3.32
7	neat	33.0	32.72	-0.28	33.14	0.14
8	neat	31.6	31.76	0.16	32.17	0.57
9	neat	30.8	32.31	1.51	32.73	1.93
10	neat	67.6	61.37	-6.23	62.18	-5.42
11	in $CHCl_3$	28.1	30.43	2.33	30.85	2.75
12	neat	62.7	59.53	-3.17	60.32	-2.38
13	neat	45.3	43.30	-2.00	43.86	-1.44
14	neat	21.3	21.10	-0.20	21.37	0.07
15	in CH_3OH	21.3	3.51	0.51	3.52	0.52
16	in CH_3OH	3.0	3.07	0.37	3.11	0.41
17	in Et_2O	2.7	-17.29	0.21	-17.41	0.09
18	in Et_2O	-17.5	-18.08	-1.48	-18.25	-1.65
19	in Et_2O	-16.6	-12.91	3.19	-13.19	2.91
20	in THF	-16.1	79.37	-4.63	80.59	-3.41
21	in THF	84.0	80.70	-1.60	82.17	-0.13

[a] [b]The predicted chemical shifts by Method 5 with scaling factors of SMD and CPCM sets, respectively. [c]THF was applied as the solvent for NMR calculations for molecules: 1, 2, 20 and 21; CH_3OH was applied as the solvent for NMR calculations for molecules: 11, 15 and 16; ET_2O was applied as the solvent for NMR calculations for molecules: 17, 18 and 19; NMR calculations for molecules: 3-10, 12-14 were conducted *in vacuo.*

Table S10. The differences between the predicted and experimental ^{11}B chemical shifts for boron containing molecules listed in Figure S4 based on Method 7 with both the SMD and CPCM models.

	Exptl.	Exptl. Value (ppm)	Linear scaled. value [a] (ppm)	Scaled-Exptl. [a] (ppm)	Linear scaled. value [b] (ppm)	Scaled-Exptl. [b] (ppm)
1	in THF	72.2	67.89	-4.31	67.94	-4.26
2	in THF	81.1	81.02	-0.08	81.83	0.73
3	neat	40.0	38.83	-1.17	38.76	-1.24
4	neat	72.0	66.90	-5.10	66.90	-5.10
5	neat	65.3	64.78	-0.52	64.77	-0.53
6	neat	55.2	51.06	-4.14	51.02	-4.18
7	neat	33.0	31.82	-1.18	31.74	-1.26
8	neat	31.6	33.38	1.78	33.29	1.69
9	neat	30.8	32.69	1.89	32.60	1.80
10	neat	67.6	64.30	-3.30	64.30	-3.30
11	in $CHCl_3$	28.1	25.27	-2.83	25.16	-2.94
12	neat	62.7	62.98	0.28	62.97	0.27
13	neat	45.3	45.44	0.14	45.39	0.09
14	neat	21.3	17.71	-3.59	17.59	-3.71
15	in CH_3OH	21.3	1.23	-1.77	1.06	-1.94
16	in CH_3OH	3.0	0.86	-1.84	0.72	-1.98
17	in Et_2O	2.7	-17.03	0.47	-17.07	0.43
18	in Et_2O	-17.5	-17.92	-1.32	-18.10	-1.50
19	in Et_2O	-16.6	-12.52	3.58	-12.79	3.31
20	in THF	-16.1	80.94	-3.06	81.29	-2.71
21	in THF	84.0	77.75	-4.55	78.24	-4.06

[a] [b]The predicted chemical shifts by Method 7 with scaling factors of SMD and CPCM sets, respectively.

[c]THF was applied as the solvent for NMR calculations for molecules: 1, 2, 20 and 21; CH_3OH was applied as the solvent for NMR calculations for molecules: 11, 15 and 16; ET_2O was applied as the solvent for NMR calculations for molecules: 17, 18 and 19; NMR calculations for molecules: 3-10, 12-14 were conducted *in vacuo*.

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