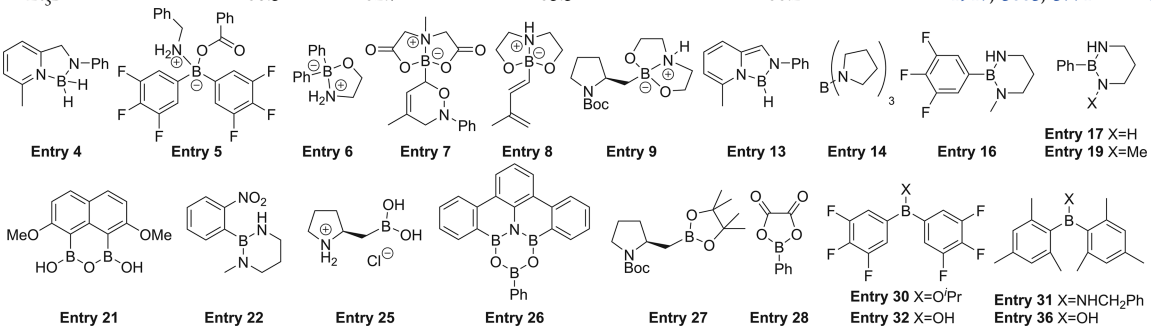
Table 1. Observed and Calculated ^{11}B NMR Shifts for a Range of Boron Compounds[†]

entry	structure	δ_{obs}	δ_{calcd} ωB97XD/ aug-cc-pvDZ	δ_{calcd} B3LYP+GD3BJ/ aug-cc-pvDZ	δ_{calcd} ωB97XD/ aug-pcSseg-1	calcd DOI	expt DOI[‡]
1[a]	$(THF)_3LiBH_4$	−41.8[17]	−43.8	−45.5	−49.0	1929, 3675, 3825	cr7n3h
2[a]	H_3BNH_3	−22[18]	−24.7	−23.7	−27.1	3894, 3895, 3896	ck62
3	H_3BNEt_3	−14[19]	−17.4	−18.3	−19.0	3817, 3715, 3775	cs4tcg
4[c]	see structure below	−2.6[20]	−5.6	−2.0	−8.5	3733, 3740, 3867	f88f6n
5	see structure below	2[6]	−1.5	−1.3	−3.4	1884, 3700, 3849	chxq
6	see structure below	6.4[33]	4.5	5.5	3.3	753, 3698, 3847	cmm8
7[b]	see structure below	10.1[21]	9.1	9.5	8.1	3741, 3704, 3928	f7j7tt
8	see structure below	10.7[21]	8.3	9.0	7.6	3920, 3706, 3846	ckzz
9	see structure below	12.4[33]	10.9	12.1	11.3	940, 3689, 3818	cmm9
10	$B(OCH_2CF_3)_3$	17[22]	15.7 (16.5)	15.2	17.4	1617, 3708, 3816	ckz2
11	$B(OPh)_3$	16.4	14.6	14.2	15.7	3877, 3893, 3898	ck94
12	$B(OMe)_3$	19*	17.1	16.7	19.2	1616, 3714, 3815	ckz7
13[c]	see structure below	19.7[20]	17.3	19.6	17.2	3735, 3739, 3866	f88f6n
14	see structure below	24*	21.8	21.3	21.7	1619, 3692, 3814	ckz8
15	$B(NMe_2)_3$	27*	26.5	26.0	26.7	1618, 3693, 3776	ckz9
16	see structure below	28.3[33]	26.7	26.9	31.0	755, 3755, 3793	cmnb
17	see structure below	28.4[33]	26.7	26.1	26.7	824, 3754, 3860	dvfzcf
18[d]	DanB-BPin	28.5[23] 25.2[23]	29.9 26.5	29.5 26.4	31.2 26.0	3073, 3921, 3929	f2p9wj
19[c]	see structure below	28.9[24]	27.5	27.1	27.6	3930, 3931, 3932	bz2sz8
20	CatBH	29*	26.8	25.9	29.2	3879, 3878, 3880	f2d8f8
21	see structure below	29.1[§]	27	26.8	27.2	3732, 3707, 3865	cmnc
22	see structure below	29.8[33]	29.1	28.7	28.7	757, 3872, 3873	cmnd
23	B_2Pin_2	30.1*	28.2	28.0	29.7	3069, 3709, 3863	ck2b
24[e]	B_2Cat_2	30.7[25]	28.5	28.0	30.2	3068, 3712, 3862	d6v9wb
25[f]	see structure below	30.7[26]	29.2	29.3	31.2	3936, 3935, 3934	fxfs7h
26[a]	see structure below	30.9[27] 28.7[27]	30.6 28.6	30.2 28.2	30.2 28.1	3826, 3876, 3864	f98mz3
27	see structure below	33[33]	31.0	30.9	32.5	1876, 3699, 3820	cmnf
28	see structure below	36[28]	34.4	34.4	35.2	3176, 3687, 3868	ckz4
29[e]	BBr_3	40.5[29]	63.3	68.5	71.3	3066, 3685, 3812	ckz5
30	see structure below	42.2[33]	40.2	40.3	41.3	942, 3691, 3819	cmng
31	see structure below	43.2[30]	44.5	44.1	45.1	949, 3701, 3850	b3h65j
32	see structure below	43.5[33]	41.2	41.7	42.8	943, 3690, 3778	cmnh
33	Ph_2BO^iPr	44.8[33]	43.0	43.1	43.8	934, 3696, 3794	d6bsbf
34	Ph_2BOH	45.7[33]	43.4	43.8	45.0	719, 3695, 3777	cmn2
35[g]	BCl_3	46.4[31]	48.6	49.2	52.7	3067, 3697, 3798	cppdj4
36	see structure below	50.2[32]	47.8	49.0	50.1	939, 3694, 3813	ckz6
37	Et_3B	86.5[7c]	82.7	85.5	88.2	1917, 3663, 3771	ck95



[†]Abbreviations: Pin = Pinacolato; Dan = naphthalene-1,8-diaminato; Cat = Catecholato. Data obtained in $CDCl_3$ unless otherwise stated. [a]THF. [b]Acetone. [c]Benzene. [d]MeOH. [e]CH_2Cl_2. [f]D_2O. [g]PhMe. *NMR spectrum collected in this work using a commercial sample. [§]Novel compound, see Experimental Section for details. FAIR data for these calculations referenced against BF_3·OEt_2 are available[16] with individual entries resolved as, e.g., https://doi.org/10.14469/hpc/1929. [‡]Short DOI resolved as, e.g., https://doi.org/cr7n3h.

the relatively recent double-ζ aug-pcSseg-1 basis,[14] which is both modestly larger than aug-cc-pVDZ in terms of basis functions, and computationally 2−3 times slower for the overall calculation. It is recognized that ^{1}H NMR shieldings are sensitive to the Boltzmann conformer populations and we also evaluated this sensitivity of ^{11}B shifts for one system where they might be expected to be maximal. To facilitate this, preliminary minimization of conformer geometries was undertaken using

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