Base Promoted Ammonia Borane Hydrogen Release

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Supporting Information

Figure 1S. Toepler pump apparatus used for some H₂-release measurements.

Figure 2S. DFT optimized geometries (B3LYP/6-31G(d)) and GIAO calculated (B3LYP/6-311G(d)) ^{11}B NMR chemical shifts. The shifts for the corresponding neutral species were previously reported in: Bluhm, M. E.; Bradley, M. G.; Butterick III, R.; Kusari, U.; Sneddon, L. G. *J. Am. Chem. Soc.* **2006**, *128*, 7748-7749

Tables of Cartesian Coordinates for DFT Optimized Geometries (B3LYP/6-31G(d)).

Cartesian Coordinates for NH_2BH_3 (A)

	X	Y	Z
N	-0.773299	-0.000000	-0.134999
B	0.791599	-0.000000	0.012799
H	-1.135099	-0.804499	0.381400
H	-1.135099	0.804499	0.381400
H	1.259600	1.009599	-0.542400
H	1.259600	-1.009500	-0.542600
H	1.206199	-0.000100	1.203099

Cartesian Coordinates for straight chain $\text{NH}_2\text{BH}_2\text{NH}_2\text{BH}_2\text{NH}_2\text{BH}_2\text{NH}_2\text{BH}_3$ (B)

	X	Y	Z
N	1.959700	0.758999	1.187400
B	2.540399	0.412200	-0.198300
N	1.293600	-0.033100	-1.148400
B	0.438000	-1.324199	-0.793400
N	-0.208900	-1.079400	0.647899
B	-1.770800	-0.859699	0.824700
N	-2.317500	0.158000	-0.263600
B	-1.968999	1.736400	-0.269600
H	2.621800	0.566400	1.930099
H	1.690000	1.733499	1.274600
H	3.295600	-0.544500	-0.124400
H	3.079500	1.353000	-0.788600
H	1.666900	-0.159100	-2.085399

H	0.660999	0.766799	-1.215500
H	1.179299	-2.286599	-0.761700
H	-0.431200	-1.475000	-1.641799
H	0.363400	-0.328299	1.081500
H	0.006900	-1.898000	1.208599
H	-2.009999	-0.428400	1.935800
H	-2.320700	-1.938300	0.636300
H	-3.330500	0.091499	-0.210599
H	-2.079099	-0.229699	-1.175400
H	-2.334400	2.210500	0.790599
H	-2.574799	2.233699	-1.213899
H	-0.765400	1.877400	-0.419700

Cartesian Coordinates for branched chain $\text{NH}_2\text{BH}_2\text{NH}_2\text{BH}(\text{NH}_2\text{BH}_3)_2$ (C)

	X	Y	Z
N	0.936900	-1.183599	0.363600
N	-3.477799	0.052300	-0.022599
B	-2.135199	-0.649400	0.192800
N	-0.967499	0.439900	-0.199000
B	0.448600	-0.075100	-0.630100
N	1.511099	1.101200	-0.554800
B	1.424499	2.188700	0.643000
B	2.350199	-1.921000	0.066400
H	0.204500	-1.889200	0.394999
H	0.967599	-0.795899	1.306100
H	-3.907000	0.364899	0.842100
H	-4.148900	-0.556700	-0.475500
H	-1.892199	-0.982400	1.350600
H	-1.999500	-1.589500	-0.576400
H	-0.870600	1.111000	0.562499
H	-1.391400	0.972999	-0.955799
H	0.388799	-0.524300	-1.750799
H	1.519300	1.602100	-1.438399
H	2.418199	0.634999	-0.505100
H	0.455499	2.902500	0.431400
H	1.299700	1.582000	1.695699
H	2.453100	2.843799	0.631900
H	2.261599	-2.477400	-1.011600
H	3.231400	-1.069400	0.053500
H	2.550500	-2.713099	0.974099

Cartesian Coordinates for branched chain $\text{NH}_2\text{BH}_2\text{NH}(\text{BH}_2\text{NH}_3)\text{BH}_2\text{NH}_2\text{BH}_3$ (D)

	X	Y	Z
B	0.952800	1.127599	-0.632599
B	-3.608900	-0.082999	-0.197800
N	-2.090899	0.391100	0.108600
B	-0.943000	-0.681100	0.233600
N	0.470500	0.036699	0.461900
B	1.593199	-0.997600	0.780699
N	1.653900	-1.898799	-0.575000
N	1.751000	2.201099	0.111999
H	-0.009499	1.651199	-1.183400
H	-4.299799	0.933600	-0.234500
H	-3.970399	-0.817499	0.707500
H	-3.621200	-0.655200	-1.274800
H	-1.807799	1.056199	-0.608300
H	-2.124200	0.935900	0.968200
H	-0.910399	-1.311300	-0.815700
H	-1.180600	-1.407399	1.179100
H	0.390799	0.606400	1.304599
H	1.332799	-1.745900	1.699600
H	2.697300	-0.496499	0.891300
H	0.750399	-2.344899	-0.726400
H	1.785399	-1.215200	-1.331499
H	2.398799	-2.585799	-0.574399
H	1.818200	3.047100	-0.444999
H	2.704399	1.902899	0.300900
H	1.584100	0.505399	-1.529600

Cartesian Coordinates for $\text{Et}_3\text{BNH}_2\text{BH}_3^-$

	X	Y	Z
H	2.898393	0.064802	-1.374654
H	3.374397	-1.870369	-1.058731
H	3.290745	-0.598384	0.498209
H	0.979668	-1.751368	-1.252881
H	1.254571	-2.016425	0.307674
B	2.818632	-0.871854	-0.595970
B	-0.024587	-0.301398	-0.025209
N	1.257141	-1.272733	-0.393218
C	-1.248822	-1.414974	0.182725
H	-0.913282	-2.166525	0.924831
H	-1.386741	-1.992316	-0.752259
C	0.267263	0.495040	1.385183
H	0.604829	-0.228949	2.150129
H	-0.689964	0.880711	1.778684
C	-0.219236	0.678012	-1.336068
H	0.740499	1.175473	-1.540536

H	-0.413257	0.065351	-2.237708
C	-2.636932	-0.933171	0.639745
H	-3.113391	-0.288521	-0.109021
H	-3.334342	-1.765121	0.833144
H	-2.571604	-0.348085	1.566375
C	1.267229	1.665540	1.362140
H	1.395657	2.131444	2.353965
H	2.250996	1.333497	1.017624
H	0.937041	2.458782	0.677612
C	-1.308357	1.763716	-1.266141
H	-1.292437	2.438136	-2.138278
H	-2.317952	1.335748	-1.217677
H	-1.190909	2.392540	-0.373580

Cartesian Coordinates for Et₃BNH₂BH₂NH₂BH₃⁻ (Figure 17)

	X	Y	Z
H	-1.973376	1.031556	0.884937
H	-2.201170	0.815859	-1.126664
H	-0.820510	-1.339560	0.655743
H	-0.852136	-1.250299	-0.957451
B	-2.066478	0.275274	-0.052926
B	0.836476	-0.192348	-0.092427
N	-0.768299	-0.670796	-0.118477
C	1.605095	-1.636615	-0.386310
H	1.200371	-2.068877	-1.323103
H	1.334269	-2.370456	0.397727
C	1.108688	0.872984	-1.310904
H	0.702173	0.466378	-2.255249
H	2.197316	0.926333	-1.485537
C	1.069508	0.408922	1.420464
H	0.321383	1.193611	1.605925
H	0.850119	-0.370906	2.175262
C	3.137576	-1.647815	-0.521249
H	3.631333	-1.364183	0.415665
H	3.529675	-2.638214	-0.802335
H	3.476580	-0.938600	-1.287172
C	0.592853	2.314007	-1.146182
H	0.839618	2.949048	-2.012247
H	-0.493703	2.336795	-1.019284
H	1.029156	2.795498	-0.260936
C	2.454242	0.997297	1.747594
H	2.482709	1.479006	2.737705
H	3.241083	0.232662	1.745465
H	2.750655	1.756872	1.012585
H	-3.347816	-1.408267	-0.518157
H	-3.215754	-1.163142	1.079698

H	-5.045222	0.442455	-0.884607
H	-5.589647	-0.981050	0.446384
H	-4.870481	0.792194	1.104587
N	-3.326438	-0.671772	0.190345
B	-4.834247	-0.038808	0.214854

Complete reference 36:

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