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	-1.00232	0.07462	-0.31999
B	0.37161	-0.07459	0.31998
H	-1.07957	1.06076	-0.83002
H	-1.1637	-0.73367	-1.06781
H	0.44885	-1.06076	0.83002
H	0.53294	0.73372	1.0678
H	1.1637	-0.00642	-0.45888

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	4.83915	-7.08363	0.55536
B	4.04723	-5.81867	0.63796
N	4.71739	-4.68092	-0.11815
B	6.12183	-4.15855	-0.38453
N	7.14514	-5.25359	-0.64623
B	7.81478	-5.80583	-1.89592
N	6.86838	-5.91175	-3.08408
B	5.56174	-6.62455	-3.40064
H	4.64891	-7.68727	1.35354
H	4.57285	-7.62573	-0.26468
H	3.93492	-5.43606	1.93205
H	2.79937	-6.02348	0.14485
H	4.55264	-3.99248	0.66638

H	3.98298	-4.06692	-0.57237
H	6.53447	-3.46904	0.70359
H	6.10324	-3.33483	-1.46369
H	7.48761	-5.71844	0.24269
H	7.96047	-4.62539	-0.40746
H	8.29278	-7.05189	-1.65743
H	8.85169	-5.00237	-2.23194
H	7.48213	-6.6109	-3.58306
H	7.22845	-5.29785	-3.86726
H	4.93762	-6.97826	-2.24771
H	5.87102	-7.73391	-4.10912
H	4.74944	-5.83549	-4.1489

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	8.11989	-2.98745	-1.45092
N	5.13131	-4.15499	1.49617
B	5.48785	-3.50977	0.19668
N	6.25317	-4.47744	-0.69122
B	7.71521	-4.41609	-1.1107
N	7.97359	-5.37588	-2.26415
B	7.14003	-5.7923	-3.46474
B	9.46991	-2.38674	-1.80517
H	8.16679	-2.72851	-0.42805
H	7.30721	-2.31198	-1.38275
H	4.12383	-4.13382	1.64686
H	5.53275	-3.64545	2.28175
H	4.34154	-3.07764	-0.39389
H	6.29275	-2.44075	0.42327
H	5.71618	-5.34468	-0.98084
H	6.48	-5.13285	0.10497
H	8.46838	-4.7865	-0.04457
H	8.9412	-5.79457	-2.15198
H	8.5512	-4.67519	-2.79922
H	5.88131	-6.14199	-3.08736
H	7.07778	-4.72484	-4.29295
H	7.74295	-6.82482	-4.10384
H	10.0935	-2.00539	-0.66698
H	10.20506	-3.33411	-2.44471
H	9.31824	-1.30176	-2.60595

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	8.119890	-2.987450	-1.450920
B	5.131310	-4.154990	1.496170
N	5.487850	-3.509770	0.196680

B	6.253170	-4.477440	-0.691220
N	7.715210	-4.416090	-1.110700
B	7.973590	-5.375880	-2.264150
N	7.140030	-5.792300	-3.464740
N	9.469910	-2.386740	-1.805170
H	8.166790	-2.728510	-0.428050
H	7.307210	-2.311980	-1.382750
H	4.123830	-4.133820	1.646860
H	5.532750	-3.645450	2.281750
H	4.659060	-4.902540	1.072160
H	4.341540	-3.077640	-0.393890
H	6.292750	-2.440750	0.423270
H	5.716180	-5.344680	-0.980840
H	6.480000	-5.132850	0.104970
H	8.468380	-4.786500	-0.044570
H	8.941200	-5.794570	-2.151980
H	8.551200	-4.675190	-2.799220
H	5.881310	-6.141990	-3.087360
H	7.077780	-4.724840	-4.292950
H	7.742950	-6.824820	-4.103840
H	10.093500	-2.005390	-0.666980
H	9.318240	-1.301760	-2.605950

Cartesian Coordinates for Et₃BNH₂BH₃⁻

	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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