Stability of η^2-H_2 borane complexes – a theoretical investigation

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Cartesian coordinates:

Geometries for **BH_2R** on the basis of ωB97xD/aug-cc-pVTZ:

R = H: Energy: -26.6085243

B	0.000000	0.000016	0.000000
H	-0.577480	-1.042136	0.000000
H	1.191262	0.020871	0.000000
H	-0.613782	1.021183	0.000000

R = F: Energy: -125.9403003

F	-0.012709	0.979913	0.177093
B	0.005903	1.657858	1.309584
H	0.093637	2.848135	1.246676
H	-0.066073	1.041325	2.330915

R = Cl: Energy: -486.2873196

Cl	-0.017466	0.817440	-0.094358
B	0.007692	1.712844	1.401477
H	0.094922	2.895506	1.343858
H	-0.063388	1.104534	2.418593

R = OH: Energy: -101.918348

O	-0.027873	0.953368	0.103271
B	0.003964	1.664447	1.251513
H	0.092892	2.860319	1.225446
H	-0.060145	1.046990	2.271254
H	0.026317	1.493237	-0.685470

R = SH: Energy: -424.872246

S	-0.046306	0.672784	-0.036299
B	0.005000	1.701163	1.409024
H	0.091411	2.882165	1.319027
H	-0.051942	1.138175	2.454344
H	0.036991	1.624073	-0.980082

R = NH_2: Energy: -82.0470692

N	-0.017934	0.939822	0.109466
B	0.004476	1.652653	1.300763
H	0.080705	2.844285	1.260641
H	-0.053071	1.055131	2.333749
H	0.027015	1.377348	-0.793316
H	-0.080586	-0.061657	0.069734

R = PH_2: Energy: -368.590903

B	1.302016	0.000001	0.050532
H	1.892618	1.033524	0.023009
H	1.892617	-1.033522	0.023012
P	-0.555675	0.000001	-0.111360
H	-0.980385	1.081049	0.684717
H	-0.980386	-1.081042	0.684723

R = $P(O)H_2$: Energy: -443.81499

B	1.659517	0.390046	-0.000057
P	-0.134032	-0.335108	0.000023
H	1.861831	1.559057	0.000269
H	2.547657	-0.404350	-0.000284
H	-0.045880	-1.264134	-1.075898
H	-0.045694	-1.263760	1.076273
O	-1.325627	0.556196	-0.000053

R = AsH_2: Energy: -2263.204140

B	-1.642716	0.000000	0.049984
H	-2.234751	-1.032155	0.009466
H	-2.234752	1.032154	0.009465
As	0.345624	0.000000	-0.062162
H	0.653243	-1.134223	0.886394
H	0.653243	1.134224	0.886392

R = CH_3: Energy: -65.945486

B	-0.017900	0.871226	0.000000
H	0.014064	1.484744	1.026464
H	0.014064	1.484744	-1.026464
C	-0.018552	-0.682851	0.000000
H	-0.439906	-1.140898	0.894013
H	-0.439906	-1.140898	-0.894013
H	1.051147	-0.947313	0.000000

R = CF_3: Energy: -363.702719

B	-0.452497	1.566653	0.000000
H	-0.570822	2.115492	1.044185

H	-0.570822	2.115492	-1.044185
C	-0.044396	0.017536	0.000000
F	-0.452902	-0.672286	-1.076429
F	1.312911	-0.007857	0.000000
F	-0.452902	-0.672286	1.076429

R = CCl_3: Energy: -1444.779074

B	-0.570842	1.683803	0.000000
H	-0.709211	2.221490	1.048025
H	-0.709211	2.221490	-1.048025
C	-0.264785	0.148458	0.000000
Cl	-0.568116	-0.797263	-1.446046
Cl	1.484061	0.783118	0.000000
Cl	-0.568116	-0.797263	1.446046

R = SiH_3: Energy: -317.306749

B	-0.008861	1.442651	0.000000
H	0.018870	2.061412	1.019905
H	0.018870	2.061412	-1.019905
Si	-0.009222	-0.573626	0.000000
H	-0.647003	-1.162402	1.206205
H	-0.647003	-1.162402	-1.206205
H	1.425604	-0.981932	0.000000

R = SiF_3: Energy: -615.286437

B	-0.545301	1.952931	0.000000
H	-0.693644	2.535630	1.025864
H	-0.693644	2.535630	-1.025864
Si	-0.015750	0.013123	0.000000
F	-0.545682	-0.782325	-1.271604
F	1.572571	-0.104238	0.000000
F	-0.545682	-0.782325	1.271604

Geometries for **η^2-H_2 BH_2R** on the basis of ωB97xD/aug-cc-pVTZ:

R = H, optimum: Energy: -27.7966144

B	-0.630632	-1.044205	-0.825731
H	0.008130	-0.202083	-0.268262
H	-0.333777	-2.178489	-0.547443
H	-1.788230	-0.867314	-1.063696
H	-0.200265	-0.672353	-2.108575
H	0.028690	-1.444437	-1.979617

R = H, TS_{ROT}: Energy: -27.7965312

H	-0.545155	-0.000002	1.142496
B	-0.201309	-0.000007	-0.000453
H	-0.341228	1.006169	-0.639302

H	-0.341245	-1.006167	-0.639321
H	1.139780	0.405489	0.076655
H	1.139788	-0.405480	0.076701

R = PH_2: Energy: -369.763715156

B	0.000000	0.000000	0.000000
P	0.000000	0.000000	1.961146
H	1.110321	0.000000	-0.468013
H	-0.799051	-0.597962	-0.656624
H	0.109506	1.309555	-0.510032
H	-0.650959	1.244020	-0.235384
H	-1.202797	-0.715220	2.173832
H	0.826692	-1.141779	2.078129

R = $P(O)H_2$: Energy: -445.008422312

O	0.000000	0.000000	0.000000
P	0.000000	0.000000	1.494639
B	1.754581	0.000000	2.326762
H	2.345814	1.008234	2.048615
H	1.919392	-0.406165	3.435373
H	2.688810	-0.470924	1.446887
H	2.212107	-1.113222	1.660435
H	-0.738549	-1.057311	2.086176
H	-0.651527	1.095613	2.119057

R = CH_3: Energy: -67.122430

B	-0.801152	-1.078709	-0.844301
H	-0.173971	-0.251682	-0.233095
H	-0.443271	-2.204293	-0.607897
C	-2.327617	-0.800604	-1.196481
H	-0.006115	-0.561220	-1.992571
H	-0.112170	-1.331840	-2.140273
H	-2.517225	0.206485	-1.571030
H	-2.754748	-1.515532	-1.901393
H	-2.898051	-0.899852	-0.268982

R = CF_3: Energy: -364.893518284

C	0.000000	0.000000	0.000000
F	0.000000	0.000000	1.354011
B	1.478257	0.000000	-0.637280
F	-0.741428	1.072277	-0.365849
F	-0.685293	-1.091520	-0.385119
H	2.246390	-0.805188	-0.203335
H	1.552547	0.198261	-1.812797
H	2.172844	0.927187	0.151613
H	1.893401	1.331283	-0.496473

R = CCl_3: Energy: -1445.961057659

C	0.000000	0.000000	0.000000
Cl	0.000000	0.000000	1.792592
B	1.493343	0.000000	-0.602350
Cl	-0.947128	1.416941	-0.555352
Cl	-0.786848	-1.491948	-0.582960
H	2.253526	-0.793364	-0.133657
H	1.590882	0.198047	-1.776344
H	2.175612	0.968314	0.203362
H	1.913645	1.360727	-0.447274

R = SiH_3: Energy: -318.501085790

B	0.000000	0.000000	0.000000
Si	0.000000	0.000000	2.030432
H	1.116078	0.000000	-0.426256
H	-0.818384	-0.758867	-0.426256
H	-0.411325	1.048553	-0.706829
H	-0.476683	1.215165	0.151007
H	-1.354255	0.170530	2.620985
H	0.520334	-1.326373	2.445638
H	0.877081	1.045858	2.620986

R = SiF_3: Energy: -616.485248250

B	1.913395	0.231523	0.014428
H	2.275263	0.669758	-1.035180
H	2.289716	0.711013	1.039233
Si	-0.061271	0.010677	0.001396
H	2.758802	-0.796619	-0.003062
H	1.951607	-1.094214	0.050698
F	-0.643815	-0.740474	1.280843
F	-0.743839	1.444991	-0.036219
F	-0.610631	-0.793076	-1.260555

Geometries for **BHR_2** on the basis of ωB97xD/aug-cc-pVTZ:

R = SiH_3: Energy: -608.007494

Si	0.018205	-0.580111	-0.013731
B	0.031597	1.433510	-0.001533
Si	0.045522	2.492455	1.711194
H	0.031259	2.018153	-1.042951
H	-0.583902	-1.161038	1.214800
H	-0.648510	-1.180224	-1.197799
H	1.456897	-0.976231	-0.041622
H	0.711804	3.816011	1.606653
H	-1.393080	2.722112	2.035548
H	0.648393	1.746284	2.846568

R = SiF_3: Energy: -1203.963675

Si	0.095333	0.010768	-0.023673
F	-0.224736	-0.845426	1.273794
B	-0.754304	1.828457	0.051266
F	-0.364770	-0.859338	-1.267925
F	1.669965	0.198193	-0.124788
Si	-0.807240	2.947168	1.718980
H	-1.245992	2.282463	-0.931564
F	-0.525184	4.479113	1.414620
F	-2.252110	2.829946	2.368513
F	0.251726	2.497130	2.811615

Geometries for **η^2-H_2 BHR_2** on the basis of ωB97xD/aug-cc-pVTZ:

R = SiH_3: Energy: -609.207008

B	-0.031990	0.021482	-0.005306
Si	0.022759	0.038290	2.016175
Si	1.916139	-0.031344	-0.557284
H	-0.729779	-0.782755	-0.543974
H	-0.074975	1.097061	-0.683847
H	-0.698063	1.105512	0.057245
H	-1.325226	-0.106718	2.624644
H	0.857959	-1.099465	2.481612
H	0.625274	1.295469	2.535432
H	2.123040	0.146311	-2.018656
H	2.724336	1.003161	0.141975
H	2.433678	-1.369961	-0.178729

R = SiF_3: Energy: -1205.171774

B	0.004853	0.014112	-0.004202
Si	0.021248	0.006634	1.985861
F	1.481021	0.027516	2.609771
F	-0.752292	1.247654	2.610420
F	-0.710913	-1.301894	2.493634
Si	1.373638	-1.260559	-0.681525
H	-1.103593	-0.094623	-0.424294
H	0.535375	0.955660	-0.716352
H	0.277085	1.275096	0.094795
F	1.099057	-1.686547	-2.186423
F	2.834338	-0.632425	-0.642088
F	1.402204	-2.596879	0.172619

Geometries for **pentavalent H_2/BHR_2** on the basis of ωB97xD/aug-cc-pVTZ:

R = SiH_3: Energy: -609.224278

B	0.031021	-0.313962	-0.021356
H	-0.200997	-1.490488	0.073086
H	-0.283874	0.206498	-1.078029
Si	-1.964781	0.061016	0.007944

Si	1.997703	0.054772	0.004397
H	2.666921	-0.620918	-1.136422
H	-2.595963	-0.649041	-1.127950
H	-2.556758	-0.453832	1.264604
H	2.609810	-0.444156	1.262427
H	2.269876	1.512196	-0.096022
H	-2.235862	1.512207	-0.105212
H	-0.290942	0.358071	0.949291

R = SiF_3: Energy: -1205.190481

B	-0.002533	-0.008619	-0.018649
Si	-1.957818	-0.000320	-0.000033
Si	1.933331	0.000341	0.003007
H	0.336677	0.171997	-1.174036
H	0.334052	0.903859	0.716770
H	0.336008	-1.099513	0.405642
F	2.514489	1.372166	-0.522921
F	2.501662	-0.222828	1.460096
F	2.528836	-1.141679	-0.912162
F	-2.554908	-1.147973	-0.915829
F	-2.522163	-0.220985	1.464449
F	-2.536557	1.377517	-0.528287

Geometries for **BR_3** on the basis of ωB97xD/aug-cc-pVTZ:

R = SiH_3: Energy: -898.710902

B	0.023402	-0.007325	-0.048991
Si	0.946441	1.766016	-0.257861
Si	1.052549	-1.720913	0.160563
Si	-1.983512	-0.052621	0.048119
H	2.300171	1.692467	-0.866952
H	0.275200	-2.926720	-0.230883
H	-2.597546	1.217197	0.518407
H	0.135103	2.749505	-1.023925
H	2.353335	-1.741412	-0.558417
H	-2.406400	-0.272892	-1.366780
H	1.090433	2.280730	1.135696
H	1.330076	-1.811617	1.624445
H	-2.519345	-1.172370	0.866579

R = SiF_3: Energy: -1792.642194

B	-0.001063	0.011235	-0.000842
Si	0.008540	0.011222	2.006639
Si	1.734386	0.011175	-1.009865
Si	-1.743579	0.011308	-0.997433
F	1.460300	0.011158	2.640424
F	1.562105	0.011183	-2.584571
F	-3.019391	0.011377	-0.058608

F	-0.740529	1.304321	2.535315
F	2.565345	1.304366	-0.622647
F	-1.825308	1.304435	-1.910545
F	-0.740637	-1.281820	2.535299
F	2.565256	-1.282074	-0.622651
F	-1.825425	-1.281833	-1.910516

Geometry for **η^2-H_2 BR_3** on the basis of ωB97xD/aug-cc-pVTZ:

R = SiF_3: Energy: -1793.856502

B	0.010286	-0.125855	0.053058
Si	-0.151331	0.051369	2.029703
F	1.286317	0.028380	2.696886
Si	1.493845	-1.237289	-0.682166
F	2.829080	-0.399700	-0.834997
F	1.815148	-2.469291	0.262805
F	1.111953	-1.828131	-2.105763
F	-0.865184	1.395838	2.482522
F	-0.997500	-1.142468	2.650858
Si	0.130253	1.657531	-0.837957
H	-1.114292	-0.166177	-0.554135
H	-0.870177	-1.010161	-0.224018
F	-1.234306	2.461199	-0.777538
F	1.235474	2.500615	-0.087839
F	0.530500	1.547617	-2.366393

Geometries for **pentavalent H_2/BR_{23}** on the basis of ωB97xD/aug-cc-pVTZ:

R = SiH_3: Energy: -899.932758

B	0.587399	0.034959	0.126500
Si	-0.474449	-0.053825	1.838314
Si	2.102248	0.051600	-1.204165
Si	-0.112777	1.874995	-0.402729
H	0.082348	-0.957011	-0.335607
H	1.503195	-0.190895	0.894269
H	1.586518	0.362668	-2.560926
H	3.130227	1.055564	-0.843700
H	2.724497	-1.293061	-1.226046
H	0.016409	0.928172	2.832981
H	-1.907601	0.219695	1.564813
H	-0.347262	-1.418739	2.401004
H	-1.225403	1.634113	-1.353390
H	-0.634187	2.659678	0.748528
H	0.909032	2.722824	-1.073608

R = SiF_3: Energy: -1793.873196

B	0.615673	0.338696	0.161037
Si	-0.151485	2.079511	-0.429017

Si	-0.402664	-0.190435	1.765580
Si	2.046539	-0.091532	-1.127015
H	0.163519	-0.708082	-0.257627
H	1.539513	0.199655	0.938490
F	1.506692	-0.006453	-2.607939
F	3.272663	0.891611	-0.991360
F	2.576810	-1.558179	-0.874915
F	-0.099229	0.755442	2.990978
F	-1.954509	-0.146211	1.479863
F	-0.017037	-1.662926	2.188492
F	-1.335571	1.799685	-1.441158
F	-0.731872	2.931808	0.775657
F	0.911151	2.998145	-1.164828