Computational Study of the Release of H₂ from Ammonia Borane Dimer (BH₃NH₃)₂ and Its Ion Pair Isomers

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Supporting Information CCSD(T) total energies, MP2 zero-point energies, Cartesian coordinates of the MP2/aVTZ optimized geometries, and atomization energy components for the ion pairs (**DADB** and **IonP-N**) and the ions (BH₃NH₂BH₃⁻ and NH₃BH₂NH₃⁺), and figures showing important MP2/aVTZ geometry parameters of the transition structure **dim-ts6**, **dim-ts7**, **dim-ts8** for release of one H₂ molecules from **dim**, and the various products.

Table S-1. CCSD(T)/aVnZ total and zero-point energies of three isomers of the ammonia borane dimer, and the NH₃BH₂NH₃⁺ and BH₃NH₂BH₃⁻ ions.

Structure	Total Energy ^a				ZPE
	aVDZ	aVTZ	aVQZ	CBS ^b	
dim	-165.995673	-166.163632	-166.207333	-166.231052	89.89 ^c
DADB	-165.977593	-166.145464	-166.189205	-166.212954	89.14 ^d
IonP-N	-165.968472	-166.136217	-166.180116	-166.203944	89.28 ^d
NH ₃ BH ₂ NH ₃ ⁺	-138.635303	-138.770197	-138.806590	-138.826516	65.96 ^c
BH ₃ NH ₂ BH ₃ ⁻	-109.011802	-109.122892	-109.151609	-109.167170	55.98 ^c

^a Total CCSD(T) energies, in Hartrees, with different basis sets are based on MP2/aVTZ optimized geometries.

^b Extrapolated energies at a complete basis set limit, see text.

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^c Unscaled zero-point energies, in kcal/mol, obtained from harmonic vibrational frequencies calculated at the MP2/aVTZ level.

^d Unscaled zero-point energies, in kcal/mol, obtained from harmonic vibrational frequencies calculated at the MP2/aVDZ level.

Table S-2. Components for calculated atomization energies in kcal/mol.

Structure	$\Delta E_{\text{CBS}}^{\text{a}}$	ΔE_{ZPE}	$\Delta E_{\text{CV}}^{\text{b}}$	$\Delta E_{\text{SR}}^{\text{c}}$	$\Delta E_{\text{SO}}^{\text{d}}$	$\Sigma D_0(0\text{K})$
DADB	1222.46	86.92 ^e	3.99	-0.82	-0.06	1138.63
IonP-N	1216.80	87.06 ^e	3.97	-0.83	-0.06	1132.83
$\text{NH}_3\text{BH}_2\text{NH}_3^+$	730.44	63.87 ^f	2.58	-0.72	-0.03	668.39
$\text{BH}_3\text{NH}_2\text{BH}_3^-$	898.84	54.00 ^f	3.14	-0.51	-0.06	847.41

^a Extrapolated by using Equation (2) with CCSD(T)/aVnZ, where $n=\text{D, T and Q}$.

^b Core/valence corrections were obtained by CCSD(T)/cc-pwCVTZ.

^c Scalar relativistic correction is based on a CISD/cc-pVTZ calculation.

^d See text.

^e Scaled zero-point energy by 0.9751. See text

^f Scaled zero-point energy by 0.9684. See text

Table S-3. CCSD(T) total and zero-point energies of equilibrium and transition structures related to the H₂-release pathways from ammonia borane dimers.

Structures	Total Energy ^a		ZPE ^b
	aVDZ	aVTZ	
2AB	-165.970245	-166.138514	88.04
dim-ts1	-165.904990	-166.073681	83.24
dim-ts2	-165.916121	-166.085530	85.24
dim-ts3	-165.913925	-166.083164	85.43
dim-ts4	-165.909376	-166.078276	84.08
dim-ts5	-165.911499	-166.080996	86.04
dim-p1 + 2H ₂	-165.970025	-166.140847	73.70
2(BH ₂ NH ₂) + 2H ₂	-165.964471	-166.135791	73.32
dim-p2 + H ₂	-165.978569	-166.147961	81.65
AB + BH ₂ NH ₂ + H ₂	-165.967358	-166.137153	80.68
DB + 2A	-165.938944	-166.107506	86.25
AB + A + B	-165.922605	-166.088858	82.02
DBA-com + A	-165.944203	-166.111894	83.78
BBA-com + A	-165.954405	-166.122503	86.09
BAA-com + B	-165.9384956	-166.1045074	84.51
2AB-com1	-165.9730224	-166.1400748	88.00
2AB-com2	-165.9714453	-166.1386629	87.86
2AB-com3	-165.958648	-166.126166	87.26
2AB-p1 + H ₂	-165.984461	-166.155764	82.01
2AB-p2 + A + H ₂	-165.9522198	-166.1233381	78.48
DBA-ts + A	-165.933133	-166.100515	84.55

2AB-ts1	-165.9502267	c	86.43
2AB-ts2	-165.9231013	-166.0901032	83.30
2AB-ts3	-165.9255221	-166.0919607	86.62
2AB-ts4	-165.914159	-166.081795	83.01
2AB-ts5	-165.910299	-166.076957	87.56
2AB-ts6	-165.9030518	c	84.26
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DADB-p1 + H₂	-165.974685	-166.145454	82.94
DADB-p2 + H₂	-165.945483	-166.114899	80.42
DADB-p3 + H₂	-165.994645	-166.165585	84.18
DADB-ts1	-165.938201	-166.106569	85.10
DADB-ts2	-165.887586	-166.056680	84.40
DADB-p1-ts + H₂	-165.972489	-166.143064	83.48
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zwt-n-p + H₂	-165.936004	-166.104826	80.93
zwt-n-ts1	-165.933564	-166.101649	85.27
zwt-n-ts2	-165.868783	-166.037562	83.27

^a Total energies, given in hartree, were based on MP2/aVTZ optimized geometries.

^b Unscaled zero-point energies were obtained from harmonic vibrational frequencies at the MP2/aVDZ method.

^c High energy so CCSD(T)/aVTZ calculation not done.

Table S-4: Geometries of the structures considered optimized at the MP2/aug-cc-pVTZ level of theory, given in Cartesian coordinates (Å).

1) dim

B	1.775139	-0.465777	0.216710
N	0.659431	-1.651747	0.197959
H	1.474437	0.252922	1.147180
H	2.849061	-0.988633	0.366964
H	1.677196	0.093838	-0.855655
H	-0.282413	-1.271421	0.072409
H	0.834197	-2.304664	-0.558333
H	0.669725	-2.175617	1.066449
N	-0.659431	1.651747	-0.197959
B	-1.775139	0.465777	-0.216710
H	0.282413	1.271421	-0.072409
H	-0.669725	2.175617	-1.066449
H	-0.834197	2.304664	0.558333
H	-1.474437	-0.252922	-1.147180
H	-1.677196	-0.093838	0.855655
H	-2.849061	0.988633	-0.366964

2) dim-ts1

B	1.642030	0.671226	0.190279
N	1.312062	-0.742156	-0.251134
H	0.670937	1.067192	1.112183
H	2.492134	0.770487	1.030323
H	1.637275	1.507112	-0.666642
H	-0.064427	-1.032988	0.498989
H	1.200490	-0.863097	-1.247947
H	1.963817	-1.440447	0.079667
N	-1.312055	0.742154	-0.251134
B	-1.642036	-0.671228	0.190273
H	0.064400	1.032989	0.498972
H	-1.200460	0.863096	-1.247945
H	-1.963815	1.440447	0.079652
H	-0.670945	-1.067179	1.112199
H	-2.492146	-0.770482	1.030313
H	-1.637276	-1.507116	-0.666644

3) dim-ts2

N	1.480719	0.767453	-0.241877
B	1.896551	-0.709881	0.333341
N	-1.336660	-0.720746	-0.332489
B	-1.912068	0.628098	0.240655
H	1.706865	-1.471688	-0.587184
H	3.053267	-0.630248	0.661114
H	1.152510	-0.905309	1.269009
H	0.503572	0.770205	-0.527035
H	1.594258	1.485762	0.465227
H	2.049039	1.022889	-1.041848
H	-2.355989	-0.598750	0.614737
H	-1.592194	-1.031872	-1.253183
H	-0.488307	-1.133903	0.030129
H	-2.814653	0.125192	1.101058
H	-1.159747	1.217959	0.959305
H	-2.579447	1.231722	-0.540750

4) dim-ts3

N	1.784958	0.759515	-0.030514
B	2.000363	-0.866270	-0.103907
N	-1.165040	-0.096743	0.371535
B	-2.658995	-0.087724	-0.239475
H	0.798393	0.956896	0.139484
H	2.331081	1.170714	0.718406
H	2.058411	1.208466	-0.897769
H	1.284606	-1.234380	-1.009729
H	3.171458	-1.041789	-0.325211
H	1.642684	-1.277382	0.975523
H	-1.748480	0.935618	-0.257972
H	-1.141655	-0.173979	1.376533
H	-0.537000	-0.763978	-0.059261
H	-2.620211	1.165257	-0.695843
H	-2.770589	-0.748840	-1.222290
H	-3.514967	-0.066037	0.587892

5) dim-ts4

N	1.056292	0.811258	-0.115433
B	1.980851	-0.512821	0.140871
N	-0.987121	-0.794488	-0.137435
B	-2.040669	0.267308	0.172430

6) dim-ts5

N	1.125822	0.693062	-0.407001
B	1.726300	-0.503590	0.380804
N	-1.202226	-0.627300	-0.495825
B	-1.632119	0.514864	0.544355

H	1.553368	-1.008716	1.172742
H	-0.684984	1.329281	-0.061825
H	1.768976	-1.249871	-0.808536
H	3.144492	-0.199326	0.232667
H	1.224125	1.456539	0.650555
H	1.369768	1.281806	-0.958678
H	-1.453923	1.587221	-0.084062
H	-2.292843	0.420357	1.322816
H	-2.879776	0.429958	-0.654943
H	-1.115013	-1.308491	-1.000299
H	-0.033983	-0.177700	-0.216275
H	-0.785317	-1.450876	0.609408

7) dim-p1

N	1.548445	-0.764609	-0.152921
B	1.707343	0.839244	0.162990
N	-1.653808	0.644666	-0.100740
B	-2.032930	-0.665312	0.163117
H	1.048542	1.027063	1.160717
H	2.886983	1.021906	0.325176
H	1.266994	1.402424	-0.811325
H	0.571355	-1.030554	-0.249685
H	2.031913	-1.017812	-1.007798
H	1.939159	-1.320115	0.600722
H	-2.281970	1.307310	-0.523106
H	-0.739719	1.024201	0.105642
H	-1.228439	-1.405762	0.654794
H	-3.129344	-1.038721	-0.110043

9) 2AB-com1

N	0.095204	-0.714209	-0.101016
B	0.601476	0.789315	-0.133271
B	2.702145	-0.014725	0.142974
N	-2.729806	0.052051	0.079030
H	0.397410	-1.220568	-0.927075
H	0.307355	1.332810	0.890968
H	1.852521	0.897470	-0.339175
H	0.185249	1.304837	-1.137331
H	0.493192	-1.195976	0.700439
H	-0.935485	-0.708812	-0.045167
H	2.681430	-0.875521	-0.702533
H	2.368772	-0.365050	1.244232
H	3.651125	0.716069	0.110436
H	-3.263742	-0.085952	0.928898
H	-2.436673	1.023644	0.073808
H	-3.377047	-0.060796	-0.692110

H	0.214929	0.266760	-0.771158
H	0.688917	-0.961531	1.151819
H	0.830064	1.474734	0.172526
H	1.713205	1.017301	-1.165436
H	2.203748	-1.333355	-0.324175
H	2.292479	-0.235572	1.392767
H	-0.831004	0.461838	1.484177
H	-2.760049	0.373299	0.957884
H	-1.492437	1.586116	-0.031975
H	-1.666948	-0.487108	-1.387996
H	0.409330	-1.144052	0.402866
H	-1.538316	-1.535131	-0.187318

8) dim-p2

N	-0.952517	-1.573806	0.000000
B	-2.063024	-0.734121	0.000000
N	0.952516	1.573805	0.000000
B	2.063024	0.734122	0.000000
H	-3.154489	-1.207955	0.000000
H	-1.895805	0.448430	0.000000
H	0.000000	-1.247027	0.000000
H	-1.032488	-2.576262	0.000000
H	0.000000	1.247026	0.000000
H	1.032486	2.576261	0.000000
H	3.154489	1.207957	0.000000
H	1.895806	-0.448430	0.000000

10) 2AB-com2

N	-0.274313	-1.089926	-0.516198
B	-1.109878	-0.624063	0.753347
B	-1.375618	1.407683	-0.222651
N	2.201207	0.293650	0.084780
H	-0.712772	-0.743911	-1.365884
H	-1.113139	0.650166	0.842967
H	-2.215526	-1.069604	0.729525
H	-0.463150	-0.867827	1.737835
H	0.689972	-0.712022	-0.461152
H	-0.227076	-2.102589	-0.560274
H	-2.065020	0.838072	-1.024588
H	-0.261109	1.662484	-0.612777
H	-1.920181	2.285184	0.384355
H	1.701338	1.177579	0.094957
H	2.471136	0.099494	1.042005
H	3.054748	0.438810	-0.440521

11) 2AB-com3

N	2.159116	-0.415529	0.153398
B	0.645939	-0.719449	-0.268922
B	0.290170	1.498309	-0.015896
N	-2.918189	-0.338986	-0.038957
H	2.670981	-1.277567	0.313702
H	0.042116	0.340064	-0.636758
H	0.083913	-1.243704	0.643592
H	0.663036	-1.315623	-1.307770
H	2.634460	0.121220	-0.566633
H	2.171987	0.150315	0.999150
H	-0.753028	1.999619	-0.325325
H	1.253188	1.915983	-0.610622
H	0.443248	1.330829	1.164923
H	-3.788897	-0.200173	0.458471
H	-2.425145	0.546380	-0.023857
H	-2.362892	-0.980031	0.514128

14) 2AB-ts2

N	-2.326652	0.299428	0.069236
N	0.296605	-0.975521	-0.597170
B	0.982107	-1.055243	0.698165
B	1.518488	1.450906	0.029739
H	-1.754299	1.059487	0.422123
H	1.435114	1.021191	-1.212095
H	-3.040598	0.716471	-0.515606
H	-2.801741	-0.102209	0.868660
H	0.420483	1.782958	0.379114
H	2.323238	2.322918	-0.128126
H	0.940380	0.296812	-0.931077
H	-0.702794	-0.764871	-0.584123
H	0.559477	-1.634773	-1.315003
H	1.996180	-1.674678	0.754231
H	1.952004	0.477021	0.643867
H	0.379901	-0.745988	1.674055

16) 2AB-ts4

B	-1.034253	-0.863571	0.515875
N	-2.100999	-0.358748	-0.386829
H	-1.557114	1.083162	-0.212197
H	-0.205599	0.455431	0.927869
H	-1.337188	-1.024762	1.657065
H	-0.133418	-1.471845	0.033672
H	-2.050857	-0.624380	-1.359501

13) 2AB-ts1

N	-1.934899	-0.827527	-0.003762
B	-2.058608	0.789809	0.024842
B	0.633757	0.521277	-0.040953
N	2.936193	-0.206406	0.017070
H	-2.833782	-1.276070	0.132721
H	-0.915172	1.218078	-0.112165
H	-2.501632	1.085060	1.103294
H	-2.735015	1.104135	-0.919801
H	-1.542812	-1.137159	-0.887465
H	-1.294023	-1.132815	0.723645
H	1.087889	1.619942	-0.107948
H	0.468942	-0.122017	-1.038015
H	0.461770	0.008943	1.028178
H	3.246506	-1.165843	0.110387
H	3.330914	0.317031	0.788595
H	3.341609	0.162814	-0.834026

15) 2AB-ts3

N	-0.206783	0.949559	-0.017623
B	0.214571	-0.554093	-0.103970
N	2.290704	-0.206915	0.046706
B	-2.589667	-0.376776	0.054502
H	-1.229602	0.950714	-0.293680
H	0.233211	-1.178110	0.900412
H	-1.586579	-1.046760	-0.262898
H	0.332566	-0.989673	-1.200011
H	-0.167475	1.315879	0.927404
H	0.317791	1.555664	-0.637372
H	-2.599847	0.586468	-0.733365
H	-2.420544	0.038838	1.190265
H	-3.588560	-1.035354	-0.077616
H	2.636348	0.158553	0.928047
H	2.580746	-1.177712	0.001673
H	2.779979	0.277333	-0.699097

17) 2AB-ts5

N	-1.728574	-0.437893	0.016357
B	0.000035	-0.846547	-0.065042
N	1.728642	-0.437775	0.016359
B	-0.000107	1.731544	0.003993
H	-2.277370	-1.255585	0.264646
H	-0.000015	0.662419	-0.679989
H	0.000073	-1.520888	-1.059751

H	-3.050860	-0.411403	-0.049353
B	-0.078985	1.409484	0.145112
H	-1.314986	1.889993	0.061671
H	0.302736	1.103575	-0.941759
H	0.417773	2.356674	0.678322
N	2.962477	-0.390167	-0.240617
H	2.888350	0.616614	-0.161515
H	2.033478	-0.757411	-0.074216
H	3.543532	-0.702803	0.527124

18) 2AB-ts6

N	-0.603643	0.092277	0.474882
B	-0.543799	1.636389	-0.214761
B	-1.412692	-1.339562	-0.189251
N	2.146484	-0.349889	-0.019030
H	-0.027961	1.446361	-1.291212
H	2.195299	0.530055	-0.522126
H	-1.501071	-0.005591	-0.368192
H	-0.934933	0.166660	1.427701
H	-1.699661	1.982885	-0.303532
H	0.115678	2.292307	0.548537
H	2.873534	-0.334871	0.685526
H	2.380530	-1.084193	-0.676072
H	0.385722	-0.224604	0.415731
H	-2.188575	-0.699323	-0.943843
H	-0.597846	-1.905221	-0.838707
H	-2.018148	-1.845319	0.695285

20) 2AB-p2

N	-0.561952	-0.000031	0.713084
B	-1.233015	-0.948786	-0.316301
B	-1.232896	0.948838	-0.316273
N	2.293237	-0.000031	-0.047042
H	-1.753490	0.000070	-1.103205
H	-2.192656	1.524793	0.091389
H	-0.457075	1.505043	-1.032423
H	0.459748	-0.000091	0.706996
H	-0.953027	-0.000022	1.640913
H	-0.457265	-1.505067	-1.032469
H	-2.192847	-1.524632	0.091343
H	2.288832	-0.811932	-0.653473
H	2.289566	0.812802	-0.652226
H	3.178781	-0.000799	0.443733

H	0.000048	-1.420310	1.003310
H	-1.845388	0.281720	0.725315
H	-2.067582	-0.046859	-0.856600
H	1.021076	2.295907	-0.320253
H	-0.000028	1.432916	1.186358
H	-1.021442	2.295686	-0.320165
H	2.277479	-1.255426	0.264693
H	2.067634	-0.046773	-0.856618
H	1.845400	0.281879	0.725285

19) 2AB-p1

N	-0.561952	-0.000031	0.713084
B	-1.233015	-0.948786	-0.316301
B	-1.232896	0.948838	-0.316273
N	2.293237	-0.000031	-0.047042
H	-1.753490	0.000070	-1.103205
H	-2.192656	1.524793	0.091389
H	-0.457075	1.505043	-1.032423
H	0.459748	-0.000091	0.706996
H	-0.953027	-0.000022	1.640913
H	-0.457265	-1.505067	-1.032469
H	-2.192847	-1.524632	0.091343
H	2.288832	-0.811932	-0.653473
H	2.289566	0.812802	-0.652226
H	3.178781	-0.000799	0.443733

21) DADB

B	-1.399314	0.000021	-0.265823
N	-0.527289	1.275131	0.130025
H	-0.921829	2.104294	-0.303236
H	1.901481	0.994005	-0.712326
H	-1.536887	0.000020	-1.456229
H	-2.423055	0.000026	0.361812
H	-0.484119	1.445009	1.130595
H	0.468349	1.176920	-0.182999
B	2.252761	-0.000019	-0.068475
H	1.901414	-0.994045	-0.712285
H	1.696743	0.000049	1.029620
H	3.450788	-0.000066	0.051824
N	-0.527330	-1.275127	0.130025
H	-0.921965	-2.104272	-0.303184
H	0.468298	-1.177009	-0.183049
H	-0.484116	-1.444969	1.130599

22) DADB-ts1

B	-0.909886	0.640139	-0.110768
N	0.227584	-0.371180	-0.198184
H	1.459397	0.278163	-0.250003
H	2.697232	-0.192221	1.294130
H	-1.079077	1.213338	-1.155206
H	-0.798954	1.354345	0.850552
H	0.421467	-0.932702	0.624036
H	0.252922	-0.975942	-1.010799
B	3.036157	0.017969	0.152606
H	2.209367	0.882797	-0.346552
H	3.013225	-0.965799	-0.549737
H	4.029773	0.687101	0.042195
N	-2.346407	-0.154919	0.150165
H	-3.101097	0.522933	0.210618
H	-2.569673	-0.799906	-0.601899
H	-2.334180	-0.679953	1.019608

24) DADB-p1

N	1.638905	1.066432	0.000000
B	0.000000	0.773977	0.000000
N	-0.218595	-0.752975	0.000000
H	1.777845	2.072875	0.000000
H	2.105122	0.695382	0.822589
H	2.105122	0.695382	-0.822589
H	-0.383820	1.278502	1.017985
H	-0.383820	1.278502	-1.017985
H	0.172382	-1.215237	0.815195
H	0.172382	-1.215237	-0.815195
B	-1.821509	-1.173751	0.000000
H	-1.829791	-2.387136	0.000000
H	-2.285021	-0.699183	1.010374
H	-2.285021	-0.699183	-1.010374

26) DADB-p1-ts

N	0.655755	-0.369026	-0.391431
B	2.048661	0.087020	0.359828
B	-0.517545	0.652496	-0.257537
N	-1.846784	-0.189055	0.238078
H	1.772398	0.099630	1.541653
H	-0.824996	1.128286	-1.319006
H	-0.340666	1.443690	0.623283
H	0.454824	-1.285103	-0.001863
H	0.873674	-0.537274	-1.367838
H	2.872279	-0.759061	0.078175

23) DADB-ts2

N	0.925380	-1.186579	-0.247015
B	1.199811	0.191007	0.326123
N	0.236149	1.287531	-0.222424
B	-2.179529	-0.328316	0.089347
H	1.671014	-1.757502	-0.603333
H	-1.696458	-0.706331	-0.976864
H	2.344075	0.494882	0.430315
H	0.774713	0.052508	1.594912
H	0.713565	-0.797738	1.116389
H	-0.016433	-1.407224	-0.556120
H	-2.236746	0.912071	0.053545
H	-1.445381	-0.656647	1.017650
H	-3.296658	-0.747940	0.247669
H	0.357608	1.372345	-1.230457
H	-0.790226	1.017713	-0.074942
H	0.388817	2.203739	0.189955

25) DADB-p2

N	-0.826302	-1.207712	0.004024
B	-1.390492	0.038824	-0.009859
N	-0.408820	1.228121	-0.001799
B	2.202068	-0.195071	0.009127
H	-1.380850	-2.047095	0.008929
H	1.708466	0.153402	1.076586
H	-2.552327	0.272952	-0.023029
H	0.189826	-1.346153	0.000309
H	1.770847	0.531009	-0.911390
H	1.860975	-1.342261	-0.252874
H	3.401203	-0.084354	0.020689
H	-0.250493	1.560697	0.949085
H	0.577066	0.922279	-0.329825
H	-0.736744	2.017890	-0.550395

27) DADB-p3

N	0.811170	0.706584	-0.120600
B	-0.732735	0.864689	0.139342
N	-1.363904	-0.610933	-0.061605
B	1.431736	-0.781799	0.078566
H	1.015366	-1.455751	-0.846810
H	-1.267995	1.596711	-0.653376
H	-0.931193	1.148866	1.290899
H	1.300670	1.327734	0.514899
H	1.063148	1.025861	-1.049934
H	2.634620	-0.698853	0.069070

H	2.324250	1.182387	-0.069636
H	-2.616753	0.465420	0.342301
H	-2.142256	-0.911600	-0.411870
H	-1.691137	-0.617384	1.146811

28) IonP-N

N	1.383348	0.000088	0.000027
B	0.596776	-1.389515	0.006040
B	0.596487	1.389545	-0.006056
N	-2.017041	-0.000082	0.000002
H	1.371215	2.312206	0.059197
H	-1.354333	-0.718874	-0.383620
H	2.006162	-0.002608	0.803020
H	2.006045	0.002929	-0.803058
H	-0.073007	1.437499	-1.024585
H	-0.127482	1.410111	0.995102
H	-1.355007	0.719163	0.383722
H	-2.587718	-0.408670	0.731999
H	-2.588059	0.407959	-0.732020
H	1.371627	-2.312039	-0.059630
H	-0.072452	-1.437904	1.024712
H	-0.127448	-1.409962	-0.994966

30) IonP-N-ts2

N	1.371082	0.248770	-0.036661
B	0.343728	1.391630	-0.042106
B	1.070058	-1.231483	-0.165455
N	-2.077737	-0.229483	0.003930
H	0.848744	2.474338	0.114567
H	-1.453862	-0.944804	-0.389988
H	0.965458	-0.621674	1.048391
H	2.344427	0.495300	0.040471
H	-0.375121	1.365092	-1.042185
H	-0.434788	1.244160	0.967173
H	-1.373764	0.508077	0.419460
H	-2.695013	-0.627040	0.703209
H	-2.604242	0.208860	-0.744504
H	1.990327	-1.986660	-0.244241
H	0.594280	-1.503443	1.176573
H	0.071202	-1.547949	-0.782002

H	1.012370	-1.195939	1.147633
H	-2.322511	-0.639185	0.267379
H	-1.339992	-0.925128	-1.026278
H	-0.790357	-1.268328	0.472410

29) IonP-N-ts1

N	1.333317	0.597494	0.000010
B	2.522574	-0.545307	0.000004
B	-0.067251	-0.031874	-0.000032
N	-2.882742	-0.111070	0.000007
H	-0.866741	1.047514	0.000031
H	-2.641477	-1.096884	-0.001184
H	1.492363	1.182285	0.813459
H	1.492387	1.182325	-0.813405
H	-0.325459	-0.618332	-1.015890
H	-0.325460	-0.618452	1.015764
H	-1.665227	0.541423	-0.000022
H	-3.436597	0.086471	0.825428
H	-3.437816	0.088211	-0.824175
H	3.567551	0.070929	0.000000
H	2.357921	-1.192274	1.009502
H	2.357913	-1.192277	-1.009490

31) IonP-N-p

N	-1.146273	0.075824	-0.265872
B	-1.119581	-1.222805	0.213110
B	-0.411089	1.361851	0.217644
N	1.845285	-0.280124	-0.100754
H	-1.140496	2.319568	0.262801
H	1.164774	-0.871748	0.394516
H	-1.817744	0.243894	-1.003890
H	0.139768	1.143594	1.284151
H	0.483579	1.662637	-0.625234
H	1.270142	0.618147	-0.341341
H	2.186352	-0.753673	-0.930151
H	2.613169	-0.035866	0.515282
H	-1.819338	-2.086451	-0.227676
H	-0.319944	-1.505229	1.084154

Figure S-1: Selected MP2/aVTZ geometrical parameters of the transition structure **dim-ts6**, **dim-ts7**, **dim-ts8** for release of one H₂ molecules from **dim**. Bond lengths are given in Å and bond angles in degrees.

dim-ts6
(101.3 kcal/mol at MP2/aug-cc-pVTZ)

dim-ts7
(101.4 kcal/mol at MP2/aug-cc-pVTZ)

dim-ts8
(199.9 kcal/mol at MP2/aug-cc-pVTZ)

Figure S-2. Selected MP2/aVTZ geometrical parameters of the products. Bond lengths are given in Å and bond angles in degrees.

DADB-p3

IonP-N-p