Electronic Supplementary Material (ESI) for RSC Advances

Supporting Materials

Table S1 Cartesian coordinates and total energies (a.u.) at the MP2/aug-cc-pvdz level of the relevant structures in the H_2-release from AlH_3PH_3

AlH_3				PH_3			
Energy = -243.7133604				Energy = -342.6140538			
Al	0.000000	0.000000	0.000000	P	0.000000	0.000000	0.128045
H	0.000000	1.586877	0.000000	H	0.000000	1.202235	-0.640227
H	1.374276	-0.793439	0.000000	H	-1.041166	-0.601118	-0.640227
H	-1.374276	-0.793439	0.000000	H	1.041166	-0.601118	-0.640227
AlH_3PH_3				alp-ts			
Energy = -586.3490281				Energy = -586.2951395			
P	0.000000	0.000000	1.186296	P	-1.336627	0.000074	0.048135
H	0.000000	-1.241385	1.869331	H	-1.119896	1.056186	-0.886636
H	-1.075071	0.620692	1.869331	H	-1.120603	-1.056373	-0.886412
H	1.075071	0.620692	1.869331	H	0.064138	-0.000815	1.142848
Al	0.000000	0.000000	-1.42869	Al	1.351058	0.000030	-0.055211
H	0.000000	1.588672	-1.609811	H	1.811557	-1.438270	-0.502849
H	-1.375831	-0.794336	-1.609811	H	1.038949	-0.001353	1.629111
H	1.375831	-0.794336	-1.609811	H	1.811498	1.439128	-0.500344
AlH_2PH_2							
Energy = -585.1825402							
Al	1.210441	-0.000019	0.010946				
H	1.985800	1.383851	-0.008345				
H	1.986346	-1.383607	-0.008354				
P	-1.139212	-0.000033	-0.118603				
H	-1.310163	-1.056181	0.826956				
H	-1.309545	1.056680	0.826502				

Table S2 Cartesian coordinates and total energies (au) at the MP2/aug-cc-pvdz level of the relevant structures in the H_2-release from BH_3PH_3

BH_3				PH_3			
Energy = -26.4867297				Energy = -342.6140538			
B	0.000000	0.000000	0.000000	P	0.000000	0.000000	0.128045
H	0.000000	1.201984	0.000000	H	0.000000	1.202235	-0.640227
H	1.040949	-0.600992	0.000000	H	-1.041166	-0.601118	-0.640227
H	-1.040949	-0.600992	0.000000	H	1.041166	-0.601118	-0.640227
BH_3PH_3				bp-ts			
Energy = -369.1376326				Energy = -369.0852497			
B	0.000000	0.000000	-1.403450	P	0.761958	-0.032403	-0.104893
H	1.010419	0.618226	-1.682373	H	0.684483	1.321641	0.321488
H	-1.040609	0.565935	-1.682373	H	0.992267	-0.53505	1.210675
H	0.030190	-1.184162	-1.682373	H	-0.741597	-0.947827	-0.210747
P	0.000000	0.000000	0.560646	H	-1.697344	0.346177	1.187612
H	-0.031923	1.252769	1.218225	H	-1.885671	-1.038201	-0.259719
H	-1.068968	-0.654030	1.218225	H	-1.629203	0.807881	-0.907599
H	1.100891	-0.598738	1.218225	B	-1.430462	0.106287	0.046337
BH_2PH_2							
Energy = -367.9491181							
B	-1.316046	0.000010	0.051578				
H	-1.910424	1.043442	0.019506				
H	-1.910360	-1.043457	0.019382				
P	0.562636	-0.000009	-0.112373				
H	0.980767	1.087947	0.694309				
H	0.980698	-1.087842	0.694512				

Table S3 Cartesian coordinates and total energies (au) at the MP2/aug-cc-pvdz level of the relevant structures in the H_2-release from AlH_3PH_3+AlH_3

alalp-com1				alalp-com2			
Energy = -830.0940338				Energy = -830.0632826			
H	0.617896	1.950900	1.489225	H	-0.239669	-0.880443	1.075406
H	-1.125901	1.065977	-0.388475	H	3.341622	-1.429894	0.000002
H	1.123730	2.150274	-1.273197	H	-0.239669	-0.880446	-1.075404
H	-1.847037	-1.198784	-1.393280	H	-0.443808	0.973129	-0.000002
H	-3.455253	0.189194	0.415249	H	3.060361	0.937182	-1.376455
H	-1.070529	-0.986153	1.161062	H	3.060360	0.937186	1.376453
H	0.808683	-1.836294	-0.760745	H	-3.301894	1.680290	-0.000002
H	2.782414	-0.964342	-0.463801	H	-3.310341	-0.701558	-1.373852
H	1.556946	-1.480428	1.260933	H	-3.310342	-0.701554	1.373854
Al	-2.052247	-0.431944	-0.000537	Al	2.996256	0.129706	0.000000
Al	0.424924	1.487901	-0.012269	P	0.374441	-0.188994	0.000000
P	1.450949	-0.841186	0.007967	Al	-3.321889	0.093449	0.000000
alalp-tsalal				alalp-tslew			
Energy = -829.9906196				Energy = -830.0288768			
H	-0.052621	-1.559846	-0.000021	H	-0.303107	1.487469	-1.086574
H	3.348710	-0.278331	1.383429	H	3.375640	0.971334	0.000003
H	-0.548634	2.001428	-1.111504	H	-0.303107	1.487465	1.086578
H	-2.428056	-1.256623	-1.436748	H	-0.808828	-0.835504	-0.000005
H	-2.428024	-1.256640	1.436758	H	2.298655	-1.165355	1.370633
H	-0.548621	2.001427	1.111504	H	2.298656	-1.165349	-1.370637
H	0.800592	-1.207623	-0.000008	H	-1.510528	-1.691319	-0.000006
H	0.900031	0.367923	-0.000003	H	-3.024362	0.004115	1.447490
H	3.348714	-0.278324	-1.383427	H	-3.024367	0.004124	-1.447486
Al	-1.852733	-0.922525	0.000001	Al	2.498684	-0.362418	0.000000
P	-0.771015	1.164225	0.000001	P	0.078974	0.659913	0.000000
Al	2.558358	-0.307996	0.000000	Al	-2.512781	-0.329556	0.000000
alalp-tsalp				$AlH_3AlH_2PH_2$+H_2			
Energy = -830.0659317				Energy = -830.0783449			
H	0.577578	2.025507	1.450188	H	0.274949	1.995786	1.350384
H	-0.963175	1.001587	-0.481734	H	-1.086536	0.903488	-0.57836
H	1.232689	2.113912	-1.305347	H	0.995445	2.169477	-1.345737
H	-1.246057	-1.476964	-0.888748	H	-1.711490	-1.737297	-1.263268
H	-3.477288	0.079358	-0.555945	H	-3.536850	-0.159978	-0.540873
H	-1.636563	-0.596487	1.516085	H	-1.669744	-0.793448	1.488921
H	-0.323419	-1.461335	-0.557245	H	-1.014050	-1.728719	-0.936975
H	2.370872	-1.245638	-0.85352	H	2.688231	-0.68854	-0.654775
H	1.755896	-1.441014	1.247385	H	1.994202	-0.908905	1.334549
Al	-2.03569	-0.213955	0.026551	Al	-2.101085	-0.165953	0.112808
Al	0.686218	1.398324	0.000473	Al	0.657391	1.323499	-0.043099

P	1.283507	-0.959715	0.005171	P	1.455592	-0.939998	0.015995
$AlH_3PH_2AlH_2+H_2$							
Energy = -830.0831199							
H	1.037443	-2.295512	0.378000				
H	-3.285538	0.459277	-0.376332				
H	0.225189	1.916201	1.092471				
H	2.690435	-0.657760	1.354458				
H	2.539030	-0.714698	-1.456958				
H	0.217999	1.889486	-1.077664				
H	0.510025	-2.064966	-0.129275				
H	-1.429690	-1.441250	-1.148075				
H	-1.870482	-1.045660	1.483690				
Al	1.971604	-0.379457	-0.023711				
P	0.030611	1.011815	0.019470				
Al	-2.055725	-0.483801	-0.008009				

Table S4 Cartesian coordinates and total energies (au) at the MP2/aug-cc-pvdz level of the relevant structures in the H_2-release from AlH_3PH_3+BH_3

balp-com				balp-tsbp			
Energy = -612.892835				Energy = -612.837809			
H	-0.617799	-1.407535	-1.417743	H	-1.116064	1.640669	1.412484
H	-2.638031	-0.352836	0.001267	H	-1.658186	-0.228753	-0.636517
H	-0.616762	-1.407151	1.417835	H	-0.70286	1.966833	-1.354279
H	-2.748809	1.351183	1.044597	H	-0.775205	-2.035181	-0.642353
H	-2.75006	1.349522	-1.044909	H	-2.661227	-1.898838	-0.176128
H	-1.095599	1.013676	-0.000812	H	-1.272778	-1.17476	1.175633
H	2.230137	1.011632	1.071566	H	0.002138	-1.554455	-0.367177
H	2.747748	-0.768385	-0.000796	H	2.360518	0.102028	-0.842903
H	2.229817	1.013074	-1.070722	H	1.940079	-0.378329	1.261578
Al	-0.839802	-0.736928	0.000024	Al	-0.58209	1.159863	0.006489
P	1.735245	0.224941	-0.000037	P	1.309431	-0.336679	-0.003834
B	-2.370378	0.880555	-0.000006	B	-1.638142	-1.293451	0.028562
$BH_3AlH_2PH_2$+H_2							
Energy = -612.8480829							
H	-0.641776	1.821235	1.379164				
H	-1.848548	0.232099	-0.549705				
H	-0.287809	2.001377	-1.378263				
H	-1.84113	-1.806289	-0.797422				
H	-3.332276	-1.073838	-0.129612				
H	-1.777672	-0.911873	1.203514				
H	-1.170568	-1.679017	-0.35272				
H	2.350036	-0.058632	-0.768607				
H	1.891024	-0.448053	1.262255				
Al	-0.152292	1.21711	-0.002265				
P	1.305983	-0.674345	-0.017812				
B	-2.190246	-0.756853	0.085603				

Table S5 Cartesian coordinates and total energies (au) at the MP2/aug-cc-pvdz level of the relevant structures in the H_2-release from BH_3PH_3+AlH_3

albp-com				albp-tslew			
Energy = -612.8735671				Energy = -612.7294306			
H	-1.034605	-1.372187	0.877731	H	-1.624183	-0.845893	1.229830
H	0.685258	1.186161	-0.454191	H	2.268934	-0.502568	-1.393473
H	-1.574609	-1.028118	-1.229567	H	-1.624463	-0.845682	-1.229845
H	-2.784260	-0.142424	0.376933	H	-2.619119	0.518395	0.000216
H	-1.056176	2.022077	-0.821611	H	2.268481	-0.502879	1.393627
H	-0.483860	1.752095	1.134167	H	-0.008755	-1.467685	-0.000239
H	3.127617	0.492674	-0.643961	H	-1.645850	1.278565	0.000143
H	1.067235	-1.330746	-0.841964	H	-0.094560	1.764989	-1.082152
H	1.687352	-0.347509	1.587015	H	-0.094502	1.764952	1.082166
B	-0.456164	1.354473	-0.006050	P	-1.128326	-0.391287	-0.000026
P	-1.437833	-0.347421	-0.003022	Al	1.604301	-0.113631	0.000010
Al	1.862644	-0.214852	0.007002	B	-0.151401	1.236862	-0.000002
albp-tsalb1				albp-tsalb2			
Energy = -612.7760806				Energy = -612.8124818			
Al	-1.989580	0.010768	0.003955	Al	-1.750053	-0.258950	-0.061592
H	-0.015907	1.390393	-0.387040	H	0.074397	1.483893	-1.269415
H	-1.702236	0.210075	1.561452	H	2.880965	0.203929	-0.012734
H	1.656171	-1.429817	-1.037241	H	0.391189	1.964114	0.683130
H	2.038296	1.686191	-0.925327	H	-0.954545	0.693510	1.065212
H	1.466345	1.732738	1.143011	H	1.508559	-1.008202	1.159655
H	1.040362	-1.400894	1.134000	H	1.527571	-1.192635	-1.013728
H	-0.840338	1.239312	-0.749839	H	-1.724349	0.225508	1.632548
H	-0.538157	-0.712119	-0.601692	H	-3.052214	0.328726	-0.731272
H	-3.453991	-0.222675	-0.576721	H	-1.212246	-1.758585	-0.037298
B	1.514599	1.226620	0.054552	P	1.520453	-0.203693	-0.005420
P	1.242733	-0.584419	0.007681	B	0.100913	1.096295	-0.118819
albp-tsalp1				albp-tsalp2			
Energy = -612.8134632				Energy = -612.8164997			
H	0.539895	-1.367973	1.093336	H	-1.296238	-1.498787	-1.035881
H	3.308765	-0.167352	0.000109	H	1.850895	0.504611	1.550844
H	0.539983	-1.368153	-1.093184	H	-1.387889	1.566291	-1.138286
H	-0.345647	0.869252	-0.000253	H	0.794016	-1.261526	-0.212005
H	2.254148	1.275061	-1.023403	H	-1.097318	-1.45886	1.137362
H	2.254048	1.27523	1.023278	H	1.776042	1.076709	-1.323466
H	-1.126332	1.658211	-0.000403	H	1.90545	-1.403233	-0.303148
H	-2.416652	-0.217752	-1.448177	H	-0.935729	1.777446	0.845548
H	-2.416465	-0.21704	1.44845	H	-2.782295	1.059432	0.290505
B	2.390359	0.627158	-0.000003	Al	1.679102	0.257391	0.009883
P	0.729959	-0.486968	0.000011	P	-0.839929	-0.650213	0.002768

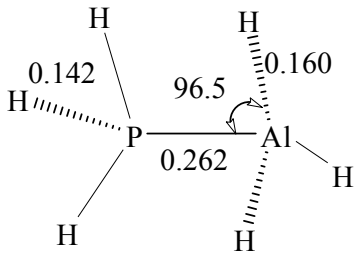
Al	-1.960994	0.186865	0.000008	B	-1.611266	1.209005	0.003705
albp-tsalp3				$AlH_2BH_2PH_3+H_2$			
Energy = -612.8402397				Energy = -612.8450928			
B	0.221466	1.152447	0.055139	H	1.209695	-1.482144	-1.090949
H	-0.340201	1.024043	-1.031245	H	-2.245037	-1.553986	-0.009255
H	0.207003	-1.269423	-0.426489	H	2.679082	-0.319946	0.005006
H	-0.749966	-1.429278	-0.626674	H	3.424725	2.56758	-0.010808
Al	-1.805392	-0.174401	0.010312	H	-3.263727	0.951186	0.000681
H	2.610183	0.05526	-0.907828	H	1.204907	-1.494641	1.081075
H	2.263608	-0.433814	1.205984	H	2.675485	2.463472	-0.009454
H	-0.526593	0.774358	0.987281	H	0.233895	1.475195	1.028681
H	0.531929	2.291842	0.280455	H	0.237072	1.485368	-1.01037
H	-2.797941	0.428739	-1.062181	P	1.283144	-0.584334	0.000431
H	-2.310078	-0.805632	1.379475	Al	-1.956957	0.031434	-0.001489
P	1.564988	-0.275408	-0.013902	B	0.007437	0.852856	0.00566
$AlH_2PH_2BH_3+H_2$				$AlH_3BH_2PH_2+H_2$			
Energy = -612.8680247				Energy = -612.8743314			
H	0.834317	-1.565684	1.087766	B	0.228431	-0.496435	0.637558
H	3.02985	0.530791	0.00001	H	-0.562276	0.501939	0.798591
H	0.834318	-1.565681	-1.087773	H	-2.672122	2.3772	0.454424
H	-0.507554	1.989327	0.000009	H	-2.971321	2.004841	1.041475
H	1.529589	1.499756	-1.017505	Al	-1.772111	-0.233569	-0.265664
H	1.529576	1.49976	1.017501	H	2.388825	0.824749	0.969251
H	-1.249828	2.185514	-0.000023	H	2.635756	-0.95727	-0.07632
H	-2.319379	0.147888	-1.404337	H	-0.318468	-1.265622	-0.228452
H	-2.319367	0.14789	1.404348	H	0.251866	-1.096169	1.682119
B	1.881341	0.918392	0.000001	H	-2.94894	-0.89505	0.544229
P	0.672809	-0.672619	-0.000002	H	-1.822079	0.522453	-1.644996
Al	-1.604643	0.048289	0.000002	P	1.860937	0.233433	-0.218299
cyclic-$AlH_2BH_3PH_2+H_2$							
Energy = -612.8792263							
H	1.304682	1.500953	-1.117611				
H	-1.792817	-0.687099	1.433076				
H	1.827709	-1.427604	-1.038804				
H	-3.1751	1.840256	0.378452				
H	1.304245	1.501336	1.117354				
H	-1.792497	-0.687645	-1.433453				
H	-3.175917	1.839596	-0.377189				
H	0.176631	-1.773529	0.000394				
H	1.827543	-1.427205	1.039654				
Al	-1.145911	-0.562255	-0.00014				
P	0.794644	0.81665	-0.000111				
B	1.294539	-1.123899	0.000324				

Table S6 Cartesian coordinates and total energies (au) at the MP2/aug-cc-pvdz level of the relevant structures in the H_2-release from BH_3PH_3+BH_3

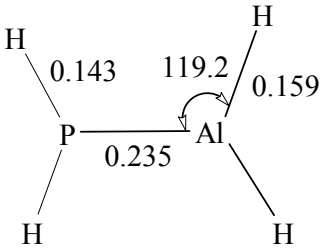
bbp-com1				bbp-com2			
Energy = -395.6488159				Energy = -395.6262089			
H	1.517325	0.740083	-0.355217	H	-0.179141	-0.633771	1.242751
H	1.287821	-1.290815	-0.749563	H	2.864165	-0.517421	0.460926
H	-2.292451	0.289219	0.250209	H	0.107991	-1.430182	-0.756583
H	0.386825	1.675856	1.095994	H	-0.617804	0.598106	-0.495995
H	0.084023	1.892102	-0.928119	H	2.443223	0.641362	-1.180634
H	-1.182077	-0.913586	-1.209813	H	2.167058	1.39729	0.708918
H	3.023604	-0.302783	-0.314825	H	-3.089452	0.961292	-0.948359
H	-0.885726	-1.252295	0.949937	H	-2.943876	-0.954129	-0.145503
H	1.688456	-0.715256	1.191838	H	-2.894944	0.706165	1.109205
B	0.375969	1.169808	0.002093	B	2.23378	0.414188	-0.004213
P	-0.994269	-0.217103	0.000751	B	-2.976231	0.238514	0.005012
B	1.881279	-0.543005	0.009567	P	0.390336	-0.268815	0.000085
bbp-tslew				bbp-tsbb			
Energy = -395.4987052				Energy = -395.5452977			
H	1.059445	-0.792948	-1.234828	H	-0.600783	1.291568	-0.262866
H	1.059416	-0.793155	1.234696	H	-1.879255	0.115889	1.183624
H	2.28814	0.382792	0.000049	H	1.005484	-1.396056	-1.092209
H	-0.568106	-1.484733	-0.000152	H	1.383232	1.718746	-0.953941
H	1.293409	1.139284	0.000094	H	0.893017	1.757559	1.130165
H	-0.616002	1.728576	1.060431	H	0.455856	-1.419248	1.100099
H	-0.615995	1.728703	-1.060216	H	-1.47379	1.020557	-0.617274
P	0.682847	-0.248696	-0.000025	H	-1.194436	-0.589375	-0.617678
B	-0.579162	1.161773	0.000074	H	-3.293677	-0.176797	-0.333516
B	-1.447406	-0.525558	-0.000015	B	0.879895	1.25872	0.036787
H	-2.00502	-0.679674	1.061215	P	0.736466	-0.571581	0.015399
H	-2.005151	-0.679487	-1.061203	B	-2.148422	-0.008546	0.009735
bbp-tsbp1				bbp-tsbp2			
Energy = -395.6093632				Energy = -395.5997264			
H	-0.262841	-1.204566	1.14524	H	0.513029	-1.179619	-0.495781
H	2.637257	-0.260173	0.230517	H	1.575237	-0.688487	1.193113
H	-0.007145	-1.481351	-0.992752	H	0.144312	1.910626	-0.962972
H	-0.906378	0.591954	-0.791138	H	-2.174695	0.101416	-0.749333
H	1.78917	1.053082	-1.102018	H	-1.572473	-0.449074	1.280038
H	1.586609	1.370139	0.91435	H	0.467209	1.726084	1.076281
H	-1.952412	1.291485	-0.857496	H	1.384494	-1.299416	-0.795244
H	-2.572059	-0.47921	-0.079107	H	1.433722	0.686804	-0.447087
H	-1.647644	1.050347	1.105912	H	3.042756	-0.422631	-0.259611
B	1.773881	0.570353	0.017501	P	-1.029996	-0.293539	-0.017245
B	-1.857839	0.470104	0.077018	B	0.246268	1.207489	0.015763

P	0.117016	-0.4756	-0.003073	B	1.881001	-0.404013	0.06809
$BH_3BH_2PH_2+H_2$				$BH_3PH_2BH_2+H_2$			
Energy = -395.6057209				Energy = -395.6257217			
H	1.200942	-1.322525	-0.464265	H	0.158718	-1.340441	-1.097187
H	1.678771	-0.644056	1.204989	H	0.157855	-1.341477	1.096296
H	0.129042	1.841823	-1.004864	H	3.246111	-0.500304	0.377193
H	-2.224725	0.312386	-0.643682	H	-2.657511	-0.462889	-0.000763
H	-1.621172	-0.289733	1.298836	H	3.260234	-0.47656	-0.379655
H	0.410523	1.694923	1.039705	H	1.662721	1.314071	1.048525
H	1.8838	-1.246186	-0.901599	H	1.66298	1.315075	-1.046097
H	1.46239	0.693264	-0.456645	P	-0.078488	-0.480586	-0.000138
H	3.186058	-0.245486	-0.149383	B	1.314858	0.850256	0.000973
P	-1.125231	-0.351309	-0.032964	B	-1.852687	0.448334	-0.000228
B	0.143555	1.162234	-0.00513	H	-1.812609	1.103819	1.025185
B	2.011014	-0.26719	0.119403	H	-1.812036	1.10455	-1.025156

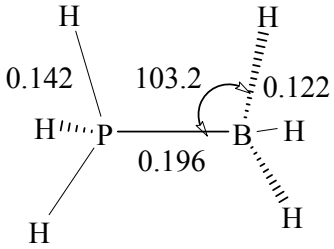
Figure S1 Selected MP2/aVDZ geometry parameters of the complexes and products for H_2-release from AlH_3PH_3, BH_3PH3 without or with the presence of AlH_3, BH_3. Bond lengths in nanometers and bond angles in degrees.



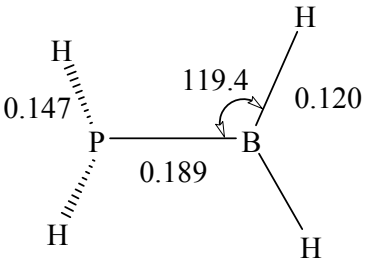
alp



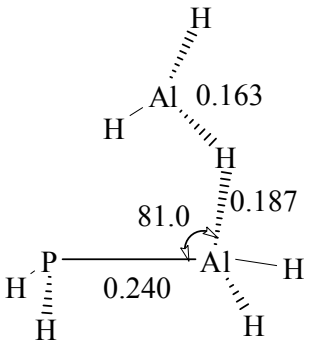
AlH_2PH_2



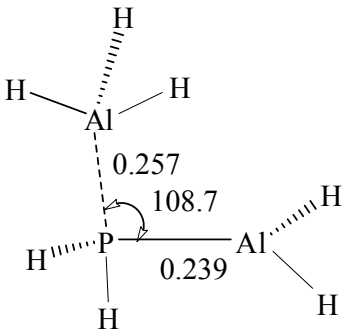
bp



BH_2PH_2



$AlH_3AlH_2PH_2$



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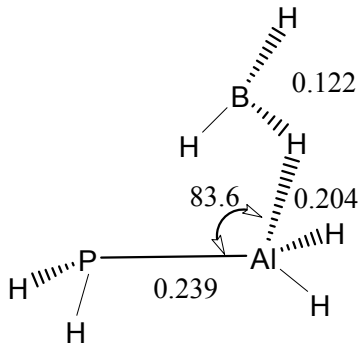
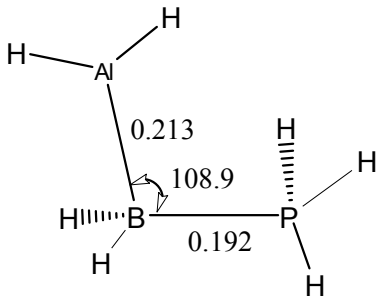


$BH_3AlH_2PH_2$



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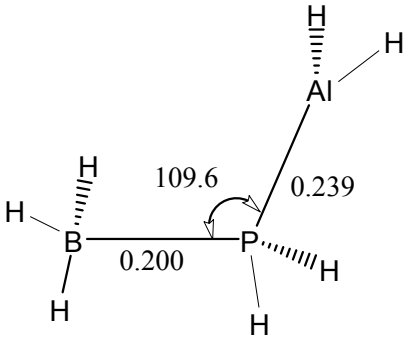

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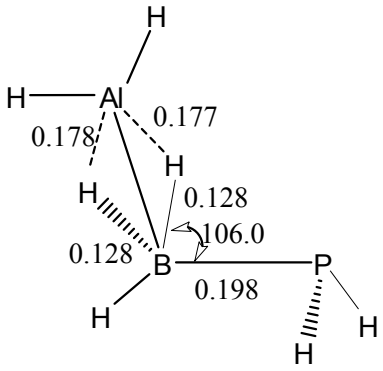

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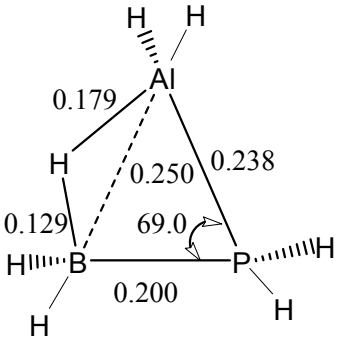
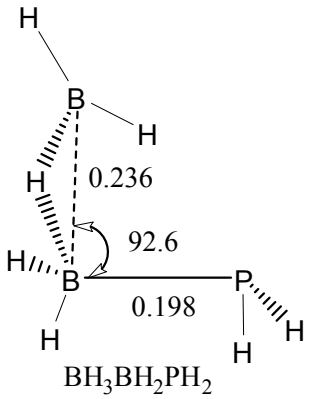


cyclic-$AlH_2BH_3PH_2$



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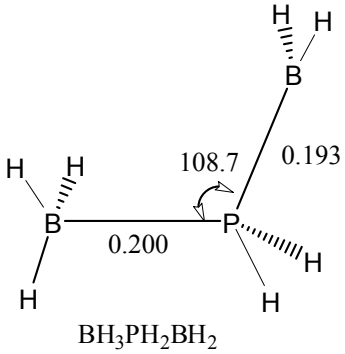

$BH_3PH_2BH_2$