

**SUPPORTING INFORMATION**

**Title:** Catalytic Dehydrogenation of Amine-Boranes using Geminal Phosphino-Boranes

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# **Catalytic Dehydrogenation of Amine-Boranes using Geminal Phosphino-Boranes**

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## 1. Computational details

All calculated structures were optimized at  $\omega$ -B97X-D level of theory,<sup>[1]</sup> with the Gaussian09 suite, revision D01.<sup>[2]</sup> Geometry optimizations were performed using the 6-311G(d,p) basis set,<sup>[3,4]</sup> and the nature of each stationary point was confirmed by frequency calculations. All calculations were performed in the gas phase at room temperature (298.15 K) and no solvent model was applied.

## 2. Cartesian Coordinates

### 2.1 Dehydrogenation of $\text{NH}_3 \cdot \text{BH}_3$

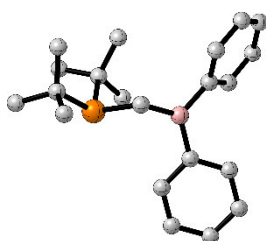
#### *t*Bu<sub>2</sub>PCH<sub>2</sub>Ph<sub>2</sub> (1)

E: -1184.48426998 a.u.

ZP correction: 0.463695 a.u.

H: -1183.995332 a.u.

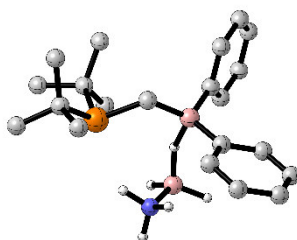
G: -1184.073406 a.u.



C	-0.485963000	0.159393000	-1.047812000	H	-4.147221000	1.305690000	-2.665795000
H	-0.552693000	0.942239000	-1.811888000	H	-2.806732000	2.212581000	-1.954275000
H	-0.766468000	-0.790999000	-1.512810000	H	-2.496489000	0.707525000	-2.839598000
P	-1.806568000	0.652748000	0.181182000	B	1.015962000	0.143498000	-0.556599000
C	-1.680763000	-0.714193000	1.491321000	C	1.782072000	1.473798000	-0.235616000
C	-1.401210000	-2.133026000	0.981531000	C	3.177586000	1.547835000	-0.379582000
C	-0.515109000	-0.277960000	2.397890000	C	1.112381000	2.648634000	0.145205000
C	-2.953880000	-0.721729000	2.349242000	C	3.870119000	2.730772000	-0.157226000
H	-2.187335000	-2.505058000	0.324571000	H	3.728083000	0.664983000	-0.686565000
H	-0.451902000	-2.198096000	0.448988000	C	1.801295000	3.827209000	0.392208000
H	-1.338198000	-2.816369000	1.836686000	H	0.034566000	2.630570000	0.268493000
H	-0.703632000	0.698434000	2.851125000	C	3.182469000	3.871787000	0.237026000
H	-0.381994000	-1.012262000	3.200315000	H	4.945995000	2.762973000	-0.289558000
H	0.435924000	-0.219167000	1.862364000	H	1.260947000	4.715710000	0.699882000
H	-2.786728000	-1.339059000	3.238636000	H	3.720317000	4.795886000	0.419797000
H	-3.221534000	0.283666000	2.688042000	C	1.784277000	-1.227296000	-0.474722000
H	-3.807055000	-1.145212000	1.815127000	C	1.572541000	-2.241640000	-1.419091000
C	-3.383307000	0.402635000	-0.854364000	C	2.681716000	-1.498225000	0.568587000
C	-3.743305000	-1.039175000	-1.222437000	C	2.229965000	-3.461461000	-1.335308000
C	-4.550172000	1.051039000	-0.090435000	H	0.883239000	-2.073467000	-2.240927000
C	-3.184980000	1.204431000	-2.152624000	C	3.315956000	-2.728507000	0.679997000
H	-2.914083000	-1.554388000	-1.715224000	H	2.872156000	-0.735662000	1.317283000
H	-4.038985000	-1.622881000	-0.348458000	C	3.096429000	-3.711411000	-0.277532000
H	-4.589847000	-1.039991000	-1.919035000	H	2.058880000	-4.222771000	-2.088414000
H	-4.340496000	2.101557000	0.128006000	H	3.988493000	-2.918727000	1.509160000
H	-5.458328000	1.007411000	-0.702583000	H	3.597446000	-4.669904000	-0.198754000
H	-4.766325000	0.548617000	0.853134000				

***t*Bu<sub>2</sub>PCH<sub>2</sub>Ph<sub>2</sub> – BHB interaction (4)**

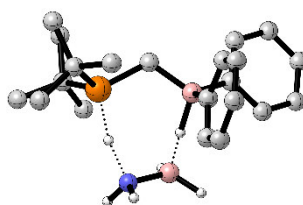
E: -1267.71771195 a.u.  
ZP correction: 0.537330 a.u.  
H: -1267.151457 a.u.  
G: -1267.237087 a.u.



C	0.429700000	-0.295556000	-0.717797000	C	-2.105863000	-1.207748000	-0.189697000
H	0.390299000	-1.255368000	-1.232661000	C	-3.471358000	-0.959384000	0.006259000
H	0.604104000	0.444017000	-1.504426000	C	-1.744933000	-2.535231000	-0.462848000
P	1.928727000	-0.397727000	0.363870000	C	-4.418101000	-1.971998000	-0.054908000
C	2.442508000	1.422958000	0.569749000	H	-3.794564000	0.055627000	0.212142000
C	2.180080000	2.306225000	-0.657279000	C	-2.684808000	-3.562218000	-0.519783000
C	1.607164000	1.974936000	1.736556000	H	-0.704345000	-2.786280000	-0.654695000
C	3.921183000	1.522940000	0.965750000	C	-4.028040000	-3.282123000	-0.313590000
H	2.651132000	1.924422000	-1.564368000	H	-5.466674000	-1.741442000	0.100295000
H	1.111171000	2.426458000	-0.845399000	H	-2.367322000	-4.576837000	-0.737212000
H	2.588272000	3.305560000	-0.468413000	H	-4.767079000	-4.074220000	-0.362110000
H	1.780940000	1.417662000	2.660121000	C	-1.608405000	1.467414000	-0.240746000
H	1.883323000	3.021318000	1.909825000	C	-1.685059000	2.000469000	-1.534322000
H	0.538656000	1.953127000	1.520970000	C	-2.083221000	2.267811000	0.802764000
H	4.134927000	2.549047000	1.283510000	C	-2.201680000	3.267382000	-1.774709000
H	4.166185000	0.860649000	1.801282000	H	-1.338406000	1.409106000	-2.377843000
H	4.590075000	1.295234000	0.133362000	C	-2.596976000	3.539905000	0.574221000
C	3.181415000	-1.307349000	-0.741313000	H	-2.046415000	1.891664000	1.820868000
C	3.582470000	-0.570802000	-2.021899000	C	-2.657386000	4.046141000	-0.717213000
C	4.430151000	-1.645953000	0.090321000	H	-2.248482000	3.649485000	-2.789164000
C	2.532687000	-2.650209000	-1.128158000	H	-2.949558000	4.136785000	1.408772000
H	2.706706000	-0.286236000	-2.611577000	H	-3.057646000	5.037425000	-0.899333000
H	4.159624000	0.331397000	-1.810628000	H	-0.764686000	0.084192000	1.378291000
H	4.206660000	-1.220889000	-2.646192000	B	-0.950792000	-0.466876000	2.505939000
H	4.161241000	-2.189644000	1.000883000	H	-0.311789000	0.201356000	3.274191000
H	5.096702000	-2.285662000	-0.498920000	H	-2.124571000	-0.579168000	2.720004000
H	4.998039000	-0.763695000	0.381999000	N	-0.262213000	-1.890265000	2.348853000
H	3.297662000	-3.314421000	-1.543543000	H	-0.205370000	-2.380219000	3.235873000
H	2.096099000	-3.155460000	-0.259416000	H	-0.785747000	-2.466013000	1.686765000
H	1.756787000	-2.537215000	-1.887669000	H	0.689383000	-1.736653000	1.972284000
B	-1.029194000	-0.015728000	-0.053145000				

***t*Bu<sub>2</sub>PCH<sub>2</sub>Ph<sub>2</sub> – TS H<sub>2</sub> abstraction (TS<sub>4.2</sub>)**

E: -1267.69490620 a.u.  
ZP correction: 0.530168 a.u.  
H: -1267.136157 a.u.  
G: -1267.220673 a.u.



C	-0.172037000	-0.630895000	-0.735942000	C	-1.934069000	-2.870245000	0.991454000
H	-0.161548000	-0.165782000	-1.727518000	C	-4.129846000	-1.760831000	0.584963000
H	-0.116263000	-1.709306000	-0.902962000	H	-3.353982000	-1.997447000	-2.059953000
P	-1.770234000	-0.316146000	0.079704000	H	-1.770996000	-2.731543000	-1.779860000
C	-2.708428000	-1.940141000	0.037885000	H	-3.235265000	-3.568543000	-1.268193000
C	-2.765181000	-2.583249000	-1.353793000	H	-1.936777000	-2.491731000	2.016020000

H	-2.412863000	-3.854466000	0.994327000	H	1.061222000	1.857138000	2.208732000
H	-0.891219000	-3.006826000	0.697427000	C	1.765942000	4.219914000	-0.108462000
H	-4.587840000	-2.745514000	0.722147000	H	2.194517000	3.816499000	-2.176469000
H	-4.133687000	-1.256607000	1.555819000	H	1.353929000	4.287080000	1.997081000
H	-4.766224000	-1.196861000	-0.100015000	H	1.904204000	5.291401000	-0.202616000
C	-2.682653000	1.100676000	-0.738617000	C	2.449684000	-1.029396000	-0.141842000
C	-3.316480000	0.706989000	-2.076560000	C	2.648132000	-1.703720000	-1.350523000
C	-3.755662000	1.619826000	0.232778000	C	3.488045000	-1.088548000	0.796309000
C	-1.671674000	2.232340000	-0.977692000	C	3.823294000	-2.400708000	-1.618092000
H	-2.583841000	0.264131000	-2.757011000	H	1.874269000	-1.684544000	-2.113759000
H	-4.143587000	0.004999000	-1.951774000	C	4.657590000	-1.792409000	0.547033000
H	-3.716937000	1.603870000	-2.560113000	H	3.369590000	-0.573462000	1.744625000
H	-3.311068000	1.934240000	1.180858000	C	4.831750000	-2.450950000	-0.666399000
H	-4.242672000	2.494071000	-0.210846000	H	3.949090000	-2.906090000	-2.570245000
H	-4.531189000	0.883291000	0.445509000	H	5.439230000	-1.825706000	1.298867000
H	-2.212519000	3.105687000	-1.355877000	H	5.748010000	-2.995930000	-0.866623000
H	-1.147375000	2.528861000	-0.066426000	H	0.831790000	-0.461377000	1.414043000
H	-0.914751000	1.964319000	-1.714922000	H	-1.442606000	-0.031201000	1.629626000
B	1.133012000	-0.158290000	0.144353000	B	0.552451000	-0.687147000	2.702280000
C	1.392477000	1.427859000	0.131773000	N	-0.808036000	-0.002743000	2.934305000
C	1.746410000	2.021158000	-1.088129000	H	0.476223000	-1.888028000	2.723216000
C	1.274175000	2.278724000	1.232621000	H	1.497719000	-0.196973000	3.262273000
C	1.925265000	3.390857000	-1.215256000	H	-1.375945000	-0.517277000	3.598190000
H	1.886539000	1.389472000	-1.962480000	H	-0.733357000	0.951228000	3.269756000
C	1.453037000	3.655668000	1.119872000				

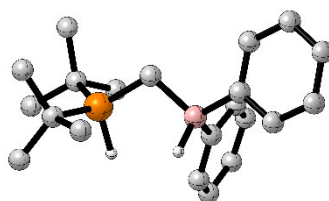
### ***t*Bu<sub>2</sub>PCH<sub>2</sub>Ph<sub>2</sub> – H<sub>2</sub> adduct (2)**

E: -1185.66935680 a.u.

ZP correction: 0.482809 a.u.

H: -1185.160983 a.u.

G: -1185.239873 a.u.



C	-0.035846000	-0.729393000	0.612405000	H	-3.913868000	-2.307135000	0.804271000
H	0.031358000	-1.790876000	0.866070000	H	-3.366267000	-3.755506000	-0.039680000
H	0.060668000	-0.156963000	1.538651000	H	-3.046379000	-1.015052000	-2.628204000
P	-1.641713000	-0.413544000	-0.083549000	H	-3.861682000	-2.532546000	-2.250183000
C	-2.697983000	0.627775000	1.036789000	H	-4.324162000	-1.060028000	-1.401880000
C	-2.794044000	0.004109000	2.435718000	H	-1.761167000	-3.658180000	-1.902724000
C	-1.973688000	1.985107000	1.129136000	H	-0.804874000	-2.200192000	-2.231514000
C	-4.099172000	0.841761000	0.453670000	H	-0.537276000	-3.108939000	-0.750470000
H	-3.330307000	-0.946345000	2.435233000	B	1.138321000	-0.267229000	-0.505437000
H	-1.808766000	-0.157837000	2.877693000	C	2.580238000	-0.850114000	-0.065625000
H	-3.339860000	0.692490000	3.087802000	C	3.588480000	-1.008767000	-1.026683000
H	-1.859577000	2.465535000	0.153988000	C	2.922604000	-1.181103000	1.250254000
H	-2.563406000	2.646829000	1.770536000	C	4.857848000	-1.465785000	-0.699625000
H	-0.975546000	1.898468000	1.561560000	H	3.363807000	-0.765084000	-2.061677000
H	-4.625057000	1.579616000	1.066727000	C	4.191768000	-1.639915000	1.595299000
H	-4.063651000	1.229772000	-0.568109000	H	2.181578000	-1.082475000	2.040755000
H	-4.694053000	-0.074094000	0.463001000	C	5.167285000	-1.784966000	0.619249000
C	-2.417959000	-1.963024000	-0.760120000	H	5.611064000	-1.575731000	-1.473744000
C	-3.039261000	-2.794768000	0.368383000	H	4.417161000	-1.883857000	2.629035000
C	-3.476171000	-1.605706000	-1.815019000	H	6.157275000	-2.144254000	0.879753000
C	-1.304599000	-2.773261000	-1.449014000	C	1.105160000	1.357631000	-0.575073000
H	-2.320558000	-3.002003000	1.166000000	C	1.560330000	2.139289000	0.496931000

C	0.547706000	2.053042000	-1.654653000	H	1.799049000	4.092431000	1.359905000
C	1.432983000	3.522127000	0.511758000	H	-0.027046000	3.941917000	-2.513588000
H	2.035084000	1.644310000	1.341543000	H	0.740856000	5.260784000	-0.557453000
C	0.410559000	3.439997000	-1.655939000	H	-1.499430000	0.403111000	-1.215022000
H	0.221914000	1.488849000	-2.525960000	H	0.820552000	-0.716801000	-1.604010000
C	0.843206000	4.180814000	-0.564155000				

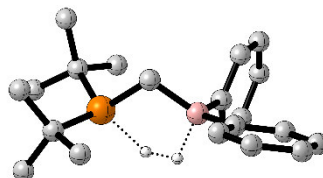
### ***t*Bu<sub>2</sub>PCH<sub>2</sub>Ph<sub>2</sub> – TS H<sub>2</sub> elimination**

E: -1185.62673695 a.u.

ZP correction: 0.478147 a.u.

H: -1185.123321 a.u.

G: -1185.201454 a.u.



C	0.209039000	-0.476643000	-0.880336000	H	0.632428000	-2.762067000	1.300303000
H	0.161656000	-1.464436000	-1.341585000	H	0.830947000	-3.234088000	-0.393514000
H	0.294973000	0.247970000	-1.692776000	B	-1.087281000	-0.103597000	0.068762000
P	1.655414000	-0.340427000	0.234776000	C	-2.408721000	-1.002127000	-0.047511000
C	2.803108000	1.009804000	-0.398866000	C	-3.681004000	-0.452336000	0.153973000
C	3.113933000	0.872894000	-1.895983000	C	-2.351682000	-2.376110000	-0.316112000
C	2.062100000	2.337412000	-0.163698000	C	-4.833070000	-1.228072000	0.088455000
C	4.110947000	1.027603000	0.401714000	H	-3.771210000	0.608973000	0.362627000
H	3.653880000	-0.044703000	-2.131406000	C	-3.494435000	-3.163037000	-0.378917000
H	2.206828000	0.901316000	-2.502486000	H	-1.388655000	-2.850962000	-0.475955000
H	3.741816000	1.716043000	-2.204285000	C	-4.744126000	-2.588521000	-0.177555000
H	1.845304000	2.499416000	0.894539000	H	-5.803328000	-0.768337000	0.245157000
H	2.694362000	3.160167000	-0.513852000	H	-3.411164000	-4.225068000	-0.585630000
H	1.114565000	2.389134000	-0.703757000	H	-5.641003000	-3.196564000	-0.228361000
H	4.677603000	1.925241000	0.133940000	C	-1.309273000	1.483276000	0.186190000
H	3.929633000	1.060699000	1.479524000	C	-1.621613000	2.224752000	-0.961780000
H	4.742220000	0.164686000	0.178665000	C	-1.179213000	2.195209000	1.380986000
C	2.488794000	-2.019120000	0.372279000	C	-1.778191000	3.604231000	-0.923562000
C	3.340793000	-2.400824000	-0.841223000	H	-1.747729000	1.708003000	-1.910133000
C	3.340976000	-2.039317000	1.652238000	C	-1.328633000	3.578033000	1.432337000
C	1.363265000	-3.056680000	0.542038000	H	-0.949811000	1.657041000	2.296812000
H	2.775493000	-2.320416000	-1.773663000	C	-1.623650000	4.289348000	0.277433000
H	4.235256000	-1.779755000	-0.923737000	H	-2.020843000	4.147360000	-1.831125000
H	3.671307000	-3.440392000	-0.739426000	H	-1.213900000	4.099464000	2.377007000
H	2.735360000	-1.816438000	2.534693000	H	-1.740803000	5.366966000	0.312254000
H	3.769210000	-3.038714000	1.782580000	H	0.353745000	-0.245674000	1.346373000
H	4.167585000	-1.329718000	1.620783000	H	-0.621475000	-0.421234000	1.354032000
H	1.804884000	-4.008182000	0.854343000				

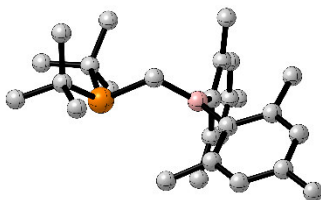
### ***t*Bu<sub>2</sub>PCH<sub>2</sub>BMe<sub>2</sub> (6)**

E: -1420.36419007 a.u.

ZP correction: 0.630541 a.u.

H: -1419.698895 a.u.

G: -1419.795924 a.u.



C	-0.487425000	-0.901155000	0.780533000	H	-0.955906000	-0.509356000	1.687294000
H	-0.043693000	-1.859579000	1.050991000	P	-1.867816000	-1.288548000	-0.447365000

C	-3.248515000	-0.045078000	0.007288000	H	5.280114000	0.025202000	1.439718000
C	-3.278365000	0.416175000	1.467748000	C	0.338915000	1.617040000	0.076261000
C	-3.007927000	1.181397000	-0.890448000	C	-0.113186000	2.498586000	1.071217000
C	-4.627056000	-0.610725000	-0.359416000	C	0.432599000	2.100274000	-1.249599000
H	-3.337479000	-0.414665000	2.174410000	C	-0.471159000	3.806630000	0.738512000
H	-2.403011000	1.017316000	1.712308000	C	0.063383000	3.405030000	-1.543835000
H	-4.157240000	1.051182000	1.627604000	C	-0.396439000	4.279583000	-0.561314000
H	-3.053161000	0.911377000	-1.948907000	H	-0.817624000	4.470997000	1.526285000
H	-3.784166000	1.930831000	-0.696243000	H	0.125560000	3.750591000	-2.572498000
H	-2.043589000	1.650623000	-0.700088000	C	2.980478000	1.230628000	1.907577000
H	-5.359182000	0.203726000	-0.334362000	H	2.560871000	2.109793000	1.414735000
H	-4.644064000	-1.035449000	-1.366671000	H	2.291940000	0.937560000	2.704051000
H	-4.963991000	-1.370523000	0.348307000	H	3.919896000	1.521787000	2.380769000
C	-2.362484000	-3.031556000	0.162394000	C	6.207340000	-2.005162000	-0.108378000
C	-2.782565000	-3.110866000	1.632232000	H	6.951272000	-1.213962000	0.011801000
C	-3.476206000	-3.598331000	-0.736446000	H	6.378509000	-2.741350000	0.683648000
C	-1.142361000	-3.944374000	-0.068748000	H	6.387172000	-2.500426000	-1.064946000
H	-2.012955000	-2.710242000	2.297792000	C	1.477131000	-2.131532000	-1.659559000
H	-3.711475000	-2.567550000	1.817846000	H	1.503007000	-3.222054000	-1.586723000
H	-2.952461000	-4.156282000	1.915515000	H	0.450944000	-1.809770000	-1.494915000
H	-3.238442000	-3.462036000	-1.795458000	H	1.729715000	-1.868013000	-2.691845000
H	-3.573914000	-4.673876000	-0.552130000	C	0.861211000	1.195356000	-2.379022000
H	-4.449093000	-3.150095000	-0.546755000	H	0.180370000	0.343149000	-2.476381000
H	-1.417758000	-4.974355000	0.182057000	H	0.855160000	1.730594000	-3.330195000
H	-0.831497000	-3.928388000	-1.116462000	H	1.866883000	0.800391000	-2.216061000
H	-0.277375000	-3.685600000	0.544401000	C	-0.179938000	2.131352000	2.536544000
B	0.668237000	0.088778000	0.328257000	H	-1.130558000	2.444480000	2.976159000
C	2.151247000	-0.455540000	0.165612000	H	-0.060232000	1.063408000	2.718174000
C	2.472793000	-1.510939000	-0.710264000	H	0.615144000	2.642302000	3.088186000
C	3.205230000	0.101267000	0.931546000	C	-0.788710000	5.690161000	-0.912708000
C	3.782415000	-1.983684000	-0.798856000	H	-1.187182000	6.219887000	-0.045284000
C	4.492947000	-0.410387000	0.830050000	H	0.071918000	6.252855000	-1.286135000
C	4.807510000	-1.456695000	-0.031418000	H	-1.551683000	5.700932000	-1.695936000
H	4.000141000	-2.785798000	-1.499897000				

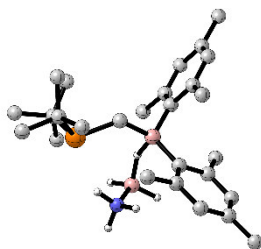
### ***t*Bu<sub>2</sub>PCH<sub>2</sub>BMe<sub>2</sub> – BHB interaction (9)**

E: -1503.58657016 a.u.

ZP correction: 0.706030 a.u.

H: -1502.842791 a.u.

G: -1502.944609 a.u.



C	0.957527000	-0.044558000	-0.460620000	H	1.825620000	0.693451000	2.627579000
H	0.794044000	-0.547075000	-1.414405000	H	5.341299000	1.127098000	1.883054000
H	1.211542000	0.977390000	-0.744863000	H	5.177257000	-0.595981000	1.546489000
P	2.519946000	-0.825123000	0.201493000	H	5.420848000	0.559502000	0.220582000
C	3.403751000	0.614045000	1.108550000	C	3.524265000	-1.189389000	-1.391198000
C	3.120597000	2.011583000	0.540234000	C	3.890403000	0.059375000	-2.201548000
C	2.902049000	0.567705000	2.557805000	C	4.788581000	-1.985458000	-1.021257000
C	4.922797000	0.401270000	1.177333000	C	2.705094000	-2.112156000	-2.307186000
H	3.421427000	2.113519000	-0.503275000	H	3.001975000	0.643960000	-2.456181000
H	2.065800000	2.281813000	0.609758000	H	4.587871000	0.710316000	-1.674125000
H	3.683618000	2.751352000	1.120484000	H	4.369917000	-0.240108000	-3.140623000
H	3.158647000	-0.380654000	3.039489000	H	4.534840000	-2.869121000	-0.428467000
H	3.367585000	1.375506000	3.133870000	H	5.277542000	-2.328925000	-1.939558000



H	5.519459000	-1.403888000	-0.465014000	H	-0.452287000	-2.543534000	1.614595000
H	3.334836000	-2.410942000	-3.151818000	H	1.112208000	-2.019916000	1.811609000
H	2.388041000	-3.023597000	-1.795863000	C	-0.406155000	2.594024000	2.158922000
H	1.826306000	-1.619765000	-2.725386000	H	0.586598000	2.146303000	2.189956000
B	-0.551257000	0.047767000	0.234764000	H	-0.330348000	3.589693000	2.600245000
C	-1.714837000	-1.108932000	0.132838000	H	-1.043781000	1.991544000	2.812203000
C	-3.013154000	-0.830657000	0.653997000	C	-2.403175000	5.498119000	-1.374526000
C	-1.547511000	-2.390920000	-0.439388000	H	-3.475759000	5.614714000	-1.187952000
C	-4.028606000	-1.779218000	0.587027000	H	-1.886423000	6.295065000	-0.834598000
C	-2.595064000	-3.317900000	-0.483205000	H	-2.237955000	5.650836000	-2.443962000
C	-3.850374000	-3.034228000	0.019617000	C	-1.830920000	0.643556000	-2.370462000
H	-5.000909000	-1.528508000	1.002941000	H	-0.960394000	-0.009619000	-2.456362000
H	-2.414178000	-4.288648000	-0.937195000	H	-2.675469000	0.009206000	-2.087952000
C	-1.076797000	1.551710000	-0.084980000	H	-2.032253000	1.054185000	-3.362100000
C	-1.624932000	1.762915000	-1.371399000	C	-3.403647000	0.478273000	1.300443000
C	-0.952437000	2.677182000	0.753814000	H	-2.654466000	0.832883000	2.005108000
C	-2.032486000	3.034191000	-1.768867000	H	-3.545155000	1.263244000	0.554732000
C	-1.375731000	3.934028000	0.321089000	H	-4.341306000	0.356009000	1.846652000
C	-1.924269000	4.139037000	-0.935914000	C	-4.980342000	-4.025956000	-0.049257000
H	-2.449931000	3.163280000	-2.764558000	H	-5.457848000	-4.149736000	0.926565000
H	-1.271978000	4.780525000	0.995255000	H	-5.750462000	-3.688464000	-0.749433000
H	-0.289422000	0.060605000	1.694093000	H	-4.630684000	-5.004995000	-0.383713000
B	-0.386587000	-0.702050000	2.723666000	C	-0.266309000	-2.854592000	-1.085746000
H	0.324561000	-0.213836000	3.555865000	H	-0.132405000	-2.385119000	-2.063323000
H	-1.537347000	-0.819356000	3.027298000	H	0.621659000	-2.627948000	-0.497062000
N	0.195446000	-2.112688000	2.278470000	H	-0.286812000	-3.934205000	-1.249925000
H	0.296067000	-2.729279000	3.078765000				

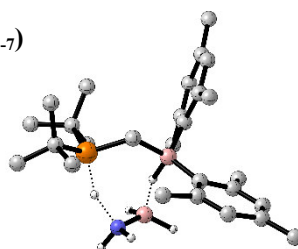
***t*Bu<sub>2</sub>PCH<sub>2</sub>BMe<sub>2</sub> – TS H<sub>2</sub> abstraction (TS<sub>9-7</sub>)**

E: -1503.56051412 a.u.

ZP correction: 0.699799 a.u.

H: -1502.823606 a.u.

G: -1502.924181 a.u.



C	0.736073000	-0.478925000	-0.628529000	C	2.307618000	-3.258681000	-1.421689000
H	0.484376000	-1.291421000	-1.301925000	H	2.950717000	-0.863581000	-2.683332000
H	1.013821000	0.352101000	-1.278506000	H	4.515079000	-0.628857000	-1.887524000
P	2.252055000	-1.015884000	0.220822000	H	4.224389000	-2.076941000	-2.850765000
C	3.231101000	0.527338000	0.689893000	H	4.016831000	-3.334239000	0.722378000
C	3.083233000	1.627810000	-0.372362000	H	4.844797000	-3.564035000	-0.819941000
C	2.636602000	1.034634000	2.007986000	H	5.166875000	-2.125061000	0.137491000
C	4.717480000	0.236396000	0.931659000	H	2.906215000	-3.977143000	-1.989966000
H	3.390442000	1.299881000	-1.367921000	H	1.842231000	-3.799503000	-0.593766000
H	2.059510000	2.003900000	-0.427274000	H	1.522664000	-2.895438000	-2.084324000
H	3.723872000	2.469102000	-0.088334000	B	-0.604846000	-0.009790000	0.287277000
H	2.767479000	0.315834000	2.820139000	C	-2.015573000	-0.852799000	0.176591000
H	3.136356000	1.967869000	2.287499000	C	-3.204145000	-0.257132000	0.686857000
H	1.577154000	1.243042000	1.907328000	C	-2.186822000	-2.123534000	-0.415462000
H	5.175925000	1.142582000	1.339428000	C	-4.449021000	-0.848798000	0.501148000
H	4.867503000	-0.560846000	1.664077000	C	-3.455342000	-2.688471000	-0.584712000
H	5.257082000	-0.014931000	0.017525000	C	-4.609119000	-2.059005000	-0.159708000
C	3.235225000	-2.134959000	-0.931730000	H	-5.327514000	-0.350100000	0.903096000
C	3.761092000	-1.371491000	-2.152981000	H	-3.532703000	-3.663088000	-1.060629000
C	4.384289000	-2.815201000	-0.167740000	C	-0.730824000	1.601234000	-0.015424000

C	-1.040159000	1.940874000	-1.362605000	H	-0.884632000	0.062571000	-2.476676000
C	-0.453406000	2.676849000	0.849280000	H	-2.515270000	0.515865000	-2.034467000
C	-0.944988000	3.251681000	-1.812285000	H	-1.683821000	1.376278000	-3.338853000
C	-0.350129000	3.983677000	0.355073000	C	-0.365120000	2.575127000	2.357599000
C	-0.563755000	4.295344000	-0.973750000	H	0.498805000	3.126328000	2.740459000
H	-1.181900000	3.468833000	-2.851041000	H	-1.257399000	3.035428000	2.794747000
H	-0.111092000	4.781678000	1.054704000	H	-0.313240000	1.560362000	2.737966000
H	-0.209154000	-0.120181000	1.578176000	C	-3.209708000	1.017330000	1.495807000
B	-0.249379000	-0.940790000	2.678479000	H	-2.425105000	1.006886000	2.251130000
H	0.437218000	-0.288042000	3.425200000	H	-3.060966000	1.902148000	0.874414000
H	-1.418495000	-1.000332000	2.937637000	H	-4.165101000	1.124184000	2.014167000
N	0.450597000	-2.248610000	2.293322000	C	-1.057769000	-3.002882000	-0.903108000
H	0.858796000	-2.684065000	3.113329000	H	-0.746680000	-2.747108000	-1.921888000
H	-0.188318000	-2.919680000	1.879330000	H	-0.180589000	-2.950116000	-0.262885000
H	1.573804000	-1.821041000	1.407070000	H	-1.380655000	-4.046292000	-0.927715000
C	-0.403708000	5.697783000	-1.498487000	C	-5.972376000	-2.665049000	-0.361294000
H	-1.183349000	5.941298000	-2.224962000	H	-5.904836000	-3.643349000	-0.842256000
H	-0.450976000	6.432614000	-0.691568000	H	-6.491251000	-2.792821000	0.593255000
H	0.561448000	5.820026000	-2.001257000	H	-6.597864000	-2.024017000	-0.989849000
C	-1.551804000	0.918322000	-2.356241000				

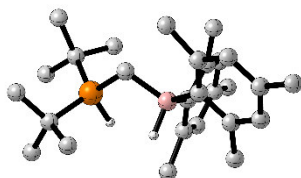
***t*Bu<sub>2</sub>PCH<sub>2</sub>BMe<sub>2</sub> – H<sub>2</sub> adduct (7)**

E: -1421.55067809 a.u.

ZP correction: 0.650071 a.u.

H: -1420.865517 a.u.

G: -1420.963306 a.u.



C	0.375129000	-1.104557000	-0.636315000	H	1.508771000	-3.873991000	2.370555000
H	0.149141000	-2.169044000	-0.717594000	H	0.850935000	-2.230605000	2.461108000
H	0.439410000	-0.707891000	-1.650336000	H	0.408321000	-3.278641000	1.120337000
P	2.007462000	-0.983667000	0.073179000	B	-0.723102000	-0.274336000	0.342612000
C	3.244513000	-0.364266000	-1.168359000	C	-2.317390000	-0.567089000	0.068887000
C	3.236189000	-1.225361000	-2.438434000	C	-3.223102000	-0.035374000	1.024411000
C	2.782198000	1.064241000	-1.516326000	C	-2.901645000	-1.310626000	-0.980538000
C	4.656464000	-0.305344000	-0.574926000	C	-4.596747000	-0.226779000	0.913956000
H	3.613182000	-2.234021000	-2.262783000	C	-4.287315000	-1.485702000	-1.060820000
H	2.237713000	-1.302778000	-2.874048000	C	-5.159322000	-0.952456000	-0.127807000
H	3.885011000	-0.754195000	-3.182818000	H	-5.250382000	0.206873000	1.667746000
H	2.721197000	1.713937000	-0.638775000	H	-4.694834000	-2.056876000	-1.891945000
H	3.502787000	1.497928000	-2.216252000	C	-0.267539000	1.314766000	0.284515000
H	1.801791000	1.078498000	-1.994067000	C	-0.462161000	2.084714000	-0.889840000
H	5.312116000	0.214257000	-1.279828000	C	0.428673000	1.961337000	1.335160000
H	4.682774000	0.248978000	0.367345000	C	0.045135000	3.376828000	-1.006466000
H	5.077099000	-1.299704000	-0.410211000	C	0.944263000	3.252172000	1.178826000
C	2.475393000	-2.520568000	1.013090000	C	0.770472000	3.980484000	0.012991000
C	2.940945000	-3.622365000	0.053817000	H	-0.126063000	3.927368000	-1.928896000
C	3.572391000	-2.193396000	2.037766000	H	1.485382000	3.704383000	2.007701000
C	1.228625000	-2.995530000	1.780920000	H	2.038322000	0.016761000	1.050579000
H	2.205866000	-3.816255000	-0.732350000	H	-0.514482000	-0.720487000	1.458469000
H	3.897022000	-3.379812000	-0.414878000	C	0.628362000	1.357660000	2.712235000
H	3.075109000	-4.550870000	0.616239000	H	1.597046000	1.650129000	3.129990000
H	3.248789000	-1.413892000	2.732802000	H	-0.141985000	1.727784000	3.396678000
H	3.781407000	-3.092950000	2.624419000	H	0.550205000	0.272734000	2.718238000
H	4.507326000	-1.877715000	1.575373000	C	-1.207337000	1.545559000	-2.088134000

H	-0.601013000	0.828591000	-2.654765000	H	-1.409834000	-1.275790000	-2.570867000
H	-2.124175000	1.033972000	-1.798169000	C	-2.742688000	0.760928000	2.213330000
H	-1.464917000	2.352815000	-2.777343000	H	-2.023513000	0.187124000	2.803643000
C	1.303400000	5.382763000	-0.126938000	H	-2.239014000	1.679361000	1.902733000
H	1.521163000	5.621360000	-1.170953000	H	-3.578667000	1.032492000	2.862143000
H	0.573875000	6.115989000	0.232123000	C	-6.648958000	-1.156649000	-0.222849000
H	2.220120000	5.520598000	0.452020000	H	-7.004767000	-1.837188000	0.557637000
C	-2.111900000	-1.963076000	-2.097937000	H	-7.186173000	-0.211591000	-0.102123000
H	-1.545905000	-2.832030000	-1.748938000	H	-6.929833000	-1.583607000	-1.188548000
H	-2.789045000	-2.319216000	-2.877418000				

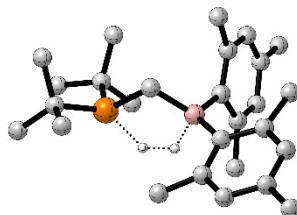
***t*Bu<sub>2</sub>PCH<sub>2</sub>BMes<sub>2</sub> – TS H<sub>2</sub> elimination (TS<sub>7-6</sub>)**

E: -1421.50508426 a.u.

ZP correction: 0.646415 a.u.

H: -1420.824417 a.u.

G: -1420.919804 a.u.



C	-0.633907000	-0.775482000	0.890760000	H	5.277715000	-0.492824000	1.058096000
H	-0.282578000	-1.728198000	1.293108000	H	3.467627000	-3.690041000	-1.086019000
H	-0.996210000	-0.196863000	1.736703000	C	0.546450000	1.583342000	0.015172000
P	-2.010571000	-1.126980000	-0.259980000	C	0.228075000	2.369512000	1.141251000
C	-3.175897000	0.366642000	-0.318123000	C	0.829659000	2.274310000	-1.186588000
C	-3.265987000	1.086580000	1.032421000	C	0.088035000	3.753427000	1.025072000
C	-2.595108000	1.338633000	-1.360806000	C	0.691588000	3.656457000	-1.266150000
C	-4.584410000	-0.016870000	-0.791219000	C	0.289195000	4.418176000	-0.174819000
H	-3.551042000	0.418757000	1.848575000	H	-0.159499000	4.330412000	1.913596000
H	-2.318361000	1.564745000	1.279090000	H	0.909531000	4.154978000	-2.207561000
H	-4.021761000	1.876130000	0.965086000	C	1.064525000	-2.700610000	-1.368057000
H	-2.553236000	0.881266000	-2.353215000	H	0.129152000	-2.702402000	-0.812821000
H	-3.243119000	2.219305000	-1.421161000	H	0.874729000	-2.182362000	-2.314057000
H	-1.598041000	1.684923000	-1.092678000	H	1.308433000	-3.739570000	-1.600593000
H	-5.148653000	0.906642000	-0.954828000	C	5.833248000	-2.946367000	0.048311000
H	-4.566523000	-0.559018000	-1.739870000	H	5.869442000	-3.718347000	-0.723644000
H	-5.134596000	-0.606510000	-0.056716000	H	6.682505000	-2.274843000	-0.101766000
C	-2.909366000	-2.692501000	0.318901000	H	5.971208000	-3.438131000	1.016803000
C	-3.595902000	-2.452945000	1.670710000	C	3.266988000	1.134341000	1.253579000
C	-3.918300000	-3.185311000	-0.731742000	H	3.040136000	1.934062000	0.547249000
C	-1.870969000	-3.814712000	0.490471000	H	2.565356000	1.229648000	2.081602000
H	-2.875824000	-2.135204000	2.429538000	H	4.267826000	1.309919000	1.653497000
H	-4.384466000	-1.700888000	1.612252000	C	1.284544000	1.546031000	-2.429818000
H	-4.055301000	-3.385751000	2.015601000	H	1.736755000	2.243921000	-3.137814000
H	-3.460687000	-3.251229000	-1.722932000	H	2.016941000	0.770052000	-2.196730000
H	-4.250959000	-4.191013000	-0.454872000	H	0.444304000	1.058689000	-2.936825000
H	-4.804986000	-2.559559000	-0.802972000	C	0.117614000	1.815507000	2.549595000
H	-2.386354000	-4.702721000	0.869752000	H	-0.920596000	1.733773000	2.889941000
H	-1.407015000	-4.086035000	-0.459610000	H	0.578929000	0.834773000	2.655291000
H	-1.083769000	-3.567728000	1.203905000	H	0.623380000	2.490278000	3.245473000
B	0.580278000	-0.035493000	0.024956000	C	0.095135000	5.906989000	-0.293014000
C	2.033130000	-0.779502000	0.017633000	H	0.823178000	6.348124000	-0.978335000
C	3.204124000	-0.229267000	0.601392000	H	-0.902437000	6.140202000	-0.679612000
C	2.184754000	-2.042027000	-0.603588000	H	0.197998000	6.400218000	0.676238000
C	4.403670000	-0.941060000	0.592371000	H	-0.779692000	-0.776612000	-1.346729000
C	3.401715000	-2.722158000	-0.595372000	H	0.104338000	-0.307208000	-1.263082000
C	4.529631000	-2.193732000	0.009653000				

### $\text{NH}_3 \cdot \text{BH}_3$

E: -83.2159633856 a.u.

ZP correction: 0.070182 a.u.

H: -83.141047 a.u.

G: -83.168195 a.u.

H	1.014309000	0.585611000	-1.239338000
H	0.000000000	-1.171223000	-1.239338000
H	-1.014309000	0.585611000	-1.239338000
B	0.000000000	0.000000000	-0.925652000
N	0.000000000	0.000000000	0.726264000
H	0.000000000	0.948689000	1.087476000
H	-0.821589000	-0.474344000	1.087476000
H	0.821589000	-0.474344000	1.087476000

### $\text{NH}_2=\text{BH}_2$

E: -82.0369654693 a.u.

ZP correction: 0.048127 a.u.

H: -81.984674 a.u.

G: -82.010580 a.u.

B	0.000000000	0.000000000	-0.776359000
H	0.000000000	1.046053000	-1.357097000
N	0.000000000	0.000000000	0.610947000
H	0.000000000	0.843683000	1.159680000

### $\text{H}_2$

E: -1.17607105465 a.u.

ZP correction: 0.010104 a.u.

H: -1.162662 a.u.

G: -1.177458 a.u.

H	0.000000000	0.000000000	0.372182000
H	0.000000000	0.000000000	-0.372182000

## 2.2 Dehydrogenation of $\text{NMe}_2\text{H} \cdot \text{BH}_3$

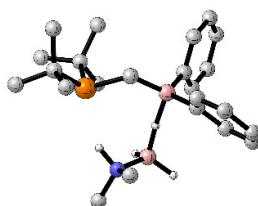
### *t*Bu<sub>2</sub>PCH<sub>2</sub>Ph<sub>2</sub> – BHB interaction

E: -1346.32774635 a.u.

ZP correction: 0.592760 a.u.

H: -1345.702993 a.u.

G: -1345.795195 a.u.



C	0.357868000	-0.205405000	-0.888704000	H	0.297200000	-1.215584000	-1.297491000
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H	0.449908000	0.460315000	-1.756389000	H	-3.530316000	-0.233378000	1.057770000
P	1.955161000	-0.248227000	0.044774000	C	-3.320511000	-2.533418000	-2.024062000
C	2.427258000	1.565043000	0.326287000	H	-1.366837000	-1.734367000	-2.323114000
C	2.021110000	2.506429000	-0.813502000	C	-4.464587000	-2.536861000	-1.240344000
C	1.683905000	1.986165000	1.604619000	H	-5.423465000	-1.690524000	0.488388000
C	3.930636000	1.706522000	0.596850000	H	-3.262790000	-3.164370000	-2.904968000
H	2.461488000	2.220389000	-1.770412000	H	-5.303442000	-3.174284000	-1.498160000
H	0.937711000	2.554250000	-0.929621000	C	-1.534110000	1.625986000	-0.025534000
H	2.365819000	3.520414000	-0.580795000	C	-1.658766000	2.378205000	-1.201222000
H	2.007226000	1.396925000	2.467198000	C	-1.905202000	2.250116000	1.168142000
H	1.892161000	3.041697000	1.812726000	C	-2.106733000	3.692410000	-1.186015000
H	0.604927000	1.880112000	1.504620000	H	-1.406562000	1.923028000	-2.155784000
H	4.128085000	2.719256000	0.964171000	C	-2.352798000	3.566963000	1.195018000
H	4.275937000	1.005521000	1.362449000	H	-1.829692000	1.703911000	2.103320000
H	4.531969000	1.564926000	-0.303295000	C	-2.451791000	4.296003000	0.017810000
C	3.142992000	-1.049399000	-1.205164000	H	-2.189880000	4.245412000	-2.115765000
C	3.436425000	-0.218018000	-2.457553000	H	-2.623309000	4.024376000	2.140929000
C	4.455206000	-1.397739000	-0.482574000	H	-2.799677000	5.323023000	0.036253000
C	2.508810000	-2.383297000	-1.642188000	H	-0.851515000	-0.231077000	1.238009000
H	2.516068000	0.077405000	-2.968583000	B	-0.761377000	-0.740980000	2.395853000
H	4.002744000	0.685810000	-2.225837000	H	-0.254038000	0.096506000	3.093412000
H	4.033015000	-0.808419000	-3.162633000	H	-1.848161000	-1.138140000	2.721894000
H	4.264084000	-2.005043000	0.407228000	N	0.243553000	-1.955670000	2.218965000
H	5.098486000	-1.978363000	-1.153202000	H	1.045818000	-1.552699000	1.693293000
H	5.015946000	-0.516675000	-0.173694000	C	-0.310461000	-3.059303000	1.409702000
H	3.265832000	-2.993227000	-2.145932000	H	0.448761000	-3.830034000	1.255821000
H	2.135825000	-2.958339000	-0.787695000	H	-1.171042000	-3.481992000	1.928956000
H	1.686419000	-2.242062000	-2.345824000	H	-0.647179000	-2.669531000	0.450842000
B	-1.064957000	0.101309000	-0.165577000	C	0.742247000	-2.431309000	3.522724000
C	-2.277294000	-0.880599000	-0.563277000	H	1.447082000	-3.253474000	3.380322000
C	-3.457247000	-0.886373000	0.193994000	H	1.234868000	-1.605349000	4.033722000
C	-2.243984000	-1.717809000	-1.682691000	H	-0.102065000	-2.771391000	4.124439000
C	-4.529312000	-1.704898000	-0.126035000				

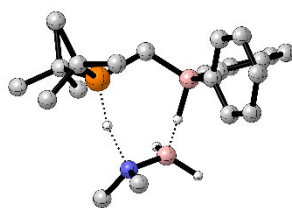
### **tBu<sub>2</sub>PCH<sub>2</sub>Ph<sub>2</sub> – TS H<sub>2</sub> abstraction**

E: -1346.30475450 a.u.

ZP correction: 0.585728 a.u.

H: -1345.687410 a.u.

G: -1345.778740 a.u.



C	-0.087770000	-0.474471000	-1.065735000	H	-4.769516000	-2.403372000	-0.300833000
H	-0.005602000	0.079940000	-2.006606000	H	-4.253057000	-1.150312000	0.831611000
H	-0.070453000	-1.530621000	-1.344456000	H	-4.757823000	-0.718343000	-0.815360000
P	-1.727153000	-0.175175000	-0.339940000	C	-2.458026000	1.441392000	-0.923443000
C	-2.786273000	-1.672285000	-0.709782000	C	-3.035219000	1.359061000	-2.340036000
C	-2.788480000	-2.045953000	-2.197864000	C	-3.540923000	1.878338000	0.077331000
C	-2.159941000	-2.824787000	0.096944000	C	-1.335067000	2.488692000	-0.898505000
C	-4.222920000	-1.458936000	-0.217392000	H	-2.305335000	0.968306000	-3.054404000
H	-3.300567000	-1.305593000	-2.813005000	H	-3.932774000	0.738612000	-2.384522000
H	-1.777385000	-2.175813000	-2.589974000	H	-3.313975000	2.364785000	-2.670299000
H	-3.312676000	-2.998964000	-2.322213000	H	-3.125666000	1.985511000	1.082762000
H	-2.129466000	-2.605933000	1.166127000	H	-3.932013000	2.854114000	-0.227398000
H	-2.760469000	-3.727667000	-0.050788000	H	-4.382259000	1.186445000	0.125456000
H	-1.141667000	-3.050837000	-0.223988000	H	-1.774127000	3.472522000	-1.090996000

H	-0.821582000	2.534494000	0.064635000	H	1.030983000	-2.957609000	0.154368000
H	-0.577814000	2.304075000	-1.659797000	C	4.339914000	-3.286376000	-0.449872000
B	1.207737000	-0.163378000	-0.085366000	H	5.695378000	-1.654436000	-0.777538000
C	1.767748000	1.342942000	-0.140071000	H	2.752518000	-4.685598000	-0.070575000
C	2.008300000	1.962533000	-1.373046000	H	5.104091000	-4.050520000	-0.543599000
C	2.127049000	2.062145000	1.003668000	H	0.750624000	-0.241707000	1.177297000
C	2.542131000	3.242055000	-1.464313000	H	-1.545386000	-0.083297000	1.183832000
H	1.783112000	1.428664000	-2.293580000	B	0.350957000	-0.757171000	2.351468000
C	2.655817000	3.346922000	0.927489000	N	-0.962817000	-0.031270000	2.635403000
H	2.002383000	1.598841000	1.977257000	H	0.181436000	-1.929172000	2.127738000
C	2.858721000	3.946791000	-0.308496000	H	1.288737000	-0.474303000	3.059822000
H	2.714132000	3.690163000	-2.437564000	C	-0.827226000	1.370553000	2.996595000
H	2.917533000	3.876905000	1.837574000	H	-0.277883000	1.901482000	2.215664000
H	3.273101000	4.946985000	-0.372819000	H	-1.813095000	1.838993000	3.107479000
C	2.349034000	-1.293229000	-0.202039000	H	-0.278166000	1.502557000	3.939822000
C	3.686225000	-0.966793000	-0.451764000	C	-1.836628000	-0.738422000	3.558807000
C	2.049356000	-2.656313000	-0.072549000	H	-1.437503000	-0.751720000	4.583590000
C	4.668385000	-1.944127000	-0.580296000	H	-2.825293000	-0.263250000	3.589992000
H	3.968128000	0.076404000	-0.549733000	H	-1.956007000	-1.775424000	3.237919000
C	3.020620000	-3.640739000	-0.189319000				

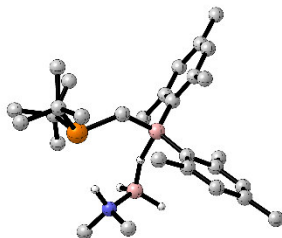
### ***t*Bu<sub>2</sub>PCH<sub>2</sub>Mes<sub>2</sub> – BHB interaction**

E: -1582.19204652 a.u.

ZP correction: 0.763357 a.u.

H: -1581.388445 a.u.

G: -1581.495617 a.u.



C	0.857089000	0.202471000	-0.750309000	H	3.309532000	-1.775046000	-3.679594000
H	0.694047000	-0.266311000	-1.719389000	H	2.478765000	-2.532986000	-2.319207000
H	1.012448000	1.255909000	-0.988156000	H	1.753681000	-1.150101000	-3.160473000
P	2.506876000	-0.481127000	-0.212030000	B	-0.601044000	0.125512000	0.028284000
C	3.296237000	0.960361000	0.779284000	C	-1.727591000	-1.040662000	-0.164633000
C	2.792829000	2.355271000	0.384887000	C	-2.965611000	-0.921396000	0.526672000
C	2.943510000	0.688126000	2.249277000	C	-1.605995000	-2.160898000	-1.017383000
C	4.830407000	0.959082000	0.715827000	C	-3.982914000	-1.853948000	0.340568000
H	2.994063000	2.585170000	-0.663115000	C	-2.653378000	-3.068801000	-1.185133000
H	1.723052000	2.482545000	0.553564000	C	-3.860319000	-2.933500000	-0.522093000
H	3.309951000	3.105682000	0.993402000	H	-4.909404000	-1.729223000	0.895029000
H	3.469193000	-0.201840000	2.608555000	H	-2.510849000	-3.912529000	-1.855506000
H	3.256526000	1.533910000	2.871731000	C	-1.209961000	1.632965000	0.021272000
H	1.878331000	0.539263000	2.410634000	C	-1.854700000	2.009819000	-1.183614000
H	5.204238000	1.669064000	1.461831000	C	-1.093591000	2.620372000	1.018420000
H	5.249787000	-0.020066000	0.961074000	C	-2.368966000	3.293490000	-1.343033000
H	5.220912000	1.275561000	-0.251602000	C	-1.622956000	3.896923000	0.819923000
C	3.454516000	-0.617886000	-1.869556000	C	-2.273616000	4.257648000	-0.348597000
C	3.618117000	0.717643000	-2.604089000	H	-2.858914000	3.547352000	-2.279935000
C	4.824161000	-1.275741000	-1.627519000	H	-1.521086000	4.632445000	1.613851000
C	2.690435000	-1.574305000	-2.798966000	H	-0.213564000	-0.230882000	1.531490000
H	2.652383000	1.203992000	-2.766136000	B	-0.156900000	-0.976541000	2.566918000
H	4.263483000	1.414149000	-2.067853000	H	0.288960000	-0.295590000	3.452075000
H	4.070313000	0.543917000	-3.587289000	H	-1.235964000	-1.455463000	2.781347000
H	4.713416000	-2.225812000	-1.096545000	N	0.882761000	-2.157370000	2.239859000
H	5.295165000	-1.486956000	-2.593857000	H	1.544669000	-1.803540000	1.529339000
H	5.511805000	-0.650209000	-1.064485000	C	-2.869694000	5.628452000	-0.532490000

H	-3.955354000	5.603131000	-0.393567000	H	-0.256445000	-1.816659000	-2.668258000
H	-2.460579000	6.339951000	0.188363000	H	0.544181000	-2.385761000	-1.203029000
H	-2.677273000	6.014548000	-1.536961000	H	-0.399617000	-3.499372000	-2.187654000
C	-2.040158000	1.061310000	-2.349934000	C	-4.991173000	-3.905091000	-0.728314000
H	-1.121392000	0.529123000	-2.606163000	H	-5.731654000	-3.497973000	-1.424286000
H	-2.798395000	0.304766000	-2.134585000	H	-4.632433000	-4.850077000	-1.142410000
H	-2.354241000	1.613208000	-3.238377000	H	-5.506855000	-4.116971000	0.211654000
C	-0.450895000	2.365801000	2.358110000	C	1.668391000	-2.530455000	3.434082000
H	0.514082000	1.875305000	2.265257000	H	0.980616000	-2.860967000	4.213545000
H	-0.296600000	3.305653000	2.892356000	H	2.363304000	-3.337179000	3.189464000
H	-1.068861000	1.722813000	2.990590000	H	2.214550000	-1.660864000	3.791752000
C	-3.283953000	0.187937000	1.500720000	C	0.230559000	-3.353233000	1.661584000
H	-2.450852000	0.401585000	2.166849000	H	-0.420538000	-3.049784000	0.847463000
H	-3.535686000	1.115629000	0.982425000	H	0.986563000	-4.058019000	1.307062000
H	-4.136470000	-0.096259000	2.121476000	H	-0.381156000	-3.819861000	2.433907000
C	-0.360211000	-2.477694000	-1.803669000				

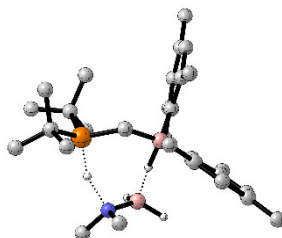
### ***t*Bu<sub>2</sub>PCH<sub>2</sub>Mes<sub>2</sub> – TS H<sub>2</sub> abstraction**

E: -1582.17034098 a.u.

ZP correction: 0.754835 a.u.

H: -1581.375237 a.u.

G: -1581.482131 a.u.



C	0.492373000	-0.546952000	-0.758957000	C	-2.238770000	-0.242549000	-0.191758000
H	0.072810000	-1.510195000	-1.034338000	C	-3.260844000	0.245507000	0.668615000
H	0.719742000	-0.031659000	-1.694434000	C	-2.673166000	-1.140130000	-1.200621000
P	2.038270000	-1.138950000	-0.030158000	C	-4.573928000	-0.202582000	0.571740000
C	3.186643000	0.248142000	0.470994000	C	-4.005448000	-1.564361000	-1.264533000
C	3.112843000	1.401492000	-0.540392000	C	-4.972913000	-1.130512000	-0.378365000
C	2.670614000	0.717099000	1.836603000	H	-5.312642000	0.193550000	1.263723000
C	4.639954000	-0.207500000	0.650000000	H	-4.292018000	-2.257515000	-2.051539000
H	3.439856000	1.097826000	-1.537652000	C	-0.411695000	1.876973000	0.039832000
H	2.106496000	1.816621000	-0.612803000	C	-0.479635000	2.478353000	-1.248644000
H	3.776383000	2.204729000	-0.204325000	C	-0.007752000	2.733599000	1.090403000
H	2.819449000	-0.046008000	2.605368000	C	-0.044624000	3.782758000	-1.464433000
H	3.207982000	1.622499000	2.135794000	C	0.436486000	4.033704000	0.829936000
H	1.614170000	0.956407000	1.799235000	C	0.454164000	4.577175000	-0.441070000
H	5.205409000	0.631973000	1.066461000	H	-0.105246000	4.193859000	-2.469446000
H	4.724241000	-1.038232000	1.355596000	H	0.765400000	4.643066000	1.668855000
H	5.121637000	-0.489202000	-0.287423000	H	-0.473459000	-0.183494000	1.376716000
C	2.813717000	-2.309684000	-1.281033000	B	-0.501541000	-1.119110000	2.424126000
C	3.456432000	-1.556006000	-2.452187000	H	0.164949000	-0.531339000	3.236736000
C	3.842206000	-3.205668000	-0.572255000	H	-1.683534000	-1.196962000	2.629479000
C	1.710359000	-3.222754000	-1.841961000	N	0.174727000	-2.400667000	1.973727000
H	2.739171000	-0.891249000	-2.941415000	H	1.351333000	-1.916326000	1.111003000
H	4.318450000	-0.961997000	-2.145989000	C	0.921706000	5.985799000	-0.695576000
H	3.801094000	-2.278357000	-3.199247000	H	1.410330000	6.072633000	-1.669333000
H	3.384661000	-3.749867000	0.259180000	H	0.079562000	6.685427000	-0.687892000
H	4.223438000	-3.944551000	-1.284468000	H	1.629116000	6.313316000	0.069868000
H	4.696997000	-2.652285000	-0.187322000	C	-1.043775000	1.775724000	-2.465544000
H	2.180640000	-4.019110000	-2.426801000	H	-0.302965000	1.144489000	-2.967532000
H	1.122239000	-3.696298000	-1.051157000	H	-1.900103000	1.152250000	-2.214232000
H	1.029919000	-2.685371000	-2.503555000	H	-1.372954000	2.514056000	-3.199477000
B	-0.689464000	0.252644000	0.099770000	C	-0.080848000	2.401980000	2.566012000

H	-0.192309000	1.346543000	2.780978000	H	-7.107186000	-0.819369000	-0.299289000
H	0.810131000	2.762717000	3.087503000	H	-6.601556000	-2.108849000	-1.400563000
H	-0.941992000	2.914003000	3.006863000	H	-6.576448000	-2.372450000	0.345378000
C	-3.001947000	1.282390000	1.730627000	C	0.895511000	-3.089549000	3.037761000
H	-2.273136000	0.932347000	2.460644000	H	0.223062000	-3.465126000	3.820701000
H	-2.620613000	2.207496000	1.295367000	H	1.445826000	-3.945064000	2.626610000
H	-3.923118000	1.513693000	2.269116000	H	1.608612000	-2.404543000	3.502087000
C	-1.815254000	-1.711004000	-2.318066000	C	-0.691397000	-3.314451000	1.237499000
H	-1.104660000	-0.994503000	-2.725603000	H	-1.242726000	-2.767985000	0.471135000
H	-1.260006000	-2.600984000	-2.000787000	H	-0.102555000	-4.110421000	0.764131000
H	-2.459098000	-2.027335000	-3.141131000	H	-1.429353000	-3.786658000	1.899525000
C	-6.390601000	-1.632820000	-0.440210000				

### NMe<sub>2</sub>H·BH<sub>3</sub>

E: -161.827446270 a.u.

ZP correction: 0.127550 a.u.

H: -161.693084 a.u.

G: -161.727723 a.u.

H	-2.049538000	-1.013345000	-0.353943000	H	1.742413000	1.214142000	-0.226772000
H	-1.549818000	-0.000012000	1.331931000	H	0.180560000	2.087402000	-0.299680000
H	-2.049540000	1.013342000	-0.353930000	H	0.652814000	1.258024000	1.190068000
B	-1.574144000	-0.000004000	0.116758000	C	0.699445000	-1.218842000	0.101676000
N	-0.001495000	0.000000000	-0.342388000	H	0.180557000	-2.087402000	-0.299661000
H	-0.014813000	0.000000000	-1.358473000	H	1.742413000	-1.214144000	-0.226792000
C	0.699438000	1.218845000	0.101676000	H	0.652842000	-1.258009000	1.190070000

### NMe<sub>2</sub>=BH<sub>2</sub>

E: -160.642943223 a.u.

ZP correction: 0.105038 a.u.

H: -160.531576 a.u.

G: -160.565216 a.u.

B	0.000123000	1.537197000	-0.000094000	H	-1.252311000	-1.294923000	-0.885625000
H	1.046845000	2.117421000	0.000058000	H	-1.252721000	-1.294098000	0.886258000
H	-1.046521000	2.117570000	-0.000066000	C	1.212476000	-0.649746000	0.000066000
N	0.000018000	0.149948000	-0.000071000	H	1.252352000	-1.294540000	0.886126000
C	-1.212582000	-0.649561000	0.000023000	H	1.252276000	-1.294856000	-0.885762000
H	-2.085154000	0.001969000	-0.000470000	H	2.085133000	0.001672000	-0.000087000

## 2.3 Amino-borane adducts

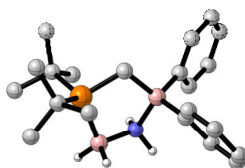
### *t*Bu<sub>2</sub>PCH<sub>2</sub>Ph<sub>2</sub> – NH<sub>2</sub>BH<sub>2</sub> adduct (3)

E: -1266.57651965 a.u.

ZP correction: 0.518590 a.u.

H: -1266.030938 a.u.

G: -1266.111809 a.u.





C	0.334597000	-0.162863000	0.852572000	B	-0.990318000	-0.021968000	-0.149585000
H	0.359631000	0.594058000	1.636475000	C	-1.751456000	1.417656000	-0.076437000
H	0.339438000	-1.126875000	1.364494000	C	-2.774219000	1.689808000	-0.997504000
P	1.832834000	-0.033750000	-0.167581000	C	-1.492702000	2.417161000	0.863871000
C	2.613452000	-1.740243000	-0.197353000	C	-3.469976000	2.890198000	-1.007421000
C	2.881983000	-2.311792000	1.201278000	H	-3.064573000	0.926067000	-1.717120000
C	1.597438000	-2.655506000	-0.907908000	C	-2.187031000	3.624361000	0.875121000
C	3.909656000	-1.723177000	-1.016951000	H	-0.731803000	2.264675000	1.621695000
H	3.619193000	-1.734431000	1.757923000	C	-3.174158000	3.871230000	-0.067559000
H	1.971476000	-2.374046000	1.800990000	H	-4.252158000	3.057544000	-1.740597000
H	3.272256000	-3.329219000	1.094618000	H	-1.952268000	4.373788000	1.624088000
H	1.460811000	-2.361972000	-1.951791000	H	-3.713926000	4.811808000	-0.065444000
H	1.982295000	-3.679857000	-0.902687000	C	-2.050206000	-1.223622000	0.123627000
H	0.624222000	-2.670306000	-0.407689000	C	-2.394345000	-1.561061000	1.440147000
H	4.244175000	-2.752723000	-1.179745000	C	-2.700695000	-1.939009000	-0.887614000
H	3.761093000	-1.260093000	-1.995952000	C	-3.318768000	-2.553920000	1.731982000
H	4.714641000	-1.197180000	-0.499141000	H	-1.931677000	-1.021407000	2.262574000
C	2.994351000	1.310558000	0.425506000	C	-3.629402000	-2.939497000	-0.611216000
C	3.841810000	0.900353000	1.633746000	H	-2.501866000	-1.715831000	-1.934110000
C	3.901398000	1.720687000	-0.746782000	C	-3.941173000	-3.253603000	0.703100000
C	2.128236000	2.520754000	0.816540000	H	-3.558618000	-2.782202000	2.765417000
H	3.225896000	0.517143000	2.451956000	H	-4.111347000	-3.469359000	-1.426458000
H	4.588577000	0.146830000	1.375862000	H	-4.664684000	-4.029990000	0.925924000
H	4.378000000	1.779389000	2.005649000	N	-0.418515000	-0.160282000	-1.674012000
H	3.315397000	2.077812000	-1.596108000	B	1.029878000	0.436083000	-1.887195000
H	4.555437000	2.535508000	-0.419619000	H	0.967929000	1.640496000	-1.928323000
H	4.538746000	0.904575000	-1.089356000	H	1.606615000	-0.045936000	-2.833934000
H	2.781982000	3.389002000	0.944795000	H	-1.055822000	0.314818000	-2.306779000
H	1.382702000	2.766177000	0.057569000	H	-0.437245000	-1.138430000	-1.948439000
H	1.612030000	2.356975000	1.764495000				

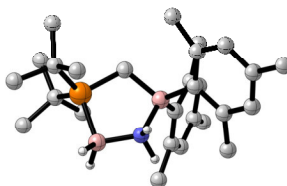
***t*Bu<sub>2</sub>PCH<sub>2</sub>Mes<sub>2</sub> – NH<sub>2</sub>BH<sub>2</sub> adduct (8)**

E: -1502.44361085 a.u.

ZP correction: 0.687143 a.u.

H: -1501.720424 a.u.

G: -1501.818432 a.u.



C	0.686423000	-0.531837000	-0.741816000	C	2.457542000	-2.822564000	-0.133349000
H	0.413057000	-1.423233000	-1.289601000	C	2.575791000	-3.088419000	-1.641030000
H	1.013614000	0.191418000	-1.489692000	C	3.726221000	-3.304663000	0.579835000
P	2.107897000	-1.020942000	0.270878000	C	1.255743000	-3.618254000	0.412114000
C	3.553768000	0.125653000	-0.050537000	H	1.671051000	-2.805064000	-2.182987000
C	4.178595000	-0.089444000	-1.432846000	H	3.419415000	-2.569864000	-2.095445000
C	3.007937000	1.561679000	0.036730000	H	2.726506000	-4.161698000	-1.796514000
C	4.616739000	-0.050095000	1.045205000	H	3.716383000	-3.048758000	1.642839000
H	4.716621000	-1.037751000	-1.495090000	H	3.791262000	-4.394505000	0.498535000
H	3.429677000	-0.059301000	-2.229014000	H	4.629180000	-2.890011000	0.126734000
H	4.901358000	0.709452000	-1.626532000	H	1.354067000	-4.663458000	0.102846000
H	2.547887000	1.762585000	1.004486000	H	1.217599000	-3.588132000	1.501412000
H	3.844061000	2.257078000	-0.087036000	H	0.300477000	-3.250355000	0.028728000
H	2.269404000	1.787476000	-0.734177000	B	-0.557561000	0.064652000	0.213113000
H	5.391553000	0.711426000	0.909758000	C	-2.070246000	-0.638305000	0.014294000
H	4.187140000	0.083013000	2.040336000	C	-3.100877000	-0.254554000	0.915820000
H	5.103872000	-1.024634000	1.006731000	C	-2.431258000	-1.667643000	-0.901238000

C	-4.338023000	-0.898457000	0.944686000	H	-2.220271000	-2.693461000	-2.772414000
C	-3.680437000	-2.289758000	-0.834008000	C	-5.970918000	-2.659049000	0.156463000
C	-4.648626000	-1.942562000	0.092871000	H	-6.381880000	-2.825249000	-0.842785000
H	-5.085367000	-0.559289000	1.657558000	H	-5.861556000	-3.638288000	0.633507000
H	-3.908889000	-3.071902000	-1.553719000	H	-6.702540000	-2.088856000	0.733076000
C	-0.533213000	1.717480000	0.033645000	C	-2.965968000	0.878891000	1.910643000
C	-0.856955000	2.216712000	-1.258851000	H	-2.417927000	1.722843000	1.498590000
C	-0.139258000	2.696445000	0.979466000	H	-3.954329000	1.237737000	2.203866000
C	-0.718714000	3.564575000	-1.578115000	H	-2.474304000	0.558107000	2.836452000
C	-0.009155000	4.041580000	0.617509000	C	0.137356000	2.425550000	2.444854000
C	-0.276161000	4.503191000	-0.657952000	H	0.925015000	1.692383000	2.609213000
H	-0.970550000	3.891936000	-2.583990000	H	0.452985000	3.344574000	2.941286000
H	0.311701000	4.753914000	1.373122000	H	-0.760557000	2.089460000	2.973065000
N	-0.133638000	-0.473784000	1.729365000	C	-0.140281000	5.957265000	-1.024561000
B	1.384270000	-0.795133000	2.069093000	H	-1.122445000	6.431503000	-1.118018000
H	1.496418000	-1.792135000	2.739571000	H	0.423671000	6.506966000	-0.267669000
H	1.943586000	0.135857000	2.585950000	H	0.372112000	6.077898000	-1.982947000
H	-0.671822000	-1.327823000	1.846290000	C	-1.381302000	1.338695000	-2.372634000
H	-0.502252000	0.155446000	2.432734000	H	-0.621982000	0.645805000	-2.743726000
C	-1.582529000	-2.169996000	-2.057631000	H	-2.235279000	0.743801000	-2.048408000
H	-1.089067000	-1.367073000	-2.601152000	H	-1.697808000	1.950218000	-3.219735000
H	-0.820544000	-2.889738000	-1.743209000				

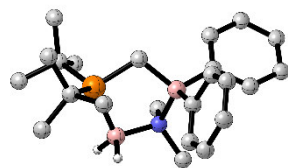
### ***t*Bu<sub>2</sub>PCH<sub>2</sub>Ph<sub>2</sub> – NMe<sub>2</sub>BH<sub>2</sub> adduct (5)**

E: -1345.17054128 a.u.

ZP correction: 0.576218 a.u.

H: -1344.565243 a.u.

G: -1344.648385 a.u.



C	-0.315620000	-0.425874000	-0.878207000	H	-4.153822000	2.696998000	0.627568000
H	-0.305810000	0.217001000	-1.760955000	H	-4.543755000	1.002973000	0.911365000
H	-0.312782000	-1.453422000	-1.252184000	H	-2.250087000	3.429437000	-0.643947000
P	-1.859139000	-0.243979000	0.069501000	H	-1.208725000	2.643813000	0.541435000
C	-2.980891000	-1.718265000	-0.327398000	H	-0.962972000	2.341785000	-1.175250000
C	-3.135902000	-1.945093000	-1.839452000	B	0.978302000	-0.121423000	0.134147000
C	-2.351651000	-2.989013000	0.263413000	C	1.370819000	1.467057000	0.050342000
C	-4.357913000	-1.544897000	0.329417000	C	1.201029000	2.489895000	0.987509000
H	-3.695891000	-1.156356000	-2.337114000	C	1.936838000	1.862485000	-1.175250000
H	-2.167185000	-2.039253000	-2.335970000	C	1.570426000	3.809206000	0.733404000
H	-3.677133000	-2.883685000	-1.997710000	H	0.718770000	2.290734000	1.935808000
H	-2.157062000	-2.893003000	1.332316000	C	2.296044000	3.173010000	-1.451371000
H	-3.050644000	-3.818606000	0.118605000	H	2.110541000	1.108300000	-1.938087000
H	-1.425417000	-3.260703000	-0.246328000	C	2.118513000	4.161653000	-0.489239000
H	-4.922961000	-2.475026000	0.213047000	H	1.414674000	4.564442000	1.497142000
H	-4.270201000	-1.341177000	1.400150000	H	2.726884000	3.421963000	-2.415758000
H	-4.944784000	-0.750371000	-0.131625000	H	2.403223000	5.188281000	-0.692005000
C	-2.753337000	1.370106000	-0.328655000	C	2.311721000	-0.984375000	-0.270755000
C	-3.504639000	1.326802000	-1.664795000	C	2.298232000	-2.130861000	-1.072650000
C	-3.720457000	1.709932000	0.818416000	C	3.566738000	-0.597363000	0.223667000
C	-1.720767000	2.501115000	-0.406506000	C	3.449887000	-2.859833000	-1.353318000
H	-2.851339000	1.029100000	-2.489370000	H	1.364036000	-2.483337000	-1.500812000
H	-4.369200000	0.662804000	-1.643360000	C	4.724261000	-1.320300000	-0.035599000
H	-3.875395000	2.332454000	-1.885692000	H	3.642471000	0.313962000	0.809584000
H	-3.196185000	1.755153000	1.775159000	C	4.671057000	-2.461188000	-0.827458000

H	3.392099000	-3.740345000	-1.985200000	H	1.212945000	0.845150000	2.925719000
H	5.672616000	-0.985093000	0.371568000	H	0.924609000	-0.720839000	3.687321000
H	5.572705000	-3.024930000	-1.041010000	H	2.321525000	-0.500256000	2.606485000
N	0.449521000	-0.666194000	1.631208000	C	0.548202000	-2.147830000	1.659260000
B	-1.063202000	-0.200927000	1.874393000	H	0.001791000	-2.532139000	2.523352000
H	-1.079283000	0.958873000	2.203551000	H	0.134958000	-2.577548000	0.754119000
H	-1.634027000	-0.909689000	2.670834000	H	1.593854000	-2.449382000	1.718234000
C	1.279392000	-0.225249000	2.779451000				

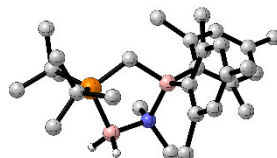
### ***t*Bu<sub>2</sub>PCH<sub>2</sub>Mes<sub>2</sub> – NMe<sub>2</sub>BH<sub>2</sub> adduct**

E: -1581.01905910 a.u.

ZP correction: 0.745254 a.u.

H: -1580.236042 a.u.

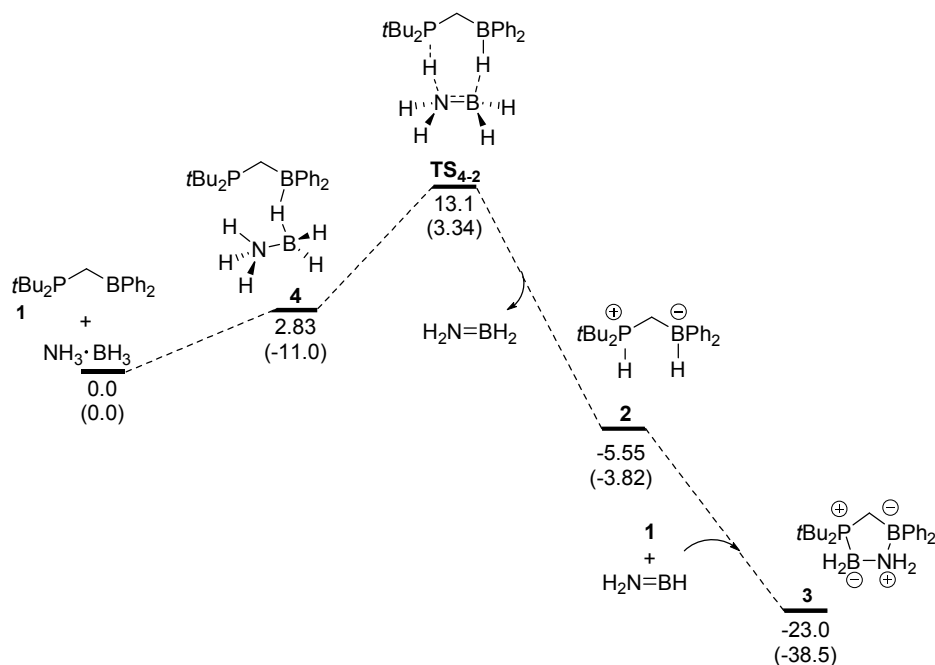
G: -1580.335934 a.u.



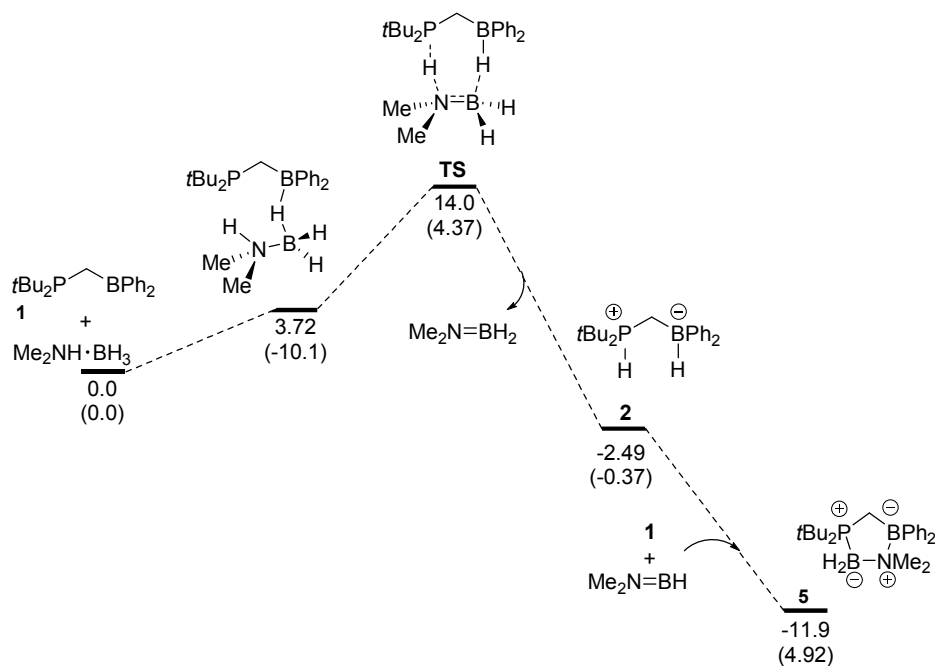
C	-0.804128000	-0.526967000	-0.789071000	C	2.228195000	-2.031829000	-0.866089000
H	-0.894518000	0.202062000	-1.595233000	C	3.117657000	-0.406793000	0.657513000
H	-0.723995000	-1.495838000	-1.271286000	C	3.498911000	-2.598330000	-0.964878000
P	-2.383133000	-0.606341000	0.113988000	C	4.371245000	-1.013144000	0.536413000
C	-3.341262000	-2.127509000	-0.491803000	C	4.592397000	-2.117853000	-0.263035000
C	-3.406051000	-2.204501000	-2.025611000	H	3.640364000	-3.449043000	-1.626289000
C	-2.636244000	-3.401934000	-0.003860000	H	5.208064000	-0.585403000	1.082906000
C	-4.756427000	-2.138714000	0.103939000	C	0.016355000	2.484374000	2.345462000
H	-3.995545000	-1.406794000	-2.472146000	H	-0.501607000	3.401497000	2.636023000
H	-2.410071000	-2.182760000	-2.474845000	H	-0.669375000	1.662366000	2.514469000
H	-3.871518000	-3.154694000	-2.307483000	H	0.865114000	2.377638000	3.030624000
H	-2.490165000	-3.408229000	1.076712000	C	1.385485000	5.667489000	-1.171299000
H	-3.260448000	-4.261294000	-0.267921000	H	1.024647000	6.368777000	-0.415723000
H	-1.674001000	-3.550707000	-0.496707000	H	2.450907000	5.862746000	-1.327621000
H	-5.229892000	-3.098184000	-0.126371000	H	0.872533000	5.889376000	-2.111550000
H	-4.734526000	-2.032231000	1.191989000	C	1.639747000	0.871558000	-2.321601000
H	-5.393490000	-1.357630000	-0.310896000	H	2.636414000	0.474416000	-2.115722000
C	-3.426919000	0.943720000	-0.155231000	H	0.979639000	0.015378000	-2.427489000
C	-4.109846000	0.983979000	-1.527678000	H	1.674380000	1.378439000	-3.288522000
C	-4.473404000	1.065126000	0.966785000	C	3.144115000	0.848194000	1.508603000
C	-2.509864000	2.167136000	-0.058585000	H	3.308536000	1.730404000	0.883495000
H	-3.392773000	0.849555000	-2.341952000	H	2.232097000	1.026543000	2.062545000
H	-4.902473000	0.242423000	-1.629843000	H	3.964149000	0.790021000	2.229032000
H	-4.569678000	1.968810000	-1.655726000	C	1.210170000	-2.701876000	-1.770402000
H	-4.000713000	1.042952000	1.950831000	H	0.386918000	-3.167751000	-1.225112000
H	-4.981724000	2.028923000	0.861647000	H	0.781885000	-2.011480000	-2.499833000
H	-5.235430000	0.287950000	0.934080000	H	1.692322000	-3.499419000	-2.338024000
H	-3.122733000	3.065743000	-0.182014000	C	5.944632000	-2.771938000	-0.359856000
H	-2.027766000	2.228648000	0.913183000	H	6.086568000	-3.248164000	-1.332962000
H	-1.734725000	2.184012000	-0.824883000	H	6.747026000	-2.044313000	-0.216744000
B	0.494682000	-0.167777000	0.238797000	H	6.060095000	-3.545753000	0.406249000
C	0.721394000	1.490373000	0.049924000	B	-1.668802000	-0.711593000	1.937455000
C	1.216103000	1.851811000	-1.243247000	N	-0.095883000	-0.932692000	1.714983000
C	0.485170000	2.585146000	0.913348000	H	-1.899205000	0.345870000	2.457475000
C	1.406364000	3.182787000	-1.608566000	H	-2.155786000	-1.616564000	2.574916000
C	0.698954000	3.907027000	0.508741000	C	0.596114000	-0.658166000	2.999320000
C	1.155392000	4.240923000	-0.749552000	H	1.654815000	-0.903567000	2.905938000
H	1.777150000	3.397304000	-2.607863000	H	0.485330000	0.372956000	3.301406000
H	0.489721000	4.702797000	1.219257000	H	0.158090000	-1.291009000	3.776644000
C	1.975735000	-0.911310000	-0.022572000	C	0.131441000	-2.393168000	1.536407000

H -0.258643000 -2.726836000 0.585563000 H -0.381895000 -2.935391000 2.332881000  
H 1.196124000 -2.617397000 1.565805000

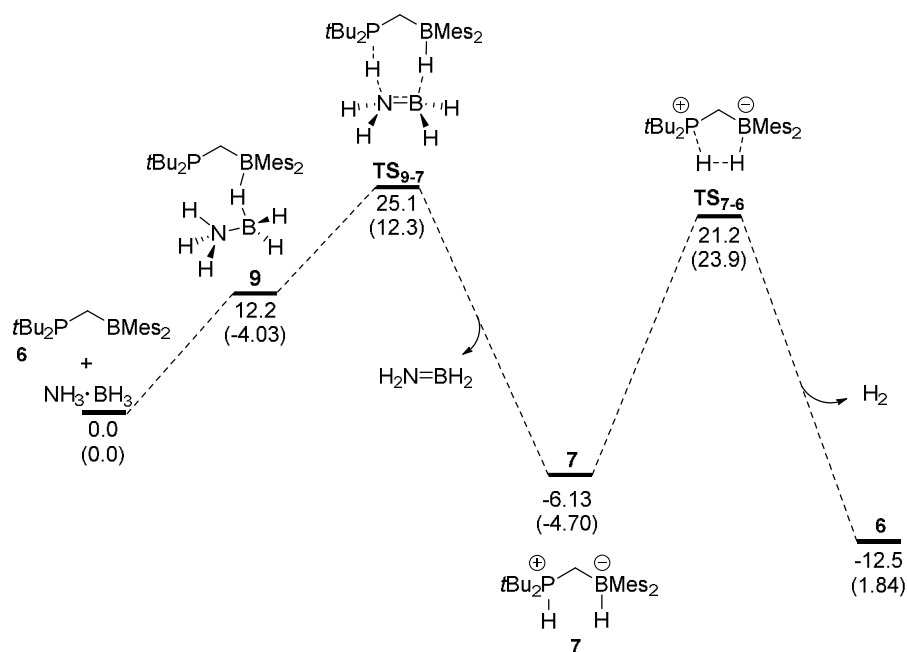
### 3. Calculated energy profiles for discussed reactions



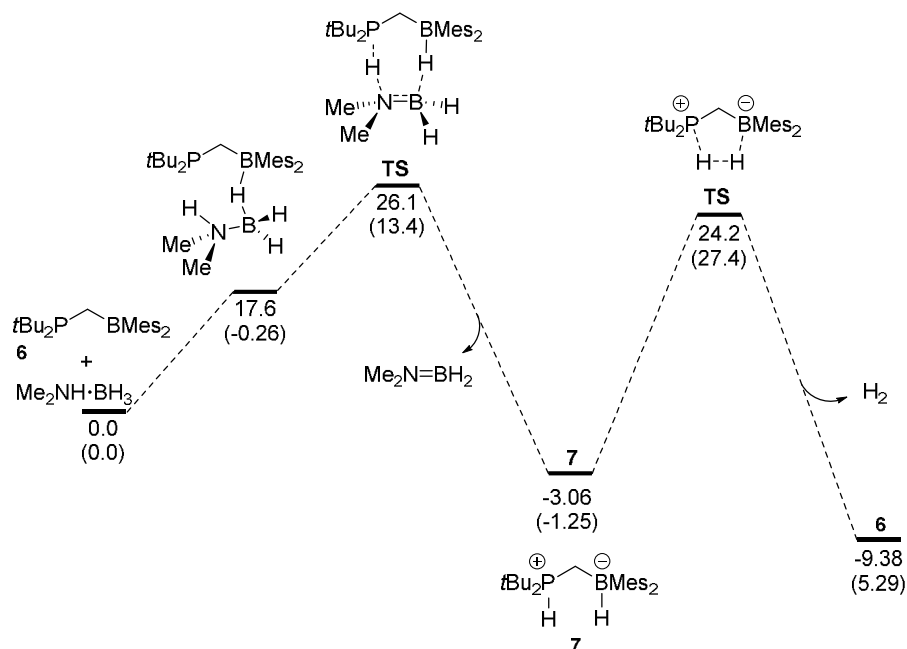
**Scheme S1.** Gibbs free energy and (energy) profile in kcal/mol for AB dehydrogenation by FLP **1** and trapping of the corresponding amino-borane species.



**Scheme S2.** Gibbs free energy and (energy) profile in kcal/mol for DMAB dehydrogenation by FLP 1 and trapping of the corresponding amino-borane species.



**Scheme S3.** Gibbs free energy and (energy) profile in kcal/mol for catalytic AB dehydrogenation by FLP 6.



**Scheme S4.** Gibbs free energy and (energy) profile in kcal/mol for catalytic DMAB dehydrogenation by FLP 6.

#### 4. Kinetic studies on catalytic dehydrogenation of Me<sub>2</sub>NH·BH<sub>3</sub> with FLP 6

**Table S1.** Consumption of Me<sub>2</sub>NH·BH<sub>3</sub> in time by **6** as catalyst at 50 °C, 60 °C, 70 °C and 80 °C.

Reaction temperature (°C)	t (min)	MeAB (%)	Conversion (%)*	TOF (h <sup>-1</sup> )**
50	0	99.7	0.3	
	10	99.4	0.6	
	35	99.4	0.6	0.27
	85	97.7	2.3	0.43
	115	95.4	4.6	0.63
	175	92.3	7.7	0.69
	235	90.7	9.3	0.62
60	0	99.5	0.5	
	20	99	1	
	60	93.4	6.6	
	95	88.6	11.4	1.89
	160	82.9	17.1	1.68
	225	79	21	1.47
	240	78.1	21.9	1.44
	1470	43	57	0.61
	1525	41.5	58.5	0.60
	1575	40.5	59.5	0.60
1620	39.5	60.5	0.59	
70	0	100	0	
	25	96.5	3.5	
	40	93	7	
	50	91.6	8.4	2.65
	95	85.3	14.7	2.44
	145	78.4	21.6	2.35
	175	76.3	23.7	2.13
	230	70.4	29.6	2.03
	6905	14.7	85.3	0.19
	8295	9.65	90.35	0.17
80	0	100	0	
	30	91.7	8.3	4.36
	55	85.5	14.5	4.15
	150	68.9	31.1	3.27
	180	66.8	33.2	2.91
	240	61.5	38.5	2.53

\*Minor amounts of other dehydrogenation products of Me<sub>2</sub>NH·BH<sub>3</sub> were observed by <sup>11</sup>B NMR spectroscopy, therefore the conversion of DMAB was calculated as the consumption of the substrate. \*\*The TOF was calculated as ([dehydrogenation products] / [FLP]<sub>0</sub>) / time (h).

## 5. References

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