Supplementary Data For:

Metal-free Lewis Acid Mediated Dehydrocoupling of Phosphines and Concurrent Hydrogenation†

Roman Dobrovetsky, Katsuhiko Takeuchi and Douglas W. Stephan

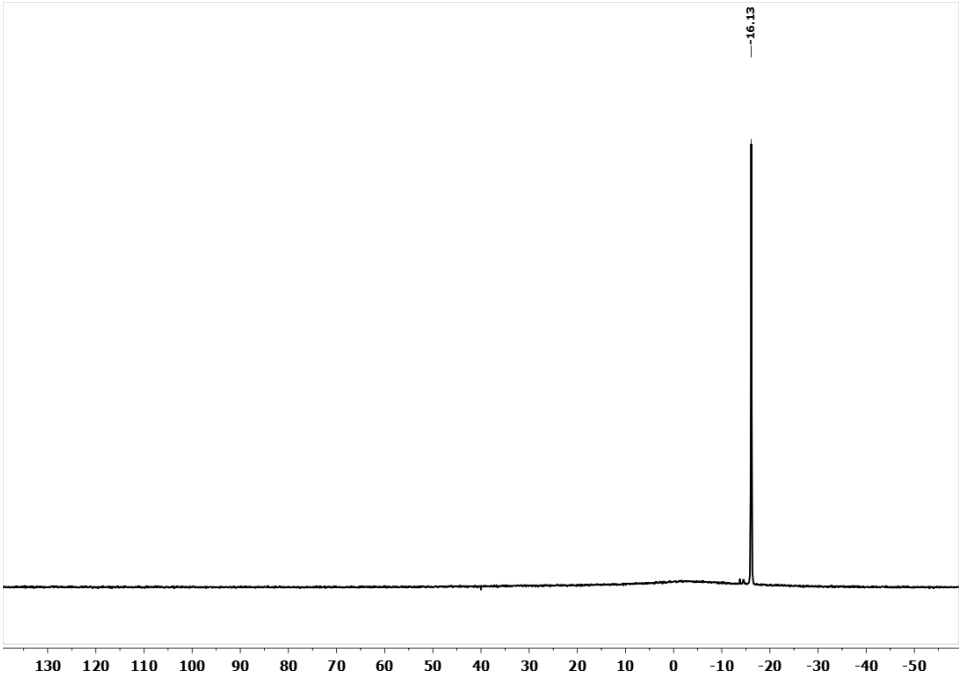
General Considerations. All manipulations were performed under an atmosphere of dry, oxygen-free N_2 by means of standard Schlenk or glovebox techniques (Innovative Technology glovebox equipped with a –35 ºC freezer). Bromobenzene was dried over CaH_2 and vacuum transferred before use. NMR spectra were obtained on a Bruker Avance 400 MHz spectrometer and spectra were referenced to residual solvent of C_6D_5Br (^1H = 6.94, 7.02, 7.30 ppm; ^{13}C = 121.79, 125.78, 128.95, 130.50 ppm), or externally (^{31}P: 85% H3PO4). Chemical shifts (δ) listed are in ppm and absolute values of the coupling constants are in Hz. All the phosphines, $Me_3SiO(Ph)C=CH_2$, *t*BuN=C(H)Ph, $[Ph_3C][B(C_6F_5)_4]$ were purchased from Aldrich and all were used without further purification. $(HC_6F_4)_3B$ was prepared by procedure described in M. Ullrich, A. J. Lough, D. W. Stephan, *Organometallics* **2010**, *29*, 3647-3654.

$[Ph_2P(H)\text{-}PPh_2][B(C_6F_5)_4]$ (1):

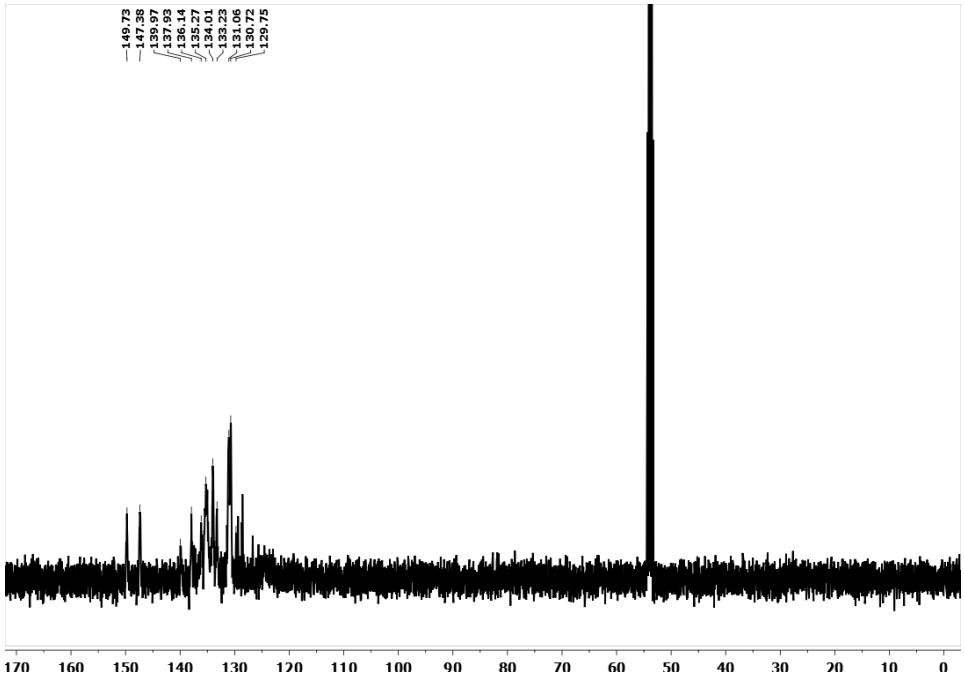
J. Young NMR tube in the glovebox was charged with Ph_2PH (18.6 mg, 0.1 mmol) and $[Ph_3C][B(C_6F_5)_4]$ (46 mg, 0.05 mmol) and dissolved in C_6D_5Br (1.5 mL). The solution was heated to 130°C for 3 h. Afterwards, C_6D_5Br was evaporated and resulting oil was washed with C_6H_6 (x1) and hexane (x3) leaving **1** as a residue in 87 % yields.

^1H NMR (400 MHz, Methylene Chloride-d_2): δ 7.66 (bs, 2H), 7.46 (bs, 6H), 7.34 (bs, 12H), 7.27 (d, *J(PH)* = 456.7 Hz, 1H). $^{11}B\{^1H\}$ NMR (128 MHz,) δ -16.13. $^{13}C\{^1H\}$ NMR (101 MHz, Methylene Chloride-d_2): δ 135.27, 134.01 , 131.06 , 130.72 (C_6H_5-P); 148.57 (d, *J(CF)* = 239.4 Hz), 138.69 (d, *J(CF)* = 257.8 Hz), 134.68 (d, *J(CF)* = 292.7 Hz), 129.75 (C_6F_5-B). $^{19}F\{^1H\}$ NMR (377 MHz,) δ -131.62 (d, *J* = 18.1 Hz), -161.84 (t, *J* = 21.1 Hz), -165.71 (t, *J* = 19.6 Hz). ^{31}P NMR (162 MHz, Methylene Chloride-d_2): δ 6.04 (d, *J(PH* = 456.8 Hz), -25.10.

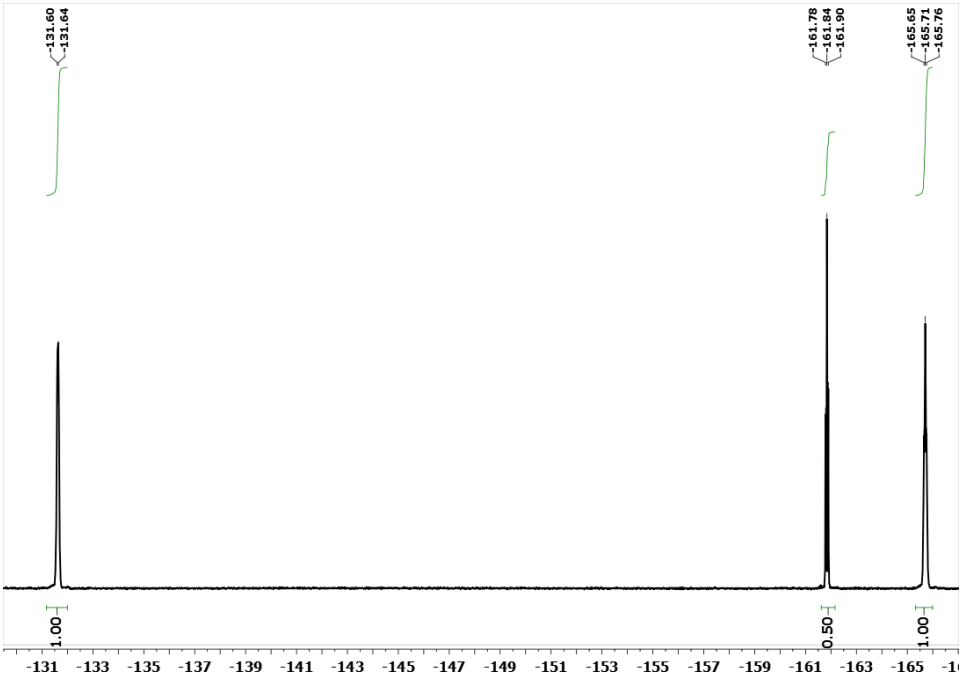
$^{11}B\{^{1}H\}$: $[Ph_2(H)P\text{-}PPh_2][B(C_6F_5)_4]$

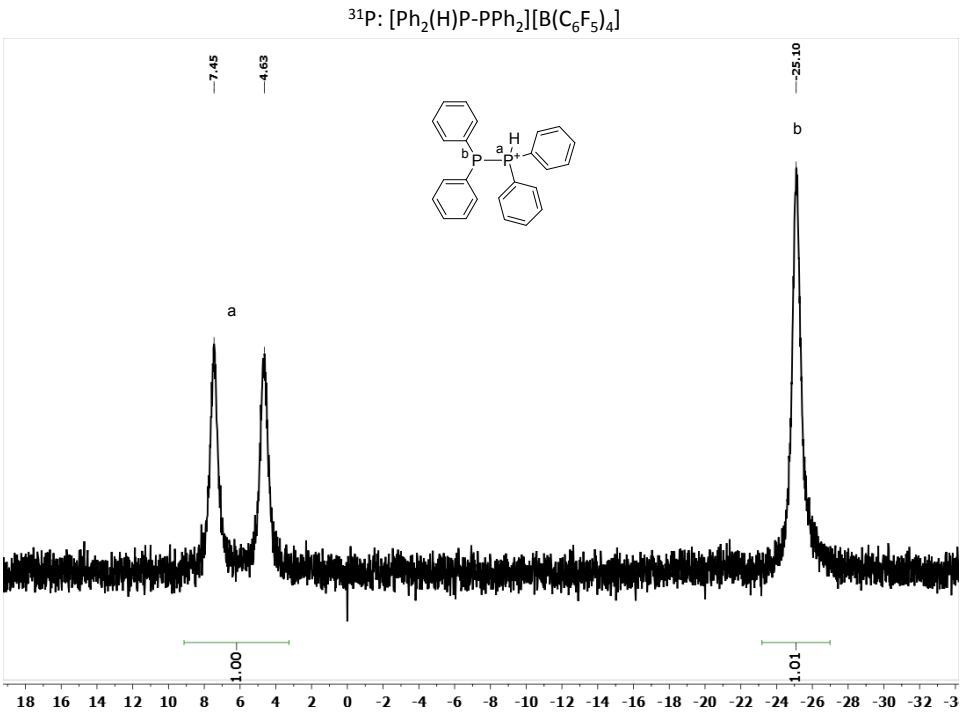


$^{13}C\{^{1}H\}$: $[Ph_2(H)P\text{-}PPh_2][B(C_6F_5)_4]$



$^{19}F\{^{1}H\}$: $[Ph_2(H)P\text{-}PPh_2][B(C_6F_5)_4]$





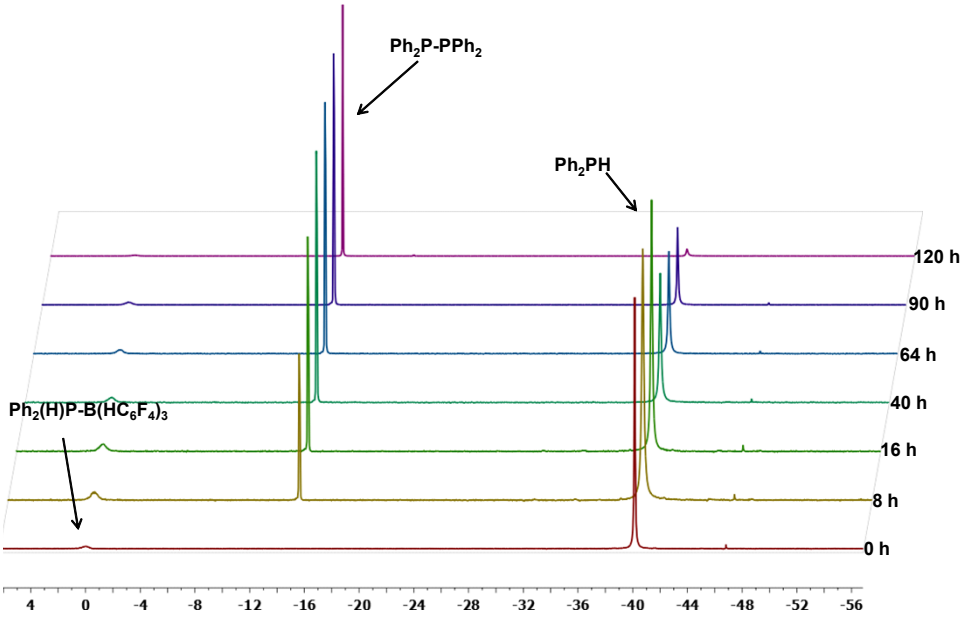
Dehydrocoupling of Ph_2PH, *p*-Tol_2Ph and $PhPH_2$:

J. Young NMR tube in the glovebox was charged with R_3P (R_3P = Ph_2PH: 39 mg, 0.21 mmol; R_3P = *p*-Tol_2PH: 42 mg, 0.2 mmol; R_3P = $PhPH_2$; 22 mg, 0.2 mmol) and 10 mol% of $(HC_6F_4)_3B$ (9 mg, 0.02 mmol; 9 mg, 0.02 mmol; 9 mg, 0.2 mmol, respectively) and dissolved in C_6D_5Br (0.5 mL). The J. Young NMR tube was degassed and the solution was heated to 130 °C. Every 12h J. Young NMR tube was degassed to remove H_2 which is formed during the reaction to drive the equilibrium to the dehydrocoupling products, and reaction propagation was monitored by ^{31}P NMR. After 120 h the reaction reached 88 % conversion to Ph_2P-PPh_2 in the case of Ph_2PH, 80% conversion to (*p*-Tol)$_2$P-P(*p*-Tol)$_2$ in the case of *p*-Tol_2PH, and 98% conversion to Ph_5P_5 in the case of $PhPH_2$, the conversion was calculated by integration of ^{31}P NMR. All of the dehydrocoupling products were isolated by crystallization form mixture DCM/Pentane (1:10) at room temperature.

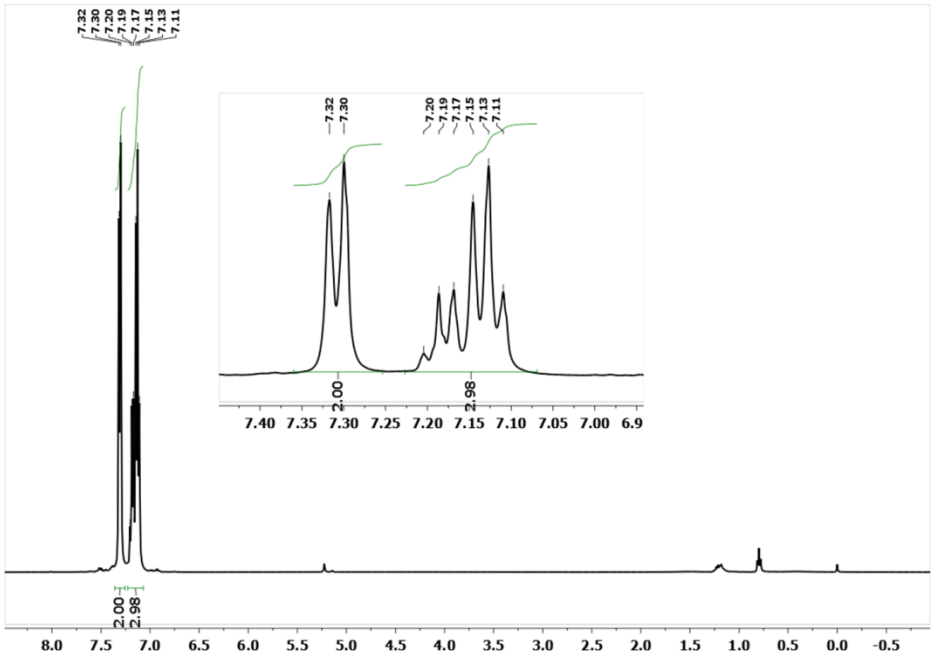
$(Ph_2P)_2$ (3)

^1H NMR (400 MHz, Methylene Chloride-d_2) δ 7.31 (d, J = 6.9 Hz, 2H), 7.18 (d, J = 7.2 Hz, 1H), 7.13 (t, J = 7.2 Hz, 2H). ^{13}C NMR (101 MHz, Methylene Chloride-d_2) δ 136.17 (t, J = 5.1 Hz), 134.69 (t, J = 13.1 Hz), 129.14, 128.61 (t, J = 3.4 Hz). ^{31}P NMR (162 MHz, C_6D_5Br): δ -16.0.

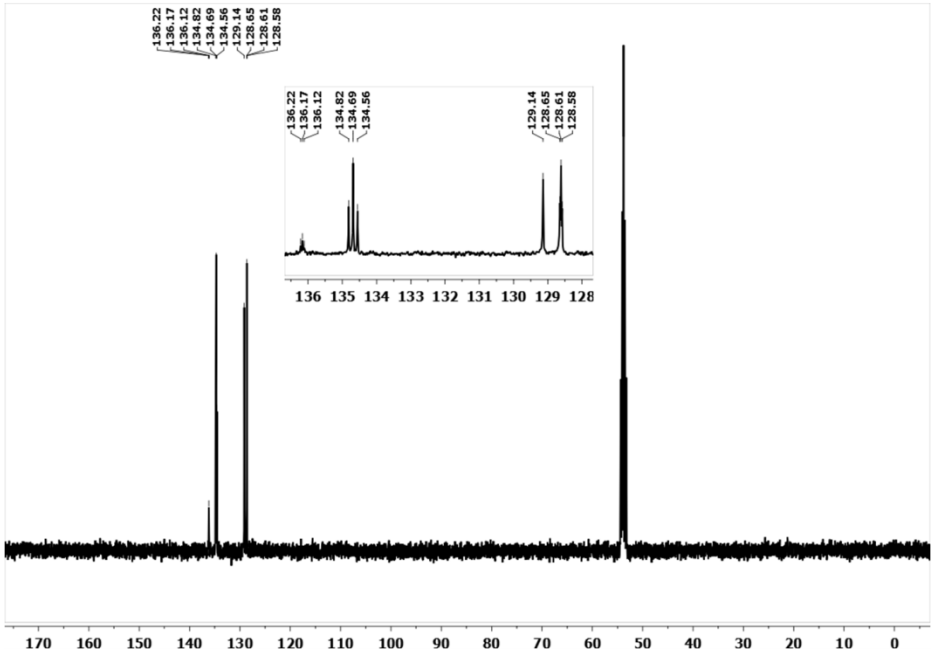
$^{31}P\{^{1}H\}$: Propagation of Ph_2PH dehydrocoupling



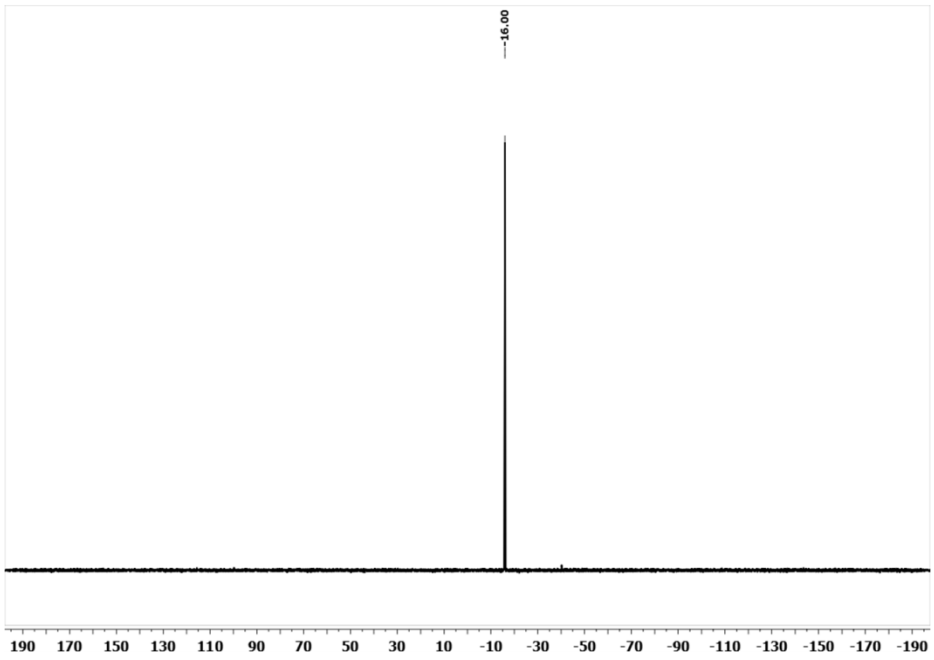
^{1}H: Ph_2PPPh_2



$^{13}C\{^{1}H\}$: Ph_2PPPh_2



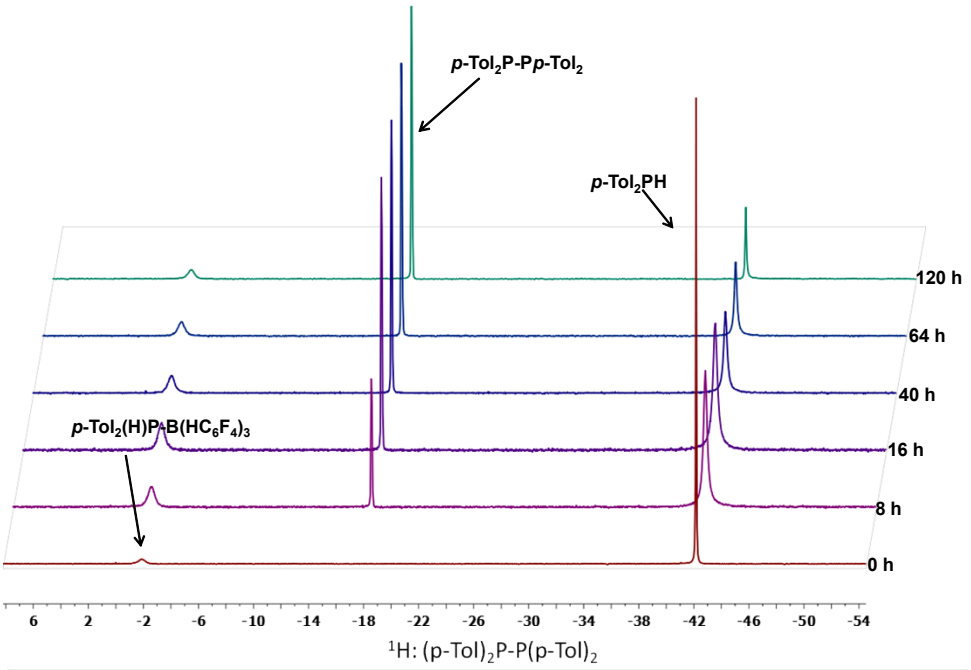
^{31}P: Ph_2PPPh_2



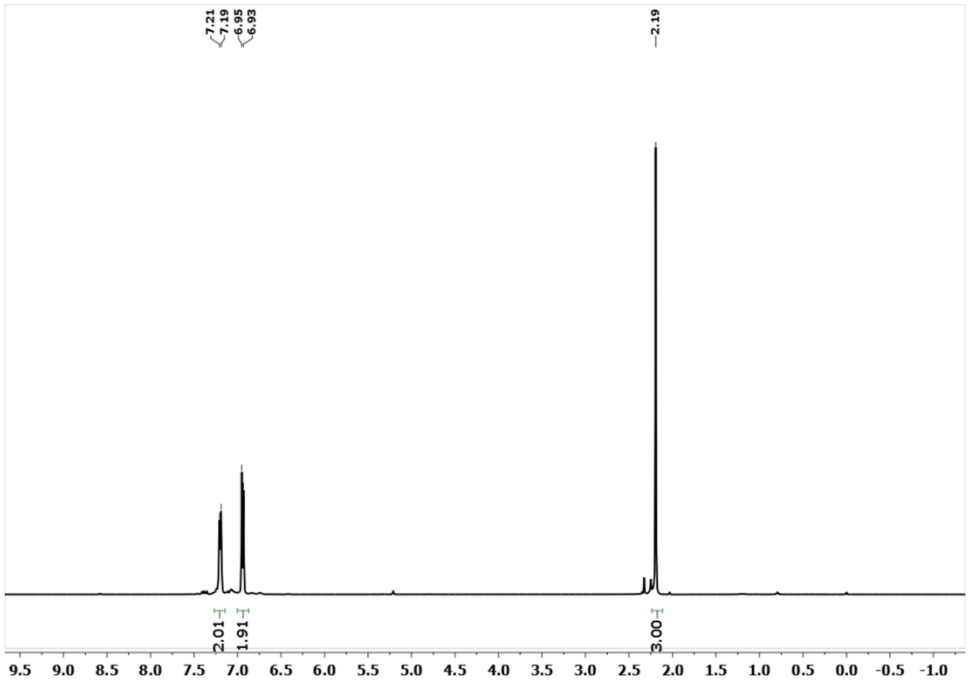
(pTol$_2$P)$_2$ (4):

^{1}H NMR (400 MHz, Methylene Chloride-d_2) δ 7.20 (d, J = 7.6 Hz, 2H), 6.94 (d, J = 7.7 Hz, 2H), 2.19 (s, 3H). ^{13}C NMR (101 MHz, Methylene Chloride-d_2) δ 139.24 , 134.62 (t, J = 12.4 Hz), 132.89 , 129.37 , 21.36. ^{31}P NMR (162 MHz, Methylene Chloride-d_2) δ -18.84.

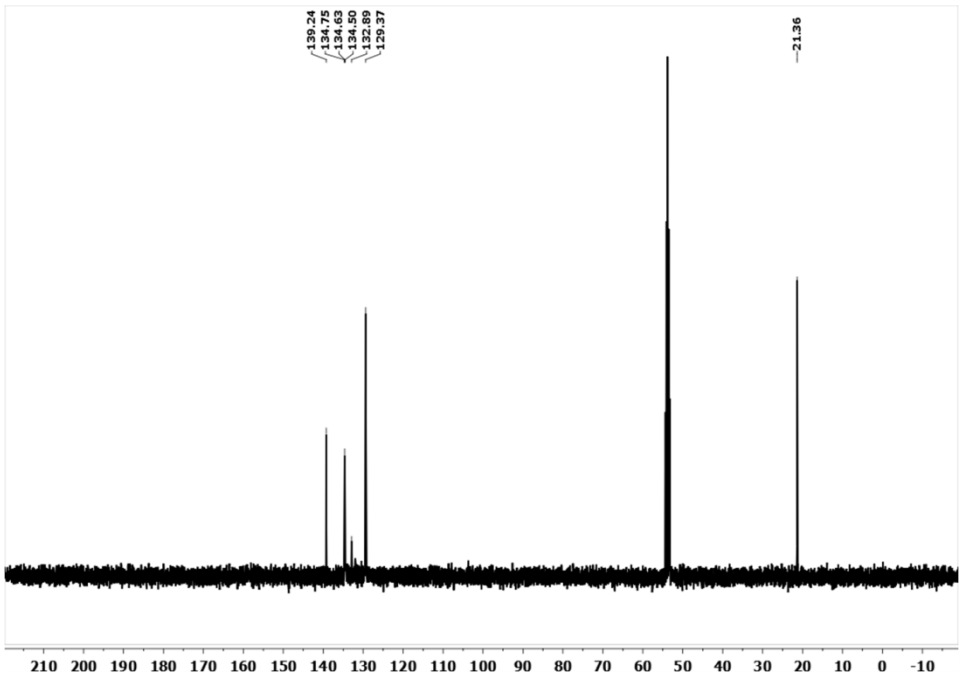
$^{31}P\{^{1}H\}$: Propagation of *p*-Tol_2PH dehydrocoupling



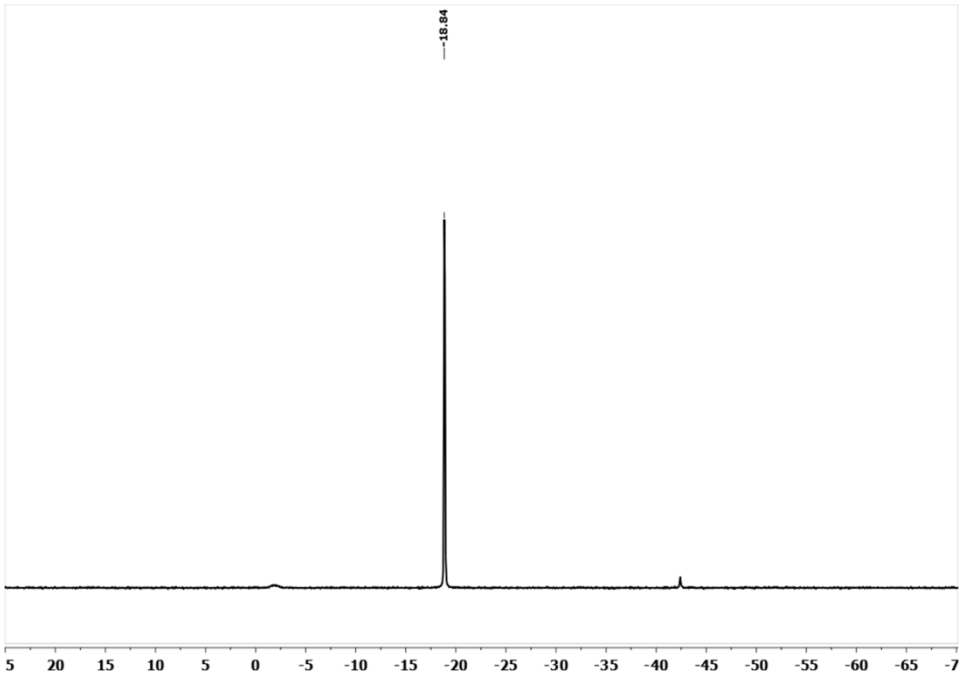
^{1}H: (p-Tol)$_2$P-P(p-Tol)$_2$



^{13}C: (p-Tol)$_2$P-P(p-Tol)$_2$



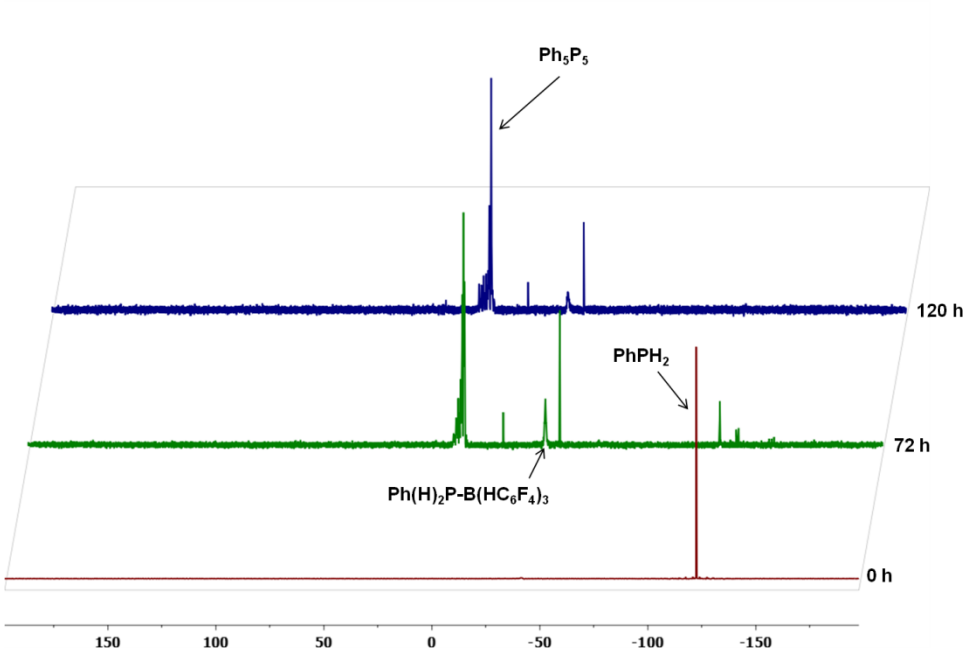
^{31}P{H}: (p-Tol)$_2$P-P(p-Tol)$_2$



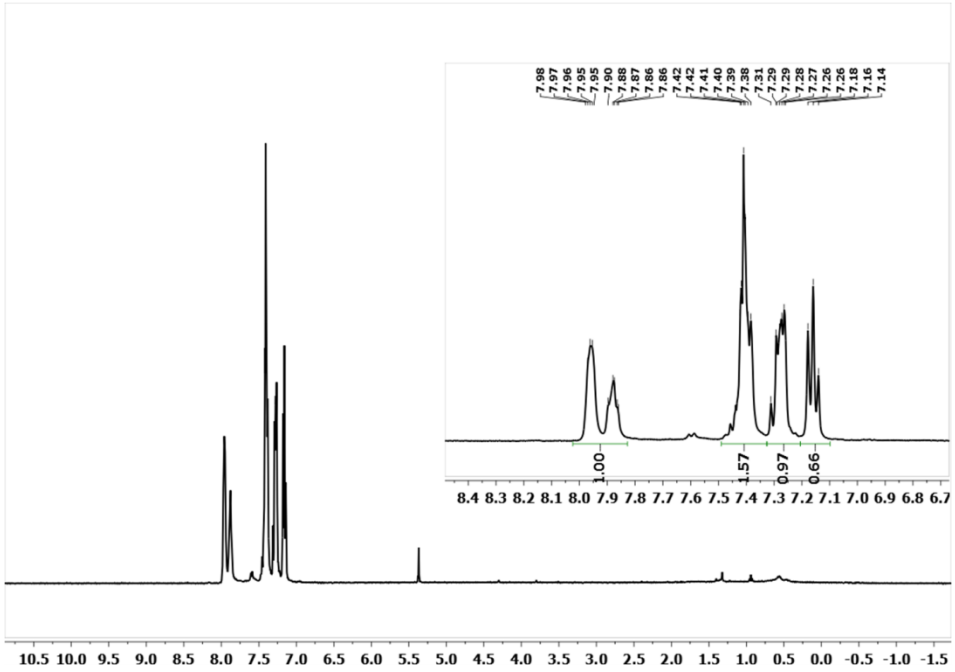
(PhP)$_5$ (5)

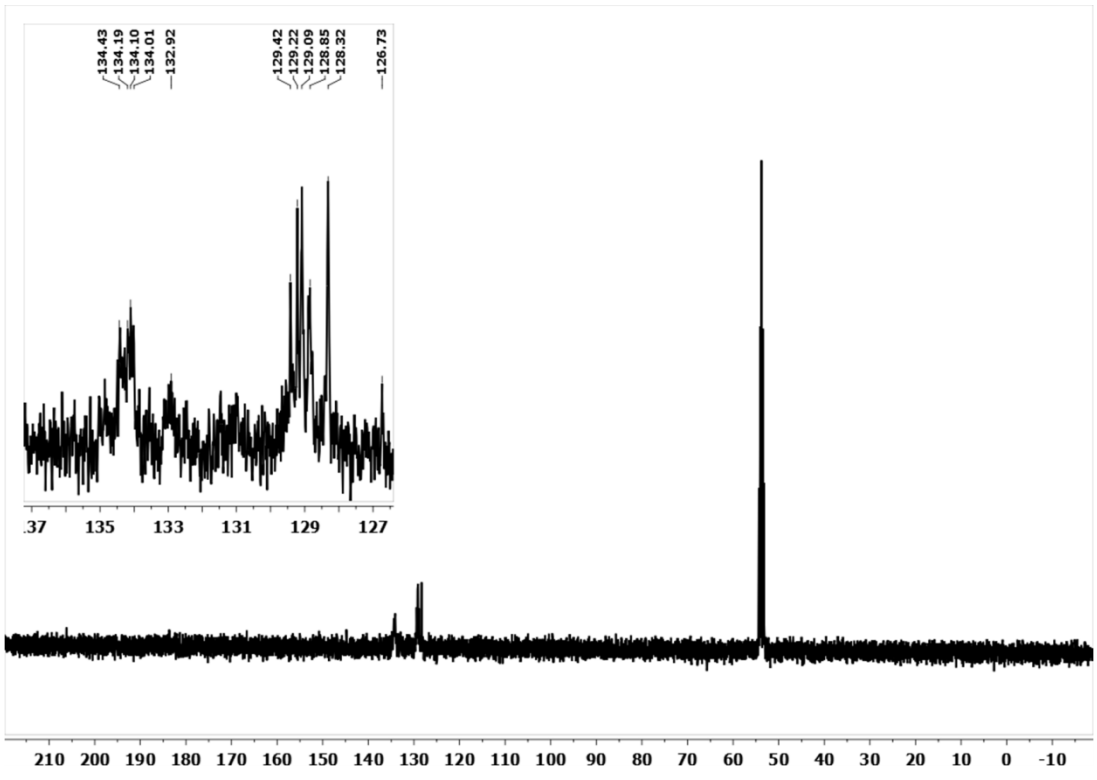
^{1}H NMR (400 MHz, Methylene Chloride-d_2) δ 7.96 (dd, J = 6.3, 3.2 Hz, 1H), 7.92 – 7.82 (m, 1H), 7.40 (dt, J = 8.2, 3.8 Hz, 2H), 7.33 – 7.22 (m, 1H), 7.16 (t, J = 7.6 Hz, 1H). ^{13}C NMR (101 MHz, Methylene Chloride-d_2) δ 135.30 – 133.57 (m), 132.92 , 129.14 (dd, J = 35.5, 22.3 Hz), 128.32 , 126.73. ^{31}P NMR (162 MHz, Methylene Chloride-d_2) δ 0.88 – -8.27 (m).

$^{31}P\{^{1}H\}$: Propagation of $PhPH_2$ dehydrocoupling

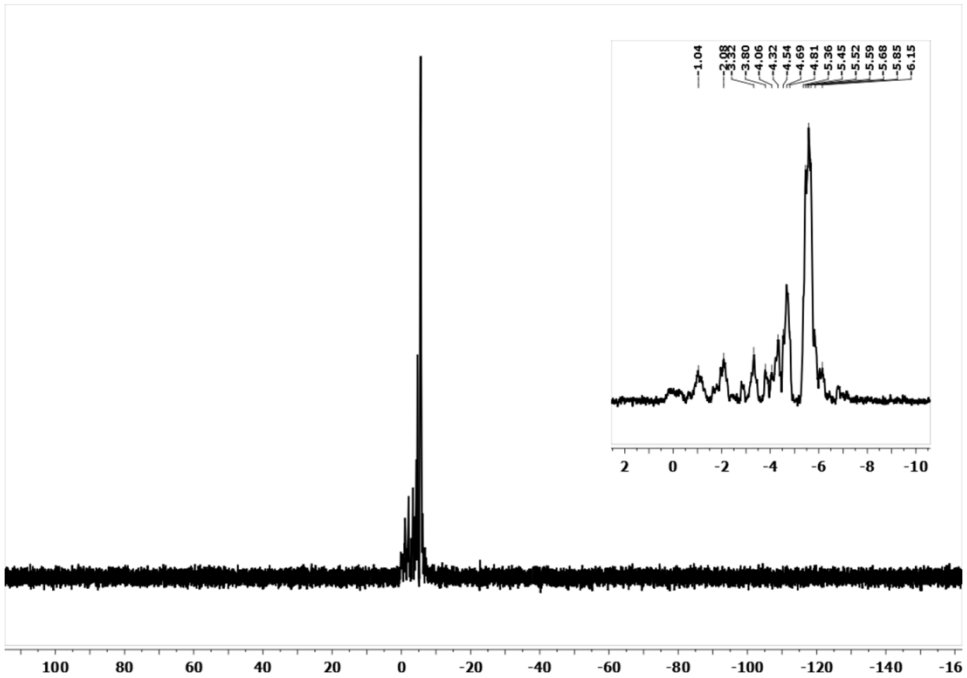


^{1}H: Ph_5P_5





^{31}P: Ph_5P_5



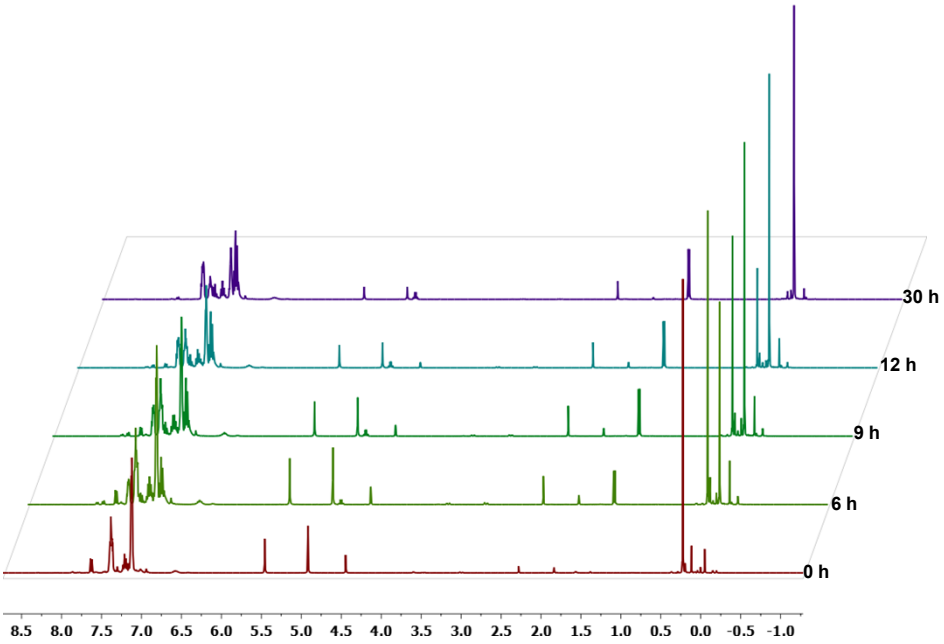
Transfer hydrogenation of $Ph(Me_3SiO)C=CH_2$:

20 mL Schlenk bomb in the glovebox was charged with Ph_2PH (65 mg, 0.31 mmol), 10 mol% of $(HC_6F_4)_3B$ (10 mg, 0.02 mmol) and $Ph(Me_3SiO)C=CH_2$ (23 mg, 0.11 mmol) dissolved in C_6D_5Br (5 mL). The flask was transferred to the Schlenk line evacuated and sealed with teflon stopcock.

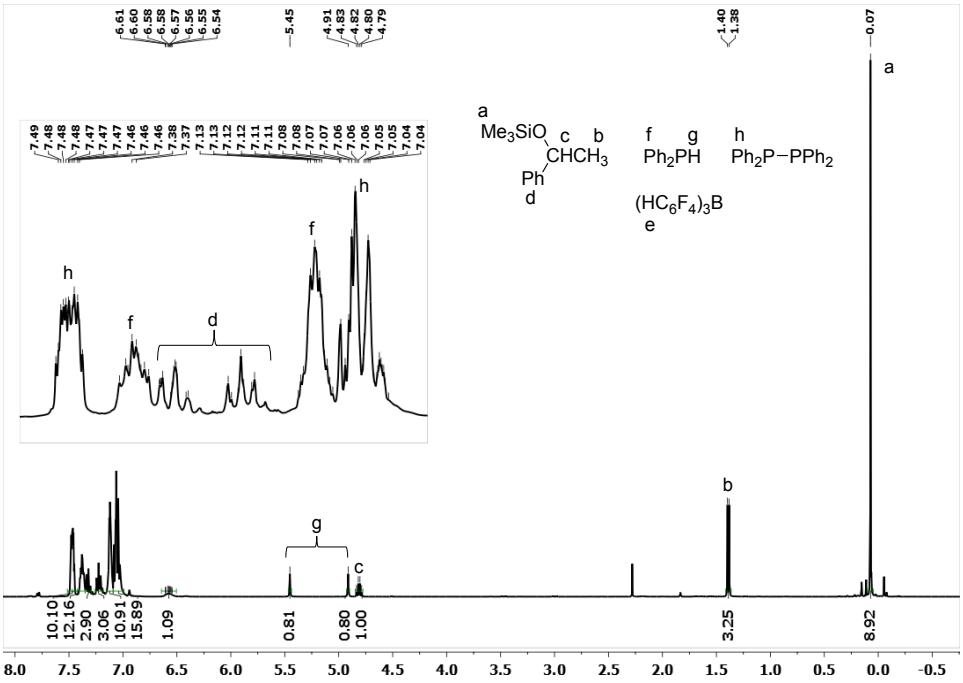
The solution was heated to 130 °C and the propagation of the reaction was followed by ^{1}H and $^{31}P\{^{1}H\}$ NMR. After 30 h all the starting $Ph(Me_3SiO)C{=}CH_2$ was converted to $Ph(Me_3SiO)CHCH_3$.

^{1}H NMR of $Ph(Me_3SiO)CHCH_3$ compared with ^{1}H NMR reported by Brunet, J. J.; Besozzi, D.; Caubere, P. *Synthesis* **1982**, *9*, 721-3. ^{1}H NMR (C_6D_5Br, 400 MHz): δ 7.35 – 7.19 (m, 5H, **Ph**$(Me_3SiO)CHCH_3$), 4.81 (q, J = 6.3 Hz, 1H, $Ph(Me_3SiO)C\mathbf{H}CH_3$), 1.39 (d, J = 6.4 Hz, 3H, $Ph(Me_3SiO)CHC\mathbf{H}_3$), 0.07 (s, 9H, $Ph(\mathbf{Me}_3SiO)CHCH_3$).

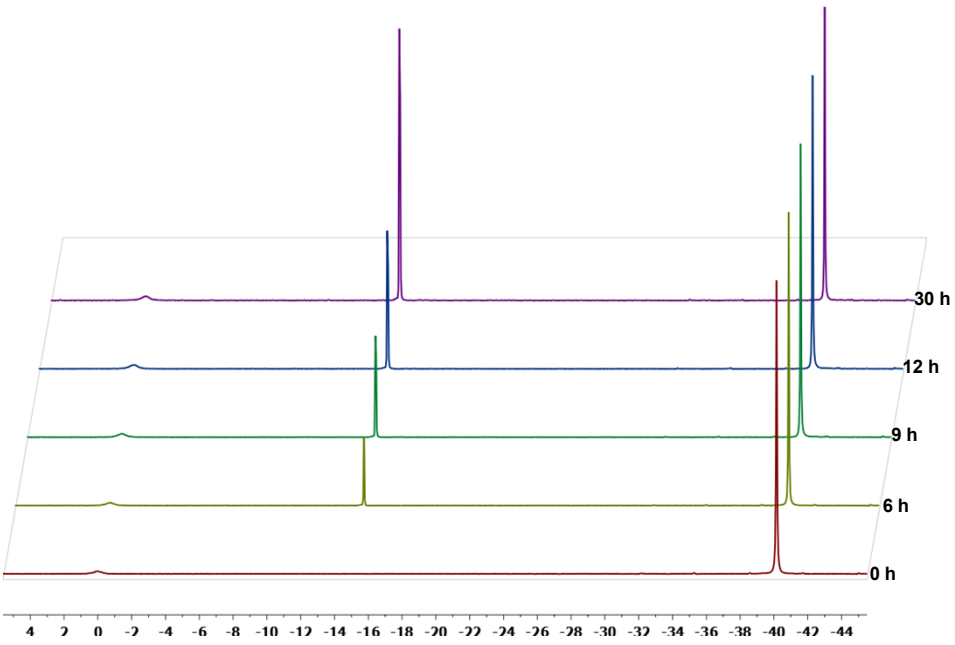
^{1}H: Propagation of Ph_2PH dehydrocoupling in the presence of $(Me_3SiO)PhCCH_2$



^{1}H: Ph_2PPPh_2 Ph_2PH and $Ph(Me_3SiO)CHCH_3$



^{31}P{^{1}H}: Propagation of Ph_2PH dehydrocoupling in the presence of $(Me_3SiO)PhCCH_2$



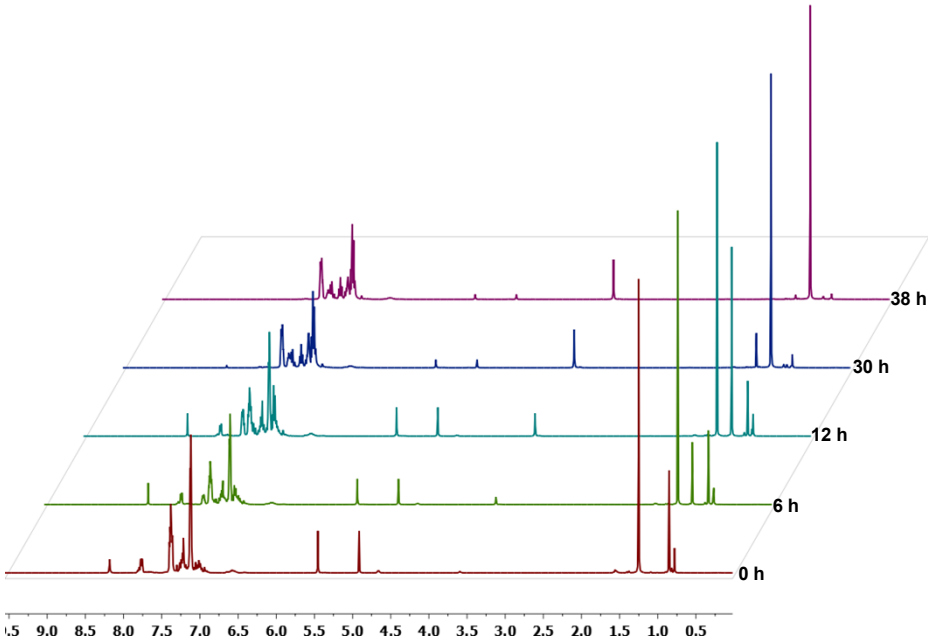
Transfer hydrogenation of Ph(H)C=N*t*Bu:

J. Young NMR tube in the glovebox was charged with Ph_2PH (43.0 mg, 0.2 mmol), $(HC_6F_4)_3B$ (10 mg, 0.02 mmol), Ph(H)C=N*t*Bu (14 mg, 0.08 mmol), and dissolved in C_6D_5Br (1.5 mL). The

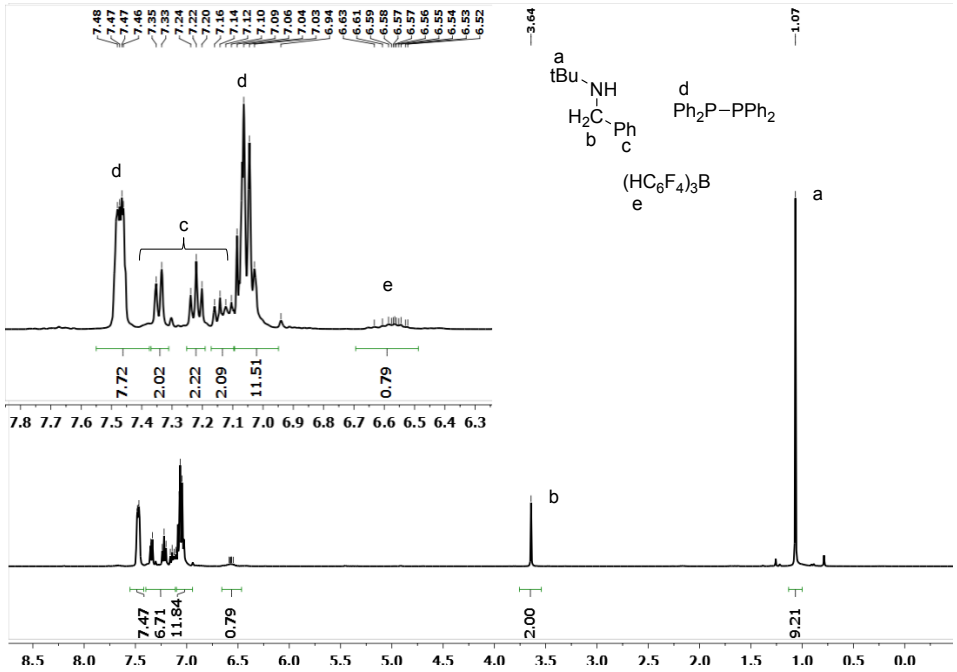
solution was heated to 130 °C and the propagation of the reaction was followed by ^{1}H and $^{31}P\{^{1}H\}$ NMR. After 35 h the conversion to the hydrogenated $PhCH_2N(H)tBu$ was 96.7 % and after 38 h all the starting $Ph(H)C{=}NtBu$ was converted to $PhCH_2N(H)tBu$.

^{1}H NMR of $PhCH_2N(H)tBu$ compared with ^{1}H NMR reported by Froyen, P.; Juvvik, P. *Tetrahedron Lett.* **1995**, *36*, 9555-9558. ^{1}H NMR (C_6D_5Br, 400 MHz): δ 7.25 and 7.23 (m, 4H, o and m–Ph–H); 7.15 (tt, 1H, p–Ph–H, 3*JHH* = 6.9 Hz, 4*JHH* = 1.6 Hz); 3.65 (s, 2H, CH_2); 1.11 (s, 9H, tBu–CH_3).

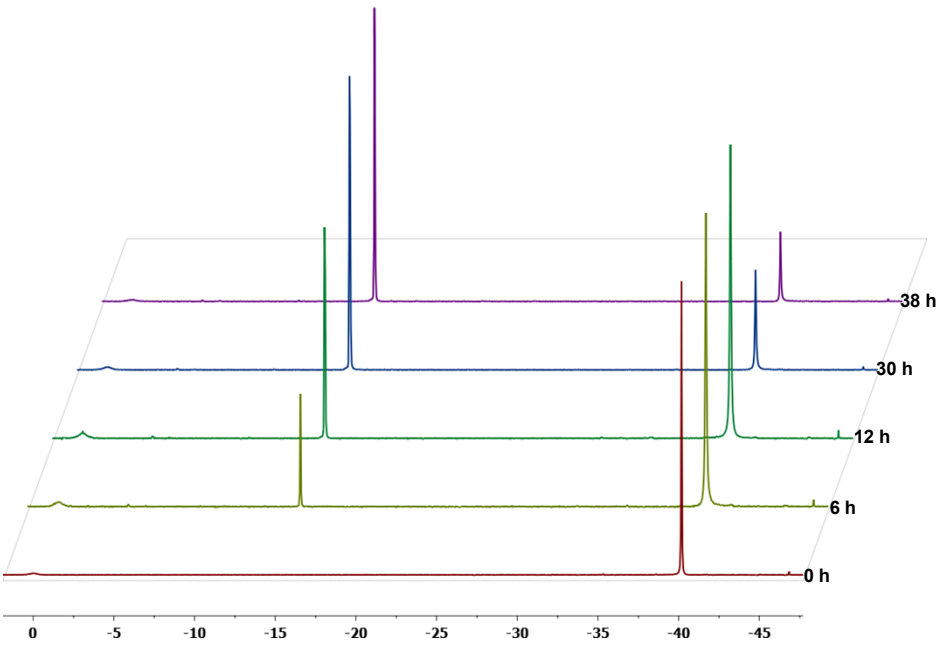
^{1}H: Propagation of Ph_2PH dehydrocoupling in the presence of $Ph(H)C{=}N(tBu)$



^{1}H: Ph_2PPPh_2 and $PhCH_2N(H)(tBu)$



^{31}P{^{1}H}: Propagation of Ph_2PH dehydrocoupling in the presence of $Ph(H)C{=}N(tBu)$

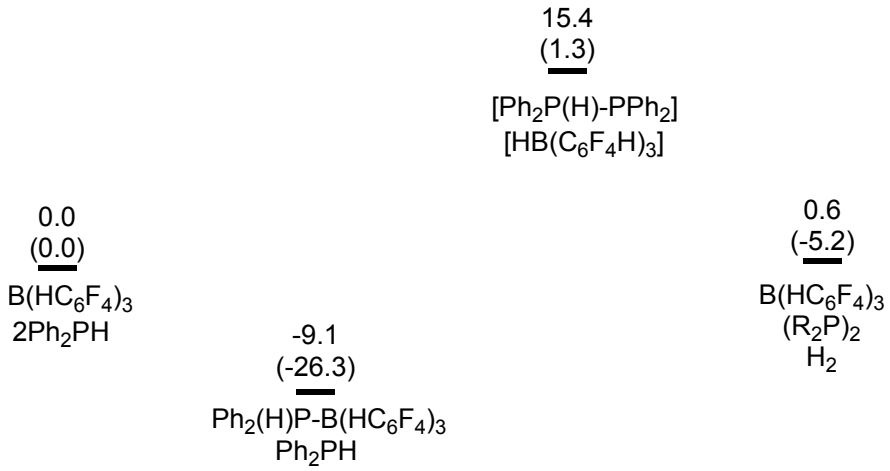


Tests for Radical Reactions

We have performed the dehydrocoupling reaction in the presence of 1,4-cyclohexadiene in a stoichiometric reaction; no benzene was observed. In addition, the reaction was also done in presence of Et_3SiH. Should radicals be generated one would expect abstraction of hydrogen from silane generating $Et_3Si\text{-}SiEt_3$ dimer. However, only P-P dehydrocoupling product were observed with traces of Si-P coupling. Further the reaction was done in the presence of $Ph_2C{=}CH_2$ yet no radical dimerization of the olefin was observed.

DFT calculations

DFT calculations were performed using Gaussian 09.2 Geometry optimization of all the molecules was carried out using the wB97XD/def2-TZV basis sets in conjunction with the conductor-like polarizable continuum solvation model (CPCM) implemented in the Gaussian 09 software. Thermal energy corrections were extracted from the results of frequency analysis performed at the same level of theory. Frequency analysis of all calculated molecules contained no imaginary frequency showing that these are energy minima.



Gibbs free energy diagram reaction pathways of dehydrocoupling (calculated at wB97XD/def2-TZV basis sets in conjunction with the conductor-like polarizable continuum solvation model (CPCM); values given in kcal mol^{-1} relative to the energy of the $2Ph_2PH$ and $B(HC_6F_4)_3$; enthalpies are given in parentheses). Transition states were not allocated for this energy diagram.

Coordinates of optimized structures:

Ph_2PH:

P	0.04440400	1.73350400	-0.31971000
H	-0.02478100	1.78963100	-1.75798300
C	1.45125300	0.49635000	-0.16564200
C	1.38660400	-0.78334100	-0.72019400
C	2.59582500	0.88037100	0.53212600
C	2.45374600	-1.66432600	-0.58181800
H	0.49957000	-1.09713400	-1.25493100
C	3.66683400	-0.00166700	0.67114400
H	2.65324700	1.86771800	0.97162400
C	3.59654500	-1.27419700	0.11455100
H	2.39424900	-2.65300100	-1.01610800
H	4.54954400	0.30588400	1.21493900
H	4.42498500	-1.96080400	0.22296800
C	-1.43399900	0.61768100	-0.06877900
C	-1.76857400	0.23692200	1.23347100
C	-2.21665100	0.16381800	-1.13121400
C	-2.86021700	-0.59251800	1.46808400
H	-1.17638400	0.58917200	2.06875600
C	-3.31716800	-0.65807600	-0.89544700
H	-1.97039100	0.44439300	-2.14700200
C	-3.63827000	-1.04092700	0.40290700
H	-3.10585800	-0.88346100	2.48027000
H	-3.91649100	-1.00283900	-1.72712800
H	-4.48930700	-1.68265200	0.58510700

Sum of electronic and zero-point Energies= -804.879663 (Ha)

Sum of electronic and thermal Energies= -804.868794 (Ha)

Sum of electronic and thermal Enthalpies= -804.867850 (Ha)

Sum of electronic and thermal Free Energies= -804.919066 (Ha)

$(HC_6F_4)_3B$:

B	0.00089400	-0.00218200	0.00024600
C	-1.02965800	-1.18109100	0.00114400
C	-2.17895000	-1.15450700	0.78559500
C	-0.85108200	-2.31700700	-0.78294100
C	-3.08563900	-2.19587800	0.79462000
C	-1.76342900	-3.35352700	-0.79185900
C	-2.89101400	-3.30729700	0.00125300
H	-3.60146100	-4.11895700	0.00117100
C	-0.50607700	1.47939900	-0.00034900
C	-1.57215600	1.89295200	-0.79340300
C	0.08225900	2.45970400	0.79303900
C	-2.01643500	3.20020600	-0.80230800
C	-0.36938400	3.76442000	0.80241400
C	-1.42256700	4.15196700	0.00032700
H	-1.77263800	5.17220500	0.00085900
C	1.53757900	-0.30251700	-0.00098200
C	2.09414000	-1.30597800	0.78643800
C	2.42799200	0.42074400	-0.78891800
C	3.45027100	-1.56508700	0.79451700
C	3.78269100	0.15408500	-0.79900300
C	4.31158300	-0.84040200	-0.00283000
H	5.37048300	-1.04596600	-0.00349100
F	0.25113000	-2.41254000	-1.60054800
F	-1.54535800	-4.44302300	-1.59595300
F	-2.41942400	-0.07531700	1.60413600
F	-4.19440300	-2.12360200	1.59865800
F	0.23714900	4.68700200	1.61614200
F	1.12997700	2.12689100	1.62023200
F	-2.19544300	0.98694100	-1.62015000
F	-3.06191400	3.55670400	-1.61530800
F	1.28326000	-2.05341700	1.60884600

F	3.94734200	-2.55588100	1.60220400
F	4.61323100	0.88814400	-1.60681400
F	1.95427500	1.41837700	-1.60925500

Sum of electronic and zero-point Energies= -1910.160594 (Ha)

Sum of electronic and thermal Energies= -1910.134360 (Ha)

Sum of electronic and thermal Enthalpies= -1910.133415 (Ha)

Sum of electronic and thermal Free Energies= -1910.220379 (Ha)

$Ph_2(H)P\text{-}B(HC_6F_4)_3$:

P	-0.13008600	-0.91678100	-1.39504300
C	-1.34291100	0.50982500	0.89430900
C	-1.55238600	0.25230400	2.24231700
C	-2.50862500	0.74962000	0.17293200
C	-2.81616800	0.18587400	2.80254800
C	-3.77202400	0.68377900	0.71699700
C	-3.95117800	0.39447000	2.05236900
H	-4.93416400	0.34054900	2.49162900
C	1.38744300	0.07564700	1.00149700
C	1.45783200	-1.21343600	1.52025400
C	2.52070600	0.84241600	1.25290600
C	2.55109300	-1.71887500	2.18611500
C	3.62698100	0.34857300	1.92444500
C	3.66815000	-0.94098300	2.40090600
H	4.53140200	-1.32313100	2.92135000
C	0.31950300	1.99919900	-0.60520000
C	-0.21839700	3.18551600	-0.11431000
C	1.10905200	2.16848600	-1.73381900
C	-0.03182900	4.40853500	-0.73046900
C	1.30417200	3.38131200	-2.36140800
C	0.73116900	4.53248700	-1.87002800
H	0.87907000	5.48676200	-2.34909400

C	-1.73371200	-1.83146200	-1.40929300
C	-2.47974300	-1.84475300	-2.58800200
C	-2.21655600	-2.47688800	-0.27061900
C	-3.70513100	-2.50079700	-2.62637700
H	-2.11676300	-1.34198900	-3.47412400
C	-3.44262400	-3.13097500	-0.31524500
H	-1.65076300	-2.46982600	0.64719600
C	-4.18827000	-3.14252400	-1.49031600
H	-4.27995000	-2.50683500	-3.54147500
H	-3.81443800	-3.62671100	0.57017300
H	-5.14331400	-3.64789800	-1.52022400
C	1.22131300	-2.18399800	-1.51177200
C	2.55811000	-1.78562600	-1.47214800
C	0.89953200	-3.53683000	-1.60210800
C	3.56632800	-2.74230200	-1.51876400
H	2.82177600	-0.74224600	-1.39828400
C	1.91310400	-4.48850700	-1.64747800
H	-0.13175200	-3.85748300	-1.62859800
C	3.24638100	-4.09382700	-1.60466100
H	4.59989300	-2.42797200	-1.48531500
H	1.65817600	-5.53654200	-1.71655400
H	4.03180400	-4.83580700	-1.63545000
B	0.09691200	0.56397600	0.13981300
F	-2.40980900	1.06720700	-1.17539200
F	-4.86869100	0.90989300	-0.08685300
F	-2.93643200	-0.08726500	4.14887200
F	-0.48709900	0.07499500	3.10469300
F	2.60036000	2.16045200	0.84380600
F	4.71100400	1.17736400	2.12095100
F	2.52522700	-3.01904700	2.64140400
F	0.36955800	-2.05738200	1.36410400

F	-0.95165200	3.19454100	1.05877900
F	-0.61136500	5.53114000	-0.17902200
F	2.10066700	3.43887300	-3.48485100
F	1.78556100	1.07587900	-2.26276300
H	-0.15808300	-0.29643600	-2.67165900

Sum of electronic and zero-point Energies= -2715.081712 (Ha)

Sum of electronic and thermal Energies= -2715.044102 (Ha)

Sum of electronic and thermal Enthalpies= -2715.043158 (Ha)

Sum of electronic and thermal Free Energies= -2715.153941 (Ha)

$[Ph_2(H)P\text{-}PPh_2]^+$:

P	-0.03321500	0.93660300	-1.08626800
P	0.03642400	-0.79305900	0.45630200
H	0.06544900	-0.30760900	1.79132400
C	1.44337300	1.88941400	-0.45758900
C	1.34728500	3.10557200	0.21772600
C	2.70245000	1.37091400	-0.77806600
C	2.50396900	3.78405800	0.59083900
H	0.38383800	3.53787900	0.44358500
C	3.85378300	2.04420300	-0.38761700
H	2.79048200	0.44738900	-1.33551400
C	3.75573900	3.25084400	0.29981500
H	2.42317000	4.72952000	1.10821000
H	4.82300800	1.63156900	-0.62907500
H	4.65098700	3.77931300	0.59562600
C	-1.54861600	1.77659400	-0.39994200
C	-1.73919400	2.10290100	0.94548500
C	-2.56142000	2.04078100	-1.32406500
C	-2.92820000	2.69241900	1.35755400
H	-0.96688800	1.91359400	1.67872600
C	-3.74832800	2.63749900	-0.90906500

H	-2.42644800	1.78336000	-2.36604200
C	-3.93304900	2.96000900	0.43078400
H	-3.06976600	2.94077300	2.39972700
H	-4.52548700	2.84351900	-1.63097900
H	-4.85680300	3.41826000	0.75452200
C	1.58095100	-1.75555400	0.25992100
C	1.70367300	-2.67961800	-0.77588300
C	2.64269700	-1.50123200	1.12630700
C	2.90594900	-3.35736500	-0.94032300
H	0.87846400	-2.87965900	-1.44609800
C	3.84200500	-2.18196100	0.95006000
H	2.54899200	-0.78026600	1.92702600
C	3.97319100	-3.10734000	-0.08079700
H	3.00808900	-4.07968300	-1.73706200
H	4.66851600	-1.98980200	1.61860800
H	4.90693300	-3.63446000	-0.21508800
C	-1.48216700	-1.79891500	0.27525900
C	-2.01522700	-2.02632200	-0.99303000
C	-2.09960900	-2.31208900	1.41523900
C	-3.17136100	-2.78860700	-1.11735300
H	-1.54892400	-1.61526100	-1.87835700
C	-3.25469700	-3.07258900	1.27872600
H	-1.69074600	-2.12916700	2.39927300
C	-3.78897300	-3.31035900	0.01527300
H	-3.58975100	-2.96890400	-2.09671700
H	-3.73670200	-3.47457200	2.15793700
H	-4.68988000	-3.89849100	-0.08569700

Sum of electronic and zero-point Energies= -1609.005572 (Ha)

Sum of electronic and thermal Energies= -1608.982950 (Ha)

Sum of electronic and thermal Enthalpies= -1608.982006 (Ha)

Sum of electronic and thermal Free Energies= -1609.061976 (Ha)

[$HB(HC_6F_4)_3$]:

H	0.00049300	-0.00497900	-1.95229400
C	0.41949600	1.50849300	-0.29807300
C	-0.12829100	2.59519900	-0.97354100
C	1.31595300	1.84974900	0.70668900
C	0.19830000	3.90546900	-0.68589500
C	1.65658900	3.15797200	0.99938100
C	1.10163300	4.21385300	0.30989400
H	1.36080300	5.23503400	0.53684700
C	1.09914000	-1.12455200	-0.29987700
C	2.31926900	-1.17968600	-0.96782200
C	0.94373700	-2.08281100	0.69372600
C	3.29317800	-2.11665000	-0.68578800
C	1.90864500	-3.03164200	0.97982600
C	3.10524500	-3.06585400	0.29743400
H	3.86079600	-3.80026800	0.52374000
C	-1.52038900	-0.39176100	-0.29710200
C	-2.25570300	0.20956100	0.71604500
C	-2.19619100	-1.40017800	-0.97721800
C	-3.56028400	-0.14249800	1.01007600
C	-3.49679400	-1.76424100	-0.69004500
C	-4.20815500	-1.13900200	0.31291500
H	-5.22424000	-1.41671800	0.54114000
F	2.60036000	-0.25504200	-1.95747700
F	4.48473800	-2.11229000	-1.39288000
F	1.68394700	-3.96204000	1.98129200
F	-0.20475500	-2.11723500	1.46754100
F	1.90707600	0.86891200	1.48614700
F	-1.05829500	2.38374800	-1.97543500
F	-0.38588800	4.93740800	-1.40240300

F	2.56536700	3.42317800	2.01059600
F	-1.55591800	-2.09706600	-1.98599600
F	-4.10815900	-2.77554100	-1.41347300
F	-4.23555900	0.50795600	2.02971200
F	-1.68945200	1.19776200	1.50383800
B	-0.00025500	-0.00386800	-0.74326500

Sum of electronic and zero-point Energies= -1910.912386 (Ha)

Sum of electronic and thermal Energies= -1910.886033 (Ha)

Sum of electronic and thermal Enthalpies= -1910.885089 (Ha)

Sum of electronic and thermal Free Energies= -1910.972069 (Ha)

Ph_2P-PPh_2:

P	-0.75488800	-0.38492700	-0.89089500
P	0.75520500	-0.38480300	0.89106000
C	-1.51444000	1.28317500	-0.52145100
C	-2.32994000	1.52194500	0.58584300
C	-1.17435500	2.34356700	-1.36169400
C	-2.80316900	2.80446100	0.84401200
H	-2.59987400	0.70802000	1.24541900
C	-1.64382900	3.62792300	-1.10099000
H	-0.53697800	2.16790800	-2.21822200
C	-2.45862700	3.86016000	0.00275000
H	-3.43535900	2.98032700	1.70374300
H	-1.37274700	4.44257600	-1.75842600
H	-2.82528900	4.85693500	0.20643000
C	-2.07465600	-1.55045000	-0.25175700
C	-1.80547700	-2.57843500	0.65178300
C	-3.36516600	-1.43322100	-0.77855300
C	-2.80778200	-3.47246600	1.02402700
H	-0.81981600	-2.69072200	1.08406500
C	-4.36656600	-2.32031600	-0.40133100

H	-3.59277600	-0.64305700	-1.48260300
C	-4.08991900	-3.34490600	0.50147900
H	-2.58337800	-4.26250200	1.72756000
H	-5.36052400	-2.21281200	-0.81362600
H	-4.86745300	-4.03697600	0.79395000
C	1.51436300	1.28344500	0.52149900
C	2.32936100	1.52250700	-0.58609500
C	1.17440500	2.34368200	1.36200300
C	2.80219000	2.80515900	-0.84433900
H	2.59921200	0.70871200	-1.24586500
C	1.64349000	3.62816400	1.10123300
H	0.53746600	2.16779000	2.21881000
C	2.45776400	3.86069700	-0.00283800
H	3.43398900	2.98124200	-1.70431400
H	1.37252300	4.44268700	1.75887800
H	2.82409300	4.85758000	-0.20658700
C	2.07504700	-1.55015000	0.25179300
C	1.80562900	-2.57856500	-0.65119500
C	3.36577200	-1.43248100	0.77794800
C	2.80790900	-3.47258600	-1.02351800
H	0.81979200	-2.69118700	-1.08298900
C	4.36714300	-2.31958100	0.40065500
H	3.59357300	-0.64198700	1.48156400
C	4.09025800	-3.34459900	-0.50159400
H	2.58331500	-4.26295200	-1.72662200
H	5.36127000	-2.21174400	0.81245700
H	4.86777500	-4.03666700	-0.79411700

Sum of electronic and zero-point Energies= -1608.607489 (Ha)

Sum of electronic and thermal Energies= -1608.585103 (Ha)

Sum of electronic and thermal Enthalpies= -1608.584159 (Ha)

Sum of electronic and thermal Free Energies= -1608.662579 (Ha)

H_2:

H	0.00000000	0.00000000	0.37109100
H	0.00000000	0.00000000	-0.37109100

Sum of electronic and zero-point Energies= -1.163140 (Ha)

Sum of electronic and thermal Energies= -1.160780 (Ha)

Sum of electronic and thermal Enthalpies= -1.159835 (Ha)

Sum of electronic and thermal Free Energies= -1.174626 (Ha)