Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supporting Information for

Essential role of phosphines in organocatalytic β-boration reaction

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Contents

1. Instrumentation and chemicals

All reactions and manipulations were carried out under a nitrogen atmosphere by using Schlenk-type techniques. The solvents were distilled over dehydrating reagents and were deoxygenated before use. Bis(pinacolato)diboron was used as purchased from Allychem.

NMR spectra were obtained using Varian Mercury 300 or 400 spectrometer. ^{1}H NMR and $^{13}C\{^{1}H\}$ NMR chemical shifts are reported in ppm (δ) relative to tetramethylsilane, referenced to the chemical shifts of residual solvent resonances. $^{31}P\{^{1}H\}$ NMR chemical shifts are reported in ppm (δ) relative to H_3PO_4. $^{11}B\{^{1}H\}$ NMR chemical shifts are reported in ppm (δ) relative to $BF_3(CH_3)_2O$.

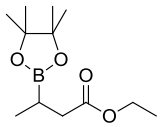
Gas chromatography with achiral HP-5 column was used to calculate conversions.

2. General Procedure for the phosphine assisted β-boration of α,β-unsaturated carbonyl compounds

The phosphine, trycyclohexylphosphine (5.6 mg, 0.02 mmol) and bis(pinacolato)diboron (140 mg, 0.55mmol) were transferred into an oven-dried Schlenk tube under nitrogen. Methanol (2 mL) was added. The substrate (0.5 mmol) was added, and the reaction mixture was stirred at 70 °C oil bath temperature for 6 hours. The reaction mixture was cooled to room temperature. An aliquot of 0.2 mL was taken from the solution. It was diluted with CH_2Cl_2 (1 mL) and analyzed by GC to determine conversion. After the GC analysis the same aliquot was gently concentrated on a rotary evaporator at RT, and analyzed by ^{1}H-NMR to confirm the conversion previously observed by gas chromatography. The analytical samples were combined with the rest of the reaction mixture, all the volatiles were removed in vacuum, and the crude product was purified by column chromatography.

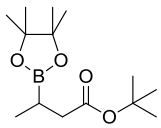
3. Characterization of the *β*-borated products

All the spectroscopic data of the follow products have been reported previously:[1]



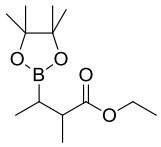
Ethyl 3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)butanoate: (purified with deactivated silica, petroleum ether: EtOAc, 15:1). White solid. Yield: (86%).

^{1}H NMR(300 MHz, $CDCl_3$) = δ 4.12 (q, *J* = 7.2 Hz, 2H), 2.43 (dd, *J* = 16.3, 7.6 Hz, 1H), 2.36 (dd, *J*1= 16.3, *J*2=6.6 Hz, 1H), 1.41−1.34 (m, 1H), 1.27(s, 6H), 1.25 (CH_3 overlapped, 3H), 1.22 (s, 6H), 1.00 (d, *J* = 7.5 Hz, 3H). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) = 173.9, 83.4, 60.4, 38.0, 25.1, 25.0, 15.5, 14.7, 13.8.



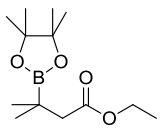
Tert-butyl 3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)butanoate: (purified with deactivated silica, petroleum ether: EtOAc, 15:1). White solid. Yield: (80%).

^{1}H NMR (300 MHz, $CDCl_3$): δ = 2.34 (dd, *J1*= 16.6, *J2*= 8.7 Hz, 1 H), 2.27 (dd, *J1*= 16.6, *J2*= 7.8 Hz, 1 H), 1.36-1.25 (m, obs., 1 H), 1.25 (s, 12 H), 1.22 (s, 9 H), 0.97 (d, *J*= 7.44 Hz, 3 H).



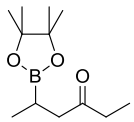
Ethyl 2-methyl-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)butanoate: (purified with deactivated silica, petroleum ether: EtOAc, 15:1). White solid. Yield: (34%).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 4.1 (q, *J*= 7.2 Hz, 2H), 2.6 (m, 1H), 2.5 (m,1H), 1.3 (m, 15H), 1.2 (d, *J*= 7.23 Hz, H), 1.1 (d, 3H), 0.9 (m, 3H).



Ethyl 3-methyl-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)butanoate: (identified from crude)

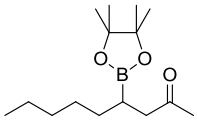
^{1}H NMR (400 MHz, $CDCl_3$): δ =4.16 (q, *J*=8.2 Hz, 2H), 2.33 (t, *J*=8.2 Hz, 2H), 2.18 (s, 3H), 1.25 (s, 12H), 1.90 (s, 3H), 1.00 (s, 3H).



5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)hexan-3-one:

(purified with deactivated silica, petroleum ether: EtOAc, 15:1). White solid. Yield: (90%).

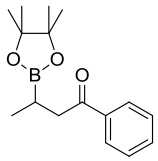
^{1}H NMR (400 MHz, $CDCl_3$): δ = 2.52 (broad d, *J* = 6.9 Hz, 2H, CH_2), 2.38 (dq, *J1*= 7.4, *J2*= 2.2 Hz, 2H, CH_2), 1.28-1.24 (m, 1H, CH), 1.23 (s, 6H, pinacolate 2 CH_3), 1.21 (s, 6H, pinacolate 2 CH_3), 1.03 (t, *J*= 7.3, 3H, CH_3), 0.94 ppm (d, *J*= 7.5 Hz, 3H, CH_3). ^{13}C{^{1}H} NMR (75.4 MHz, $CDCl_3$): δ = 211.7, 82.9, 46.2, 35.6, 25.00 24.7, 24.6, 15.0, 7.9. ^{11}B NMR: ($CDCl_3$, 128.3 MHz) δ = 34.08.



4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)nonan-2-one:

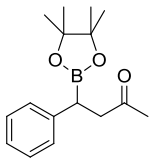
(purified with deactivated silica, petroleum ether: EtOAc, 15:1). White solid. Yield: (85%).

^{1}H NMR (300 MHz, $CDCl_3$): δ = 2.52 (d, *J* = 7.2 Hz, 2H, CH_2), 2.07 (s, 3H, CH_3), 1.28-1.21 (m, 9H, 4 CH_2, CH), 1.20 (s, 6H, pinacolate 2 CH_3), 1.80 (s, 6H, pinacolate 2 CH_3), 0.84 (t, *J*= 6.8 Hz, 3H, CH_3) ^{13}C{^{1}H} NMR (75.4 MHz, $CDCl_3$): δ = 209.2, 82.9, 45.8, 31.9, 30.3, 29.6, 28.5, 24.9, 24.7, 24.6, 22.5, 14.00. ^{11}B NMR: ($CDCl_3$, 128.3 MHz): δ = 38.7.



1-phenyl-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)butan-1-one: (purified with deactivated silica, petroleum ether: EtOAc, 15:1). White solid. Yield: (87%).

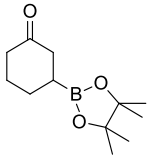
^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.96 (d, *J* = 7.2 Hz, 2H), 7.51 (t, *J*= 6.9 Hz, 1H), 7.42 (t, *J*= 6.9 Hz, 2H), 3.12 (d, *J*= 6.9 Hz, 2H), 1.40 (m, 1H), 1.26 (s, 6H), 1.25 (s, 6H), 1.06 (d, *J*= 7.5 Hz, 3H).



4-phenyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)butan-2-one:

(purified with deactivated silica, petroleum ether: EtOAc, 15:1). White solid. Yield: (91%).

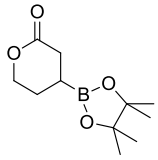
^{1}H NMR (400 MHz, $CDCl_3$): 7.45 (dd, *J1*= 6, *J2*= 4 Hz, 2H), 7.25-7.21 (m, 3H), 3.05 (dd, *J1*= 20, *J2*= 12Hz, 1H), 2.85 (dd, *J1*= 20, *J2*= 4 Hz, 1H), 2.71 (dd, *J1*=12, *J2*=4Hz, 1H), 1.94 (s, 3H), 1.29-1.19 (m, 12H).



3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)cyclohexanone:

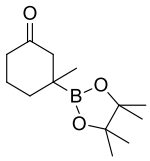
(purified with deactivated silica, petroleum ether: EtOAc, 15:1). White solid. Yield: (89%).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 2.38-2.24 (m,4H), 2.08-2.01 (m,1H), 1.88-1.83 (m,1H), 1.78-1.68 (m,1H), 1.66-1.56 (m,1H), 1.48-1.38 (m,1H), 1.22 (s, 12H).



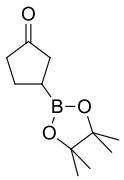
4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)tetrahydropyran-2-one: (purified with deactivated silica, petroleum ether: EtOAc, 15:1). White solid. Yield: (88%).

^{1}H NMR (300 MHz, CDCl3): δ 4.50–4.20 (m, 2H), 2.64 (dd, J = 17.8, 6.9 Hz, 1H), 2.51 (dd, J = 17.8, 10.1 Hz, 1H), 2.14–1.90 (m, 1H), 1.90–1.74 (m, 1H), 1.66–1.44 (m, 1H), 1.25 (s, 12H); ^{13}C{^{1}H} NMR(75.4 MHz, CDCl3): δ 171.8, 84.0, 70.1, 31.0, 24.9, 24.8, 24.1, 17.7 (C–B).



3-methyl-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)cyclohexanone: (purified with deactivated silica, petroleum ether: EtOAc, 15:1). White solid. Yield: (69%).

^{1}H NMR (300MHz, CDCl3): δ 2.51 (dt, *J* = 13.8, 1.3 Hz, 1H), 2.40–2.14 (m, 2H), 2.10–1.89 (m, 3H), 1.87–1.66 (m, 1H), 1.52–1.36 (m, 1H), 1.21 (s, 12H), 1.03 (s, 3H); ^{13}C{^{1}H} NMR (75.4 MHz, CDCl3): δ 212.2, 83.6, 50.8, 41.3, 34.3, 24.8, 24.7, 24.3, 24.0.



3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)cyclopentanone: (purified with deactivated silica, petroleum ether: EtOAc, 15:1). White solid. Yield: (86%).

^{1}H NMR (300 MHz, $CDCl_3$): δ = 2.42–2.02 (m, 5H), 1.94–1.76 (m, 1H), 1.74–1.56 (m, 1H), 1.26 (s, 12H); ^{13}C{^{1}H} NMR (75.4 MHz, $CDCl_3$): δ = 221.4, 83.7, 40.4, 39.1, 25.4, 24.9.

4. NMR spectroscopic studies: interactions in the PR_3 with substrate and MeOH in the absence and presence of B_2pin_2

4.1 PR_3 +MeOH without and with B_2pin_2 in the medium

4.1.1 PBu_3

Although PBu_3 can be considered a strongly basic phosphine ($pK_{a,\ protonated\ phosphine}$ = 8.43), it is still a much weaker base than MeO^- ($pK_{a,\ methanol}$ = 15.2). Accordingly, we found that PBu_3 could not be protonated by MeOH either in THF (1 mL, [PBu_3] = 0.5 M, [MeOH] = 0.5 - 4 M) (Figure ESI-1), or in MeOH as solvent (0.5 mL, [PBu_3] = 0.5 M) (Figure ESI-2), either at RT or at 45ºC. In all experiments only the free phosphine was detected by $^{31}P\{^1H\}$-NMR spectroscopy (-31.2 ppm, s) (85% H_3PO_4 as an internal pattern).

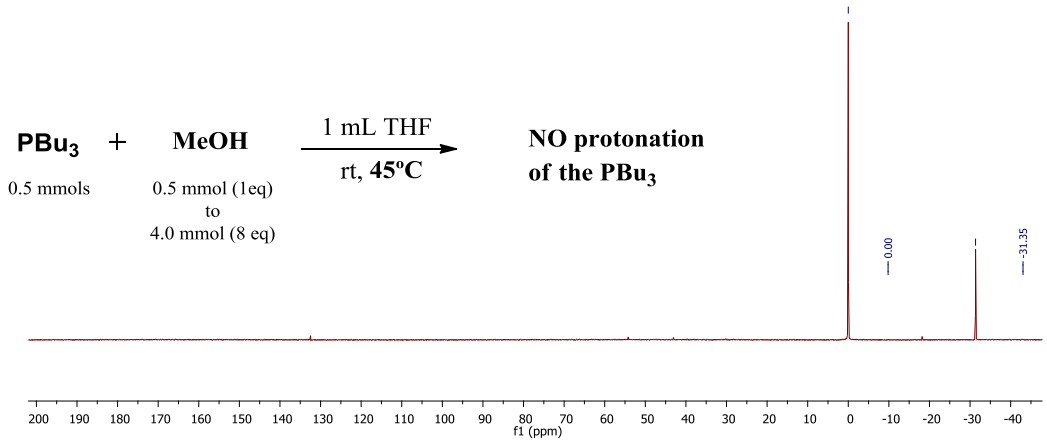


Figure ESI-1 $^{31}P\{^1H\}$-NMR spectra of a solution of PBu_3 (0.5 mmol) + MeOH (2.0 mmol) in 1 mL THF, measured at 45ºC.

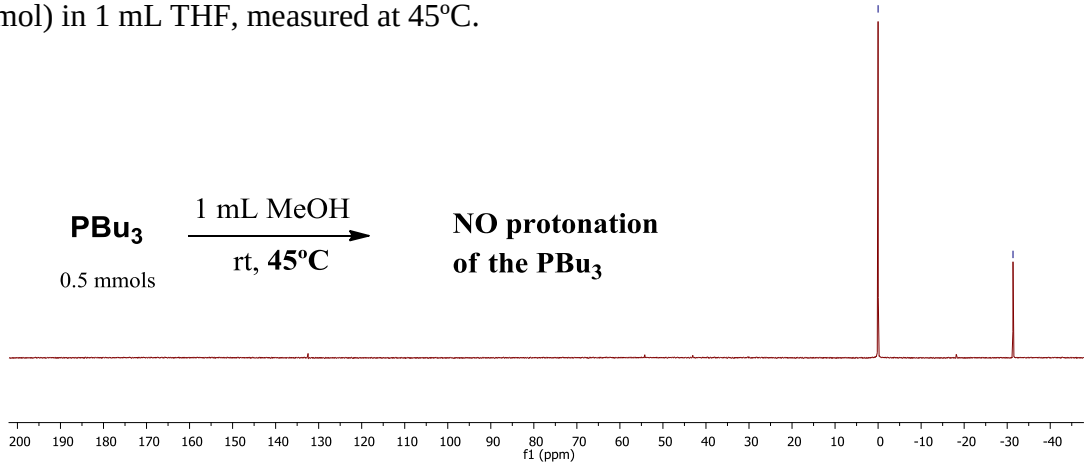


Figure ESI-2. $^{31}P\{^1H\}$-NMR spectra of a solution of PBu_3 (0.5 mmol) in 1 mL MeOH, measured at 45ºC.

In order to identify the protonated phosphine, a control experiment was carried out using the strongly acidic HBF_4 as the proton source, which quantitatively protonated the phosphine in THF (1 mL, [PBu_3] = 0.5 M, [HBF_4] = 0.55 M; $^{31}P\{^1H\}$-NMR: s, +12.0 ppm; ^{31}P-NMR: d, +12.0 ppm, $^1J_{P\text{-}H}$ = 500 Hz) (Figure ESI-3).

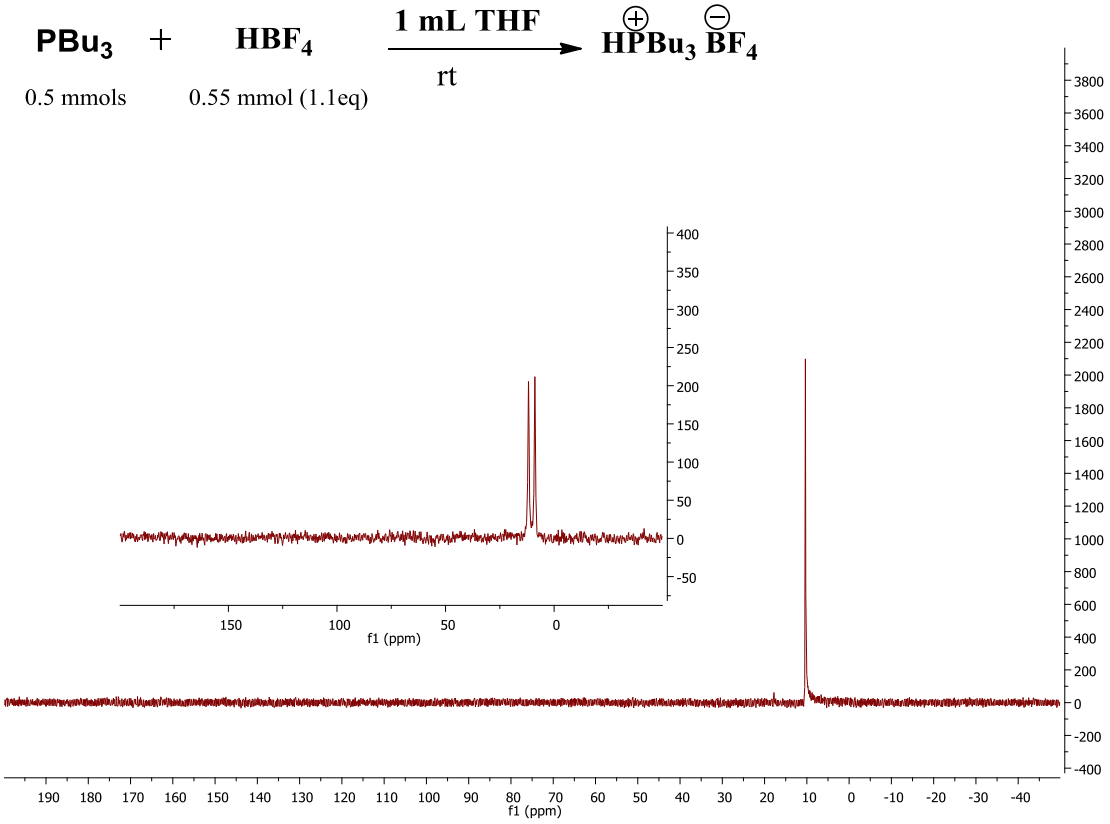


Figure ESI-3. $^{31}P\{^1H\}$-NMR and ^{31}P-NMR (small one) spectra of a solution of PBu_3 (0.5 mmol) + HBF_4 (0.55 mmol) in 1 mL THF , measured at rt.

Apart from the base, there is one more factor that can influence the methoxide-methanol equilibrium in the system, and that is the diboron reagent. We observed in our previous study that even the Verkade base ($pK_{a,\ protonated\ Verkade\ base}$ = 26) could not deprotonate MeOH quantitatively in THF (1 mL, [Verkade base] = 0.5 M, [MeOH] = 0.5 M, extent of deprotonation: 8%).[2] However, in the presence of B_2pin_2 the deprotonation became virtually complete (1 mL THF, [Verkade base] = 1 M, [MeOH] = 0.5 M, [B_2pin_2] = 0.5 M extent of deprotonation: >90%), and the MeO^- established the expected Lewis acid-base interaction with the diboron. Thus, the diboron reagent increases the Brönsted acidity of the MeOH, presumably because the conjugate base, MeO^-, will be stabilized via the formation of the $MeO^-\rightarrow B_2pin_2$ adduct. This also explains that in the base-catalyzed boron conjugate addition relatively weak bases, such as Cs_2CO_3, can also be used to initiate the reaction. Despite these facts, when PBu_3 and B_2pin_2 were dissolved in MeOH (0.5 mL, [PBu_3] = 1 M, [B_2pin_2] = 1 M) both the phosphine and the diboron reagent remained intact ($^{31}P\{^1H\}$- and $^{11}B\{^1H\}$-NMR spectroscopy, Figure ESI-4).

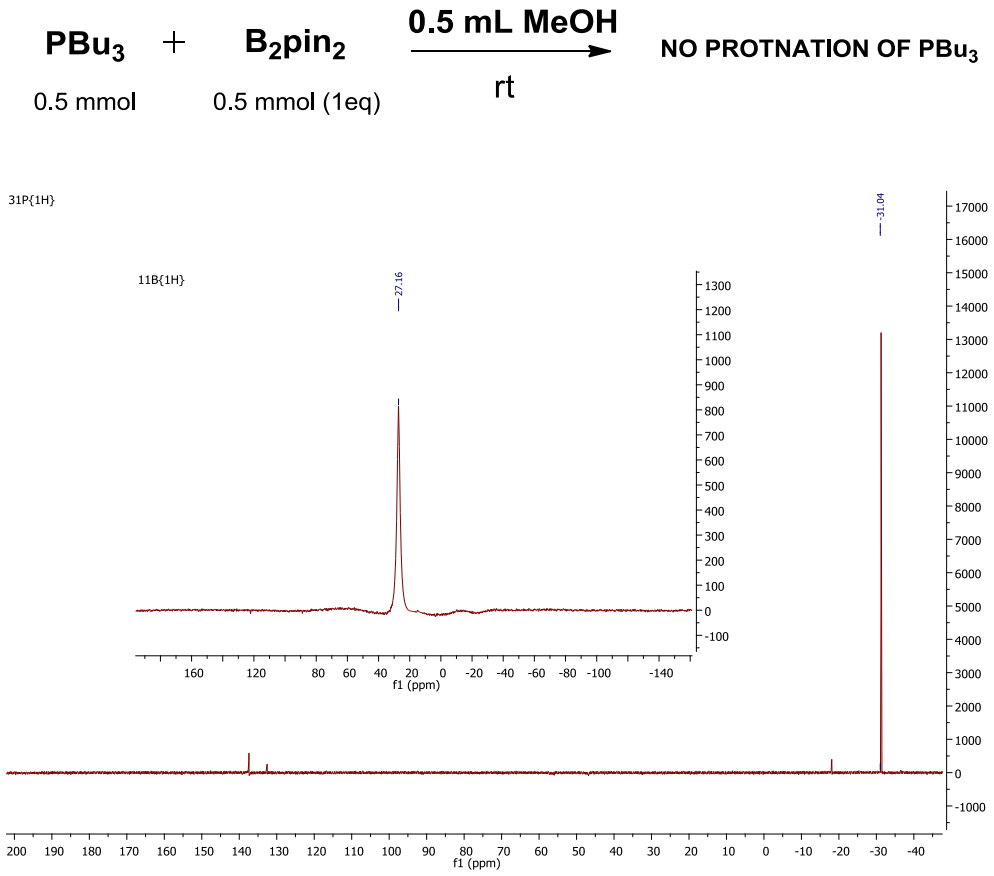
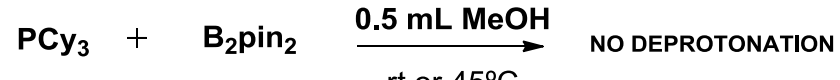


Figure ESI-4. $^{31}P\{^{1}H\}$ and $^{11}B\{^{1}H\}$ NMR (small one) spectra of a solution of PBu_3 (0.5 mmol) + B_2pin_2 (0.5 mmol) in 0.5 mL MeOH, measured at rt.

4.1.2 PCy_3

In order to test the influence of the properties of the phosphine in the possible deprotonation of MeOH in presence of B_2pin_2, we performed the same experiment (above described) using PCy_3. Although PCy_3 is a stronger base than PBu_3 (pKa(PCy_3) =9.7)[3] deprotonation of MeOH could not be observed, either at RT or at 45ºC (Figure ESI-5).



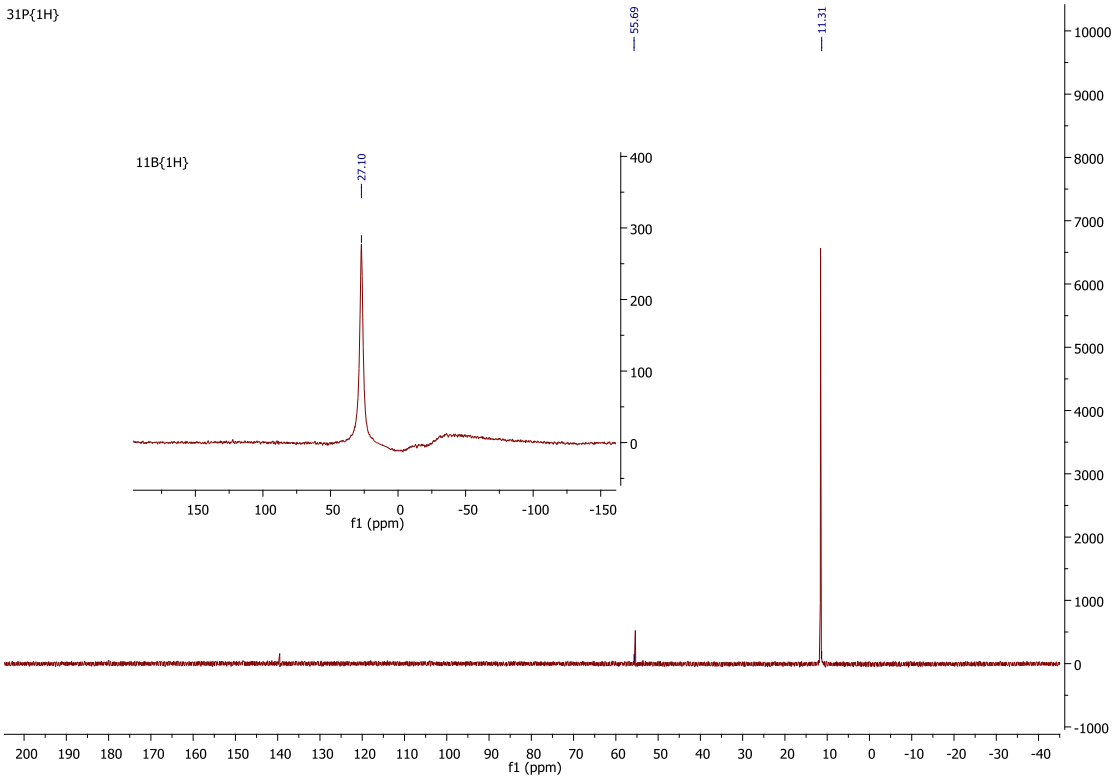


Figure ESI-5. $^{31}P\{^1H\}$ and $^{11}B\{^1H\}$ NMR (small one) spectra of a solution of PCy_3 (0.5 mmol) + B_2pin_2 (0.5 mmol) in 0.5 mL MeOH, measured at 45ºC.

4.1.3 PMe_3

The strongly basic trialkyl phosphine PMe_3 (pka=8.6) was also tested showing the same behavior, no deprotonation of MeOH was observed (Figure ESI-6) under the conditions described above.

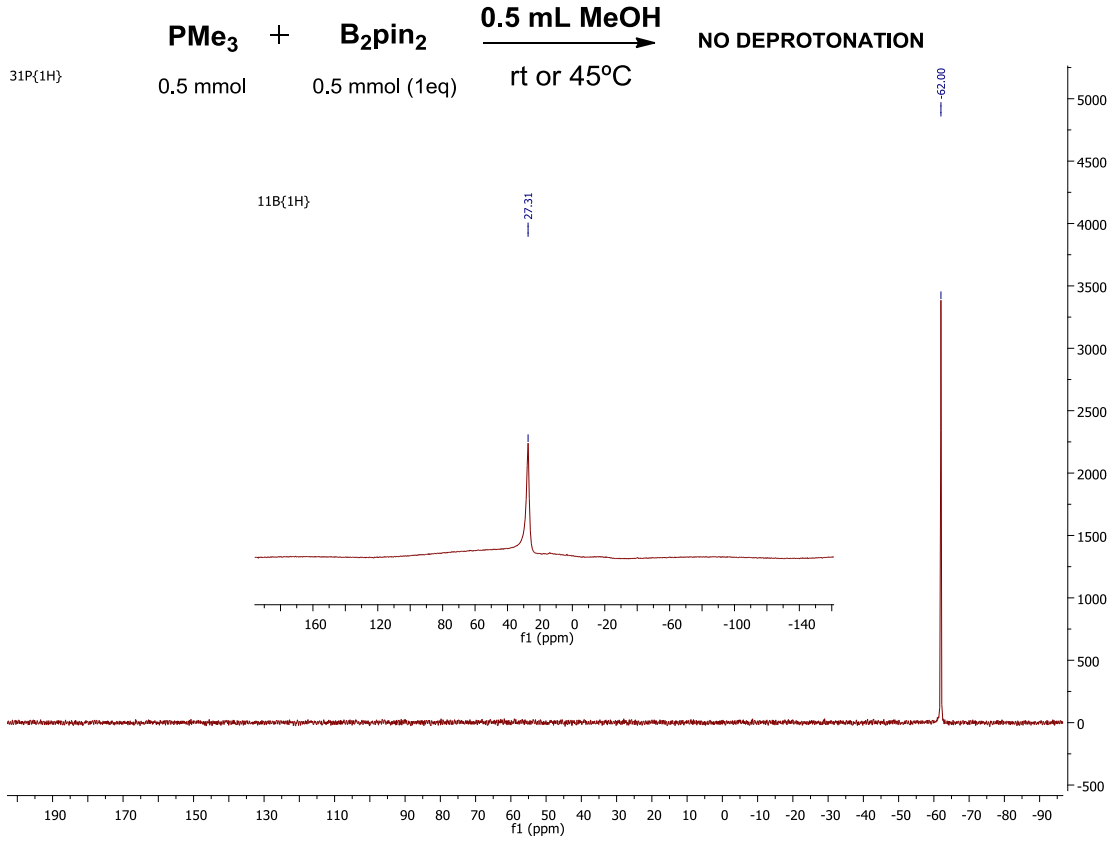


Figure ESI-6. $^{31}P\{^1H\}$ and $^{11}B\{^1H\}$ NMR (small one) spectra of a solution of PMe_3 (0.5 mmol) + B_2pin_2 (0.5 mmol) in 0.5 mL MeOH, measured at 45ºC.

4.2 PR_3-substrate-MeOH without and with B_2pin_2 in the medium

4.2.1. PBu_3

Next, we focused our attention on possible interactions between the phosphine and the substrate. Addition of trivalent phosphines as nucleophiles to α,β-unsaturated compounds has already been reported.[4] We observed in $^{31}P\{^1H\}$-NMR spectroscopy, that when PBu_3 and (*E*)-hex-4-en-3-one were dissolved in THF (1 mL, [PBu_3] = 0.5 M, [(*E*)-hex-4-en-3-one] = 0.5 M), no interaction took place between the phosphine and the activated olefin (Figure ESI-7).

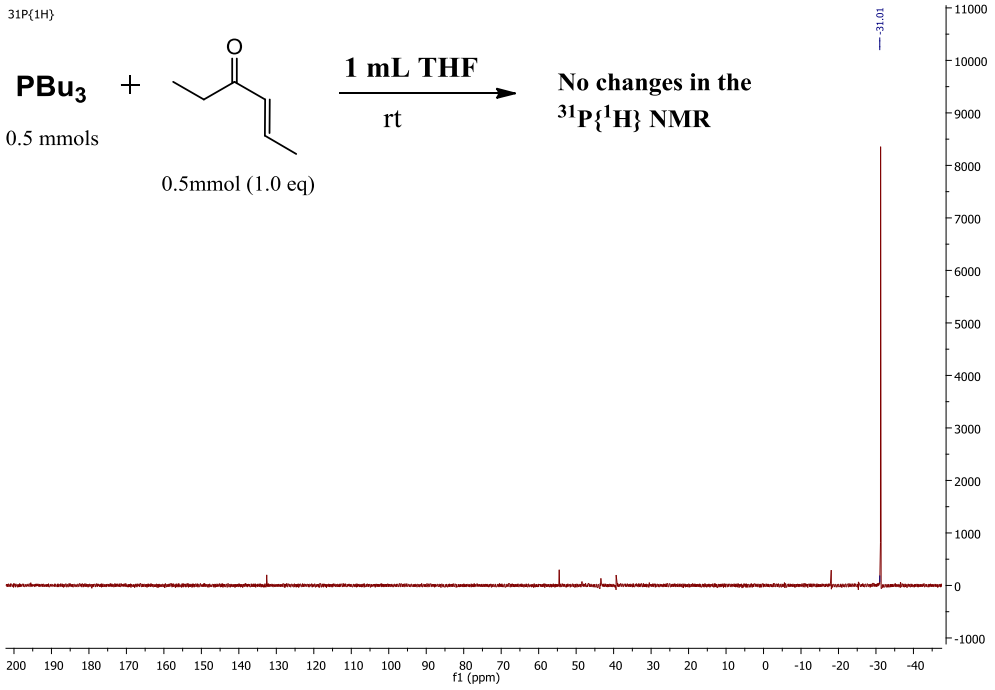
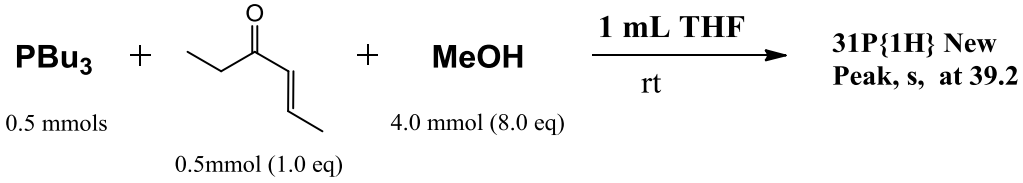


Figure ESI-7. $^{31}P\{^1H\}$-NMR spectra of a solution of PBu_3 (0.5 mmol) + (*E*)-hex-4-en-3-one (0.5 mmol) in 1 mL THF, measured at rt.

However, under similar conditions, but in the presence of MeOH (1 mL THF, [PBu_3] = 0.5 M, [(*E*)-hex-4-en-3-one] = 0.5 M, [MeOH] = 4 M) a new resonance appeared in the $^{31}P\{^1H\}$-NMR spectrum of the reaction mixture at +39.2 ppm. The relative intensity of the new signal with respect to the intensity of the signal of the free phosphine was 6.5% (Figure ESI-8).



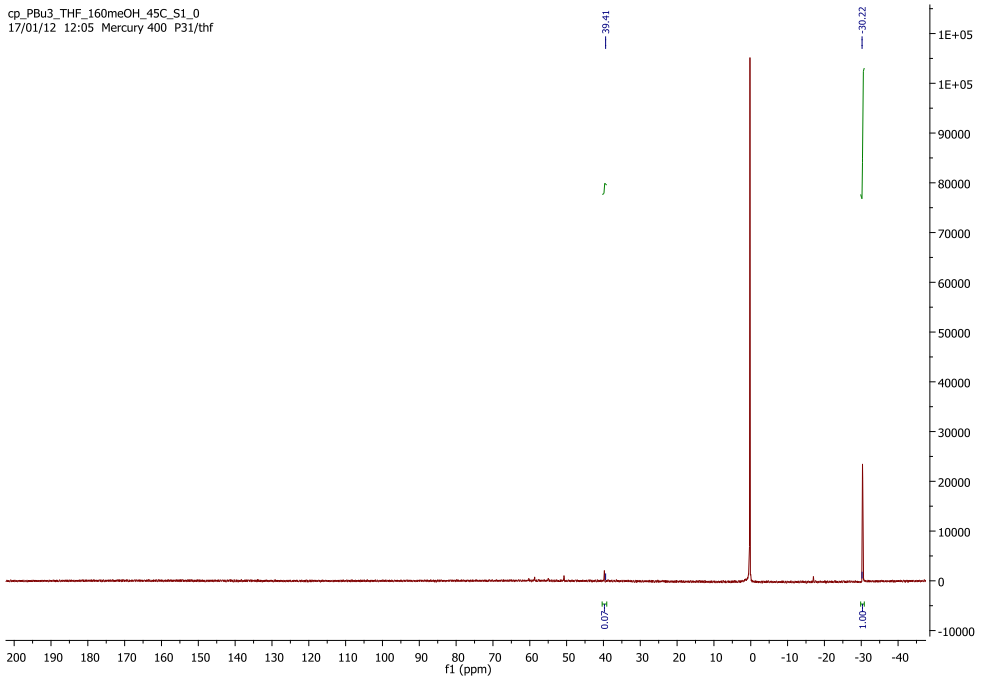
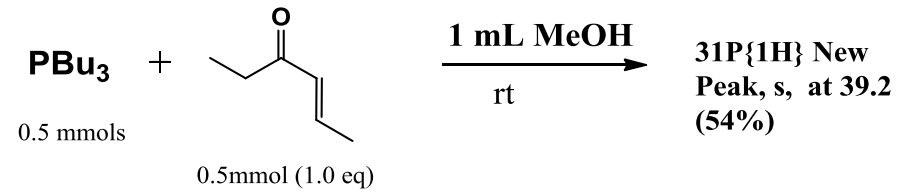


Figure ESI-8. $^{31}P\{^1H\}$-NMR spectra of a solution of PBu_3 (0.5 mmol) + (*E*)-hex-4-en-3-one (0.5 mmol) + MeOH (4.0 mmols) in 1 mL THF, measured at rt.

Increasing the temperature to 45 °C hardly changed the ratio between the new signal and that of the phosphine (8% after 3 hours), but when the interaction was studied in pure MeOH (0.5 mL, [PBu_3] = 1 M, [(*E*)-hex-4-en-3-one] = 1 M; or 1 mL, [PBu_3] = 0.5 M, [(*E*)-hex-4-en-3-one] = 0.5 M), the relative intensity of the new peak increased to 35 %, or 54%, respectively (Figure ESI-9).



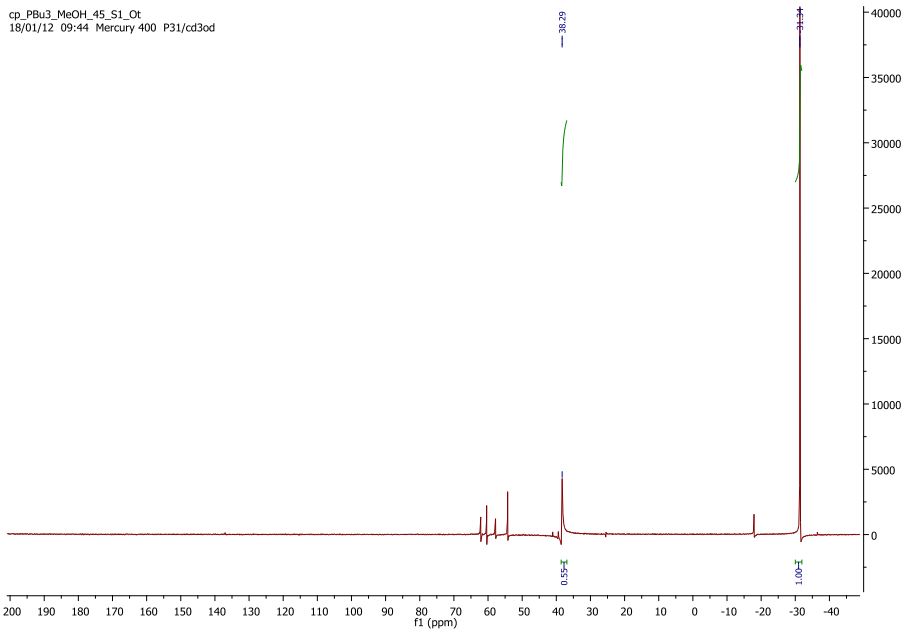


Figure ESI-9. $^{31}P\{^{1}H\}$-NMR spectra of a solution of PBu_3 (0.5 mmol) + (*E*)-hex-4-en-3-one (0.5 mmol) in 1 mL MeOH, measured at rt.

We assigned the new peak to the phosphonium salt, tributyl(4-oxohexan-2-yl)phosphonium methanolate, derived from the nucleophilic attack of the phosphine at the *β*-carbon of the substrate, followed by the protonation of the zwitterionic betaine form by MeOH. We should note that we also considered that the signal at +39.2 ppm might belong to the betaine derivative. The change of the solvent, from THF to MeOH, not only meant the introduction of a proton source, but also a substantial increase in the polarity of the reaction medium. Considering the fact that in the presumed reaction neutral species form ionic ones (either the zwitterionic betaine, or the phosphonium methoxide), the increase in the polarity of the medium should increase the reaction rate (in both cases). In order to find out whether the new species was zwitterionic, or an ion pair derived from the protonation by the alcohol, several experiments were carried out.

4.2.1.1.PBu$_3$-substrate interaction: solvent effect

The reaction was repeated in a strongly polar aprotic solvent, DMF, and a less polar protic solvent, benzyl alcohol (1 mL, [PBu_3] = 0.5 M, [(*E*)-hex-4-en-3-one] = 0.5 M). We found that, although the DMF is much more polar than the benzyl alcohol (even more polar than MeOH), it assisted the reaction much less efficiently, namely: 8% (Figure ESI-10) conversion was observed in dimethylformamide, while 24% in benzylalcohol (Figure ESI-11). Thus, the protic nature of the solvent seems to be more important than its polarity (Table S1).

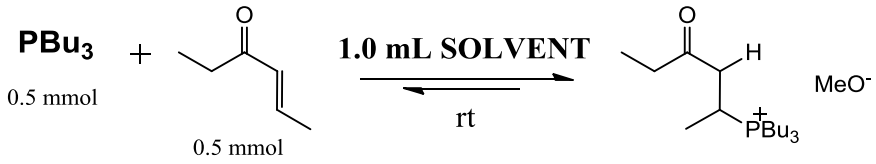


Table S1. Phosphonium salt formation from PBu_3 and (*E*)-hex-4-en-3-one in different solvents[a]

Entry	Solvent (pKa)	Polarity (dielectric constant, [ºC])	Phosphonium salt (%)
1	THF	7.5 [25 ºC]	0
2	DMF	38 [25 ºC]	8.2[b]
3	MeOH(15.5)	33 [25 ºC]	54
4	$PhCH_2OH$(15.4)	13 [20 ºC]	24

[a]Solvent: 1 mL, [PBu_3] = 0.5 M, [(*E*)-hex-4-en-3-one] = 0.5 M
[b]Common solvent, not dried

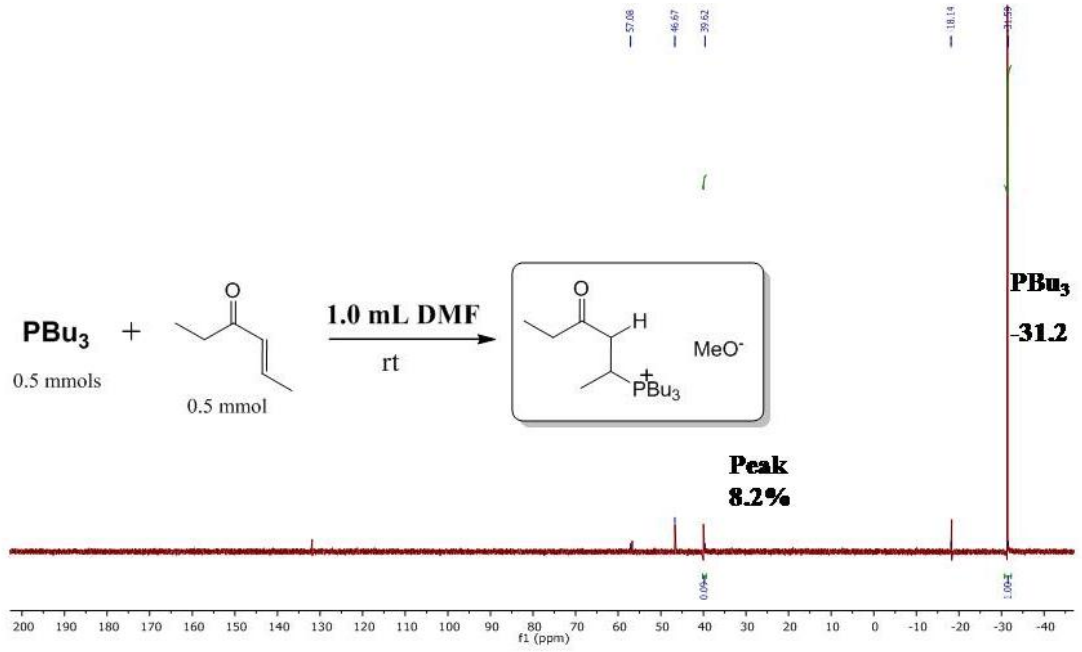


Figure ESI-10. $^{31}P\{^{1}H\}$-NMR spectra of a solution of PBu_3 (0.5 mmol) + (*E*)-hex-4-en-3-one (0.5 mmol) in 1 mL DMF, measured at rt.

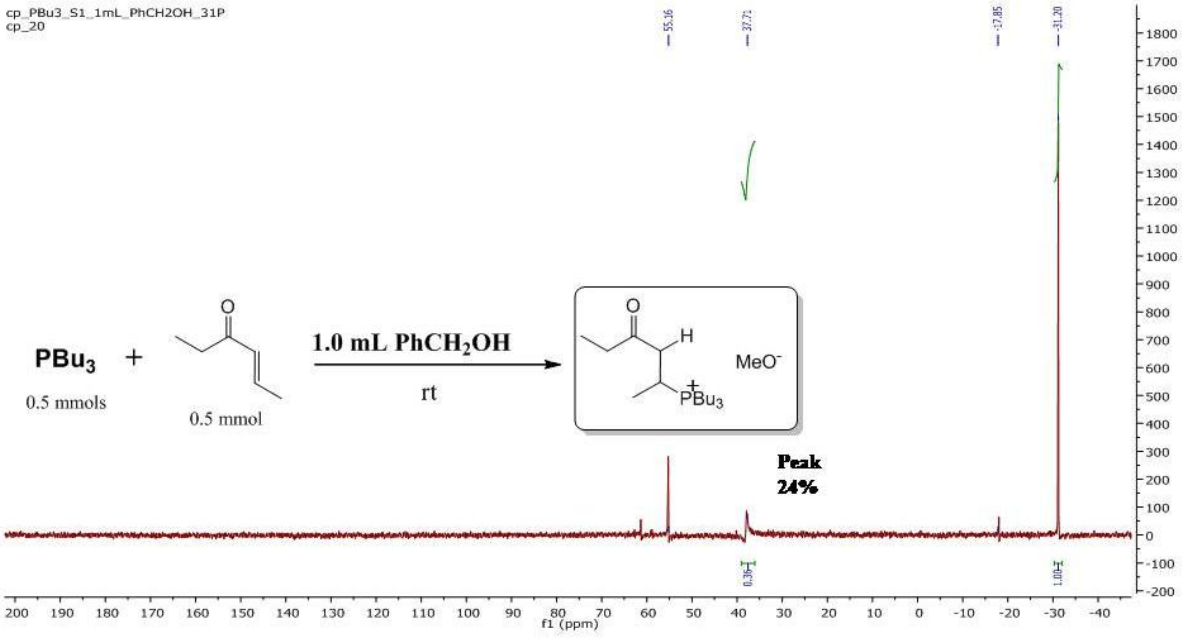


Figure ESI-11. $^{31}P\{^{1}H\}$-NMR spectra of a solution of PBu_3 (0.5 mmol) + (*E*)-hex-4-en-3-one (0.5 mmol) in 1 mL $PhCH_2OH$, measured at rt.

Furthermore, in a reaction carried out in MeOH, the addition of the strong acid HBF_4 shifted the equilibrium towards the formation of the species observed at +39.2 ppm from 54% to 63% (MeOH 1 mL, [PBu_3] = 0.5 M, [(*E*)-hex-4-en-3-one,] = 0.5 M, [HBF_4] = 0.55 M), and the rest of the phosphine became protonated (+12 ppm, s) (Figure ESI-12). The equilibrium could also be shifted changing the substrate concentration. When the substrate concentration was doubled the conversion into the hypothetical phosphonium salt increased from 54% to 95% (MeOH 1 mL, [PBu_3] = 0.5 M, [(*E*)-hex-4-en-3-one] = 1 M).

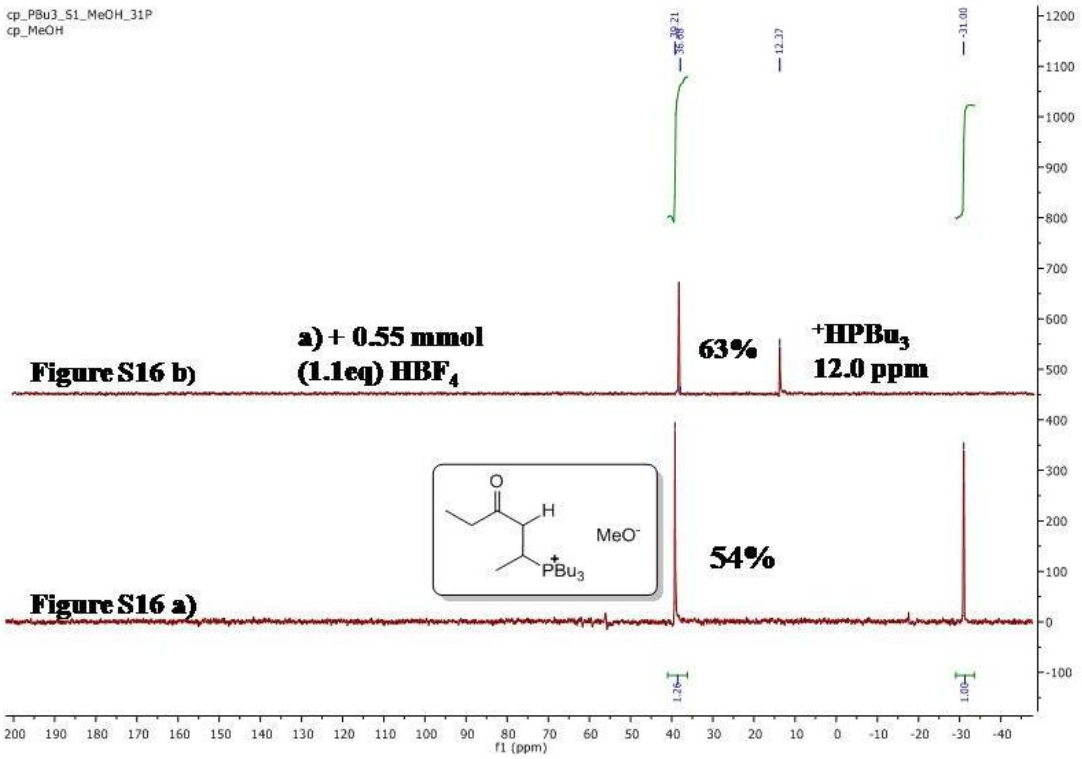


Figure ESI-12. $^{31}P\{^1H\}$-NMR spectra of a solution of a) PBu_3 (0.5 mmol) + (*E*)-hex-4-en-3-one (0.5 mmol) in 1 mL MeOH, measured at rt ; b) solution a plus HBF_4 (0.55 mmol), measured at rt.

Finally, and most importantly, the addition of one equivalent of B_2pin_2 to the MeOH solution of the mixture of phosphine and substrate (MeOH 0.5 mL, [PBu_3] = 1 M, [(*E*)-

hex-4-en-3-one] = 1 M, [B_2pin_2] = 1 M), shifted almost quantitatively the equilibrium towards the formation of the phosphonium salt, the relative intensity of the $^{31}P\{^1H\}$ resonance at +39.2 ppm increased to 90% (Figure ESI-13) Apparently, the addition of the Lewis acid increased the Brönsted acidity of the MeOH, most probably due to the fact that the conjugate base could be stabilized via the Lewis acid-base interaction with the diboron reagent. Indeed, the formation of the $MeO^- \rightarrow B_2pin_2$ adduct was confirmed by $^{11}B\{^1H\}$-NMR: the majority of the signal of bis(pinacolato)diboron (broad s, 30 ppm) disappeared, and two new broad singlets appeared at +37 ppm and +5.5 ppm, which correspond to the sp^2 and sp^3 boron atoms of the adduct, respectively.

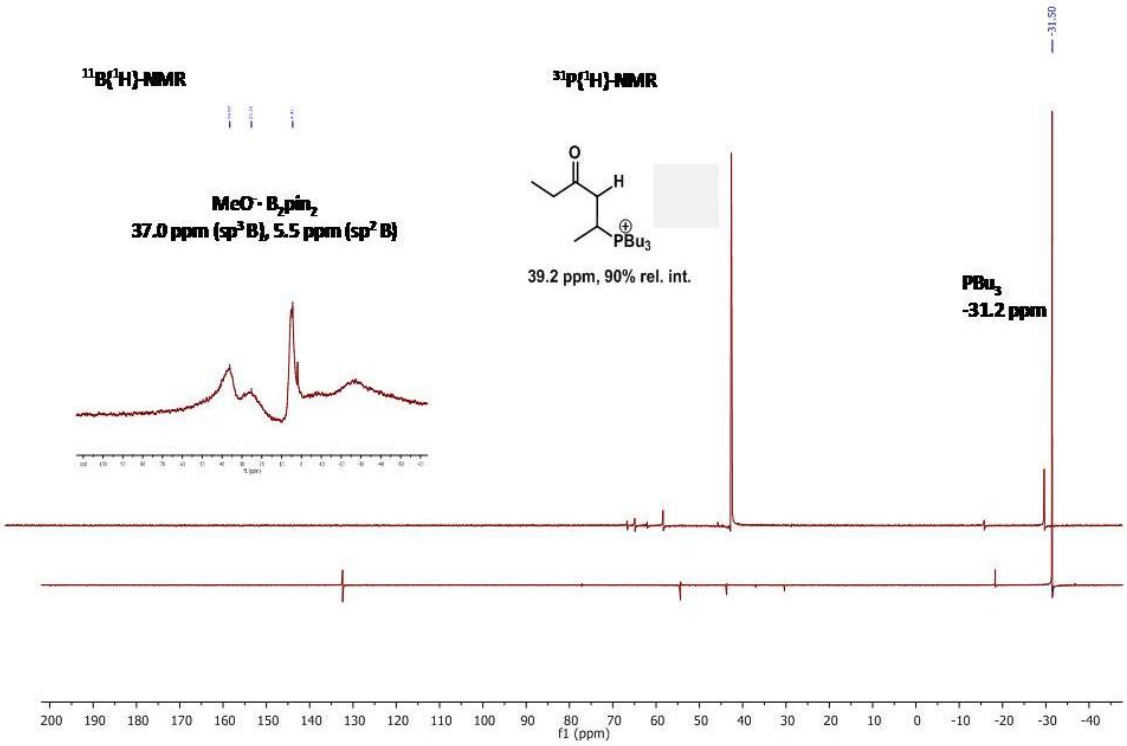
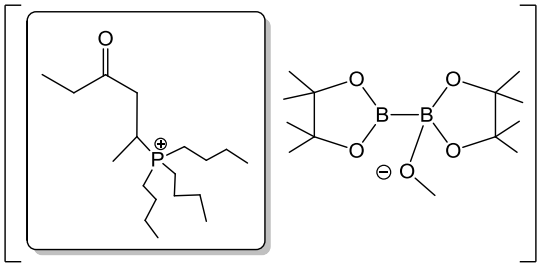


Figure ESI-13. $^{31}P\{^1H\}$ and $^{11}B\{^1H\}$ -NMR spectra of a solution of PBu_3 (0.5 mmol) + (*E*)-hex-4-en-3-one (0.5 mmol) + B_2pin_2 (0.5 mmol) in 0.5 mL MeOH, measured at rt.

The protonated phosphonium cation formed in this experiment was characterized by **ESI-MS experiments**. Mass= 301.2659 (Figure ESI-14)

301.2659	1	788607	C18 H38 O P	M*+



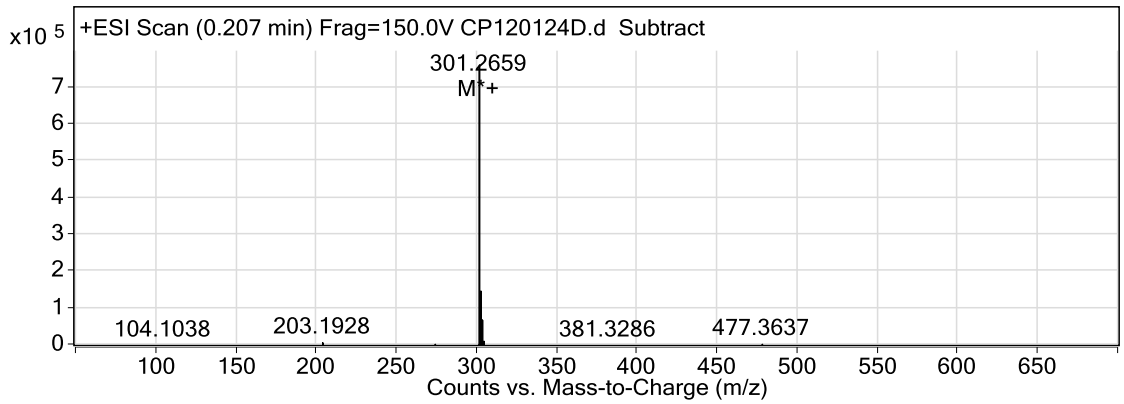


Figure ESI-14. ESI^+-MS of a solution of PBu_3 (0.5 mmol) + (*E*)-hex-4-en-3-one (0.5 mmol) + B_2pin_2 (0.5 mmol) in 0.5 mL MeOH.

4.2.2. PCy_3

We performed the same experiments using PCy_3: one equivalent of B_2pin_2 to the MeOH solution of the mixture of phosphine and substrate (MeOH 0.5 mL, [PCy_3] = 1 M, [(*E*)-hex-4-en-3-one] = 1 M, [B_2pin_2] = 1 M) (Figure ESI-15). However, in this case we could not observe the formation of the new species neither by $^{31}P\{^1H\}$ NMR nor by $^{11}B\{^1H\}$ NMR. Based on our theoretical calculations (see computational section 8 Table S3), the fact that this adduct was not observable by NMR spectroscopy under the described conditions at rt could be attributed to its low thermodynamic stability (energy of this species higher than the reactants in free form).

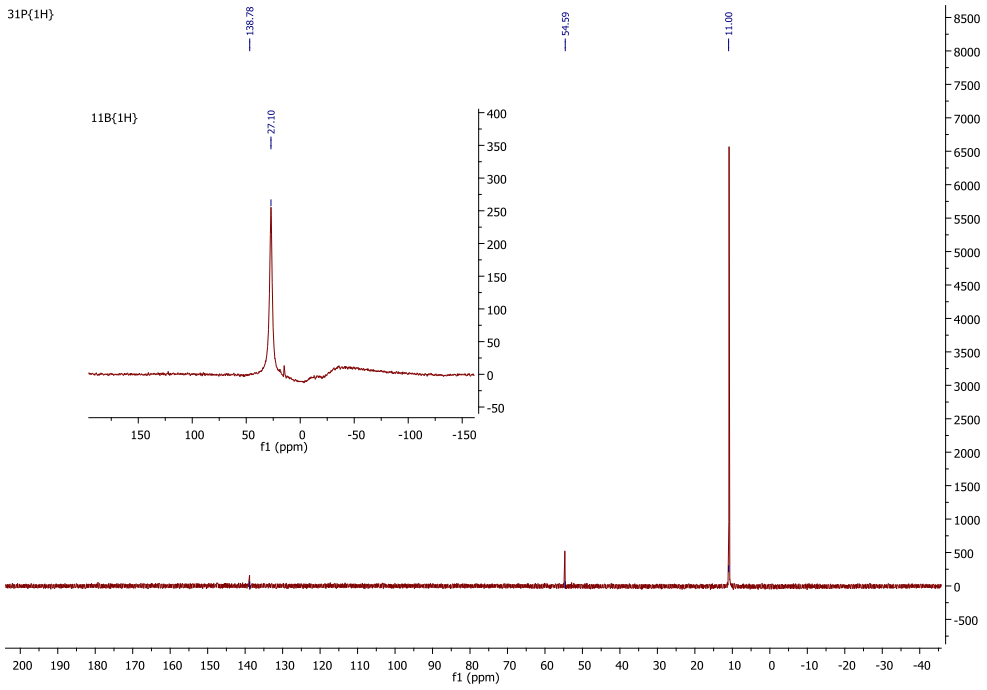


Figure ESI-15. $^{31}P\{^1H\}$ and $^{11}B\{^1H\}$ -NMR spectra of a solution of PCy_3 (0.5 mmol) + (*E*)-hex-4-en-3-one (0.5 mmol) + B_2pin_2 (0.5 mmol) in 0.5 mL MeOH, measured at rt

4.2.2.PPh_3

As observed in the case of PCy_3, upon the addition of one equivalent of B_2pin_2 to the MeOH/THF solution of the mixture of PPh_3 and substrate (MeOH 0.25 mL and 0.25 mL THF, [PPh_3] = 1 M, [(*E*)-hex-4-en-3-one] = 1 M, [B_2pin_2] = 1 M), there is no change either in the $^{31}P\{^1H\}$ NMR spectrum or in the $^{11}B\{^1H\}$ NMR spectrum of the reaction mixture (Figure ESI-16). As we concluded from our theoretical results (see section 10 Table S3) the fact that this phosphonium salt of PPh_3 was not observable by NMR spectroscopy might also be attributed to its low stability and also to the more energetically demanding pathway to its formation, with respect to PMe_3. Note that in this case, due to the low solubility of PPh_3 in MeOH,[5] the addition of a less polar cosolvent (THF) was required to completely dissolve the phosphine.

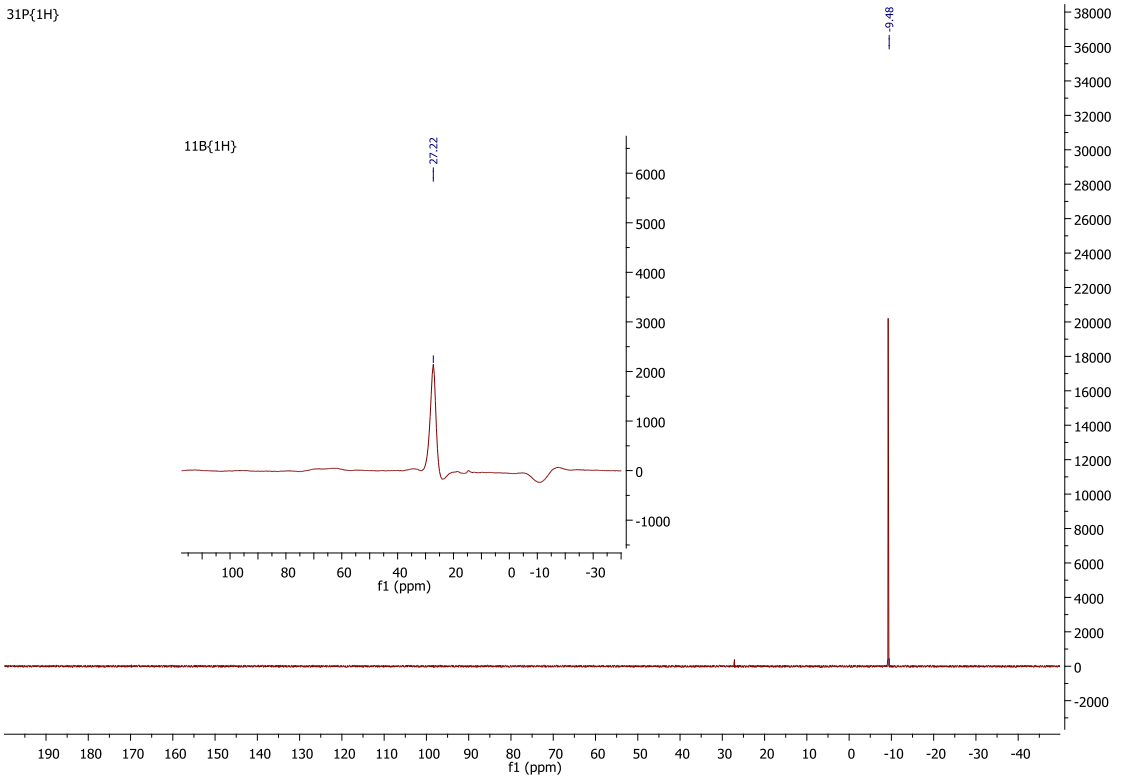


Figure ESI-16. $^{31}P\{^1H\}$ and $^{11}B\{^1H\}$ -NMR spectra of a solution of PPh_3 (0.5 mmol) + (*E*)-hex-4-en-3-one (0.5 mmol) + B_2pin_2 (0.5 mmol) in 0.25 mL MeOH+ 0.25 mL THF, measured at rt

4.2.3.PMe_3

The addition of one equivalent of B_2pin_2 to the MeOH solution of the mixture of phosphine and substrate (MeOH 0.5 mL, [PMe_3] = 1 M, [(*E*)-hex-4-en-3-one] = 1 M, [B_2pin_2] = 1 M) results in the quantitative formation of the phosphonium salt (Figure ESI-17). In the $^{31}P\{^1H\}$ NMR spectrum the peak of the free phosphine (-62 ppm) completely disappeared and a new peak appeared at +30.1 ppm. In the $^{11}B\{^1H\}$ NMR spectrum we also observed the corresponding changes: the signal of B_2pin_2 (broad s, 30.5 ppm) completely disappeared and two new broad peaks at +35 ppm and +1.3 ppm could be observed. These two new boron signals correspond to the well known $[B_2pin_2 \cdot MeO]^-$ anionic adduct, i.e., to the sp^2 and sp^3 boron atoms of the adduct, respectively.[2]

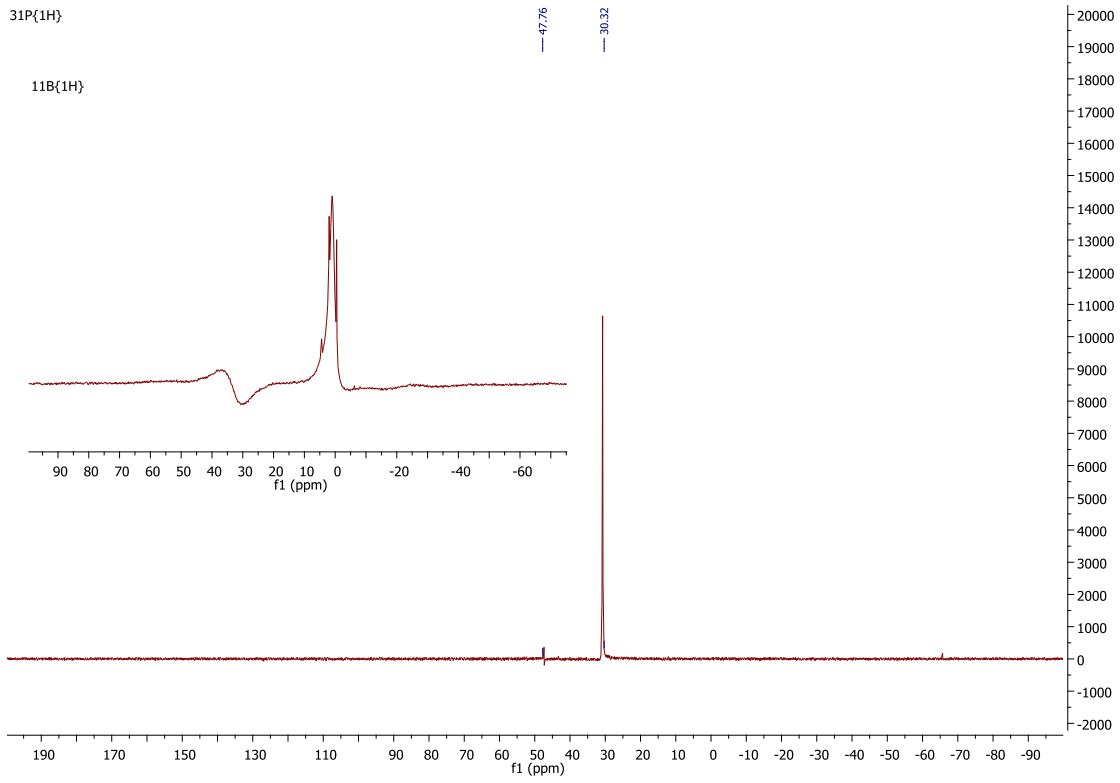
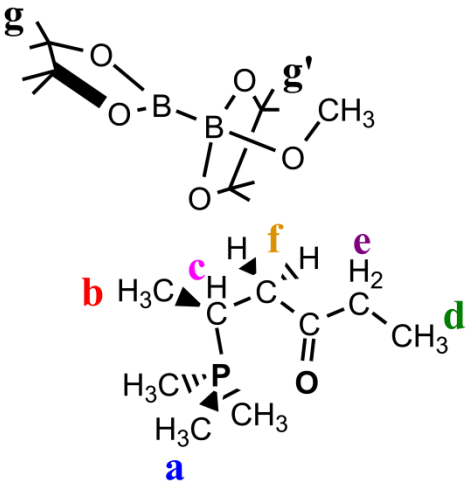


Figure ESI-17. $^{31}P\{^1H\}$ and $^{11}B\{^1H\}$ -NMR spectra of a solution of PMe_3 (0.5 mmol) + (*E*)-hex-4-en-3-one (0.5 mmol) + B_2pin_2 (0.5 mmol) in 0.5 mL MeOH, measured at rt

5. Stoichiometric experiments

Stoichiometric experiments in Schlenck and in NMR tube were performed, and progress of the reactions was monitored by ^{1}H NMR, ^{11}B{^{1}H} NMR, ^{31}P{^{1}H} NMR, ^{1}H - ^{31}P correlation NMR and CG-MS. As we mentioned above, when mixing 1eq. of PMe_3 with 1eq. of B_2pin_2 and 1eq. of [(*E*)-hex-4-en-3-one in 1 mL of MeOH ([reactants]=0.25 M), we observed complete formation of the phosphonium salt (anion is the $[B_2pin_2{\cdot}MeO]^-$ adduct, and the cationic counterpart is the trimethyl (4-oxohexan-2-yl) phosphonium cation), (Figures ESI-18 to ESI-22). Upon increasing the temperature to 70ºC, no conversion to the desired β-borated product was observed even after heating overnight.



^{1}H NMR (MeOH, 400 MHz): 1.03 (t, J=7.3 Hz, 3H), 1.15 (s, 12H), 1.15 (s, 12H), 1.24 (dd, J=13.8 , 6.8 Hz , 3H), 1.83 (d, J=14.1 Hz, 9H), 2.24 (m, 2H), 2.51 (m, 2H), 2.9 (dd, J=15.5, 5.0 Hz, 1H).

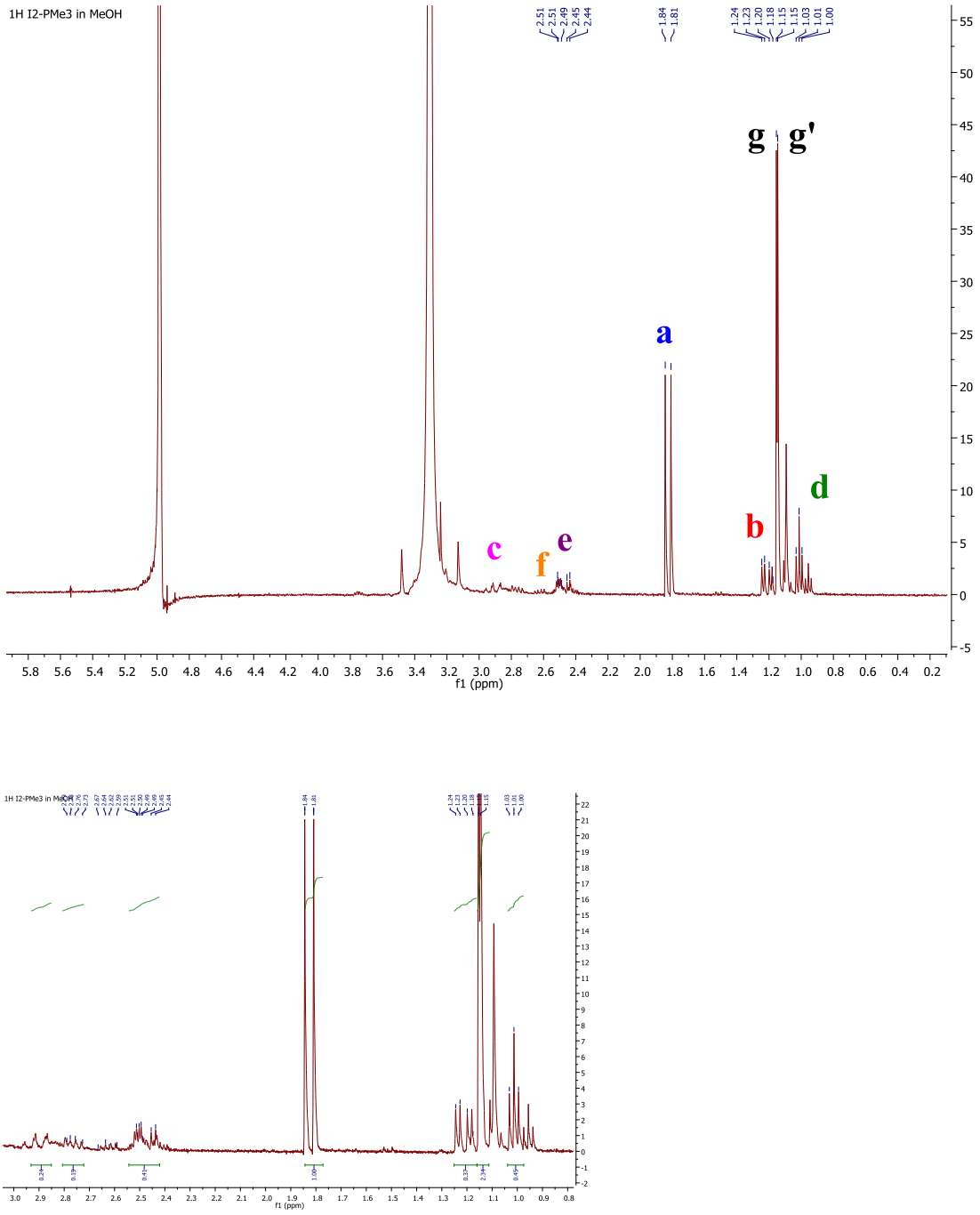


Figure ESI-18. ^{1}H-NMR spectra of a solution of PMe_3 (0.25 mmol) + (*E*)-hex-4-en-3-one (0.25 mmol) + B_2pin_2 (0.25 mmol) in 1.0 mL MeOH

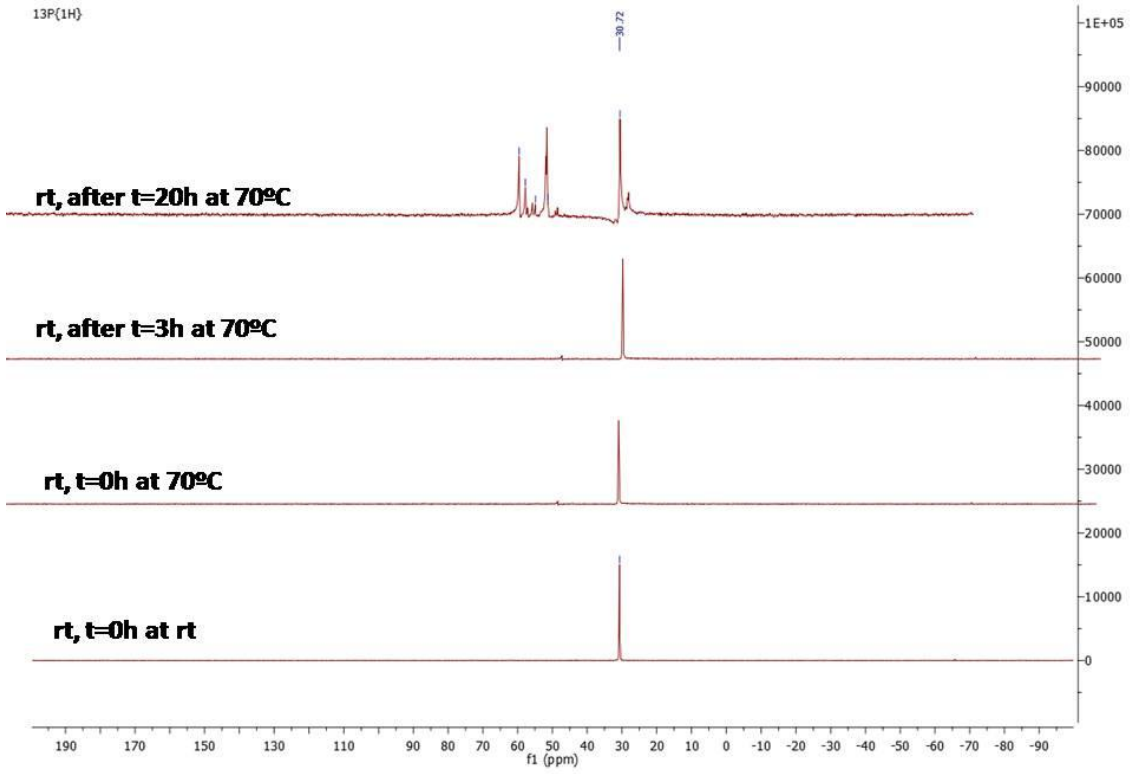


Figure ESI-19. $^{31}P\{^{1}H\}$ -NMR spectra of a solution of PMe_3 (0.25 mmol) + (*E*)-hex-4-en-3-one (0.25 mmol) + B_2pin_2 (0.25 mmol) in 1.0 mL MeOH, measured at rt after heating at 70ºC during *t* time.

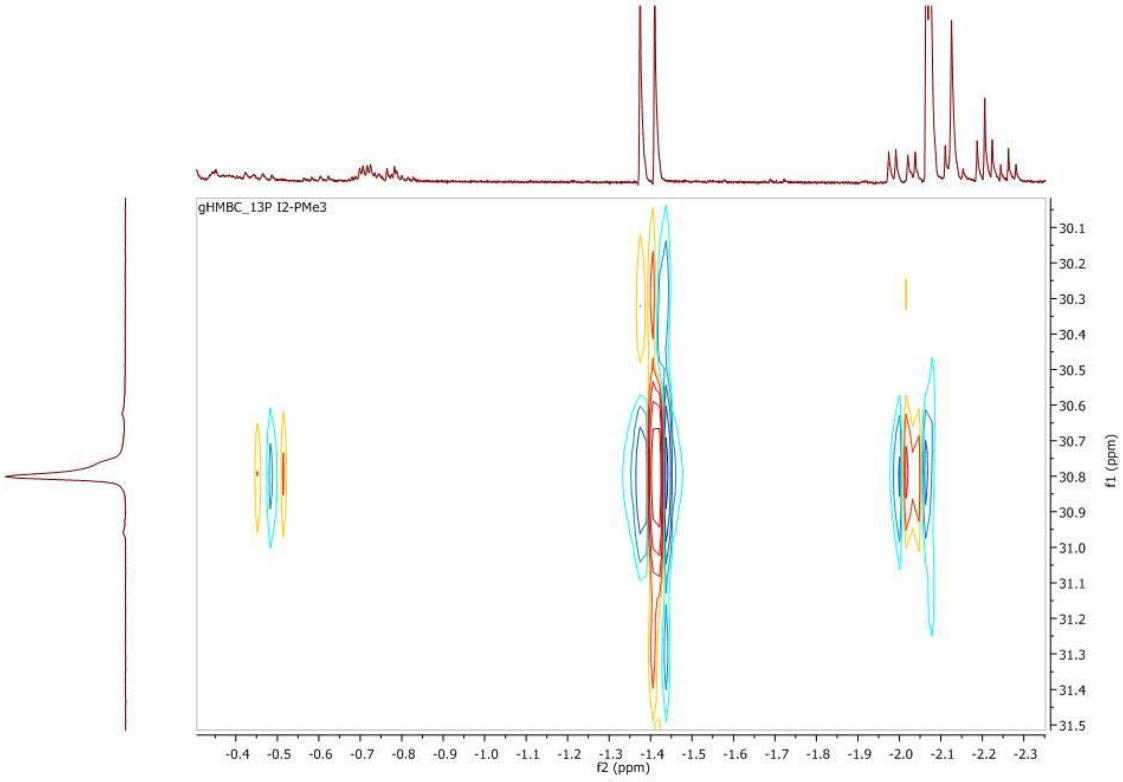


Figure ESI-20. ^{1}H-$^{31}P\{^{1}H\}$ correlation NMR spectra of a solution of PMe_3 (0.25 mmol) + (*E*)-hex-4-en-3-one (0.25 mmol) + B_2pin_2 (0.25 mmol) in 1.0 mL MeOH

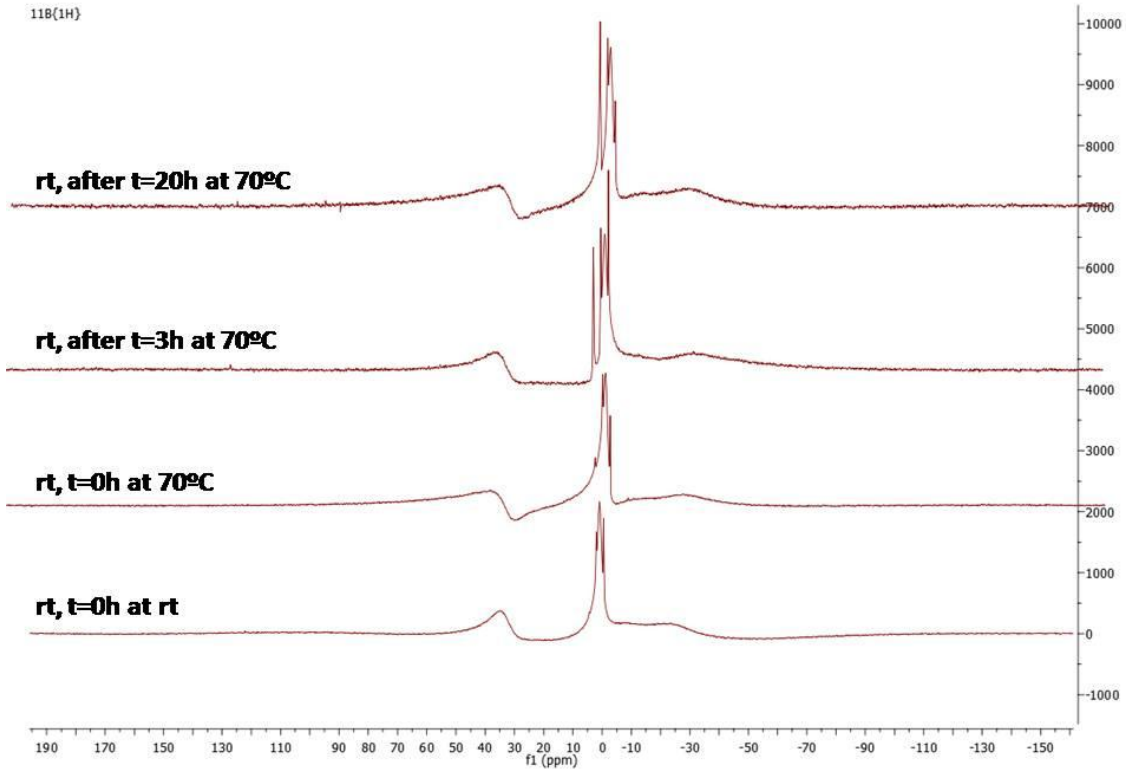


Figure ESI-21. $^{11}B\{^{1}H\}$ -NMR spectra of a solution of PMe_3 (0.25 mmol) + (*E*)-hex-4-en-3-one (0.25 mmol) + B_2pin_2 (0.25 mmol) in 1.0 mL MeOH, measured at rt after heating at 70ºC during *t* time.

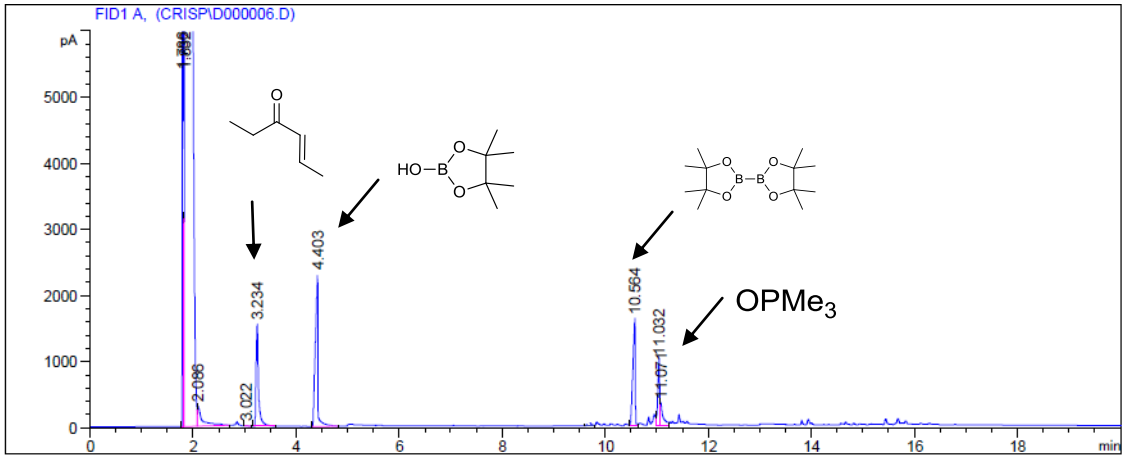


Figure ESI-22. ***GC*** analysis of the reaction mixture (0.1 mL sample diluted in 2 mL of CH_2Cl_2) containing PMe_3 (0.25 mmol) + (*E*)-hex-4-en-3-one (0.25 mmol) + B_2pin_2 (0.25 mmol) in 1.0 mL MeOH, after heating at 70ºC during 20h.

Temperature of injector: 250ºC; Temperature of detector: 275ºC; Temperature: 80ºC (for 3 min); Temperature gradient: 15ºC/min; Final oven temperature: 250ºC (for 5 min).

However, addition of an excess of substrate enabled the observation of the formation of the β-borated product. After 1h at 70ºC, with 3 eq. of substrate, 1 eq of PMe_3 and 1eq. of B_2pin_2 in 1 mL of MeOH ([reactants]= 0.25M, except for [(*E*)-hex-4-en-3-one]=0.75 M) complete conversion was observed by $^{11}B\{^1H\}$ NMR and GC (Figure ESI-23 to ESI-25) .

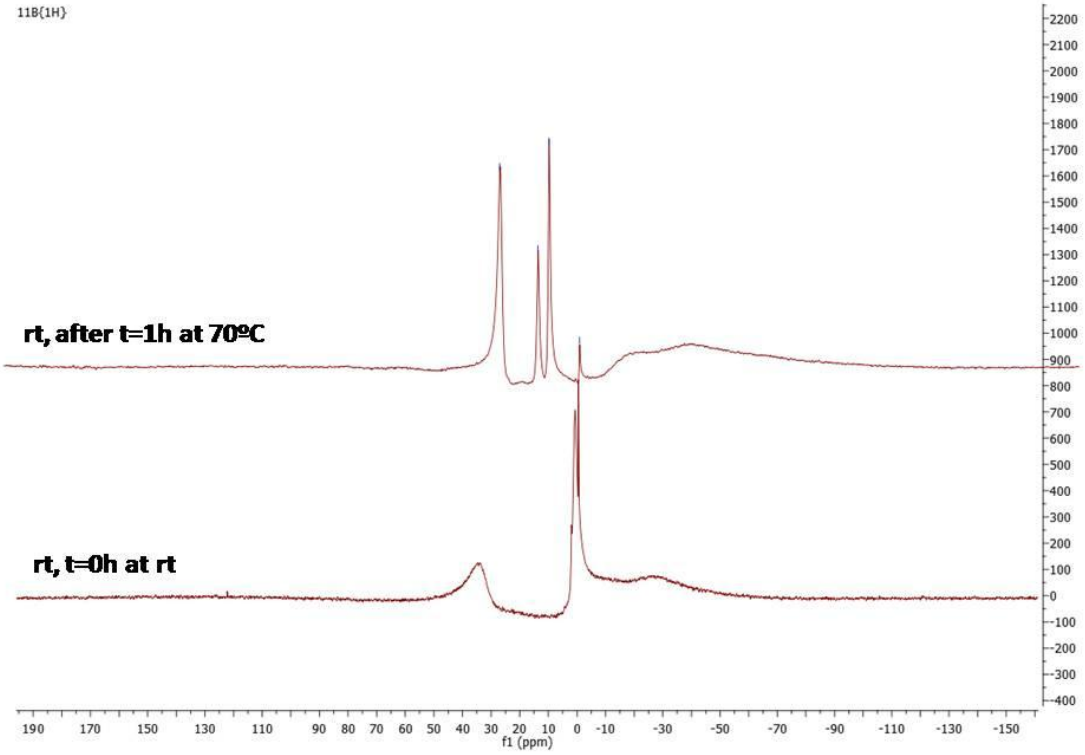


Figure ESI-23. $^{11}B\{^1H\}$ -NMR spectra of a solution of PMe_3 (0.25 mmol) + (*E*)-hex-4-en-3-one (0.75 mmol) + B_2pin_2 (0.25 mmol) in 1.0 mL MeOH, measured at rt after heating at 70ºC during *t* time.

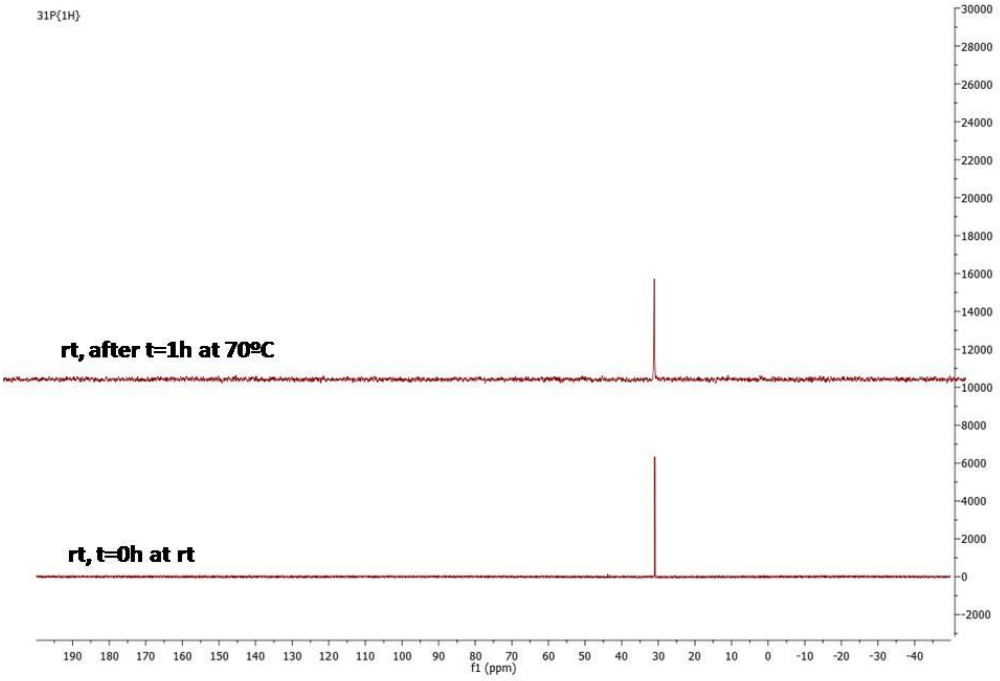


Figure ESI-24. $^{31}P\{^{1}H\}$ -NMR spectra of a solution (same as in Figure S25) of PMe_3 (0.25 mmol) + (*E*)-hex-4-en-3-one (0.75 mmol) + B_2pin_2 (0.25 mmol) in 1.0 mL MeOH, measured at rt after heating at 70ºC during t time.

Figure ESI-25. GC of 0.1 mL sample (diluted in 2 mL of CH_2Cl_2) containing of PMe_3 (0.25 mmol) + (*E*)-hex-4-en-3-one (0.75 mmol) + B_2pin_2 (0.25 mmol) in 1.0 mL MeOH, after heating at 70ºC during 1 h.

Temperature of injector: 250ºC; Temperature of detector: 275ºC; Temperature: 80ºC (for 3 min); Temperature gradient: 15ºC/min; Final oven temperature: 250ºC (for 5 min).

6. Computational Details

Molecular structures for all the species were optimized without constraints by using Density Functional Theory (DFT) based methods as implemented in the Amsterdam Density Functional (ADF v2009.01) package.[6,7] A triple-ζ plus polarization Slater basis set was used on all atoms. Relativistic corrections were introduced by scalar-relativistic zero-order regular approximation (ZORA).[8] For geometry optimizations we used the local VWN correlation potential[9] together with the Becke's exchange[10] and the Perdew's correlation[11,12] (BP86) generalized gradient corrections. Stationary points in the potential energy hypersurface were characterized either as minima or transition states by means of harmonic vibrational frequencies calculations. Standard corrections to Gibbs free energy at 298 K were evaluated, too. Nuclear Magnetic Resonance chemical shifts were computed at the same level of theory doing single point calculations with all electrons basis sets. Solvent effects were introduced by using the continuous solvent model COSMO[13] PKa values were obtained based on the Born-Haber cycle[14] using the known solvation energy of the proton.[15] Also, dispersion effects were evaluated. Single point energy metahybrid M06[16] levels were performed.

7. Computed ^{11}B NMR and ^{31}P NMR chemical shifts.

References:

	BP86	
	TZP	**TZ2P***
BF_3ET_2O	**94.3**	**93.9**
H_3PO_4	**290.9**	**289.4**

* Triple-ζ plus double polarization Slater basis set.

Table S2: Computed ^{11}B NMR and ^{31}P NMR chemical shifts for different species.

	^{11}B				^{31}P	
	TZP		**TZ2P**		**TZP**	**TZ2P**
	B-O	**B**	**B-O**	**B**	**--**	**--**
B_2pin_2	68.1	68.1	66.2	66.2	--	--
	26.2	**26.2**	**27.7**	**27.7**	**--**	**--**
PMe_3	--	--	--	--	354.18	352.3
	-	**--**	-	**--**	**-63.3**	**-63.0**
$[I2\text{-}PMe3]^+$	--	--	--	--	260.4	260.1
	--	**--**	**--**	**--**	**30.4**	**29.3**
$[B_2pin_2{\cdot}MeO]^-[I2\text{-}PMe_3]^+$	92.8	61.5	91.9	60.9	259.5	259.23
	1.5	**32.9**	**2.0**	**33.0**	**31.4**	**30.1**

***With solvent included calculated vaule is =30.5

8. Computed relative energies (in kcal·mol^{-1}) for the considered species involved in the catalytic system at different levels of theory.

8.1. Formation of I2 species

Table S3. Computed relative energies for the species involved in the formation of I2 species at BP86 level of theory.

	BP86			
Phosphine	**TS1**	**I1**	**TS2**	**I2**
PMe_3	10.9 (22.9)	-6.0 (8.3)	-1.1 (38.5) 4.9 (30.2)	-9.1 (31.5)
PPh_3	16.6 (30.6)*	2.2 (18.7)	17.6 (59.4) 15.4 (40.4)	6.0 (51.6)
PCy_3	12.5 (26.2)	-0.4 (16.4)	9.5 (54.5) 9.9 (45.0)	0.6 (45.7)

*Dispersion had to be included in the calculation

Table S4. Computed relative energies for the species involved in the formation of I2 species at M06 level of theory (single points)

	M06			
Phosphine	**TS1**	**I1**	**TS2**	**I2**
PMe_3	12.7(24.7)	-6.9(7.4)	-10.6(28.9) -3.7 (21.5)	-28.3(12.3)
PPh_3	17.6 (31.6)	-0.9 (15.7)	-2.9 (40.5) -2.0 (24.8)	-14.4 (31.3)
PCy3	12.1(25.8)	-3.2(13.6)	-3.2 (41.9) 0.0 (28.3)	-19.9(25.2)

Energies in MeOH

Table S5. Computed relative energies for the species involved in the formation of **I2-PMe_3** species at BP86 level of theory in MeOH (single points)

	BP86			
	ΔE_{gas}	$\Delta E_{gas}+ \Delta G_{solv,MeOH}$	ΔG_{gas}	ΔG_{MeOH}
TS1	**10.9**	**-14.8***	**22.9**	**-2.8**
I1	**-6.0**	**-4.3**	**8.3**	**12.7**
TS2	**-1.0** (5.0)	**6.1** (10.4)	**38.5** (30.2)	**45.6** (32.9)
I2_c	**-9.1**	**-7.6**	**31.5**	**17.5**

***-11.4 in MeOH optimized**

Table S6. Computed relative energies for the species involved in the formation of **I2-PCy_3** species at BP86 level of theory in MeOH (single points)

	BP86			
	ΔE_{gas}	$\Delta E_{gas}+ \Delta G_{solv,MeOH}$	ΔG_{gas}	ΔG_{MeOH}
TS1	**12.5**	**-8.4***	**26.2**	**5.3**
I1	**-0.4**	**3.8**	**16.4**	**20.6**
TS2	**9.5** (9.9)	**15.9** (12.1)	**54.5** (38.1)	**61.0** (40.4)
I2_c	**0.6**	**3.7**	**45.7**	**48.8**

***-7.6 in MeOH optimized**

Table S7. Computed relative energies for the species involved in the formation of **I2-PPh_3** species at BP86 level of theory in MeOH (single points)

	BP86			
	ΔE_{gas}	$\Delta E_{gas}+ \Delta G_{solv,MeOH}$	ΔG_{gas}	ΔG_{MeOH}
TS1	**16.6**	**0.9**	**30.6**	**14.9**
I1	**2.2**	**2.8**	**18.7**	**19.3**
TS2	**10.4** (8.2)	**19.9** (17.1)	**53.7** (35.0)	**63.3** (44.0)
I2_c	**6.0**	**13.3**	**51.6**	**58.9**

8.2. TS3 and alternative pathways

Table S8. Energy barriers for TS3, TS-SN_2 and the TS-PR_3 transition states calculated at BP86 level of theory.

Phosphine	**TS-PR_3 BP86**	**TS-SN_2 BP86**	**TS3 BP86**
PMe_3	28.4 (57.3)	40.8 (40.2)	22.0 (38.2)
PPh_3	38.5 (69.6)	27.6 (25.5)	19.4 (34.8)
PCy_3	41.7 (73.2)	36.8 (35.3)	19.0 (32.9)

Table S9. Energy barriers for TS3, TS-SN_2 and the TS-PR_3 transition states calculated at M06 level of theory (single points).

Phosphine	**TS-PR_3 M06**	**TS-SN_2 M06**	**TS3 M06**
PMe_3	21.7 (50.6)	50.0 (49.4)	18.6 (34.7)
PPh_3	25.8 (56.9)	35.4 (33.1)	17.0 (32.4)
PCy_3	29.6 (61.0)	43.5 (42.1)	10.4 (24.3)

Energies in MeOH:

Table S10. Energy barriers for TS3, TS-SN_2 and the TS-PR_3 transition states calculated at BP86 level of theory in MeOH (single points).

Phosphine	**TS3 BP86 $\Delta E^{\neq}_{MeOH}$ ($\Delta G^{\neq}_{MeOH}$)**	**TS-SN_2 BP86 $\Delta E^{\neq}_{MeOH}$ ($\Delta G^{\neq}_{MeOH}$)**	**TS-PR_3 BP86 $\Delta E^{\neq}_{MeOH}$ ($\Delta G^{\neq}_{MeOH}$)**
PMe_3	13.7 (29.8)	52.7 (67.6)	28.2 (57.1)
PPh_3	10.9 (26.4)	33.1 (30.9)	43.2 (74.3)
PCy_3	13.6 (27.5)	50.9 (49.5)	45.5 (77.0)

9. Characterization of I1-PR_3 species: Laplacian study and computed pKa values.

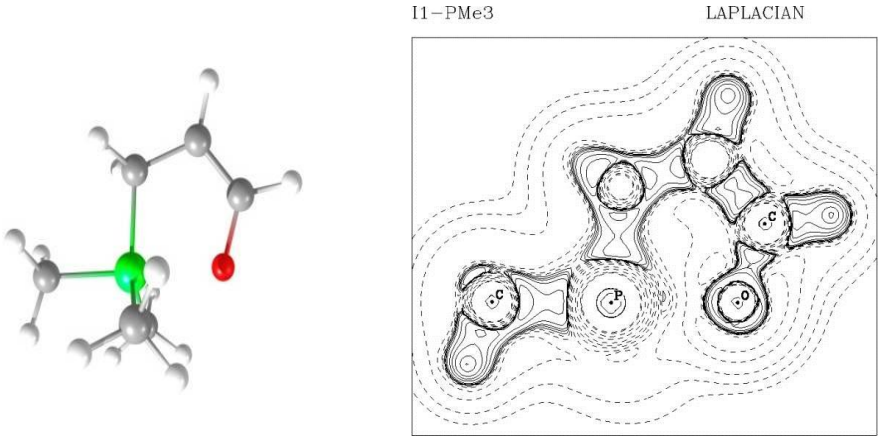
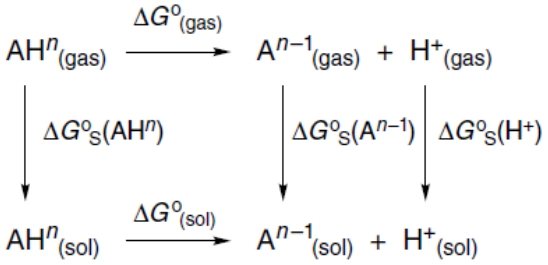


Figure ESI-26. Molecular structure for **I1-PMe_3** and illustration of its Laplacian study

Topological analysis of electronic charge density of **I1-PMe_3** revealed the existence of a P–O bond critical point. The Laplacian of the charge density indicated that the P–O bond is mainly dative like, so the five-member nature of the ring.

PKa values were obtained based on the Born-Haber cycle using the known solvation energy of the proton.



$$pK_a = -\log\left(e^{-\Delta G^{\circ}_{(sol)}/RT}\right)$$

In this particular case, molecular structures of I1-PR_3 , protonated ones ($^{+}$HI1-PR_3) and verkade's base and the respective protonated species ($^{+}$HVerkade) were calculated without constraints using Gaussian 09,[17] Revision A.02, with the hybrid B3LYP[18] functional and 6-31+G(d)[19] as a basis set. Solvent effects (dimethylsulphoxide, DMSO) were introduced by using the Polarizable Continuum Model (PCM).[20]

10. Alternative theoretical mechanistic pathways.

Alternatively, we did also consider two possible reaction paths: the intramolecular attack of the nucleophylic sp^2 boryl unit of the adduct $B_2pin_2 \cdot MeO^-$ towards the C_β of the phosphonium salt by an SN_2 type of reaction (**TS-SN2**), and the direct addition of the nucleophylic boryl unit to the alkene assisted by the phosphine (**TS-PR3**).[16] Transition state structures in Figure ESI-27 do not display large differences among the main geometrical parameters. As results collected in Table S11 show, from the energy barrier of each considered mechanism it is clear that for all the phosphines tested, the alternative reaction pathways through **TS-SN$_2$** or **TS-PR$_3$** are more energetically demanding than the intermolecular attack **TS3**.

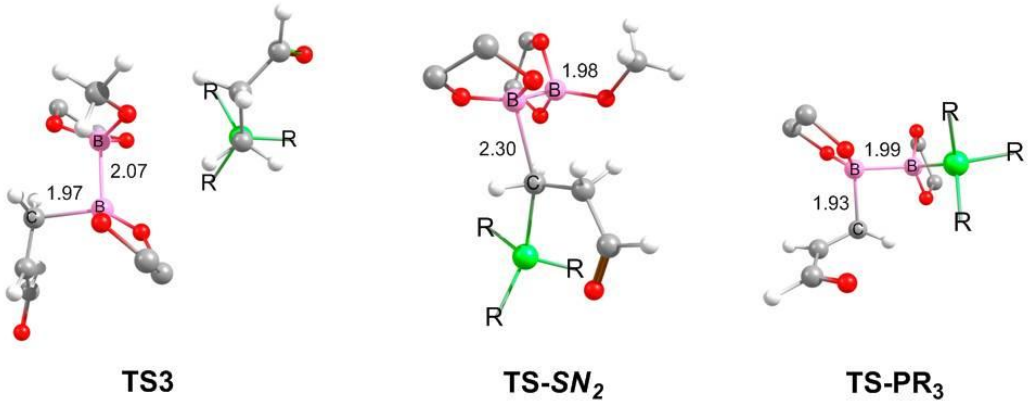


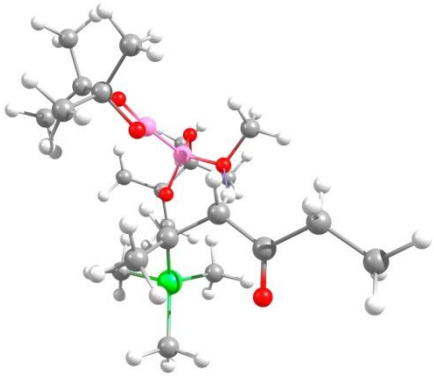
Figure ESI-27. Transition state structures for different C–B bond forming steps. Selected interatomic distances in Å.

Table S11. Comparison of the energy barriers for TS3, TS-*SN$_2$* and the TS-PR$_3$ transition states. Electronic energies and Gibbs free energies (parenthesis) in kcal.mol^{-1}.

Phosphine	**TS3** $\Delta E^{\neq}$ ($\Delta G^{\neq}$)	**TS-*SN$_2$*** $\Delta E^{\neq}$ ($\Delta G^{\neq}$)	**TS-PR$_3$** $\Delta E^{\neq}$ ($\Delta G^{\neq}$)
PMe_3	22.0 (38.2)	40.8 (40.2)	28.4 (57.3)
PPh_3	19.4 (34.8)	27.6 (25.5)	38.5 (69.6)
PCy_3	19.0 (32.9)	36.7 (35.3)	41.7 (73.2)

11. Molecular structures. Cartesian coordinates and binding energies (in kcal.mol^{-1}) for all the species. and imaginary vibrational frequencies (in cm^{-1}) for the transition state structures.

I2 ion pair : PMe3-(E)-hex-4-em-3-one



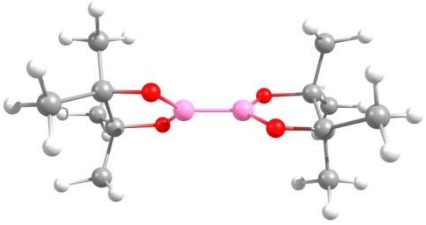
E= -9867.91kcal·mol^{-1}

	X	Y	Z
B	2.602399	0.133897	0.709285
B	1.605568	-1.300263	0.810053
C	-0.463839	0.831831	-1.812347
P	-0.449382	2.579439	-1.190787
C	0.701001	0.461267	-2.741519
O	1.573860	-2.176209	1.894083
O	0.642688	-1.689346	-0.148491
C	3.856467	-0.469574	-1.318510
O	2.975837	0.474074	-0.730895
H	3.405240	-1.481789	-1.372432
H	4.101894	-0.146722	-2.344403
H	4.795467	-0.553790	-0.746848
O	1.864767	1.361911	1.206122
O	3.785678	0.029380	1.582484
C	3.991033	1.295882	2.220621
C	2.516511	1.805088	2.418549
C	1.827393	1.124501	3.613839
H	1.943298	0.035400	3.545188

H	0.752821	1.362621	3.588248
H	2.229948	1.470204	4.578392
H	4.277723	0.300865	4.140125
C	4.766018	1.064486	3.521407
H	5.779102	0.708261	3.282706
H	4.860977	1.994734	4.105088
C	4.808320	2.218798	1.294306
H	5.747020	1.706286	1.040205
H	5.059808	3.178638	1.773461
C	2.376849	3.325860	2.539016
H	1.318437	3.600686	2.672282
H	2.759638	3.837056	1.645857
H	4.264814	2.403487	0.359894
H	2.927918	3.701239	3.415787
C	0.409954	-3.051737	1.766011
C	0.133187	-3.015157	0.223202
C	-1.336626	-3.109550	-0.178540
C	0.771144	-4.423705	2.330148
C	-0.716353	-2.420265	2.594612
H	-1.616872	-3.052470	2.612034
H	-0.363128	-2.289926	3.626482
H	-0.984104	-1.429646	2.202041
H	-0.058193	-5.136422	2.197960
H	0.974188	-4.332710	3.406494
H	1.669375	-4.831123	1.850443
H	-1.770182	-4.069485	0.142196
H	-1.929647	-2.296852	0.259672
H	-1.425227	-3.052940	-1.273493
C	0.958620	-4.042314	-0.561647
H	0.873378	-3.823446	-1.635423
H	2.019584	-3.984785	-0.284379
H	0.602732	-5.068805	-0.388930
H	1.654438	0.566777	-2.153658
H	-0.283234	0.249250	-0.891548
C	0.816546	1.239151	-4.018852
O	0.291630	2.350755	-4.148828
H	0.648982	-0.619590	-2.949582
C	-1.627384	3.667669	-2.066359
H	-2.648531	3.273370	-1.972734
H	-1.586376	4.663449	-1.601164
H	-1.342983	3.730813	-3.123226
C	1.196741	3.329814	-1.192235
H	1.130938	4.301326	-0.680413
H	1.860445	2.654812	-0.620887
H	1.541792	3.468508	-2.224151
C	-0.994046	2.478687	0.541110
H	-1.939038	1.920963	0.608931
H	-0.181504	1.955291	1.082488
H	-1.134079	3.487970	0.954244
C	-1.848994	0.456957	-2.369810

H	-1.860265	-0.619314	-2.592390
H	-2.655672	0.646065	-1.645664
H	-2.077577	1.002762	-3.295867
C	1.638807	0.614340	-5.134865
H	2.540481	0.165062	-4.686968
H	1.050455	-0.244409	-5.508317
C	1.983422	1.569658	-6.274501
H	2.550209	1.048611	-7.057721
H	1.074278	1.990153	-6.722728
H	2.590215	2.410714	-5.913021

B_2pin_2



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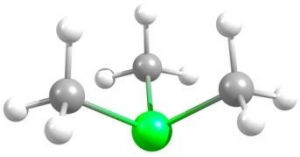
O	-1.611660	0.460787	1.056583
C	-3.011089	0.513793	0.595550
C	-3.012441	-0.513163	-0.596449
C	-3.267936	-1.957273	-0.154092
C	-3.916235	-0.146925	-1.769363
C	-3.265259	1.958198	0.153415
C	-3.914493	0.148958	1.769236
B	0.850873	-0.001597	-0.001121
O	1.613064	0.460770	-1.058039
O	1.611994	-0.462413	1.057258
C	3.011959	0.513521	-0.595136
C	3.011624	-0.513564	0.596769
C	3.265509	1.957868	-0.152410
C	3.916615	0.148824	-1.767925
C	3.267825	-1.957650	0.154762
C	3.913936	-0.147272	1.770821
H	-3.044948	2.629690	0.994336
H	-4.312054	2.109892	-0.147370
H	-3.645503	-0.823161	2.200033
H	-4.968457	0.117426	1.453379
H	-3.647083	0.825551	-2.199229
H	-4.970097	-0.115319	-1.453242

H	-3.049388	-2.629136	-0.995230
H	-4.314610	-2.107708	0.148020
H	4.311878	2.109483	0.150072
H	3.046497	2.629551	-0.993535
H	4.970361	0.118071	-1.451306
H	3.648644	-0.823687	-2.198478
H	4.968184	-0.115536	1.455907
H	3.816621	-0.907729	2.558120
H	3.048192	-2.629477	0.995635
H	2.616477	-2.236124	-0.684803
H	-2.613574	2.235955	-0.686131
H	-3.817558	0.910123	2.555885
H	-3.819769	-0.907362	-2.556765
H	-2.615565	-2.235698	0.684718
H	2.612599	2.235454	0.686261
H	3.819774	0.909622	-2.554945
H	3.644101	0.825122	2.200435
H	4.314841	-2.108090	-0.145976

PMe_3



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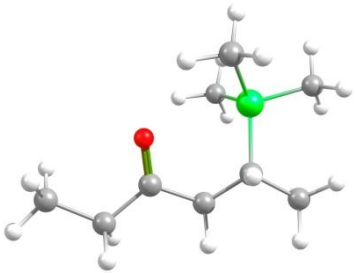
H	1.526373000	0.000000000	2.394802000
C	-0.820933000	-1.421898000	1.300044000
H	-1.877327000	-1.476638000	1.000389000
H	-0.340143000	-2.364132000	1.000389000
H	-0.763187000	-1.321878000	2.394802000
C	-0.820933000	1.421898000	1.300044000
H	-0.340143000	2.364132000	1.000389000
H	-1.877327000	1.476638000	1.000389000
H	-0.763187000	1.321878000	2.394802000

[I2-PMe3]$^{+}$



E= -3666.94 kcal·mol^{-1}

	X	Y	Z
P	1.163565	-0.205341	0.109708
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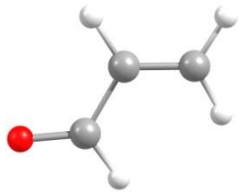
C	0.806848	-1.783081	0.943021
C	1.446389	1.130889	1.312906
H	3.132344	0.435650	-1.201645
H	3.507626	-0.758706	0.075064
H	2.715622	-1.292239	-1.432639
H	-0.135742	-1.718474	1.495646
H	0.749589	-2.577664	0.184860
H	1.637398	-2.008060	1.627956
H	0.563488	1.264708	1.948786
H	2.312110	0.855150	1.932694
H	1.680422	2.064679	0.781196
C	-0.096972	0.216769	-1.217878
C	-1.169403	1.249670	-0.811982
C	-1.978426	0.896702	0.426451
O	-1.493131	0.132218	1.259348
H	-0.711335	2.240457	-0.635463
H	-0.601540	-0.750711	-1.387833
H	-1.844763	1.398781	-1.669041
C	-3.341355	1.525198	0.576977
H	-3.240020	2.604709	0.364174
H	-3.955285	1.141620	-0.260466
C	-4.017467	1.268358	1.920851
H	-5.008817	1.737067	1.941232
H	-4.138703	0.193290	2.101108
H	-3.425054	1.680647	2.747761
C	0.580176	0.664504	-2.528287
H	1.128944	1.609007	-2.403237
H	1.266850	-0.089714	-2.929837
H	-0.195282	0.836662	-3.286772

Acrylic aldehyde



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	X	Y	Z
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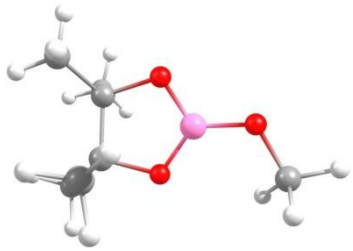
H	-2.603513	-1.475986	0.000000
C	-2.789808	0.708869	0.000000
H	-2.231769	1.648314	0.000000
C	-4.130975	0.666245	0.000000
H	-4.656676	-0.292471	0.000000
H	-4.740412	1.570175	0.000000

(pin)B-OMe



E : -3374.5 kcal·mol^{-1}

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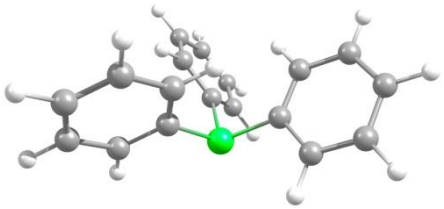
O	-1.023055	-0.694637	1.845943
C	-0.277659	1.455904	2.526291
C	-1.019652	0.159399	3.038829
C	-1.210921	2.438750	1.812537
C	0.561311	2.180357	3.574044
C	-0.236685	-0.591270	4.121216
C	-2.464214	0.374399	3.480121
H	-1.879490	2.948139	2.521301
H	-0.602963	3.198185	1.301973
H	-0.075337	2.548587	4.392727
H	1.334478	1.526000	3.995758
H	-2.510922	1.062887	4.337533
H	-2.898087	-0.586532	3.789711
H	-0.698024	-1.576660	4.271093
H	0.809178	-0.746534	3.821382
H	-1.824967	1.925882	1.059168
H	1.057709	3.046079	3.113347
H	-3.078530	0.779389	2.666534
H	-0.249968	-0.051079	5.078819
O	0.472778	-1.001796	-0.001587
C	1.543549	-0.471588	-0.800783
H	2.446253	-0.304440	-0.196690
H	1.760407	-1.210102	-1.580697
H	1.252485	0.478436	-1.270767

PPh_3



E : -5014.10 kcal·mol^{-1}

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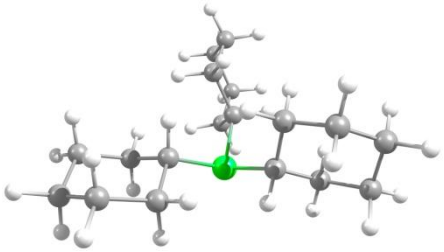
P	6.445616	0.003346	0.023165
C	7.283512	0.785382	1.480502
C	6.778023	2.026288	1.910290
C	8.329159	0.193668	2.206208
C	7.317088	2.668309	3.026923
H	5.949384	2.486715	1.367364
C	8.861151	0.831299	3.332191
H	8.724690	-0.773976	1.893540
C	8.358170	2.068728	3.744704
H	6.913632	3.630174	3.346781
H	9.670008	0.356168	3.889582
H	8.769289	2.560802	4.627780
C	7.067308	-1.741823	0.092958
C	8.160064	-2.223695	-0.644071
C	6.339922	-2.642571	0.893037
C	8.520277	-3.573896	-0.579345
H	8.728172	-1.541014	-1.277325
C	6.708103	-3.987225	0.968706
H	5.474391	-2.284997	1.455535
C	7.798124	-4.457809	0.227619
H	9.368289	-3.933933	-1.164083
H	6.134674	-4.672092	1.595139
H	8.077574	-5.511684	0.273587
C	7.389544	0.707608	-1.407924
C	6.820787	0.543752	-2.684728
C	8.580558	1.440288	-1.287932
C	7.438707	1.081305	-3.815451
H	5.882012	-0.005083	-2.789263
C	9.192231	1.990668	-2.419413
H	9.028252	1.586846	-0.303806
C	8.625571	1.811311	-3.684522
H	6.985427	0.943642	-4.798207
H	10.114538	2.563333	-2.309157
H	9.101750	2.245722	-4.565135

PCy_3

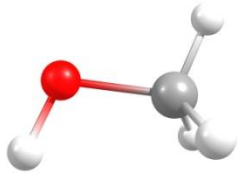


E : -6577.39kcal·mol^{-1}

	X	Y	Z
P	0.688980	-0.474898	0.006936
C	1.532663	0.184053	1.572463
C	0.718486	-0.241414	2.813267
C	3.029303	-0.104759	1.780840
H	1.406344	1.278442	1.471731
C	1.252520	0.414213	4.098182
H	0.769228	-1.339397	2.926876
H	-0.344266	0.008857	2.666798
C	3.562935	0.561015	3.062899
H	3.179480	-1.195263	1.859994
H	3.613387	0.233635	0.910491
C	2.750442	0.137432	4.295530
H	0.678643	0.058432	4.968926
H	1.089747	1.505217	4.038595
H	4.627695	0.313239	3.201271
H	3.507350	1.658659	2.950485
H	3.120426	0.654582	5.195111
H	2.898243	-0.943446	4.470845
C	1.151295	-2.327861	0.026784
C	-0.003397	-3.155269	-0.582474
C	2.499449	-2.756356	-0.583680
H	1.182161	-2.564737	1.107763
C	0.234116	-4.667493	-0.440213
H	-0.104504	-2.903426	-1.653479
H	-0.956338	-2.869672	-0.110237
C	2.736175	-4.270499	-0.429086
H	2.510415	-2.509124	-1.659259
H	3.329687	-2.199002	-0.126371
C	1.585904	-5.087457	-1.035349
H	-0.586885	-5.224610	-0.919535
H	0.211698	-4.935505	0.631555
H	3.693552	-4.549312	-0.898421
H	2.828700	-4.515154	0.644310

H	1.756511	-6.164666	-0.879636
H	1.565914	-4.926784	-2.128355
C	1.749628	0.257700	-1.381711
C	1.147991	-0.156936	-2.742601
C	1.798624	1.796709	-1.277930
H	2.781482	-0.130402	-1.317112
C	1.894786	0.474630	-3.928808
H	0.089490	0.159030	-2.768258
H	1.145154	-1.252835	-2.844646
C	2.537804	2.435510	-2.466467
H	0.764422	2.185661	-1.239995
H	2.284480	2.104496	-0.339749
C	1.937265	2.004555	-3.811808
H	1.415412	0.174154	-4.874317
H	2.927114	0.082777	-3.960583
H	2.516805	3.533038	-2.369904
H	3.600984	2.137468	-2.432627
H	2.511096	2.439849	-4.645492
H	0.909730	2.401958	-3.894082

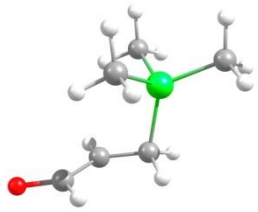
MeOH



E: -686.93kcal·mol^{-1}

	X	**Y**	**Z**
C	-0.108067000	-0.277486000	0.000000000
H	0.298890000	-1.295437000	0.000000000
H	-0.735719000	-0.152478000	-0.898299000
H	-0.735719000	-0.152478000	0.898299000
O	1.018691000	0.612195000	0.000000000
H	0.671649000	1.521355000	0.000000000

TS1-PMe$_3$

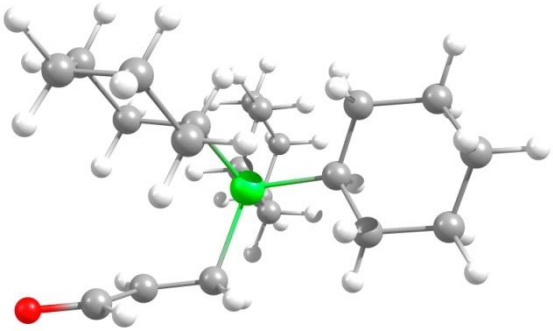


E: -2551.42kcal·mol^{-1}

Imaginary frequency: -63.62cm^{-1}

	X	Y	Z
P	1.385741000	-0.011719000	-0.020184000
C	-0.108628000	0.286722000	-1.281997000
H	2.304419000	2.232698000	-0.136107000
H	2.754629000	-1.827017000	-0.890074000
H	3.705474000	-0.873517000	0.292876000
H	3.413102000	-0.236339000	-1.357527000
H	2.491812000	1.547076000	1.512196000
H	0.884148000	2.124348000	0.953398000
H	0.592921000	-2.036419000	1.048195000
H	1.376131000	-0.943174000	2.240014000
H	-0.272546000	-0.573589000	1.615060000
C	-1.194159000	0.936391000	-0.572604000
H	-1.193280000	2.021417000	-0.448597000
H	-0.342509000	-0.734952000	-1.621903000
H	0.367142000	0.841410000	-2.103399000
O	-3.212844000	0.561799000	0.675534000
C	-2.238091000	0.170980000	-0.001715000
C	1.819254000	1.632429000	0.647798000
C	2.976963000	-0.812560000	-0.528244000
C	0.714841000	-0.990254000	1.363941000
H	-2.142998000	-0.936836000	-0.230895000

TS1-PCy$_3$



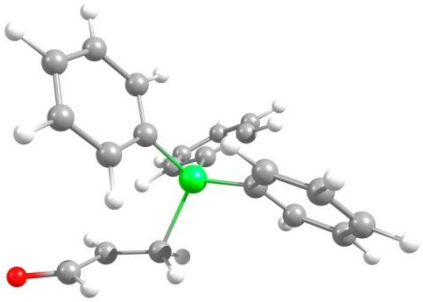
E : -7640.02 kcal·mol^{-1}

Imaginary frequency: -124.19cm^{-1}

	X	Y	Z
P	1.480330	-0.132555	-0.044869
C	-0.090573	0.273999	-1.294031
C	-0.866692	1.450833	-0.970148
H	-0.486985	2.449695	-1.199589
H	-0.674001	-0.655425	-1.209317
H	0.448408	0.269343	-2.251380
O	-2.879047	2.223998	0.096179
C	-2.106732	1.323761	-0.307069
H	-2.416427	0.240841	-0.161991
C	2.230356	-1.862217	-0.230936
C	2.845547	-2.474597	1.045849
C	1.204108	-2.829416	-0.870574
H	3.045611	-1.710307	-0.963902
C	3.458096	-3.858315	0.760993
H	2.061535	-2.584594	1.813524
H	3.609670	-1.806352	1.469128
C	1.820283	-4.212148	-1.135429
H	0.336928	-2.940970	-0.196209
H	0.816135	-2.407602	-1.809928
C	2.431441	-4.814006	0.136909
H	3.861123	-4.281412	1.694620
H	4.313894	-3.742388	0.072385
H	1.052947	-4.883111	-1.551733
H	2.605097	-4.115637	-1.906738
H	2.898538	-5.785825	-0.085214
H	1.627262	-5.010803	0.868062
C	2.856545	1.075678	-0.431893
C	4.100616	0.892898	0.465616
C	3.240941	1.046141	-1.929495
H	2.405187	2.062754	-0.219652
C	5.206972	1.907877	0.129063
H	4.504989	-0.123159	0.317511
H	3.824674	0.974586	1.527908
C	4.356966	2.057814	-2.246196
H	3.591302	0.035180	-2.204900
H	2.360772	1.260750	-2.552849
C	5.588513	1.846141	-1.355887
H	6.086840	1.715262	0.762997
H	4.857128	2.925317	0.375232
H	4.630583	1.979768	-3.309772
H	3.970437	3.080576	-2.095121
H	6.360977	2.596069	-1.585421

H	6.033430	0.859070	-1.576569
C	1.008965	0.133279	1.744524
C	0.770505	1.622759	2.097714
C	-0.223035	-0.727824	2.115404
H	1.874927	-0.229529	2.331373
C	0.391366	1.776810	3.580785
H	-0.038822	2.017984	1.464354
H	1.672083	2.219049	1.886138
C	-0.591830	-0.551560	3.598013
H	-1.076327	-0.419694	1.489960
H	-0.030887	-1.791562	1.902096
C	-0.832486	0.924510	3.943135
H	0.194730	2.838905	3.792972
H	1.247239	1.478741	4.214253
H	-1.486193	-1.152165	3.824994
H	0.225037	-0.948171	4.228544
H	-1.070487	1.032417	5.012896
H	-1.706516	1.291564	3.379556

TS1-PPh_3



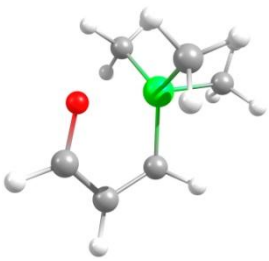
E : -6072.66 kcal·mol^{-1}

Imaginary frequency: -50.63 cm^{-1}

	X	**Y**	**Z**
P	1.595416	-0.232212	0.071077
C	-0.005697	0.051831	-1.254708
C	-1.059371	0.899998	-0.808039
H	-0.959738	1.987306	-0.842148
H	-0.290267	-1.002953	-1.387072
H	0.617368	0.401459	-2.089593
O	-3.249022	0.929877	0.174370
C	-2.241325	0.337850	-0.254324
H	-2.225095	-0.796507	-0.257773
C	2.294781	-1.862061	-0.182814

C	2.866109	-2.134795	-1.446894
C	2.021456	-2.925680	0.700720
C	3.162990	-3.447797	-1.810315
H	3.064900	-1.315833	-2.140865
C	2.320999	-4.236727	0.324286
H	1.568491	-2.715769	1.671499
C	2.885825	-4.503869	-0.930499
H	3.597895	-3.649489	-2.790245
H	2.108184	-5.055794	1.012868
H	3.103775	-5.531256	-1.225463
C	1.032760	0.007497	1.760948
C	1.749477	0.807885	2.668072
C	-0.217595	-0.528828	2.120762
C	1.229761	1.042662	3.942326
H	2.702853	1.246426	2.367781
C	-0.730527	-0.286590	3.398495
H	-0.795203	-1.110048	1.401635
C	-0.008648	0.495915	4.306194
H	1.786384	1.659850	4.648862
H	-1.706733	-0.686738	3.672681
H	-0.418745	0.695300	5.297890
C	2.827043	1.021676	-0.332243
C	2.349597	2.300619	-0.681497
C	4.205890	0.752802	-0.362822
C	3.250546	3.299919	-1.055009
H	1.276863	2.502924	-0.663864
C	5.100425	1.758503	-0.737733
H	4.565233	-0.242457	-0.097533
C	4.625032	3.030319	-1.084408
H	2.878995	4.287833	-1.330463
H	6.170966	1.550144	-0.757135
H	5.326557	3.812048	-1.380441

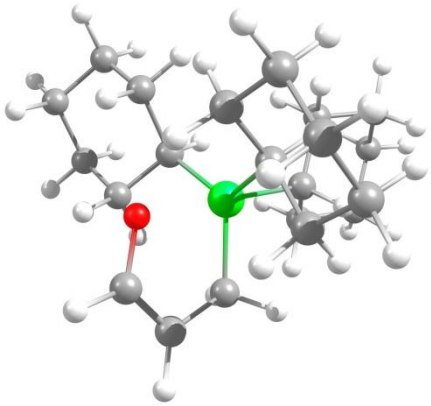
I1-PMe$_3$



E : -2568.28 kcal·mol^{-1}

	X	Y	Z
P	0.843186	-0.148424	0.210383
C	2.508399	-0.529039	-0.613885
C	0.558998	-1.828786	0.910477
C	1.497627	1.140500	1.353500
H	2.911503	0.364502	-1.114918
H	3.242490	-0.862425	0.134612
H	2.400584	-1.324831	-1.366014
H	0.289369	-1.729418	1.968564
H	-0.308717	-2.260926	0.392092
H	1.434848	-2.478304	0.785581
H	1.342461	2.115422	0.868222
H	0.924969	1.136738	2.286454
H	2.570402	0.998146	1.536768
C	0.007099	0.328054	-1.394578
C	-1.455230	0.556999	-1.180238
C	-1.826986	0.513443	0.121085
O	-0.925266	0.283464	1.073471
H	0.563057	1.218205	-1.748143
H	0.241767	-0.479021	-2.109299
H	-2.861497	0.653924	0.457068
H	-2.150455	0.735160	-1.997859

I1-PCy$_3$



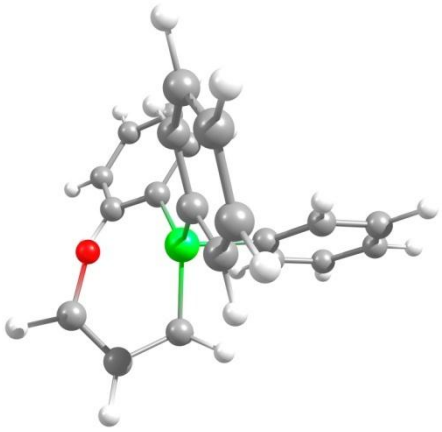
E : -7652.95kcal·mol^{-1}

	X	Y	Z
P	0.779934	-0.118748	0.374783
C	0.083856	-0.020021	-1.366028
C	-1.385565	0.261377	-1.352446

C	-1.893242	0.511548	-0.121858
O	-1.116762	0.485294	0.953212
H	0.670699	0.771601	-1.863310
H	0.362018	-0.963496	-1.866503
H	-2.955216	0.739269	0.047713
H	-1.985327	0.267020	-2.261248
C	2.544347	-0.762499	-0.169966
C	3.215747	-0.016376	-1.344982
C	3.558586	-0.872645	0.993603
C	4.535571	-0.683556	-1.777987
C	4.864920	-1.564881	0.566246
C	5.520055	-0.831828	-0.611431
C	0.403997	-1.701887	1.366891
C	-0.293372	-1.566776	2.735463
C	-0.375623	-2.681472	0.457023
C	-0.440648	-2.945482	3.405164
C	-0.541854	-4.052856	1.135841
C	-1.208465	-3.929741	2.512660
C	1.353021	1.521325	1.127174
C	0.732741	2.745383	0.419220
C	1.158076	1.615204	2.655449
C	1.318249	4.054966	0.976199
C	1.730852	2.934544	3.204526
C	1.127781	4.155490	2.496044
H	2.335652	-1.793373	-0.521421
H	3.424408	1.028946	-1.051151
H	2.548734	0.031552	-2.216684
H	3.811053	0.139265	1.357578
H	3.129003	-1.406750	1.855239
H	4.994669	-0.106797	-2.597206
H	4.308753	-1.684153	-2.187340
H	5.559672	-1.617667	1.420182
H	4.645131	-2.606698	0.272751
H	6.429628	-1.359562	-0.939606
H	5.840860	0.171241	-0.277377
H	1.395746	-2.149908	1.544324
H	-1.279613	-1.105883	2.589095
H	0.274184	-0.896965	3.397036
H	-1.364887	-2.251712	0.228789
H	0.144577	-2.816514	-0.505243
H	-0.950236	-2.828460	4.374831
H	0.559563	-3.360621	3.625443
H	-1.126867	-4.718409	0.481038
H	0.451576	-4.521960	1.255008
H	-1.276138	-4.918136	2.994817
H	-2.243406	-3.567798	2.382691
H	2.438615	1.540973	0.927105
H	-0.356696	2.727212	0.570317
H	0.910593	2.696179	-0.667059
H	0.081557	1.550668	2.877240

H	1.650054	0.767905	3.159121
H	0.844016	4.911629	0.471500
H	2.396565	4.109324	0.741184
H	1.550565	2.990551	4.290020
H	2.827093	2.941874	3.067309
H	1.578890	5.084056	2.880858
H	0.048322	4.208810	2.721740

I1-PPh$_3$

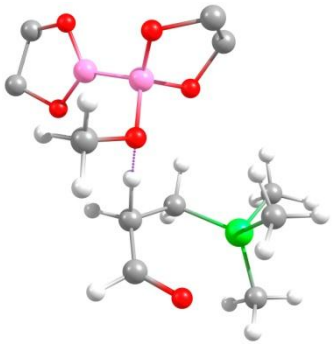


E : -6087.06kcal·mol^{-1}

	X	Y	Z
P	0.828639	-0.153956	0.230957
C	0.060730	0.180044	-1.446509
C	-1.423700	0.278272	-1.311584
C	-1.838868	0.346333	-0.025461
O	-0.940344	0.346782	0.959136
H	0.556348	1.097291	-1.813786
H	0.417968	-0.629487	-2.102753
H	-2.890011	0.393714	0.279024
H	-2.096326	0.259374	-2.166112
C	2.541444	-0.555555	-0.536872
C	3.146340	-1.821730	-0.518359
C	3.212361	0.477578	-1.221376
C	4.367033	-2.052792	-1.167109
H	2.666479	-2.647973	0.007646
C	4.423949	0.252034	-1.877241
H	2.791269	1.486503	-1.232672
C	5.006896	-1.020166	-1.854206
H	4.814180	-3.047899	-1.132552

H	4.917827	1.072167	-2.401285
H	5.954980	-1.200707	-2.364056
C	0.486872	-1.795283	0.973378
C	0.023612	-2.839190	0.156544
C	0.655633	-2.016103	2.348472
C	-0.263713	-4.090023	0.712650
H	-0.116505	-2.682566	-0.913860
C	0.379386	-3.271227	2.895386
H	0.989391	-1.203959	2.995513
C	-0.081458	-4.311270	2.080414
H	-0.629394	-4.892983	0.070921
H	0.516550	-3.433468	3.965548
H	-0.302000	-5.289165	2.511771
C	1.482060	1.161297	1.351447
C	0.847377	2.409260	1.454011
C	2.650509	0.919875	2.092066
C	1.389418	3.406611	2.269813
H	-0.076104	2.590281	0.906367
C	3.160210	1.902678	2.944458
H	3.167985	-0.035727	1.998712
C	2.538241	3.152202	3.025445
H	0.900138	4.380032	2.327183
H	4.055340	1.695404	3.532150
H	2.949281	3.926349	3.675876

TS2-PMe_3



E : -8730.50 kcal·mol^{-1}

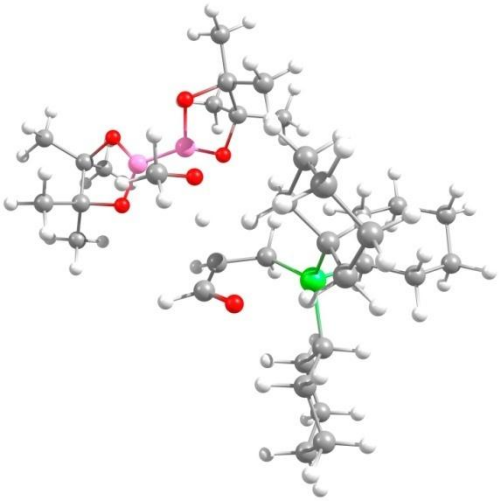
Imaginary frequency: -663.69 cm^{-1}

X	Y	Z

B	1.384476227	-0.033556149	2.000055518
C	0.254345336	0.150688730	-1.418519673
H	0.059180084	0.051199026	-0.011397450
O	-0.037295920	-0.078915801	1.204252658
H	-1.794005885	0.664636507	-1.926180457
H	1.952248804	-0.634677694	-2.579646032
H	2.005662236	-1.003023721	-0.832639192
H	0.585669097	1.193440461	-1.452505283
C	-1.028960535	-0.140498105	-1.934281010
O	-1.373480472	-1.296472104	-2.316919604
P	0.764452562	-2.611659073	-1.998509249
C	0.206012320	-3.129662358	-3.665572793
H	0.669542142	-2.469452409	-4.412920840
H	-0.881708278	-3.038685582	-3.743053716
H	0.536819795	-4.162511568	-3.847428457
H	-1.271144273	-3.098905585	-0.776022437
C	-0.211736911	-3.345515671	-0.649556360
H	-0.054015047	-4.433232247	-0.634286911
H	0.164562482	-2.905077689	0.286510187
H	2.825929235	-3.303280734	-0.884269464
C	2.381239157	-3.496478589	-1.869549587
H	3.067759021	-3.135073144	-2.649040154
H	2.239316786	-4.578791478	-1.998346309
H	-0.607654715	-2.191348084	4.065818412
H	-0.159296248	-2.469518550	2.374336907
H	1.784857963	-3.838997828	1.713583706
H	0.352830408	-3.631470012	3.641687545
C	2.714588067	-3.444574366	2.143770276
H	3.516251132	-3.538400439	1.394744912
H	2.991223733	-4.074704447	3.003362175
C	1.450046957	-1.715903643	3.639343946
O	1.132385676	-0.331042273	3.399310740
O	2.113218546	-1.197195163	1.438968464
C	3.939159388	-1.437743609	3.006983224
H	4.618214749	-1.461958569	2.141759408
H	3.847402620	-0.397586974	3.345532058
H	4.385425384	-2.039403769	3.813446892
H	2.716160955	-1.152937238	5.321171866
C	1.908860743	-1.859525870	5.092142427
H	1.066903035	-1.641318095	5.765332546
H	2.256801529	-2.883699027	5.302263257
O	2.118017235	2.320738884	0.639920449
B	2.126734783	1.525194295	1.792390688
O	2.853716742	2.131857112	2.811728282
C	2.688046860	3.631946063	0.985468281
C	3.533652265	3.309649471	2.272597770
C	3.523402205	4.396463070	3.346424577
H	2.504723829	4.611477976	3.691671394
H	3.976416099	5.328010978	2.972970215
H	4.108428799	4.055891524	4.212356967

H	5.583373400	3.736480006	1.618418231
C	4.975732042	2.888245951	1.967045928
H	5.428211903	2.493646602	2.887193844
H	5.003763953	2.095300597	1.207529276
C	1.502052794	4.564764055	1.258227527
H	0.905656517	4.204950834	2.107559388
H	0.856163647	4.587744818	0.369358860
H	2.822706944	4.313305160	-1.060571429
H	1.832383516	5.591919648	1.472043255
C	3.493188438	4.144996530	-0.205611510
H	4.265160480	3.427801004	-0.510650042
H	3.979535414	5.102845806	0.036719742
H	-1.186400655	0.735747697	2.716508620
C	-0.983948627	0.907254238	1.652701837
H	-1.913046404	0.793913024	1.076100063
H	-0.590214688	1.928301277	1.518077472
C	2.569462134	-1.982818715	2.568276262
C	0.189476294	-2.567521754	3.409194609
C	1.329276312	-0.884385187	-1.699306408

TS2-PCy_3



E : -13810.26kcal·mol^{-1}

Imaginary frequency:-680.93 cm^{-1}

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O	0.047425	0.209154	1.321604

C	-0.005457	0.146099	-1.316800
B	1.480962	0.032891	2.050396
H	-2.779789	-0.771187	-7.664292
H	-2.139829	0.370839	-6.474884
C	-2.499261	-0.664876	-6.604623
H	-4.500026	-0.148186	-5.918263
C	-3.716235	-0.889885	-5.698540
H	-4.155184	-1.880979	-5.913403
H	-1.684241	-2.668608	-6.500736
H	-0.474844	-1.431934	-6.866269
C	-1.366681	-1.639615	-6.254681
C	-0.992180	-1.574810	-4.761607
H	-0.197817	-2.309340	-4.556101
H	-0.579480	-0.579036	-4.526222
H	-2.982681	0.212570	-3.974117
C	-3.339202	-0.798182	-4.209723
H	-4.229111	-0.962554	-3.590572
H	-2.632344	-2.820851	-4.145769
C	-2.237311	-1.825315	-3.875352
P	-1.700938	-2.111672	-2.079303
O	-2.294205	0.348926	-1.857520
H	-1.095642	1.991273	-1.659236
H	0.953577	0.619418	-1.555520
H	0.636767	-1.692828	-2.314837
H	0.183294	-1.894735	-0.626898
C	-0.082322	-1.354293	-1.549559
C	-3.008230	-2.280632	-0.732179
H	-4.570821	-0.954209	-1.422252
C	-1.130532	-3.929696	-2.253714
H	-0.424642	-3.914856	-3.106118
C	-4.461414	-2.023012	-1.181476
H	-4.705752	-2.596876	-2.089609
C	-2.279111	-4.905447	-2.610450
H	-2.799844	-4.591413	-3.527445
H	-3.034298	-4.896985	-1.805341
H	-1.101113	-6.396360	-3.659167
C	-1.780605	-6.350369	-2.789856
H	-2.634928	-7.005107	-3.023083
C	-1.041257	-6.847633	-1.542626
H	-0.670471	-7.872785	-1.696152
H	-1.747056	-6.890778	-0.693954
C	0.114088	-5.903969	-1.193941
H	0.622448	-6.232136	-0.274616
H	0.868649	-5.940815	-1.999404
H	-6.470283	-2.188494	-0.376631
C	-5.439511	-2.403896	-0.054213
H	-5.385702	-3.493581	0.118696
C	-0.359783	-4.451240	-1.016738
H	-2.928635	-3.353482	-0.477143
H	-1.010810	-4.396040	-0.126351

C	-5.121072	-1.668006	1.255581
H	-5.804146	-1.999057	2.053518
H	-5.297672	-0.587291	1.115368
H	0.513287	-3.822257	-0.802791
C	-2.692312	-1.484487	0.548122
H	-2.804736	-0.413272	0.328934
H	-1.654222	-1.631751	0.875099
H	-3.423548	-1.304543	2.575987
C	-3.660208	-1.885028	1.672060
H	-3.503900	-2.946506	1.934270
H	-0.118880	2.273509	1.683528
H	-1.622374	1.427277	1.193241
C	-0.698986	1.341830	1.785297
O	2.030309	-1.201265	1.455214
H	-0.955760	1.190437	2.841637
O	1.235757	-0.250279	3.461121
C	2.431071	-2.048259	2.556155
C	3.868111	-1.676645	2.962854
H	4.518485	-1.770836	2.080925
H	3.910080	-0.637278	3.313670
H	4.257394	-2.337107	3.753307
H	2.748450	-1.278719	5.329476
H	2.097608	-2.947443	5.299022
H	1.065066	-1.586504	5.806161
C	1.862452	-1.887515	5.109994
C	1.389832	-1.667294	3.670763
C	2.388186	-3.507627	2.099234
H	3.136503	-3.668162	1.308308
H	-0.295062	-2.253234	2.423068
H	1.400674	-3.774089	1.699795
H	2.625418	-4.188358	2.932424
C	0.035032	-2.366469	3.462335
H	-0.710382	-1.887469	4.112707
H	0.076332	-3.438269	3.714320
B	2.417034	1.471943	1.793925
O	2.379055	2.280324	0.649049
O	3.344044	1.957351	2.712914
C	4.117699	3.024514	2.078149
C	3.161207	3.492199	0.921781
C	2.160826	4.567877	1.363554
H	1.404877	4.693434	0.575580
H	1.647302	4.269652	2.287763
H	2.650688	5.538403	1.531355
H	4.475700	3.114932	-0.778785
C	3.859053	3.922665	-0.365611
H	3.105926	4.198735	-1.117828
H	4.499804	4.800738	-0.188905
H	6.096257	3.136500	1.135951
C	5.417221	2.388198	1.571190
H	5.926435	1.908120	2.418152

H	3.511705	4.445720	3.619501
H	5.208914	1.615713	0.818591
C	4.426743	4.082231	3.135765
H	5.067677	3.642163	3.912827
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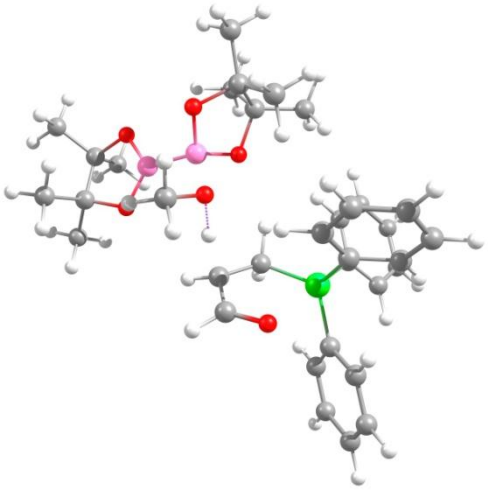
C	-1.167739	0.883198	-1.651811

TS2-PPh_3



E : -12246.10 kcal·mol^{-1}

Imaginary frequecy: -672.01 cm^{-1}

	X	**Y**	**Z**
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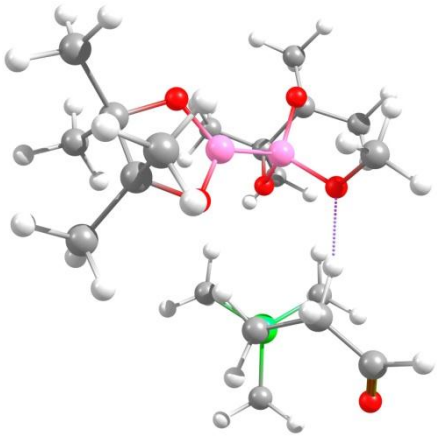
O	0.012452	0.059233	1.214219
C	0.234407	-0.012699	-1.413305
B	1.466006	0.095528	1.987997
H	-2.110834	-3.123180	-7.382826
H	-3.548926	-3.713893	-5.431279
H	0.234046	-2.362444	-7.006481
H	1.152326	-2.239927	-4.711707
C	0.118317	-2.554698	-4.861249
C	-0.397148	-2.631108	-6.158700
C	-1.712082	-3.057477	-6.369149
C	-2.518028	-3.392791	-5.276288
C	-2.015437	-3.303575	-3.977411
H	-2.656131	-3.533379	-3.126565
C	-0.689546	-2.896057	-3.764594
P	-0.006928	-2.819883	-2.067736

C	-1.126216	-3.560489	-0.827272
C	-1.488087	-4.910997	-0.971545
C	-2.358621	-5.501522	-0.053004
H	-2.643642	-6.546879	-0.175529
H	-1.090510	-5.503311	-1.796759
C	1.374680	-4.068681	-2.141625
H	-3.522624	-5.221359	1.747529
C	-2.848616	-4.757744	1.025278
C	-2.463797	-3.423759	1.184816
H	-2.826347	-2.844341	2.034079
H	-1.314008	-1.780109	0.400870
H	1.784149	-1.289086	-2.299373
C	0.970449	-1.332192	-1.555408
H	1.441734	-1.634003	-0.601560
H	0.825116	0.887539	-1.608938
C	-1.107267	-0.013835	-1.862925
H	-1.632773	0.957420	-1.966676
O	-1.757759	-1.077078	-2.065198
H	0.784495	-4.987296	-4.016114
C	2.547102	-5.919714	-3.206231
H	2.631411	-6.623728	-4.035281
C	3.481878	-5.939212	-2.168844
H	4.303805	-6.656886	-2.183187
C	3.356398	-5.035751	-1.109199
H	4.074766	-5.048056	-0.288687
H	2.231619	-3.428186	-0.245673
C	2.310409	-4.112064	-1.090604
H	-1.121309	0.978978	2.677181
C	-0.885401	1.109917	1.614458
H	-1.807592	1.033596	1.019317
H	-0.430861	2.101032	1.460837
H	2.375305	4.397804	-1.322940
C	3.249019	4.152841	-0.702024
H	3.848036	3.402432	-1.232640
H	3.851125	5.067846	-0.588967
C	2.782957	3.641689	0.657878
C	1.797247	4.633980	1.286864
H	1.448102	4.272711	2.263813
H	2.248037	5.628398	1.419965
H	0.925207	4.735524	0.625707
C	3.929205	3.205025	1.639495
O	3.318402	2.081013	2.350804
B	2.288347	1.565770	1.569466
O	2.041542	2.386771	0.461542
H	4.891689	1.895241	0.181821
C	5.168681	2.658493	0.921708
H	5.826736	2.188158	1.665160
H	5.731466	3.456944	0.415617
C	4.337699	4.255024	2.670631
H	3.490471	4.546590	3.303358

H	4.742856	5.154418	2.181293
H	5.119524	3.839988	3.322342
C	1.439341	-1.370321	3.822347
C	0.125153	-2.157891	3.701171
H	-0.651029	-1.631080	4.274824
H	-0.194557	-2.211981	2.654903
H	0.214514	-3.180144	4.100686
O	2.108644	-1.166796	1.569646
O	1.213411	-0.004517	3.413017
C	2.519351	-1.846642	2.785965
H	1.588627	-3.716878	2.134725
H	3.344400	-3.603501	1.829154
H	2.751808	-3.898838	3.474610
C	2.542248	-3.355052	2.540156
H	4.599280	-1.551063	2.297550
C	3.931948	-1.361416	3.151230
H	3.930819	-0.282619	3.351953
H	1.082713	-1.008781	5.922399
C	1.903267	-1.362038	5.280281
H	2.756826	-0.687029	5.419605
H	2.185616	-2.373145	5.614939
H	4.333586	-1.891519	4.028599
C	-1.611581	-2.817840	0.259533
C	1.499626	-4.992774	-3.193334

I2-PMe$_3$ acryl aldehyde



E : -8738.57kcal·mol^{-1}

	X	**Y**	**Z**

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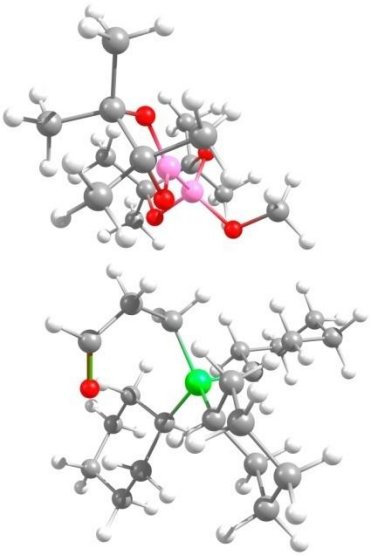
C	-0.486713000	0.769861000	-1.877056000
P	-0.546356000	2.464989000	-1.167863000
C	0.716901000	0.428822000	-2.759849000
O	1.623595000	-2.197100000	1.870657000
O	0.533635000	-1.630121000	-0.070610000
C	3.812459000	-0.500100000	-1.381189000
O	2.933331000	0.447521000	-0.792730000
H	3.388107000	-1.524599000	-1.366571000
H	3.999763000	-0.218513000	-2.431003000
H	4.776673000	-0.532098000	-0.849127000
O	1.875653000	1.363058000	1.169009000
O	3.802615000	0.027271000	1.500825000
C	4.030119000	1.299631000	2.122544000
C	2.563767000	1.814193000	2.359571000
C	1.909166000	1.143764000	3.579856000
H	2.022629000	0.053889000	3.517778000
H	0.834569000	1.383204000	3.584824000
H	2.340447000	1.496992000	4.529055000
H	4.371335000	0.318362000	4.040515000
C	4.842577000	1.075799000	3.401412000
H	5.847239000	0.715249000	3.135645000
H	4.957050000	2.010271000	3.974650000
C	4.821798000	2.211943000	1.164838000
H	5.751581000	1.695244000	0.887664000
H	5.089821000	3.174738000	1.628686000
C	2.429400000	3.335544000	2.472925000
H	1.374599000	3.612179000	2.630119000
H	2.791108000	3.841020000	1.567900000
H	4.251608000	2.391496000	0.245277000
H	3.001983000	3.715498000	3.333721000
C	0.429036000	-3.039766000	1.821906000
C	0.018104000	-2.951847000	0.311008000
C	-1.483863000	-2.990693000	0.039119000
C	0.800414000	-4.436122000	2.314871000
C	-0.601773000	-2.404675000	2.764050000
H	-1.514711000	-3.013719000	2.843143000
H	-0.156134000	-2.314995000	3.763807000
H	-0.874741000	-1.395999000	2.424737000
H	-0.057197000	-5.123046000	2.238696000
H	1.100423000	-4.381134000	3.370667000
H	1.640574000	-4.852915000	1.746312000
H	-1.916847000	-3.947811000	0.368496000
H	-2.009962000	-2.176605000	0.553825000
H	-1.667880000	-2.894492000	-1.041115000
C	0.738637000	-3.979036000	-0.570625000
H	0.563761000	-3.729098000	-1.626595000
H	1.821312000	-3.959176000	-0.388719000
H	0.368703000	-4.999397000	-0.391767000

H	1.653598000	0.509511000	-2.120585000
H	-0.458541000	0.076938000	-1.018669000
H	-1.442673000	0.631696000	-2.409768000
C	0.882427000	1.240910000	-3.987214000
O	0.298699000	2.301506000	-4.212690000
H	1.625820000	0.851347000	-4.724560000
H	0.693844000	-0.641039000	-3.023418000
C	-1.786853000	3.471038000	-2.049384000
H	-2.773973000	2.993937000	-1.969224000
H	-1.833516000	4.472425000	-1.598246000
H	-1.491724000	3.542335000	-3.104199000
C	1.052632000	3.308435000	-1.165704000
H	0.929518000	4.272903000	-0.650986000
H	1.749611000	2.669507000	-0.590560000
H	1.394188000	3.471230000	-2.195462000
C	-1.071800000	2.291522000	0.560709000
H	-1.985224000	1.682949000	0.618838000
H	-0.226897000	1.799163000	1.082655000
H	-1.257970000	3.281809000	1.000609000

I2-PCy$_3$ acryl aldehyde



E : -13819.18 kcal·mol^{-1}

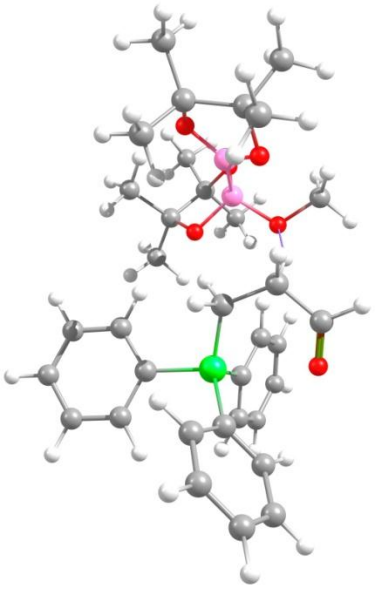
	X	**Y**	**Z**
B	1.625513000	-0.562916000	1.935882000
B	2.252455000	-1.770195000	0.832487000
C	-0.126083000	1.719611000	-0.234152000

P	-0.137299000	3.351040000	-1.075758000
C	-0.119091000	0.369892000	-0.962057000
O	2.468513000	-3.112744000	1.145408000
O	2.527206000	-1.547641000	-0.536081000
C	3.550114000	0.933202000	1.654736000
O	2.140277000	0.828852000	1.574026000
H	4.057499000	0.215206000	0.980345000
H	3.862817000	1.949067000	1.358577000
H	3.914257000	0.745441000	2.680504000
O	0.122075000	-0.453420000	1.854413000
O	1.898853000	-0.920383000	3.344548000
C	0.729935000	-0.624573000	4.117905000
C	-0.427166000	-0.930631000	3.095840000
C	-0.696694000	-2.440441000	2.966962000
H	0.244198000	-2.977662000	2.792070000
H	-1.358154000	-2.607430000	2.103351000
H	-1.187686000	-2.854968000	3.861356000
H	0.858534000	-2.567096000	5.098506000
C	0.733279000	-1.510434000	5.367325000
H	1.575659000	-1.225172000	6.015295000
H	-0.197475000	-1.394770000	5.946887000
C	0.754247000	0.859477000	4.537357000
H	1.692439000	1.048377000	5.078600000
H	-0.087135000	1.125485000	5.197939000
C	-1.742570000	-0.192571000	3.364354000
H	-2.481178000	-0.455099000	2.590458000
H	-1.597814000	0.896100000	3.348329000
H	0.744552000	1.498816000	3.646123000
H	-2.165983000	-0.474943000	4.341578000
C	2.687348000	-3.862152000	-0.090190000
C	3.178918000	-2.745393000	-1.076425000
C	2.751156000	-2.924421000	-2.531339000
C	3.696610000	-4.973624000	0.190232000
C	1.335570000	-4.468287000	-0.489452000
H	1.420371000	-5.111053000	-1.378757000
H	0.963290000	-5.077378000	0.345495000
H	0.595703000	-3.680811000	-0.688007000
H	3.938596000	-5.530200000	-0.729094000
H	3.267016000	-5.680941000	0.913695000
H	4.624400000	-4.574927000	0.618328000
H	3.181013000	-3.844772000	-2.956691000
H	1.659321000	-2.973600000	-2.629187000
H	3.114057000	-2.075862000	-3.129908000
C	4.691173000	-2.498561000	-1.001427000
H	4.927867000	-1.576000000	-1.550116000
H	5.013935000	-2.368628000	0.040120000
H	5.262851000	-3.325425000	-1.448845000
H	0.770139000	1.709540000	0.426011000
H	-0.986329000	1.760734000	0.450866000
C	-0.842297000	0.226829000	-2.244803000

O	-1.362798000	1.142816000	-2.877972000
H	-0.877229000	-0.813065000	-2.652285000
H	-0.481582000	-0.380961000	-0.229272000
C	-1.853920000	4.045999000	-1.450579000
C	-2.220172000	4.201418000	-2.944731000
C	-2.972602000	3.282252000	-0.704452000
H	-1.789632000	5.062826000	-1.017243000
C	-3.572938000	4.920550000	-3.095036000
H	-2.276658000	3.205567000	-3.406163000
H	-1.448456000	4.769885000	-3.483928000
C	-4.327547000	3.992113000	-0.868327000
H	-3.036024000	2.263676000	-1.119353000
H	-2.738909000	3.179571000	0.365400000
C	-4.692355000	4.186389000	-2.345948000
H	-3.819070000	5.009212000	-4.164461000
H	-3.487176000	5.950967000	-2.706015000
H	-5.106741000	3.411890000	-0.350822000
H	-4.285727000	4.976766000	-0.369441000
H	-5.640870000	4.737975000	-2.436626000
H	-4.852791000	3.199364000	-2.812711000
C	0.912812000	3.451975000	-2.613722000
C	1.296107000	4.904000000	-2.983228000
C	2.167624000	2.546949000	-2.605315000
H	0.225948000	3.060371000	-3.386046000
C	1.984719000	4.941242000	-4.358915000
H	1.988241000	5.305385000	-2.223995000
H	0.414374000	5.563272000	-2.987303000
C	2.855313000	2.589401000	-3.980683000
H	2.874650000	2.888882000	-1.833297000
H	1.907718000	1.511537000	-2.349720000
C	3.214665000	4.022753000	-4.397418000
H	2.268890000	5.977008000	-4.601061000
H	1.263612000	4.622255000	-5.131381000
H	3.756764000	1.958665000	-3.957174000
H	2.180666000	2.147048000	-4.734201000
H	3.661540000	4.028325000	-5.403442000
H	3.982823000	4.418588000	-3.710056000
C	0.519347000	4.538798000	0.210941000
C	-0.385358000	4.578700000	1.468320000
C	1.985269000	4.269783000	0.617642000
H	0.461004000	5.527071000	-0.287321000
C	0.116732000	5.627413000	2.476214000
H	-0.375047000	3.587188000	1.949898000
H	-1.428559000	4.801986000	1.198077000
C	2.477426000	5.320001000	1.629331000
H	2.059921000	3.265181000	1.067638000
H	2.641030000	4.278119000	-0.265265000
C	1.577833000	5.376060000	2.870818000
H	-0.531804000	5.614615000	3.365755000
H	0.022215000	6.633653000	2.029819000

H	3.513725000	5.086149000	1.916750000
H	2.498872000	6.313822000	1.146433000
H	1.926200000	6.158708000	3.562388000
H	1.647779000	4.417479000	3.411567000
H	0.914681000	0.000434000	-1.123627000

I2-PPh_3 acryl aldehyde



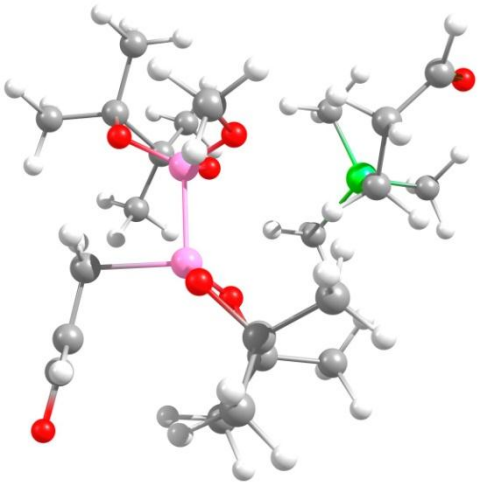
E : -12250.46 kcal·mol^{-1}

	X	Y	Z
B	2.688576	-0.389579	0.701310
B	1.687906	-1.826556	0.630998
C	-0.198226	1.271375	-0.767563
P	-0.533325	3.064251	-0.952342
C	0.425346	0.445726	-1.901967
O	1.307336	-2.543014	1.768098
O	1.155894	-2.434625	-0.521414
C	3.872172	-0.677351	-1.473997
O	3.029828	0.165532	-0.693617
H	3.403248	-1.658915	-1.669016
H	4.075196	-0.184710	-2.438689
H	4.831193	-0.853524	-0.960723
O	2.038815	0.781405	1.401050
O	3.900435	-0.682553	1.483306
C	4.202046	0.460271	2.295629
C	2.771326	1.024043	2.627265

C	2.085857	0.235678	3.755877
H	2.113571	-0.839944	3.542744
H	1.030100	0.542450	3.809736
H	2.548702	0.427002	4.736469
H	4.481998	-0.824650	4.035645
C	5.000927	-0.009533	3.515287
H	5.979910	-0.387959	3.185269
H	5.176341	0.815958	4.224296
C	5.049736	1.457250	1.480336
H	5.942326	0.930041	1.113882
H	5.379700	2.319058	2.081786
C	2.754466	2.519840	2.949336
H	1.742163	2.845682	3.228799
H	3.077691	3.118104	2.088034
H	4.483351	1.811243	0.611182
H	3.418599	2.741118	3.800137
C	0.330978	-3.561218	1.383685
C	0.636978	-3.754977	-0.142046
C	-0.571426	-4.077010	-1.017473
C	0.550582	-4.796730	2.254009
C	-1.059668	-2.970250	1.650366
H	-1.859584	-3.701145	1.458521
H	-1.115002	-2.661830	2.703343
H	-1.234396	-2.082909	1.026471
H	-0.120282	-5.616706	1.952734
H	0.334752	-4.548211	3.302931
H	1.587972	-5.147907	2.195976
H	-1.018596	-5.041065	-0.728921
H	-1.343566	-3.300302	-0.947172
H	-0.254597	-4.153500	-2.067713
C	1.761913	-4.763711	-0.405871
H	2.061336	-4.694110	-1.460935
H	2.640451	-4.540114	0.214163
H	1.438631	-5.795909	-0.204492
H	1.517786	0.272558	-1.608826
H	0.465004	1.208365	0.120121
H	-1.177594	0.868098	-0.464274
C	0.456673	1.031466	-3.250725
O	0.280685	2.225658	-3.493697
H	0.730599	0.333380	-4.076106
H	0.021396	-0.576458	-1.918566
C	-1.906656	3.480963	-2.088078
C	-1.730220	4.256933	-3.243905
C	-3.178367	2.962423	-1.785430
C	-2.820730	4.526388	-4.073272
H	-0.740387	4.625002	-3.507299
C	-4.259477	3.218037	-2.631443
H	-3.330694	2.366356	-0.884291
C	-4.083443	4.006186	-3.772957
H	-2.676433	5.131641	-4.968753

H	-5.239943	2.804745	-2.393314
H	-4.929162	4.210241	-4.431560
C	-1.195908	3.535535	0.700676
C	-2.089137	4.617670	0.813217
C	-0.770848	2.866161	1.862368
C	-2.563158	5.012772	2.064957
H	-2.429700	5.144915	-0.078765
C	-1.260967	3.262387	3.110191
H	-0.046239	2.050965	1.810764
C	-2.155372	4.330323	3.215417
H	-3.257145	5.850874	2.138394
H	-0.931113	2.733387	4.004644
H	-2.532188	4.634157	4.193364
C	0.957993	4.065365	-1.227571
C	2.226800	3.465485	-1.148784
C	0.836647	5.450023	-1.442678
C	3.364246	4.260141	-1.315725
H	2.352957	2.397710	-0.944028
C	1.982323	6.227582	-1.614736
H	-0.145537	5.922976	-1.475201
C	3.246872	5.631933	-1.555107
H	4.348165	3.794872	-1.252545
H	1.886076	7.299755	-1.789253
H	4.142226	6.241549	-1.687698

TS3-PMe_3



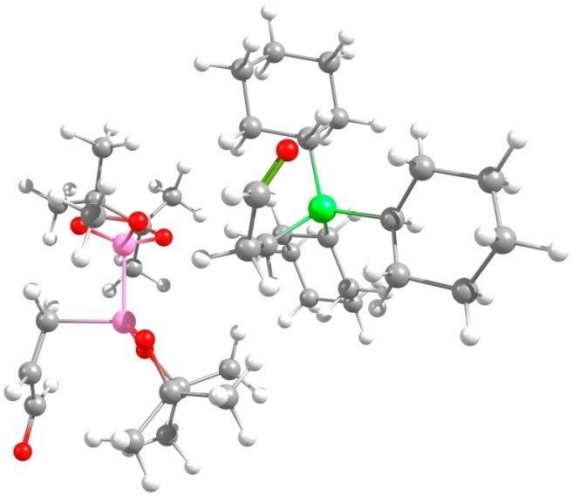
E : -9791.68kcal·mol^{-1}

Imaginary frequency:-309.02 cm^{-1}

	X	Y	Z
B	2.573614	0.082533	0.650191
B	1.505916	-1.679261	0.845001
C	2.677873	-2.217347	2.337711
C	2.022584	-3.298419	2.952861
H	-1.726604	-2.742589	2.264140
H	-0.263893	-3.737192	2.170532
H	-1.716925	-4.208872	1.251140
H	0.526154	-5.096513	0.512090
H	-0.631468	-5.116349	-0.845870
H	1.121227	-5.131903	-1.163933
H	-2.516631	-2.745184	-0.687579
H	-1.661062	-1.240490	-1.093531
H	-2.516858	-1.397746	0.466553
H	-0.671869	-3.050432	-2.487349
H	1.102681	-3.188664	-2.583995
H	0.372941	-1.651324	-2.089136
C	0.274070	-2.740899	-2.018129
C	-1.903158	-1.929314	-0.275856
C	0.373401	-3.199013	-0.556506
C	-0.656304	-2.488982	0.413459
C	0.340567	-4.727956	-0.503590
C	-1.111067	-3.355453	1.590017
O	1.667349	-2.754818	-0.061897
O	0.127266	-1.370887	0.957875
O	2.648658	0.058772	-0.808724
C	3.698133	-0.731170	-1.377022
H	-0.420923	1.360596	1.056925
H	3.742692	-0.512911	-2.455223
H	3.496894	-1.804160	-1.240314
H	4.668449	-0.483159	-0.920531
O	3.811988	0.123822	1.376306
O	1.764580	1.229456	1.082971
C	2.399797	1.808029	2.256124
H	0.658113	1.461073	3.480787
C	1.732427	1.228234	3.511404
H	1.827820	0.138921	3.557847
C	3.908344	1.384890	2.070931
H	2.148727	1.661120	4.432772
C	4.672820	1.177871	3.379308
H	4.204757	0.404571	4.001065
H	5.700695	0.857439	3.156880
H	4.725417	2.112871	3.959487
H	5.660779	1.893891	0.928764
C	4.688035	2.349605	1.159602
H	2.698110	3.776922	3.128188
H	4.869625	3.326103	1.634033
C	2.187619	3.325948	2.263468

H	2.572267	3.806846	1.355710
H	4.154106	2.503620	0.211868
H	1.115638	3.556483	2.359910
H	3.533544	-2.428574	1.697457
H	2.830082	-1.322377	2.935909
H	1.276559	-2.109837	4.587207
C	1.287714	-3.154066	4.172742
H	2.051617	-4.295034	2.503425
O	0.708477	-4.065751	4.795258
C	-1.311402	1.847433	0.619118
H	-2.118410	1.110133	0.508481
H	-1.653939	2.680546	1.249775
P	-0.833385	2.470145	-1.013356
C	-2.288880	3.279097	-1.753870
H	-3.113422	2.554344	-1.814685
O	-0.071943	3.124730	-4.016846
H	1.523505	2.168318	-4.830337
C	0.755562	2.219153	-4.020699
C	0.857401	1.150789	-2.983582
H	1.808322	1.266577	-2.417555
H	0.017925	0.284242	-1.217842
C	-0.297603	1.009301	-1.987003
H	1.003114	0.185401	-3.498778
H	-1.205707	0.620579	-2.474897
H	-2.598368	4.117023	-1.112575
H	-2.032959	3.639816	-2.757449
C	0.514691	3.660455	-0.817072
H	1.361428	3.103126	-0.385414
H	0.204031	4.448531	-0.116931
H	0.768084	4.101710	-1.789404

TS3-PCy_3



E : -14875.29kcal·mol^{-1}

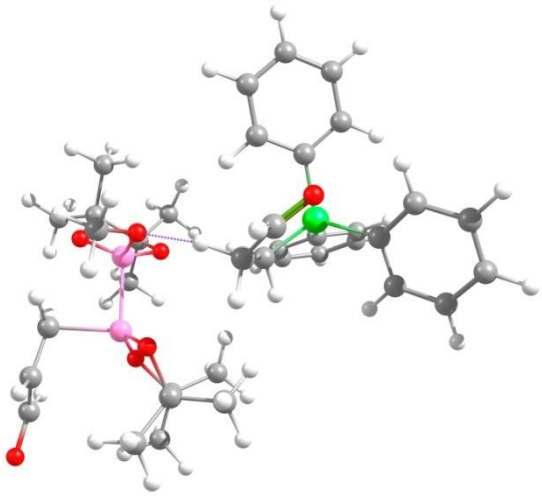
Imaginary frequency: -302.22 cm^{-1}

	X	Y	Z
B	1.363237	-2.114608	0.632111
B	2.701767	-0.568847	0.758688
C	2.850988	-3.357893	1.112025
C	2.277156	-4.636209	1.036939
H	1.555621	-4.570988	3.061493
H	2.305731	-5.211604	0.108098
H	3.049371	-2.943627	2.101103
H	3.628183	-3.095700	0.396720
O	0.999543	-6.321496	2.155206
C	1.570589	-5.210996	2.141379
H	-1.832031	-3.239952	2.768830
H	-1.091400	-4.483096	1.738329
C	-1.669376	-3.551892	1.726923
H	-2.653798	-3.750711	1.273696
H	0.109319	-4.819148	-0.132149
C	-0.532583	-4.275308	-0.832962
H	-1.538636	-4.717429	-0.793427
H	-0.132794	-4.416440	-1.847599
C	-0.939916	-2.434220	0.978534
C	-0.572237	-2.775382	-0.525081
C	-1.730869	-1.128455	1.136899
H	-1.854586	-0.921865	2.208738
H	-2.729357	-1.187005	0.676755
H	-1.172862	-0.290111	0.702610
H	-2.489093	-2.481955	-1.525551
C	-1.458877	-2.097891	-1.574584
H	-1.493393	-1.008772	-1.451216
H	-1.064578	-2.322491	-2.576624
O	0.350369	-2.211861	1.607820
O	0.786001	-2.246812	-0.657529
H	3.239341	-1.930966	-1.678587
H	3.886231	-0.419005	-2.386357
O	2.837169	-0.158995	-0.636848
H	4.664544	-1.128871	-0.943167
O	3.934237	-0.874906	1.450206
O	2.012382	0.474682	1.517293
H	0.944079	-0.116237	3.855546
C	2.014240	-0.358614	3.803515
H	2.093697	-1.403370	3.483841
H	2.447682	-0.254374	4.809728
C	4.155289	0.145639	2.440600
C	4.951288	-0.456867	3.599213
H	4.456993	-1.350994	3.999003

H	5.949060	-0.752062	3.242697
H	5.082909	0.271165	4.415487
H	5.890007	0.851479	1.372763
C	4.964129	1.278701	1.782698
H	5.236802	2.069356	2.498931
H	4.395596	1.719987	0.953575
H	3.189026	2.155716	4.217689
C	2.582190	2.024174	3.308071
H	1.540230	2.257144	3.568990
H	2.925878	2.746439	2.556286
C	2.688781	0.585260	2.798860
H	4.390370	4.249011	-0.339389
H	3.714018	4.849551	-1.857721
C	3.494233	4.704986	-0.785723
C	3.197514	6.062672	-0.135802
H	3.085360	5.926931	0.954281
H	4.044248	6.750837	-0.280651
C	1.911606	6.680550	-0.703708
H	1.682518	7.631215	-0.198042
H	2.060676	6.916987	-1.771470
H	0.504102	5.573339	0.510171
C	0.713152	5.724459	-0.562131
H	-0.187182	6.183531	-1.002984
H	1.209626	4.531926	-2.304321
C	1.029480	4.367214	-1.229189
C	2.312969	3.732625	-0.644467
H	2.167568	3.481291	0.418108
H	2.547235	2.788282	-1.153005
P	-0.425344	3.200734	-1.235798
C	-1.361343	3.378813	0.376151
C	-1.306538	3.178632	2.912397
C	-0.528654	2.948645	1.605205
H	-0.699112	2.821742	3.757361
H	0.418568	3.504183	1.640340
H	-0.248193	1.885978	1.526496
H	-1.454785	4.262365	3.066423
H	-1.543007	4.469986	0.438755
H	-3.217264	2.685252	3.832022
C	-2.669436	2.476764	2.900395
H	-2.517389	1.385388	2.858673
C	-2.740999	2.675636	0.367372
C	-3.495668	2.918134	1.686999
C	-1.679142	3.700872	-2.540392
H	-2.391753	4.313463	-1.954385
H	-3.358857	3.030192	-0.470608
H	-4.457714	2.383640	1.655415
H	-2.603925	1.589432	0.236777
H	-3.734370	3.992951	1.775193
H	-0.409055	4.020757	-4.278010
C	-1.152437	4.583420	-3.692706

H	-0.640835	5.474206	-3.297606
C	-2.315341	5.023770	-4.601541
H	-1.918054	5.624833	-5.433396
H	-2.991613	5.685307	-4.031575
C	-3.114956	3.828904	-5.139567
H	-2.471867	3.231952	-5.809307
H	-3.962386	4.179751	-5.747939
H	-4.349903	3.490604	-3.387731
C	-3.613608	2.935894	-3.995887
H	-4.137116	2.052758	-4.392874
C	-2.452312	2.481229	-3.097259
H	-1.760718	1.863873	-3.693158
H	-2.830234	1.843875	-2.285311
H	-0.759911	0.896494	-0.846907
C	1.328265	1.391457	-3.582718
H	1.777489	0.724265	-4.358475
H	0.893796	1.365599	-0.510061
C	0.562945	0.672864	-2.523642
H	1.186045	-0.163021	-2.149745
H	-0.277971	0.181151	-3.046048
O	1.463642	2.605499	-3.671011
C	0.097905	1.435850	-1.275307
C	3.698266	-0.956126	-1.443226

TS3-PPh_3



E : -13306.22 kcal·mol^{-1}

Imaginary frequency: -295.64 cm^{-1}

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B	2.688745	-0.574367	0.732742
C	2.856565	-3.335236	1.107755
C	2.309713	-4.631055	1.002233
H	1.585011	-4.639015	3.027422
H	2.347489	-5.180060	0.057436
H	3.046307	-2.950887	2.111561
H	3.655276	-3.068635	0.419411
O	1.074637	-6.377211	2.071454
C	1.616054	-5.251177	2.088973
H	-1.856348	-3.138189	2.860480
H	-1.166389	-4.430234	1.852765
C	-1.705495	-3.475813	1.824940
H	-2.696685	-3.642305	1.373546
H	0.073398	-4.836285	-0.007457
C	-0.572681	-4.303224	-0.713620
H	-1.581325	-4.738068	-0.652120
H	-0.185803	-4.472712	-1.729445
C	-0.926691	-2.409347	1.052481
C	-0.601615	-2.795100	-0.446484
C	-1.631230	-1.052134	1.197264
H	-1.705520	-0.808058	2.265728
H	-2.647183	-1.061859	0.773834
H	-1.039790	-0.261972	0.718921
H	-2.546403	-2.523471	-1.388920
C	-1.517574	-2.145023	-1.486448
H	-1.551244	-1.052054	-1.392855
H	-1.164387	-2.403557	-2.495908
O	0.385942	-2.257639	1.656154
O	0.757805	-2.275103	-0.623823
H	3.253170	-2.065242	-1.643534
H	4.062770	-0.632480	-2.348842
O	2.936487	-0.238047	-0.672544
H	4.694772	-1.355541	-0.841900
O	3.866499	-0.825657	1.524955
O	1.933270	0.502526	1.372645
H	0.720632	0.013946	3.672733
C	1.797081	-0.202674	3.705622
H	1.919410	-1.262362	3.458232
H	2.159609	-0.024280	4.729272
C	4.012649	0.259378	2.462229
C	4.737412	-0.259261	3.704517
H	4.230871	-1.136398	4.125972
H	5.760613	-0.557470	3.432407
H	4.806066	0.518779	4.481362
H	5.808510	0.927100	1.473888
C	4.850538	1.362614	1.791029

H	5.060837	2.199269	2.474871
H	4.336404	1.746214	0.900510
H	2.924159	2.362797	4.029754
C	2.359302	2.159840	3.106560
H	1.303562	2.382106	3.315999
H	2.710109	2.845749	2.325199
C	2.520939	0.697389	2.696161
C	3.777981	-1.126113	-1.406825
C	0.035101	1.505406	-1.291629
P	-0.351728	3.282551	-1.535849
C	0.681651	0.638948	-2.383161
H	1.673005	0.298317	-1.986246
H	0.665278	1.456364	-0.384632
H	-0.941749	1.092651	-0.994985
C	0.873253	1.224135	-3.728041
O	0.676183	2.401312	-4.013425
H	1.251955	0.518542	-4.504417
H	0.147757	-0.318619	-2.480952
C	-1.686919	3.610637	-2.739477
C	-1.486325	4.342412	-3.919976
C	-2.959818	3.084638	-2.452928
C	-2.555961	4.565014	-4.789160
H	-0.494262	4.717209	-4.169684
C	-4.018656	3.292407	-3.338119
H	-3.131802	2.521297	-1.533301
C	-3.819499	4.040245	-4.502466
H	-2.394805	5.138764	-5.702327
H	-5.000129	2.874791	-3.112323
H	-4.650473	4.210106	-5.190476
C	-1.088703	3.780302	0.073329
C	-1.987821	4.863166	0.113629
C	-0.726988	3.136394	1.269919
C	-2.527652	5.284795	1.328910
H	-2.284165	5.367344	-0.807258
C	-1.282579	3.559799	2.480378
H	-0.015894	2.308827	1.280403
C	-2.180126	4.629025	2.514082
H	-3.227940	6.120570	1.346789
H	-1.007280	3.046632	3.401868
H	-2.609813	4.951744	3.463776
C	1.119278	4.318423	-1.792740
C	2.399371	3.759693	-1.640570
C	0.976188	5.687969	-2.073730
C	3.526570	4.568806	-1.796415
H	2.528183	2.702581	-1.398279
C	2.110100	6.484632	-2.237264
H	-0.014361	6.135237	-2.167542
C	3.384688	5.925213	-2.103019
H	4.518630	4.132026	-1.679826
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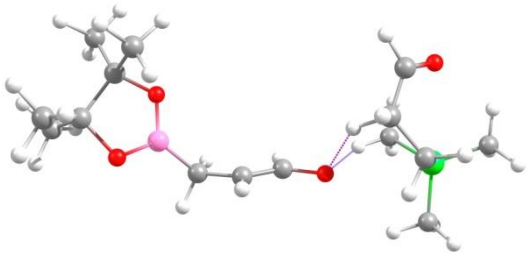
H	4.269994	6.550404	-2.232424

I3-PMe$_3$

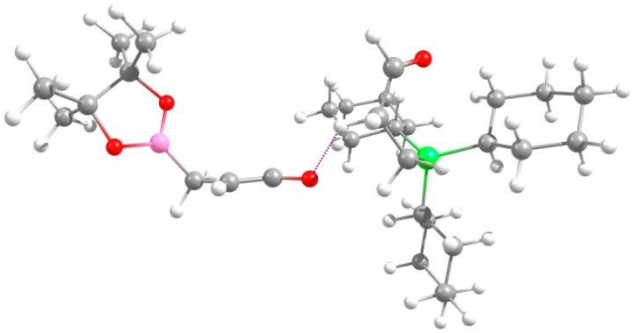


E : -6478.11kcal·mol^{-1}

	X	Y	Z
B	0.902850	-2.590832	0.925769
C	2.090077	-1.914944	1.708079
C	2.274153	-2.331776	3.156523
H	-2.416343	-3.458776	1.967619
H	-1.066691	-4.604432	1.795517
H	-2.523774	-4.781211	0.775354
H	-0.438030	-5.878251	-0.044825
H	-1.345217	-5.447051	-1.522399
H	0.414883	-5.700336	-1.595036
H	-2.912136	-3.047120	-1.163634
H	-1.905472	-1.571621	-1.179946
H	-3.000527	-1.887928	0.184280
H	-0.767451	-3.184204	-2.718723
H	0.976347	-3.498918	-2.515202
H	0.263432	-2.007717	-1.856906
C	0.084562	-3.077569	-2.031451
C	-2.320914	-2.359280	-0.539525
C	-0.155683	-3.817817	-0.709982
C	-1.223634	-3.113481	0.207880
C	-0.400663	-5.300273	-0.976118
C	-1.843153	-4.055805	1.245361
O	1.075141	-3.676786	0.073987
O	-0.409965	-2.139547	0.943865
H	2.204573	-0.366744	3.890281
C	2.355812	-1.434097	4.178687
H	2.422936	-3.394566	3.377706
O	2.605275	-1.668516	5.457118
H	3.016000	-2.108791	1.133668
H	1.932100	-0.822227	1.683097
H	1.307424	-2.226527	6.510687

C	1.070348	-2.608495	7.570115
C	-0.128259	-1.959463	8.133098
H	0.901313	-3.688150	7.433636
C	2.362869	-2.352124	8.351965
O	-0.088067	-1.031190	8.953767
H	-1.111488	-2.313454	7.745340
P	2.869650	-0.585344	8.514382
H	3.187455	-2.827236	7.800383
H	2.329173	-2.756953	9.377188
C	4.658829	-0.563669	8.159326
C	2.649060	-0.006976	10.230763
C	2.111699	0.535182	7.320484
H	4.779690	-0.867369	7.107861
H	5.186507	-1.270556	8.815231
H	5.067259	0.446110	8.307607
H	3.213270	-0.651374	10.920083
H	1.578609	-0.048197	10.470859
H	3.016955	1.025485	10.317870
H	2.204013	-0.040243	6.361859
H	2.691925	1.468979	7.294285
H	1.065810	0.729282	7.585746

I3-PCy$_3$



E : -11557.44kcal·mol^{-1}

	X	**Y**	**Z**
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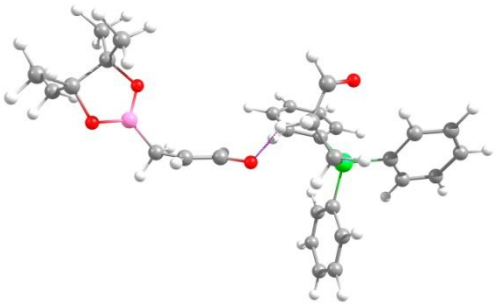
C	2.843460000	-4.371712000	3.402715000
H	-1.765422000	-4.433732000	2.307435000
H	-0.737786000	-5.851598000	2.611687000
H	-2.243061000	-6.027161000	1.661493000

H	-0.546861000	-7.815287000	1.353717000
H	-1.384206000	-7.714887000	-0.222099000
H	0.253373000	-8.405914000	-0.120080000
H	-2.297433000	-5.043431000	-0.780140000
H	-0.962984000	-3.966049000	-1.280243000
H	-2.030834000	-3.498751000	0.062728000
H	-0.302357000	-6.228650000	-2.102200000
H	1.316520000	-6.868843000	-1.713455000
H	1.018631000	-5.115817000	-1.646847000
C	0.575141000	-6.101743000	-1.451243000
C	-1.524660000	-4.347458000	-0.418659000
C	0.209675000	-6.254682000	0.030128000
C	-0.609006000	-5.033519000	0.592001000
C	-0.409433000	-7.626585000	0.282066000
C	-1.387370000	-5.367736000	1.869625000
O	1.463587000	-6.163988000	0.782303000
O	0.452638000	-4.096589000	0.972435000
H	3.060226000	-2.303899000	3.654395000
C	2.939507000	-3.270600000	4.207273000
H	2.738106000	-5.358784000	3.865540000
O	2.924753000	-3.202928000	5.517051000
H	3.778792000	-4.831746000	1.487418000
H	3.026276000	-3.229130000	1.600659000
H	1.411484000	-2.856463000	6.509326000
C	1.193248000	-2.719104000	7.619011000
C	-0.099656000	-2.056784000	7.871747000
H	1.128282000	-3.770085000	7.950615000
C	2.473923000	-2.097876000	8.191717000
O	-0.241173000	-0.911142000	8.320740000
H	-0.999926000	-2.652239000	7.586757000
P	2.855078000	-0.279756000	8.111898000
H	3.287097000	-2.556982000	7.605659000
H	2.607203000	-2.356689000	9.252402000
C	4.716306000	-0.346290000	7.882861000
C	5.404344000	0.992852000	7.545089000
C	5.419848000	-1.027883000	9.082507000
H	4.804631000	-1.014019000	7.003206000
C	6.910963000	0.793599000	7.295984000
H	5.263607000	1.711439000	8.372778000
H	4.951134000	1.440123000	6.651300000
C	6.924387000	-1.214524000	8.823467000
H	5.293975000	-0.397837000	9.980372000
H	4.962180000	-2.003223000	9.301474000
C	7.605922000	0.116588000	8.482951000
H	7.376540000	1.766769000	7.076076000
H	7.042346000	0.170561000	6.394554000
H	7.391122000	-1.672733000	9.709270000
H	7.062105000	-1.923750000	7.990025000
H	8.672134000	-0.044415000	8.262069000
H	7.563120000	0.785117000	9.361509000

C	2.513919000	0.585492000	9.757218000
C	1.253328000	1.483450000	9.812501000
C	2.477330000	-0.411191000	10.942678000
H	3.405167000	1.233621000	9.875879000
C	1.176971000	2.228755000	11.156448000
H	0.362843000	0.852807000	9.676805000
H	1.249780000	2.216508000	8.996444000
C	2.379872000	0.323261000	12.291405000
H	1.592252000	-1.057660000	10.820728000
H	3.360695000	-1.065576000	10.946100000
C	1.164892000	1.258171000	12.343070000
H	0.276378000	2.862019000	11.167447000
H	2.041219000	2.911039000	11.250654000
H	2.331134000	-0.418752000	13.103564000
H	3.301390000	0.909264000	12.455270000
H	1.146141000	1.810035000	13.295648000
H	0.240813000	0.655732000	12.306221000
C	2.040717000	0.598016000	6.680087000
C	2.279899000	2.120753000	6.527536000
C	2.331981000	-0.094177000	5.329208000
H	0.975682000	0.442465000	6.935232000
C	1.296513000	2.678153000	5.481394000
H	3.304955000	2.301113000	6.170480000
H	2.174026000	2.669125000	7.472749000
C	1.362209000	0.445717000	4.265310000
H	3.367683000	0.140990000	5.024454000
H	2.286708000	-1.194018000	5.406034000
C	1.456777000	1.972448000	4.126002000
H	1.455343000	3.762554000	5.371450000
H	0.265371000	2.544591000	5.850894000
H	1.567860000	-0.044828000	3.302938000
H	0.332621000	0.162780000	4.544529000
H	0.702470000	2.343429000	3.414687000
H	2.442546000	2.234060000	3.7021880

I3-PPh_3



E : -9989.93 kcal·mol^{-1}

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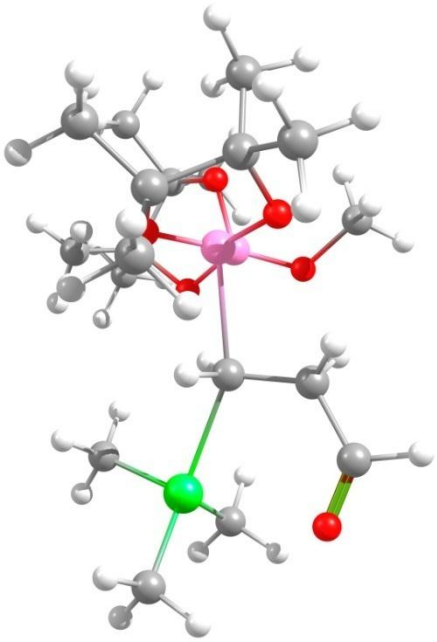
C	2.402469000	-2.804994000	2.936835000
H	-2.215864000	-3.269297000	2.059510000
H	-0.977880000	-4.518073000	1.800494000
H	-2.527783000	-4.599589000	0.911853000
H	-0.640838000	-5.871242000	-0.081251000
H	-1.627824000	-5.375335000	-1.486588000
H	0.093148000	-5.780515000	-1.697920000
H	-2.950149000	-2.859804000	-1.018716000
H	-1.832921000	-1.472917000	-1.157729000
H	-2.822099000	-1.678429000	0.305985000
H	-0.945340000	-3.175561000	-2.757814000
H	0.777016000	-3.634207000	-2.684292000
H	0.242725000	-2.086522000	-1.987671000
C	-0.037164000	-3.138196000	-2.138492000
C	-2.250807000	-2.214023000	-0.465369000
C	-0.236411000	-3.850550000	-0.795368000
C	-1.156700000	-3.047292000	0.197125000
C	-0.632394000	-5.306639000	-1.021552000
C	-1.755684000	-3.921484000	1.304663000
O	1.059060000	-3.824231000	-0.111906000
O	-0.200533000	-2.140182000	0.841497000
H	2.492956000	-0.904506000	3.797484000
C	2.486951000	-1.998388000	4.032595000
H	2.410236000	-3.891825000	3.070889000
O	2.580964000	-2.324363000	5.304479000
H	3.229077000	-2.519759000	0.939928000
H	2.314449000	-1.146211000	1.588050000
H	1.267855000	-2.481095000	6.450421000
C	1.047340000	-2.695106000	7.551988000
C	-0.223073000	-2.108815000	8.018495000
H	0.961371000	-3.795554000	7.550952000
C	2.317266000	-2.301189000	8.314601000
O	-0.314887000	-1.199238000	8.849057000
H	-1.143583000	-2.525529000	7.544959000
P	2.810616000	-0.518632000	8.500733000
H	3.157872000	-2.732713000	7.752507000
H	2.326486000	-2.691352000	9.344966000
C	4.600309000	-0.479644000	8.118443000
C	5.428818000	-1.512685000	8.591775000
C	5.159910000	0.585084000	7.397622000
C	6.799543000	-1.480970000	8.337022000
H	5.009647000	-2.346138000	9.156069000
C	6.536136000	0.614990000	7.154063000
H	4.520228000	1.381551000	7.016175000
C	7.355201000	-0.415881000	7.619954000

H	7.433737000	-2.292154000	8.695314000
H	6.963862000	1.442482000	6.587678000
H	8.427307000	-0.395410000	7.419122000
C	2.696718000	0.002289000	10.253952000
C	1.631329000	-0.413701000	11.071418000
C	3.671463000	0.875878000	10.769565000
C	1.554824000	0.034686000	12.392018000
H	0.850881000	-1.048871000	10.654832000
C	3.575777000	1.331658000	12.086062000
H	4.506572000	1.197167000	10.146085000
C	2.520554000	0.908631000	12.899901000
H	0.726861000	-0.293311000	13.021271000
H	4.331878000	2.014043000	12.475191000
H	2.450631000	1.261658000	13.930139000
C	1.987869000	0.728822000	7.465039000
C	1.675502000	0.413169000	6.133035000
C	1.746051000	2.015344000	7.979699000
C	1.090894000	1.392829000	5.325639000
H	1.920658000	-0.593789000	5.752934000
C	1.192352000	2.989948000	7.147822000
H	1.985483000	2.256881000	9.015476000
C	0.856487000	2.677384000	5.825635000
H	0.825587000	1.143720000	4.297790000
H	1.015798000	3.993105000	7.537943000
H	0.411367000	3.439924000	5.183789000

TS-*SN2*-PMe$_3$



E : -8697.79kcal·mol^{-1}

Imaginary frequency: -481.83 cm^{-1}

	X	Y	Z
B	2.964207000	0.416612000	0.769448000
B	1.377265000	-0.714301000	0.421131000
C	0.825429000	0.958306000	-1.058304000
P	-0.145905000	3.090082000	-1.723125000
C	1.464719000	0.342590000	-2.272175000
O	1.590885000	-1.941432000	-0.215750000
O	0.319334000	-0.810044000	1.330021000
C	4.607500000	-0.788609000	-0.608430000
O	3.836505000	0.389059000	-0.381868000
H	3.968494000	-1.651345000	-0.856857000
H	5.286063000	-0.587954000	-1.450561000
H	5.205008000	-1.050493000	0.278692000
O	2.645993000	1.779191000	1.166611000
O	3.379689000	-0.316733000	1.954712000
C	3.630755000	0.663069000	3.000636000
C	2.678927000	1.859681000	2.612879000
C	1.256717000	1.695912000	3.169846000
H	0.832069000	0.722922000	2.900552000
H	0.616053000	2.479283000	2.739434000
H	1.238970000	1.811631000	4.264387000
H	2.318203000	-0.383417000	4.391416000
C	3.339175000	0.016796000	4.354152000
H	4.041308000	-0.812723000	4.523488000
H	3.465078000	0.741169000	5.174260000
C	5.116473000	1.045702000	2.903894000
H	5.722639000	0.134291000	3.000961000
H	5.412987000	1.744831000	3.700661000
C	3.213562000	3.243086000	2.994864000
H	2.487568000	4.012042000	2.691152000
H	4.165851000	3.458133000	2.494963000
H	5.333335000	1.503099000	1.929618000
H	3.353599000	3.326667000	4.084040000
C	0.879856000	-2.978509000	0.555375000
C	-0.273537000	-2.150885000	1.225639000
C	-0.669921000	-2.610739000	2.626389000
C	0.423808000	-4.070545000	-0.407603000
C	1.887021000	-3.539748000	1.564598000
H	1.441849000	-4.337474000	2.177434000
H	2.739787000	-3.962572000	1.015573000
H	2.269320000	-2.743892000	2.217208000
H	-0.154561000	-4.841535000	0.124893000
H	1.303311000	-4.556834000	-0.852656000

H	-0.194648000	-3.669368000	-1.220443000
H	-1.061081000	-3.639868000	2.605787000
H	0.181900000	-2.571739000	3.315726000
H	-1.460461000	-1.955473000	3.019367000
C	-1.519725000	-2.017712000	0.342639000
H	-2.186752000	-1.263145000	0.782396000
H	-1.255646000	-1.695432000	-0.673715000
H	-2.071901000	-2.966513000	0.273302000
H	2.565603000	0.448224000	-2.176385000
H	1.376724000	1.626427000	-0.407013000
H	-0.158841000	0.630940000	-0.730648000
C	1.104379000	0.739070000	-3.679105000
O	0.341015000	1.612544000	-4.065526000
H	1.632669000	0.105280000	-4.435436000
H	1.325843000	-0.755212000	-2.260552000
C	-0.309152000	3.785296000	-0.014307000
H	-0.550061000	4.858296000	-0.030813000
H	-1.097362000	3.246673000	0.530884000
H	0.639574000	3.628007000	0.519295000
C	1.069807000	4.257991000	-2.482664000
H	2.051764000	4.111223000	-2.010555000
H	1.154659000	4.046217000	-3.555989000
H	0.752817000	5.301308000	-2.334538000
C	-1.759516000	3.581099000	-2.498110000
H	-1.745121000	3.309672000	-3.561176000
H	-2.577736000	3.036427000	-2.005635000
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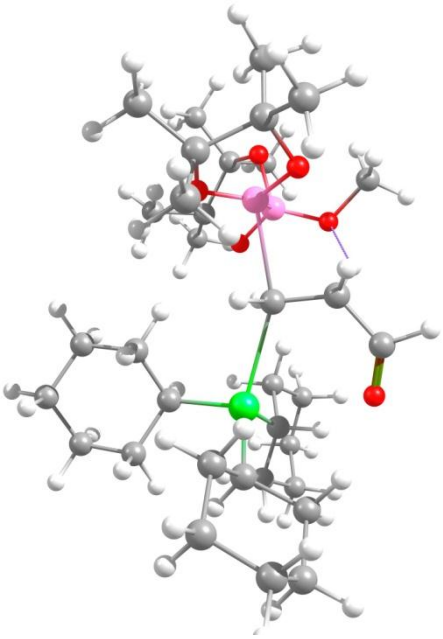
TS-*SN2*-PCy$_3$



E : -13782.42kcal·mol^{-1}

Imaginary frequency: -424.00 cm^{-1}

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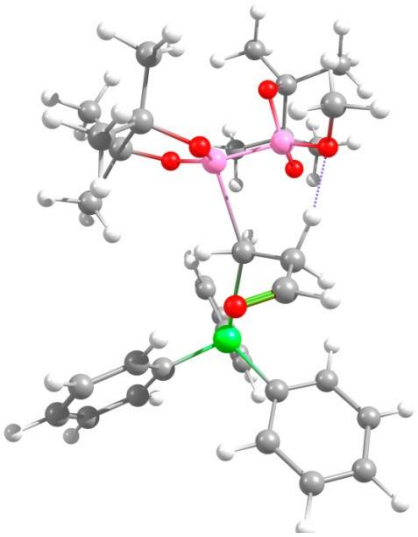
B	3.044694	0.303742	0.828299
B	1.438369	-0.725020	0.551375
C	0.891048	1.000603	-0.993828
C	1.525180	0.271449	-2.140226
O	1.586754	-1.949305	-0.108599
O	0.387059	-0.782137	1.469840
C	4.666749	-0.885371	-0.609764
O	3.868978	0.274687	-0.376328
H	4.046313	-1.786298	-0.742952
H	5.250660	-0.710436	-1.525769
H	5.357351	-1.067712	0.226998
O	2.824925	1.665022	1.299290
O	3.533430	-0.487791	1.955820
C	3.971933	0.456189	2.970017
C	3.024663	1.691181	2.732889
C	1.670042	1.535027	3.439717
H	1.196125	0.581382	3.181283
H	1.006467	2.346679	3.110117
H	1.773775	1.606383	4.533478
H	2.829836	-0.575737	4.515295
C	3.849520	-0.210391	4.339590
H	4.535846	-1.068557	4.391543
H	4.118959	0.489105	5.146631
C	5.444075	0.791141	2.675535
H	6.024609	-0.141988	2.666810
H	5.873652	1.456923	3.439477
C	3.638961	3.043140	3.106205
H	2.907851	3.841993	2.913106
H	4.537409	3.253174	2.512852
H	5.540056	1.269769	1.692141
H	3.900539	3.076904	4.175788
C	0.840503	-2.962965	0.654062
C	-0.267574	-2.093969	1.348957
C	-0.672935	-2.560381	2.744637
C	0.326869	-4.018538	-0.321371
C	1.831861	-3.586146	1.642675
H	1.358020	-4.372149	2.249095
H	2.657527	-4.038691	1.076062
H	2.260084	-2.818900	2.300947
H	-0.276541	-4.774948	0.204141
H	1.180881	-4.531714	-0.785640

H	-0.282928	-3.577739	-1.120141
H	-1.110216	-3.570414	2.707790
H	0.185458	-2.573570	3.426768
H	-1.429862	-1.877903	3.156916
C	-1.512953	-1.891139	0.478395
H	-2.143839	-1.116492	0.935366
H	-1.241153	-1.562908	-0.533860
H	-2.105119	-2.814572	0.396562
H	2.598304	0.133848	-1.844546
H	1.460656	1.696309	-0.387978
H	-0.087287	0.704729	-0.626619
C	1.611614	0.770084	-3.551356
O	1.287648	1.848010	-4.016132
H	2.072420	-0.002116	-4.221226
H	1.138698	-0.758715	-2.215480
C	1.060603	4.452199	-2.331726
C	0.568261	5.866795	-2.694659
C	2.226954	4.533947	-1.320898
H	1.446473	3.974948	-3.247094
C	1.725529	6.699547	-3.278183
H	0.182566	6.372621	-1.792722
H	-0.260144	5.822524	-3.417931
C	3.381347	5.387222	-1.874228
H	1.871500	4.994850	-0.382370
H	2.597716	3.533935	-1.052572
C	2.906034	6.784150	-2.299702
H	1.368200	7.707967	-3.541411
H	2.064066	6.228447	-4.218090
H	4.174768	5.465908	-1.114623
H	3.826601	4.870072	-2.741658
H	3.736506	7.350454	-2.750299
H	2.589884	7.349105	-1.404200
C	-0.904487	3.973461	-0.144148
C	-2.074732	4.970375	-0.297189
C	-1.229952	2.920804	0.939357
H	-0.030132	4.542459	0.220371
C	-2.443978	5.629497	1.043664
H	-2.963843	4.438868	-0.676951
H	-1.832264	5.748485	-1.035902
C	-1.601566	3.590753	2.273844
H	-2.073106	2.289700	0.605587
H	-0.375040	2.249539	1.095178
C	-2.762206	4.581521	2.118131
H	-3.302073	6.305126	0.896202
H	-1.602851	6.258409	1.384761
H	-1.844486	2.819939	3.021351
H	-0.718114	4.130199	2.659222
H	-2.982294	5.072832	3.079132
H	-3.675822	4.030984	1.829471
C	-1.707060	3.373380	-2.956212

C	-1.372381	3.288550	-4.456750
C	-2.790221	2.330889	-2.600500
H	-2.124602	4.377503	-2.764772
C	-2.637528	3.518713	-5.302239
H	-0.950233	2.298946	-4.686294
H	-0.598332	4.019821	-4.730373
C	-4.059508	2.537636	-3.444285
H	-2.384412	1.320932	-2.787109
H	-3.042204	2.373493	-1.529764
C	-3.747746	2.517770	-4.948000
H	-2.386026	3.446067	-6.372214
H	-3.006915	4.546624	-5.135589
H	-4.804937	1.765642	-3.195107
H	-4.512903	3.509160	-3.178182
H	-4.658451	2.731411	-5.529739
H	-3.421477	1.502390	-5.235079

TS-*SN2*-PPh$_3$



E : -12222.81kcal·mol^{-1}

Imaginary frequency: -420.94 cm^{-1}

	X	Y	Z
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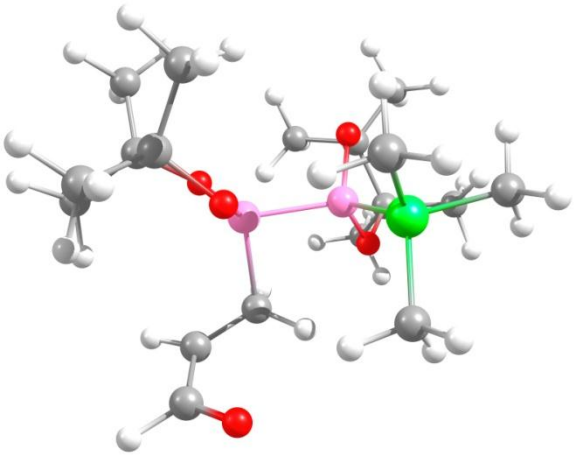
B	1.430819000	-0.694980000	0.476916000
C	0.728025000	0.941109000	-1.111078000
P	-1.025819000	2.344791000	-2.111327000
C	1.788298000	0.949663000	-2.156024000
O	1.611803000	-1.916177000	-0.165921000

O	0.364319000	-0.746481000	1.375331000
C	4.611995000	-0.928015000	-0.504436000
O	3.906255000	0.303677000	-0.337654000
H	3.941833000	-1.736736000	-0.834880000
H	5.393052000	-0.767516000	-1.261641000
H	5.080124000	-1.235698000	0.442431000
O	2.687414000	1.801367000	1.094115000
O	3.376667000	-0.262988000	2.014079000
C	3.733749000	0.786695000	2.954358000
C	2.796806000	1.978441000	2.525390000
C	1.394069000	1.880358000	3.146701000
H	0.950234000	0.895294000	2.960242000
H	0.755966000	2.643317000	2.677327000
H	1.413154000	2.072514000	4.230696000
H	2.487782000	-0.094897000	4.512409000
C	3.515260000	0.264451000	4.373753000
H	4.201356000	-0.573678000	4.566144000
H	3.720770000	1.048951000	5.119341000
C	5.221864000	1.105945000	2.731723000
H	5.802865000	0.182262000	2.863249000
H	5.594696000	1.853414000	3.448503000
C	3.377938000	3.369460000	2.793282000
H	2.662040000	4.134343000	2.458242000
H	4.317554000	3.521371000	2.247814000
H	5.386931000	1.475744000	1.711451000
H	3.560380000	3.522877000	3.868923000
C	0.854789000	-2.936548000	0.578175000
C	-0.254246000	-2.078913000	1.297761000
C	-0.591540000	-2.527094000	2.718283000
C	0.332352000	-3.965518000	-0.420892000
C	1.848311000	-3.585194000	1.547698000
H	1.374634000	-4.380085000	2.142476000
H	2.666742000	-4.031368000	0.965746000
H	2.283040000	-2.833736000	2.220237000
H	-0.281406000	-4.725966000	0.086643000
H	1.181690000	-4.476504000	-0.895403000
H	-0.266073000	-3.497144000	-1.211697000
H	-1.003076000	-3.548461000	2.720224000
H	0.292735000	-2.501812000	3.366098000
H	-1.350107000	-1.855143000	3.144830000
C	-1.539508000	-1.927766000	0.479684000
H	-2.177941000	-1.170184000	0.954355000
H	-1.329094000	-1.604883000	-0.548134000
H	-2.102789000	-2.871374000	0.433573000
H	2.091517000	1.966131000	-2.462801000
H	0.826010000	1.607809000	-0.257597000
H	0.007899000	0.128376000	-1.090042000
C	1.552111000	0.125629000	-3.373684000
O	0.589845000	-0.608204000	-3.572077000
H	2.365181000	0.193633000	-4.137724000

H	2.743896000	0.577121000	-1.669946000
C	-1.513916000	3.645575000	-0.911275000
C	-1.862716000	4.951493000	-1.296480000
C	-1.539663000	3.300440000	0.452815000
C	-2.232843000	5.893927000	-0.333773000
H	-1.843592000	5.230609000	-2.350485000
C	-1.916240000	4.245010000	1.410440000
H	-1.261163000	2.294691000	0.770360000
C	-2.260739000	5.543211000	1.019995000
H	-2.500863000	6.904723000	-0.644706000
H	-1.928353000	3.967776000	2.465038000
H	-2.545479000	6.282670000	1.770311000
C	-0.568666000	3.235098000	-3.643875000
C	0.483308000	4.173535000	-3.593357000
C	-1.136599000	2.911311000	-4.888621000
C	0.936473000	4.787778000	-4.761370000
H	0.941211000	4.430403000	-2.636160000
C	-0.672395000	3.524635000	-6.055075000
H	-1.944060000	2.180291000	-4.943487000
C	0.362137000	4.463184000	-5.996579000
H	1.745282000	5.517608000	-4.707271000
H	-1.124447000	3.265786000	-7.013574000
H	0.722817000	4.938443000	-6.910102000
C	-2.585337000	1.441865000	-2.484259000
C	-2.501632000	0.098185000	-2.891361000
C	-3.846449000	2.046349000	-2.340519000
C	-3.669292000	-0.626241000	-3.150813000
H	-1.522459000	-0.370995000	-3.012604000
C	-5.007109000	1.316849000	-2.605247000
H	-3.921122000	3.085250000	-2.017400000
C	-4.920982000	-0.021237000	-3.006021000
H	-3.596780000	-1.670208000	-3.458794000
H	-5.981517000	1.794543000	-2.493250000
H	-5.830864000	-0.591810000	-3.200609000

TS-PMe_3



E : -8014.18kcal·mol^{-1}

Imaginary frequency: -223.33 cm^{-1}

	X	Y	Z
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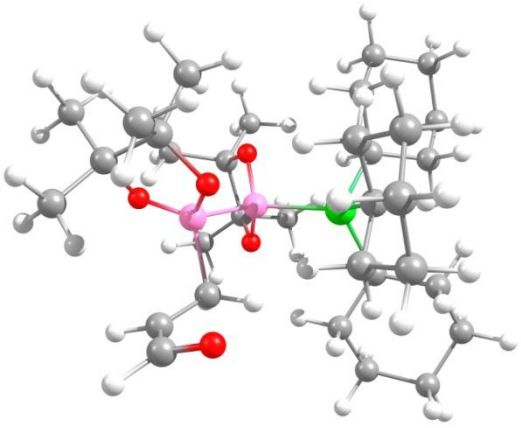
C	0.894845000	0.615802000	-1.027590000
C	-0.125199000	-0.027468000	-1.752108000
O	1.503799000	-1.930569000	0.176335000
O	0.247320000	-0.442648000	1.419981000
O	2.984137000	1.805581000	0.287078000
O	3.163413000	0.454828000	2.184577000
C	2.940835000	1.817692000	2.674757000
C	3.232868000	2.711621000	1.399843000
C	0.665104000	-2.770767000	1.030031000
C	-0.365818000	-1.745479000	1.672993000
C	0.128456000	-0.855181000	-2.894167000
O	1.250533000	-1.177111000	-3.341272000
P	4.352262000	-0.654343000	-0.199647000
C	4.521000000	-2.440007000	0.199919000
C	4.192091000	-0.564984000	-2.018517000
C	6.030214000	0.002886000	0.171668000
H	1.837031000	0.745560000	-1.555760000
H	0.629088000	1.481055000	-0.419516000
H	-0.788227000	-1.218507000	-3.422762000
H	-1.164804000	0.067516000	-1.428405000
H	5.419278000	-2.839448000	-0.291667000
H	4.607511000	-2.565048000	1.287495000
H	3.622729000	-2.956037000	-0.152036000
H	4.983603000	-1.161308000	-2.494546000
H	3.199441000	-0.926949000	-2.342002000
H	4.296538000	0.486546000	-2.323383000
H	6.795320000	-0.603557000	-0.335175000

H	6.108602000	1.043462000	-0.169727000
H	6.201870000	-0.032375000	1.257209000
C	0.033726000	-3.846238000	0.142556000
H	0.827731000	-4.469850000	-0.292137000
H	-0.633967000	-4.500650000	0.723600000
H	-0.535205000	-3.403583000	-0.684060000
C	1.589280000	-3.431613000	2.061387000
H	1.026470000	-4.075618000	2.752332000
H	2.321272000	-4.061996000	1.538096000
H	2.134083000	-2.677338000	2.643817000
C	-1.739488000	-1.736354000	0.992078000
H	-2.276862000	-2.682106000	1.154011000
H	-2.339627000	-0.920488000	1.419064000
H	-1.648585000	-1.568231000	-0.087664000
C	-0.555991000	-1.894368000	3.184592000
H	-1.239750000	-1.111453000	3.541543000
H	-1.002771000	-2.870387000	3.429335000
H	0.391769000	-1.794391000	3.727158000
C	3.890505000	2.055184000	3.850053000
H	3.802545000	3.090495000	4.214644000
H	3.624768000	1.382480000	4.677237000
H	4.937104000	1.868697000	3.578384000
C	1.492740000	1.926799000	3.167625000
H	1.332429000	1.185405000	3.961373000
H	1.291430000	2.926473000	3.580690000
H	0.772884000	1.709274000	2.372240000
C	2.300515000	3.914853000	1.227875000
H	2.417316000	4.630475000	2.055877000
H	2.550376000	4.432843000	0.291105000
H	1.249610000	3.606397000	1.175480000
C	4.686922000	3.192422000	1.304146000
H	4.854755000	3.609199000	0.301079000
H	4.900697000	3.979278000	2.042454000
H	5.395721000	2.371730000	1.463460000

TS-PCy_3



E : -13091.08kcal·mol^{-1}

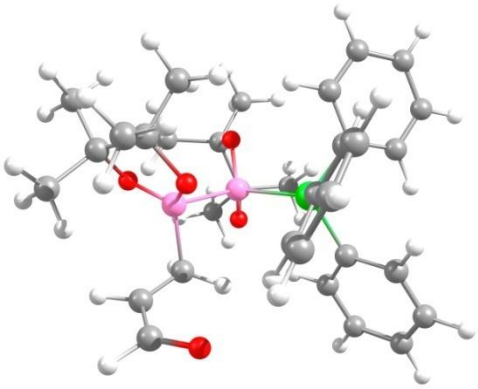
Imaginary frequency: -148.42 cm^{-1}

	X	Y	Z
P	4.544176	-0.768615	-0.347721
B	3.003692	0.363077	0.668966
B	1.162428	-0.571992	0.386661
C	1.104997	0.153564	-1.244953
C	-0.205493	-0.186485	-1.706774
O	1.312592	-1.965407	0.493836
O	0.223248	-0.101071	1.331801
O	3.038320	1.707022	0.212988
O	3.271090	0.325423	2.064483
C	3.172913	1.688267	2.602504
C	3.361129	2.601368	1.320046
C	0.525212	-2.439754	1.630430
C	-0.495370	-1.261414	1.871206
C	-0.517030	-1.337541	-2.487756
O	0.267017	-2.251020	-2.833538
C	-0.109888	-3.773942	1.237489
C	1.497621	-2.637183	2.800598
C	-1.792562	-1.412193	1.071202
C	-0.828702	-0.996394	3.338806
C	4.261526	1.858312	3.664355
C	1.803075	1.840706	3.269172
C	2.411847	3.800068	1.251610
C	4.797781	3.097117	1.103875
H	1.903644	-0.337399	-1.806399
H	1.289344	1.217168	-1.087363
H	-1.583193	-1.378566	-2.831918
H	-1.045633	0.450394	-1.415928
H	0.679341	-4.524184	1.085964

H	-0.778744	-4.142498	2.030615
H	-0.675099	-3.686060	0.301938
H	0.983295	-3.029313	3.690258
H	2.267025	-3.363672	2.505397
H	1.995953	-1.692950	3.054039
H	-2.390902	-2.260584	1.433980
H	-2.388675	-0.495076	1.182241
H	-1.586949	-1.560751	0.003058
H	-1.519200	-0.143981	3.410993
H	-1.326791	-1.871879	3.783672
H	0.066799	-0.766407	3.927997
H	4.234537	2.875970	4.083398
H	4.081754	1.151625	4.486430
H	5.267173	1.674998	3.267089
H	1.729214	1.109635	4.086172
H	1.682373	2.844864	3.701415
H	0.989190	1.633749	2.567231
H	2.600319	4.495381	2.083988
H	2.580385	4.344450	0.311769
H	1.362319	3.486351	1.285199
H	4.857474	3.590214	0.123879
H	5.096890	3.824065	1.873078
H	5.521172	2.272276	1.112059
C	4.440378	-2.544397	-0.998853
C	4.038436	-3.645784	0.007129
C	3.545395	-2.682388	-2.253097
C	4.252765	-5.035383	-0.620147
C	3.752860	-4.062196	-2.903203
C	3.456225	-5.203482	-1.920990
C	5.222950	0.242924	-1.809688
C	6.224277	-0.527639	-2.703782
C	4.154116	0.933604	-2.687993
C	6.875750	0.402779	-3.741540
C	4.806712	1.848904	-3.738838
C	5.819198	1.095888	-4.611124
C	5.951387	-0.659325	0.929853
C	5.822591	-1.658335	2.100214
C	7.404273	-0.639292	0.414004
C	6.794376	-1.306963	3.239461
C	8.382235	-0.295256	1.553913
C	8.245062	-1.254549	2.742532
H	5.491995	-2.723542	-1.299722
H	2.977648	-3.501186	0.254092
H	4.605745	-3.578731	0.941749
H	2.483912	-2.567012	-1.979373
H	3.760569	-1.902676	-2.995863
H	3.968665	-5.812299	0.107946
H	5.329742	-5.179590	-0.825324
H	3.103171	-4.141959	-3.787525
H	4.796219	-4.147424	-3.260899

H	3.680329	-6.177761	-2.384589
H	2.378407	-5.198905	-1.688816
H	5.773280	1.048500	-1.287541
H	5.688642	-1.325349	-3.240846
H	7.002156	-1.020906	-2.107637
H	3.549507	0.173826	-3.208331
H	3.472049	1.514051	-2.056698
H	7.571787	-0.179158	-4.366407
H	7.481639	1.166565	-3.221740
H	4.019673	2.298994	-4.363740
H	5.317904	2.684275	-3.227292
H	6.298750	1.780305	-5.328442
H	5.287776	0.333969	-5.208466
H	5.741141	0.338587	1.353035
H	6.074183	-2.668208	1.739470
H	4.789857	-1.679042	2.472653
H	7.668271	-1.626486	-0.003726
H	7.529477	0.097950	-0.390787
H	6.691864	-2.046262	4.049505
H	6.514728	-0.330126	3.669053
H	9.413628	-0.300890	1.167253
H	8.181320	0.736452	1.893886
H	8.923441	-0.954842	3.556706
H	8.557915	-2.266242	2.428237

TS-PPh_3



E : -11531.03kcal·mol^{-1}

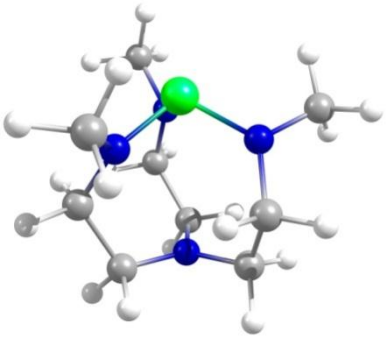
Imaginary frequency: -143.16 cm^{-1}

	X	Y	Z
B	2.988083	0.413835	0.740718
B	1.131014	-0.503501	0.399267

C	1.000036	0.555409	-1.012501
C	-0.225866	0.086203	-1.591518
O	1.354906	-1.884550	0.305344
O	0.220294	-0.212116	1.436370
O	3.072294	1.777301	0.379473
O	3.225703	0.250756	2.123016
C	3.200941	1.586876	2.745108
C	3.556744	2.535572	1.537396
C	0.660303	-2.551224	1.403020
C	-0.399893	-1.473860	1.855309
C	-0.299667	-0.782018	-2.716323
O	0.662055	-1.300036	-3.333868
P	4.433683	-0.771848	-0.347806
H	1.862871	0.447543	-1.676804
H	0.967187	1.550232	-0.562377
H	-1.340383	-0.974142	-3.081119
H	-1.170127	0.374699	-1.123526
C	0.067208	-3.856909	0.872167
H	0.882480	-4.526485	0.563928
H	-0.519352	-4.366509	1.652761
H	-0.575979	-3.683736	0.000962
C	1.711808	-2.857773	2.477578
H	1.277125	-3.410711	3.323457
H	2.494370	-3.483538	2.025482
H	2.170097	-1.932126	2.848052
C	-1.733389	-1.593703	1.109480
H	-2.284114	-2.495560	1.414216
H	-2.351293	-0.714770	1.341972
H	-1.578799	-1.629572	0.023307
C	-0.654861	-1.418646	3.360476
H	-1.372572	-0.616342	3.583241
H	-1.088119	-2.367476	3.713101
H	0.266285	-1.224373	3.923070
C	4.221993	1.601928	3.881491
H	4.282982	2.608365	4.324191
H	3.904235	0.907250	4.671702
H	5.221265	1.305614	3.540501
C	1.797383	1.822798	3.306831
H	1.572558	1.035755	4.038654
H	1.738515	2.794552	3.818496
H	1.031668	1.767836	2.526395
C	2.838370	3.884187	1.546908
H	3.135759	4.475511	2.426279
H	3.115197	4.453751	0.648296
H	1.748651	3.763760	1.555823
C	5.061929	2.751033	1.349474
H	5.234474	3.269846	0.396415
H	5.482480	3.370322	2.154778
H	5.605790	1.797712	1.326233
C	5.884836	-0.971766	0.770175

C	7.183436	-0.584114	0.402345
C	5.671057	-1.528695	2.045954
C	8.250117	-0.761352	1.289330
H	7.365066	-0.142200	-0.577862
C	6.741436	-1.711561	2.923236
H	4.665035	-1.806555	2.354734
C	8.033624	-1.327864	2.548510
H	9.253999	-0.456287	0.990780
H	6.562316	-2.148552	3.906689
H	8.868558	-1.466499	3.237648
C	5.070195	0.054161	-1.869029
C	5.884427	-0.680596	-2.751932
C	4.751258	1.387332	-2.173907
C	6.380963	-0.084581	-3.911523
H	6.116072	-1.724333	-2.537960
C	5.245537	1.974625	-3.343485
H	4.107178	1.950609	-1.500684
C	6.061142	1.244590	-4.210679
H	7.007033	-0.665265	-4.590118
H	4.980210	3.006012	-3.579938
H	6.438162	1.704478	-5.125924
C	4.055396	-2.472051	-0.937109
C	3.121812	-2.616319	-1.978078
C	4.679335	-3.607127	-0.395788
C	2.822364	-3.887960	-2.466947
H	2.584168	-1.766311	-2.406856
C	4.365010	-4.877852	-0.887435
H	5.414289	-3.508284	0.402933
C	3.437522	-5.020635	-1.923885
H	2.085340	-3.977249	-3.265280
H	4.853521	-5.754487	-0.459405
H	3.193185	-6.013824	-2.305693

Verkade base (2,8,9-trimethyl-2,5,8,9-tetraaza-1-phosphabicyclo[3.3.3]undecane)

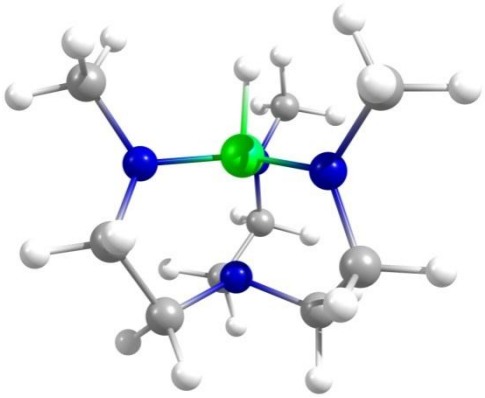


E : -4424.1kcal·mol^{-1}

	X	Y	Z
P	-1.088982	0.166168	-0.932590
N	-0.646211	0.724218	0.668560
N	0.220014	0.630478	-1.971255
N	-0.953243	-1.567019	-0.994283
C	1.551731	1.016277	-1.514257
H	2.084464	1.483318	-2.359159
H	1.462600	1.797700	-0.744654
C	2.443729	-0.134816	-0.962032
H	3.337810	0.337178	-0.501442
H	2.809757	-0.740504	-1.806550
N	1.812801	-1.038388	-0.023877
C	1.391796	-2.345891	-0.486314
H	2.235716	-2.869988	-0.979886
H	1.121445	-2.947831	0.393912
C	0.212832	-2.293337	-1.472177
H	-0.095476	-3.319019	-1.742154
H	0.564267	-1.812271	-2.397050
C	0.603142	0.668272	1.439875
H	1.228382	1.560560	1.235347

H	0.336515	0.744710	2.511573
C	1.461598	-0.597658	1.308084
H	2.372269	-0.397267	1.916574
H	0.934045	-1.429104	1.796094
C	-1.446226	1.883161	1.085271
H	-1.725452	1.793758	2.148932
H	-0.904019	2.840162	0.957288
H	-2.364947	1.931931	0.485735
C	-1.948035	-2.311212	-0.232463
H	-2.265761	-3.212373	-0.783430
H	-1.600385	-2.622137	0.770965
H	-2.833483	-1.673392	-0.085822
C	-0.064958	0.690814	-3.400630
H	-1.147426	0.570164	-3.555470
H	0.228163	1.665945	-3.827411
H	0.439835	-0.103650	-3.983264

Protonated Verkade base (protonated 2,8,9-trimethyl-2,5,8,9-tetraaza-1-phosphabicyclo[3.3.3]undecane)

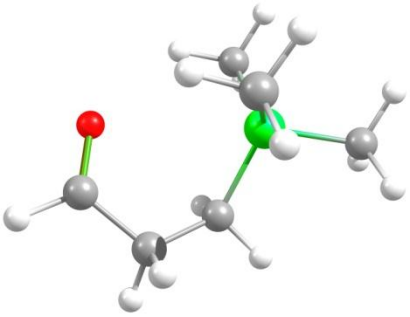


E : -4402.7 kcal·mol^{-1}

	X	Y	Z
P	-0.539348	-0.116151	-0.733590
N	-0.570833	0.564155	0.831687
N	0.284487	0.700194	-1.972099
N	-0.932983	-1.756890	-0.860024
C	1.738845	0.618871	-2.090259
H	2.031299	0.578949	-3.151154
H	2.232736	1.505658	-1.650974
C	2.168277	-0.664732	-1.391109
H	3.239413	-0.684045	-1.145925
H	1.935262	-1.530546	-2.024157
N	1.341456	-0.770047	-0.153611
C	1.127393	-2.179469	0.289465
H	2.074509	-2.737924	0.283406
H	0.737526	-2.138515	1.313494
C	0.080276	-2.783662	-0.633667
H	-0.372637	-3.661864	-0.148659
H	0.519774	-3.133707	-1.587470
C	0.696205	1.124862	1.299572
H	0.898179	2.113565	0.845771
H	0.648518	1.272123	2.387855
C	1.813737	0.123226	0.956957
H	2.730379	0.638731	0.646477
H	2.058309	-0.505695	1.820126
C	-1.761736	1.320719	1.248054
H	-1.827334	1.305461	2.344390
H	-1.739125	2.371953	0.911916

H	-2.667050	0.842922	0.857000
C	-2.076413	-2.191023	-1.673450
H	-1.758719	-2.538595	-2.670041
H	-2.599887	-3.011816	-1.163406
H	-2.786628	-1.366954	-1.803332
C	-0.365143	1.722838	-2.800042
H	-1.450768	1.697599	-2.653128
H	-0.006484	2.733313	-2.547571
H	-0.162024	1.534116	-3.864686
H	-1.831411	0.320347	-1.136907

[H-I1-PMe$_3$]$^+$



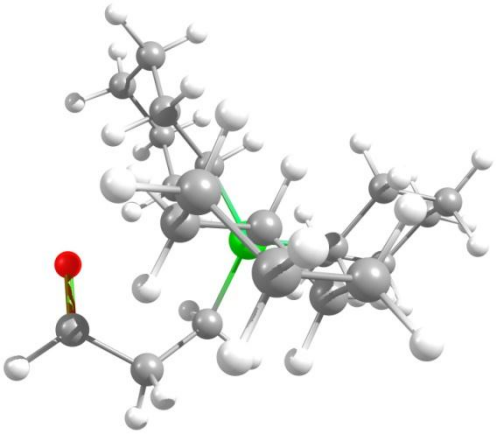
E : -409923.23 kcal·mol^{-1}

(Optimized as described in section 11)

	X	**Y**	**Z**
P	0.892820	0.013630	0.004720
C	2.484010	-0.868620	-0.124000
C	0.605120	0.371640	1.765460
C	1.051310	1.561230	-0.935260
H	2.685210	-1.132270	-1.167560
H	3.296830	-0.231530	0.238820
H	2.460630	-1.785470	0.473720
H	-0.296510	0.976180	1.886330

H	0.507940	-0.558790	2.333850
H	1.462380	0.929060	2.157310
H	1.287060	1.332980	-1.979860
H	0.117040	2.123290	-0.885290
H	1.867840	2.156210	-0.513010
C	-0.383210	-1.115080	-0.718690
C	-1.764610	-1.212320	-0.047600
C	-2.502700	0.100900	0.062220
O	-1.954010	1.174140	-0.099840
H	-0.498000	-0.804940	-1.764310
H	0.071310	-2.111940	-0.734130
H	-3.575880	0.047040	0.322860
H	-2.383980	-1.919180	-0.616460
H	-1.701720	-1.644730	0.962930

[H-I1-PCy$_3$]$^+$



E : -777468.67 kcal·mol^{-1}

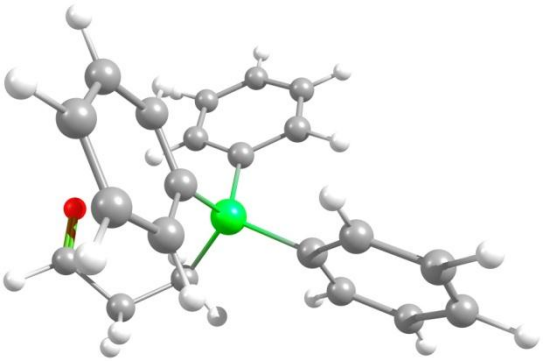
(Optimized as described in section 11)

	X	**Y**	**Z**
P	-0.024140	-0.115580	0.397060
C	0.255670	0.170250	2.216930
C	1.622920	0.583050	2.785870
C	2.140720	1.930570	2.345910
O	1.607030	2.610220	1.493170
H	-0.497530	0.903540	2.520660
H	-0.028410	-0.777560	2.687900

H	3.062440	2.279560	2.851970
H	1.540890	0.608680	3.883270
C	-1.311570	-1.472360	0.377680
C	-2.639400	-1.058680	1.060160
C	-1.583720	-2.044220	-1.035000
C	-3.612220	-2.251040	1.126920
C	-2.569820	-3.226780	-0.964530
C	-3.879070	-2.841230	-0.264130
C	1.475990	-0.807590	-0.476090
C	2.728740	0.101780	-0.530880
C	1.869740	-2.212330	0.051460
C	3.799210	-0.525500	-1.442960
C	2.966140	-2.837710	-0.833020
C	4.195220	-1.929200	-0.966490
C	-0.804400	1.337950	-0.501300
C	-1.536530	2.317860	0.447760
C	0.100680	2.108370	-1.490210
C	-2.362790	3.332790	-0.364390
C	-0.739280	3.118350	-2.295240
C	-1.496360	4.090090	-1.379830
H	-0.862890	-2.270050	0.987170
H	-3.111510	-0.249880	0.487810
H	-2.461760	-0.674540	2.071900
H	-2.012580	-1.262220	-1.677140
H	-0.657120	-2.376560	-1.516600
H	-4.549220	-1.922050	1.591590
H	-3.192320	-3.026160	1.784530
H	-2.768630	-3.586150	-1.981060
H	-2.094490	-4.060030	-0.426470
H	-4.534040	-3.716390	-0.182980
H	-4.418760	-2.103730	-0.876440
H	1.108790	-0.924040	-1.506920
H	3.151900	0.205430	0.474770
H	2.481280	1.106940	-0.874890
H	2.240790	-2.125670	1.082880
H	1.010330	-2.889070	0.080630
H	4.675740	0.132750	-1.468710
H	3.416970	-0.575010	-2.473120
H	3.249050	-3.810770	-0.414150
H	2.546470	-3.037760	-1.829740
H	4.918310	-2.375690	-1.658750
H	4.702450	-1.853860	0.006930
H	-1.568310	0.823790	-1.103600
H	-0.791840	2.850410	1.048510
H	-2.199830	1.784500	1.138630
H	0.878840	2.643580	-0.936590
H	0.595420	1.418190	-2.183550
H	-2.843370	4.033830	0.328500
H	-3.174200	2.807710	-0.889980
H	-0.077320	3.667760	-2.975130

H	-1.455600	2.574330	-2.928910
H	-2.120440	4.763380	-1.979070
H	-0.775210	4.723320	-0.843660
H	2.402370	-0.165140	2.586820

[H-I1-PPh$_3$]$^+$



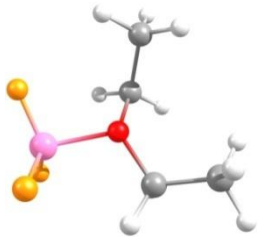
E : -770780.04 kcal·mol^{-1}

(Optimized as described in section 11)

	X	**Y**	**Z**
P	-0.127940	0.008780	0.430340
C	0.323120	0.005710	2.241560
C	1.518600	-0.848200	2.686610
C	2.867330	-0.288630	2.291410
O	3.011280	0.751620	1.682370
H	0.494560	1.050890	2.514790
H	-0.572240	-0.328580	2.772730
H	3.745570	-0.884980	2.606710
H	1.457720	-1.888600	2.342750
C	-1.758950	-0.780990	0.255190
C	-2.044420	-1.603180	-0.848240
C	-2.772540	-0.498390	1.189750
C	-3.320550	-2.150530	-0.999350
H	-1.280640	-1.820920	-1.587720
C	-4.044150	-1.048760	1.031270
H	-2.588790	0.160180	2.034380
C	-4.318390	-1.878380	-0.060660
H	-3.531150	-2.789170	-1.852210
H	-4.819490	-0.827040	1.758740

H	-5.308960	-2.307780	-0.180210
C	1.076610	-0.915430	-0.567450
C	1.188410	-2.310670	-0.410790
C	1.903930	-0.248520	-1.484510
C	2.123610	-3.023220	-1.160950
H	0.536860	-2.847340	0.274290
C	2.835320	-0.970850	-2.233480
H	1.828750	0.825820	-1.614490
C	2.948170	-2.353390	-2.071570
H	2.202560	-4.099780	-1.040070
H	3.471820	-0.449500	-2.942260
H	3.673940	-2.911130	-2.656520
C	-0.251230	1.730030	-0.136100
C	0.747840	2.662590	0.202640
C	-1.336900	2.122160	-0.938740
C	0.648640	3.975980	-0.258120
H	1.599770	2.365490	0.806600
C	-1.422340	3.438700	-1.394490
H	-2.114880	1.413270	-1.203530
C	-0.433190	4.365040	-1.054130
H	1.420030	4.693820	0.005380
H	-2.264680	3.739000	-2.010800
H	-0.505450	5.389790	-1.407420
H	1.510040	-0.914710	3.785560

$Et_2O \cdot BF_3$

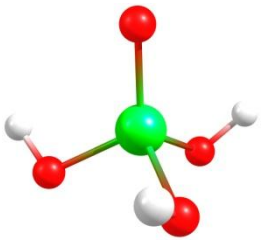


E : -2345.4 kcal·mol^{-1}

	X	Y	Z
B	-2.161457	0.311553	0.976206
F	-3.361879	0.849736	0.581138

F	-1.091847	0.676733	0.182851
F	-2.194384	-1.022075	1.299930
O	-1.866171	1.058202	2.454809
C	-2.074700	2.530024	2.439924
H	-1.262480	2.969958	3.031371
H	-1.967876	2.847282	1.395505
C	-0.595572	0.624326	3.076216
H	-0.452140	-0.394994	2.704920
C	-3.437315	2.866464	3.007829
H	-3.526632	2.534168	4.050683
H	-3.578249	3.956998	2.977185
H	-4.229664	2.396946	2.413066
C	-0.693248	0.657642	4.587356
H	0.250003	0.284820	5.012334
H	-0.853214	1.674253	4.973147
H	-1.509475	0.012458	4.937391
H	0.207396	1.262365	2.681783

H_3PO_4



E : -1044.57kcal·mol^{-1}

	X	Y	Z
P	-1.231836	1.546299	-0.078917
O	0.244912	1.660711	-0.030358

O	-1.931344	0.718746	1.119436
O	-2.078277	2.921407	-0.039167
H	-1.603101	3.609094	-0.546689
O	-1.857249	0.827475	-1.385247
H	-1.229642	0.150619	-1.707719
H	-1.379711	0.797851	1.922957

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