Electronic Supplementary Information

Hydrosilylation and hydrogermylation of white phosphorus

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1. General information

Unless stated otherwise, all reactions and manipulations were performed under an N_2 atmosphere (< 0.1 ppm O_2, H_2O) through use of MBraun Unilab and GS MEGA Line gloveboxes and standard Schlenk line techniques. All glassware was oven-dried (160 °C) overnight prior to use. PhH was distilled from Na/benzophenone and stored over molecular sieves (3 Å). MeCN was distilled from CaH_2 and stored over molecular sieves (3 Å). *n*-Hexane, PhMe, Et_2O and THF were purified using an MBraun SPS-800 system and stored over molecular sieves (3 Å). EtOH was degassed and dried by standing over at least three sequential batches of molecular sieves (3 Å). C_6D_6 was distilled from K and stored over molecular sieves (3 Å). CD_3CN, CD_3OD and D_2O were used without purification. All reagents and starting materials were purchased from major suppliers. Liquids were degassed (if not supplied under inert atmosphere) but were otherwise used as supplied, unless stated otherwise. 1,4-Cyclohexadiene (1,4-CHD) was supplied containing 0.1% BHT as stabilizer and was used as received. BnBr, EtBr, BuBr, PhC(O)Cl and *t*BuC(O)Cl were distilled, degassed, and stored over molecular sieves (3 Å). Solids were dried under vacuum (with the exception of paraformaldehyde) but otherwise used as supplied, unless stated otherwise. Red phosphorus (≥97.0%) was purchased from Sigma-Aldrich.

NMR spectra were recorded at room temperature on Bruker Avance 400 spectrometers (400 MHz). Chemical shifts, δ, are reported in parts per million (ppm); ^{1}H NMR and ^{13}C NMR shifts are reported relative to $SiMe_4$ and were referenced internally to residual solvent peaks, while ^{31}P NMR and ^{119}Sn shifts were referenced externally to 85 % H_3PO_4 (aq.) and $SnMe_4$ (90% in C_6D_6), respectively. Except where stated otherwise, integrals for ^{31}P{^{1}H} and ^{31}P spectra are provided for the purposes of qualitative comparison only, and should not be considered quantitatively accurate. The abbreviations s, d, t, q, m are used to indicate singlets, doublets, triplets, quartets and multiplets, respectively.

Reactions driven by light were performed using apparatus that has been described in previous publications, in which reaction vessels are illuminated from beneath by LEDs while placed in a metal block through which cooling water is constantly circulated to maintain near-ambient temperature. [16]

LEDs used for the optimization reactions:

- 365 nm, 3 W: 4.3 V, 700 mA, Osram OSLON SSL 80.
- 365 nm, 10 W: 14 V, 700 mA, Osram OSLON SSL 80.
- 390 nm, 40 W: Kessil PR160L.
- 455 nm (±15 nm): 3.7 V, 700 mA, Osram OSLON SSL 80.

2. Computational investigations

2.1. General methods

All calculations were carried out with the ORCA program package.[43,44] Unless stated otherwise, all calculations were carried out on isolated molecules (in the gas phase). Density fitting techniques, also called resolution-of-identity approximation (RI)[45], were used for GGA calculations and the RIJCOSX[46] approximation was used for hybrid-GGA DFT calculations. Atom-pairwise dispersion corrections with the Becke-Johnson damping (D3BJ)[47,48] were used for all DFT calculations. Pictures were rendered with the software Avogadro.[49] All geometries were obtained at the PBE-D3BJ/def2-TZVP level of theory.

2.2. Mechanisms of P_4 hydroelementation by Me_3EH (E = Si, Ge, Sn)

The calculated mechanisms for the hydroelementation of the first P–P bond in P_4 by $Me_3E^\bullet$ addition and subsequent HAT and the aggregation of P_4 with the initial intermediate $(Me_3E)P_4^\bullet$ are combined in Figure S1 for ease of comparison. While the *endo* attack of the $Me_3E^\bullet$ radical to P_4 would give the alternative *endo* isomer of intermediate $(Me_3E)P_4^\bullet$, only the *exo* pathway was considered, as in the case of $Me_3Sn^\bullet$ the *endo* attack was calculated to be much less feasible, in line with chemical intuition.[28]

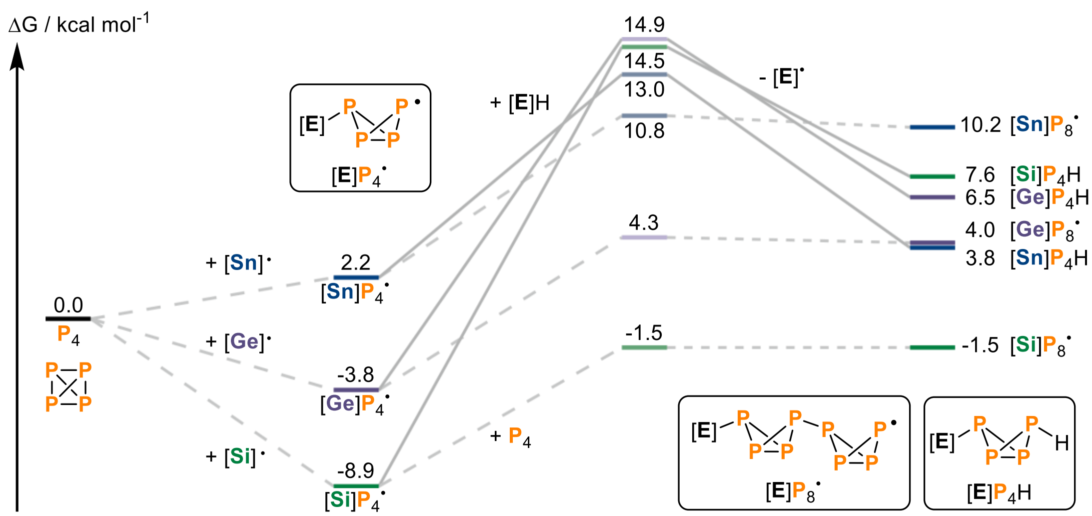


Figure S1. Calculated mechanisms for hydroelementation of the first P–P bond in P_4 and for agregation of further P_4 with the first P-centred radical intermediate (relative free energies in kcal mol^{-1}). [**E**] = Me_3Si, Me_3Ge or Me_3Sn.

2.3. Mechanisms of P_4 hydrogermylation and hydrosilylation by R_3GeH (R = Me and Ph) and R'_3SiH (R' = Me, Ph, Me_3Si), respectively.

Analogous studies on the first P–P bond hydroelementation step were performed for non-truncated model radicals such as $Ph_3Ge^\bullet$ (Figure S2a) and $R'_3Si^\bullet$ (R' = Ph and Me_3Si; Figure S2.b). In all cases, the addition of these radicals to P_4 was found to be barrierless and downhill, forming the corresponding 'butterfly' P_4 radical intermediates. Interestingly, the subsequent HAT process exhibited lower energy barriers with respect to the truncated models Me_3EH (E = Ge, Si), which is consistent with the calculated lower E–H bond dissociation energies (see Section 2.5).

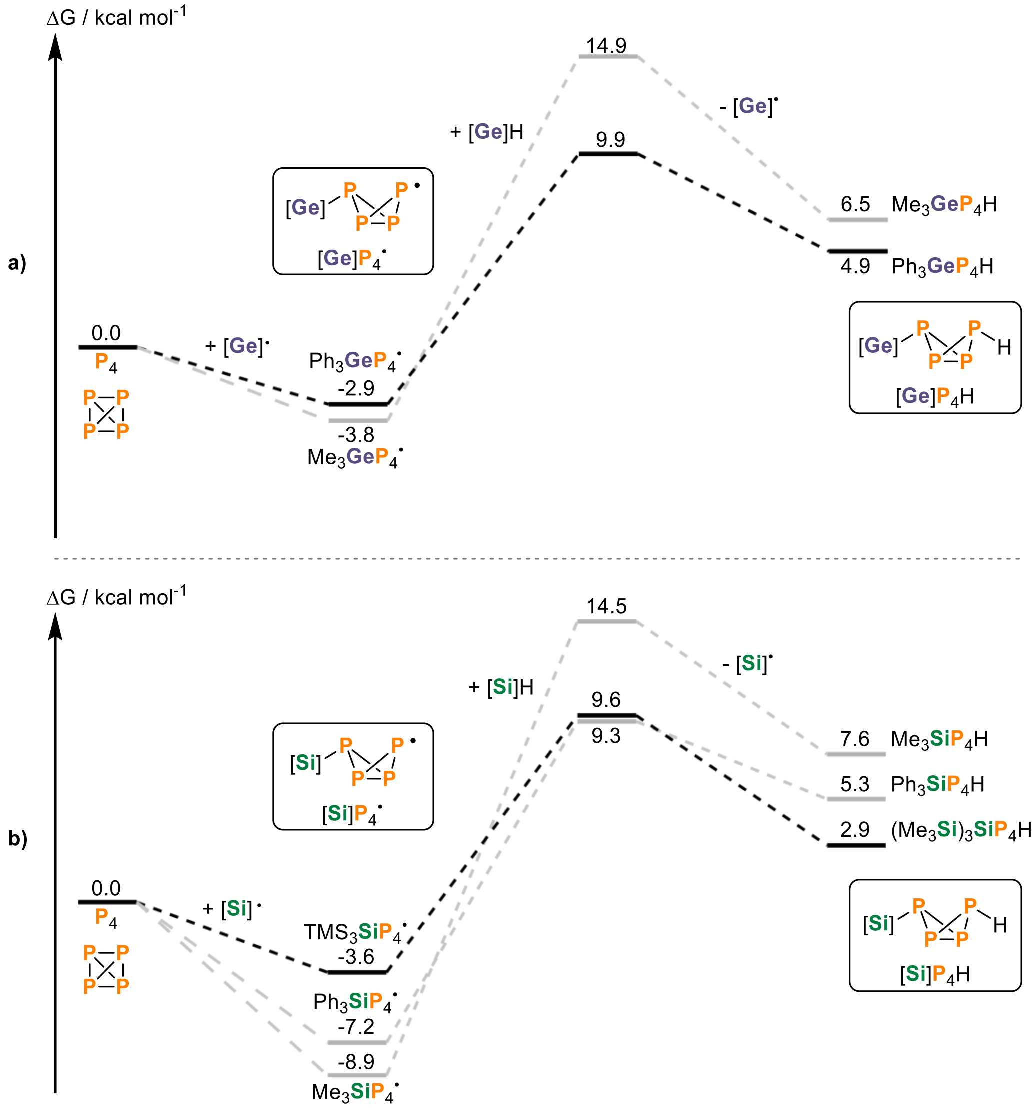


Figure S2. Calculated mechanisms for hydroelementation of the first P–P bond in P_4 by a) Me_3GeH and Ph_3GeH; b) Me_3SiH, Ph_3SiH, and $(Me_3Si)_3SiH$ (relative free energies in kcal mol^{-1}).

2.4. Mechanisms of HAT process from intermediate $(Me_3Si)P_4^{\bullet}$ with different HAT donors

The HAT process from the intermediate $(Me_3Si)P_4^{\bullet}$ with different HAT donors such as thiols RSH (R = Ph, Me_3Si, *i*Pr_3Si) and 1,4-cyclohexadiene (1,4-CHD) was calculated to be energetically favoured and with smaller activation barriers in all cases. Relaxed surface scans for the silyl substituted thiols R_3SiSH (R = Me, *i*Pr) revealed no identifiable transition state.

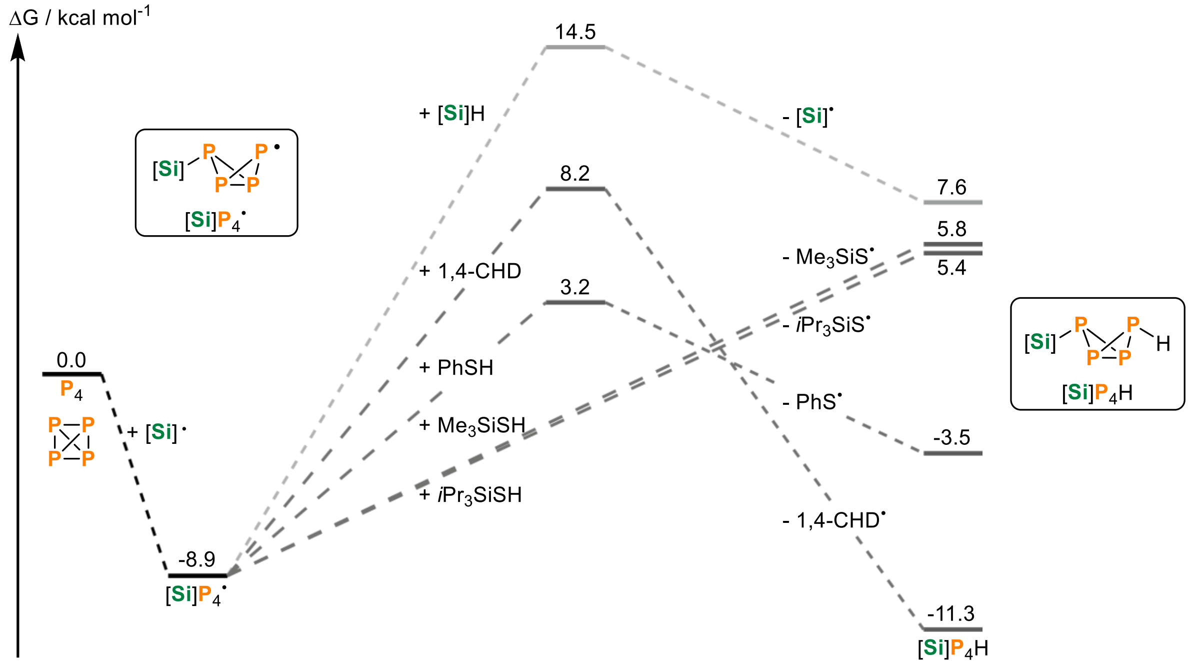


Figure S3. Calculated mechanisms for the HAT step to form $(Me_3Si)P_4H$ from the intermediate $(Me_3Si)P_4^{\bullet}$ with different HAT donors (relative free energies in kcal mol^{-1}). [**Si**] = Me_3Si. 1,4-CHD = 1,4-cyclohexadiene.

2.5. Calculated bond dissociation energies

Bond dissociation energies (BDE, Table S1) were calculated according the following equation

$$BDE = H(X^{\bullet}) + H(H^{\bullet}) - H(X\text{–}H)$$

wich corresponds to the enthalpy of the homolysis reaction

$$X\text{–}H \rightarrow X^{\bullet} + H^{\bullet}$$

$H(H^{\bullet}) = -0.49584461$ Eh. Enthalpy values for all other relevant molecules (X–H and X$^{\bullet}$) are given in Section 6.

Table S1. Calculated bond dissociation energies.

Entry	X–H	BDE (kcal mol^{-1})
1	Me_3Sn–H	75.3
2	Me_3Ge–H	84.9
3	Bu_3Ge–H	84.3
4	Ph_3Ge–H	81.6
5	Me_3Si–H	91.2
6	Ph_3Si–H	87.3
7	TMS_3Si–H	81.1
8	Me_3SiS–H	88.7
9	*i*Pr_3SiS–H	88.2
10	PhS–H	79.1
11	1,4-CHD–H	72.0

3. Hydrogermylation of white phosphorus (P_4)

3.1. Hydrogermylation of P_4 using Bu_3GeH and LED irradiation (0.01 mmol scale)

To provide the most direct comparison to the hydrostannylation of P_4 with Bu_3SnH, we first tested the reactivity of Bu_3GeH towards P_4 under the same reaction conditions. Thus, Bu_3GeH and P_4 were combined in a 6:1 molar ratio in PhMe and irradiated with blue LED light (455 nm) for one day. Unfortunately, and in sharp contrast to the efficient reaction of P_4 with R_3SnH, the $^{31}P\{^1H\}$ NMR spectrum of the resulting orange suspension showed only unconsumed P_4 at −521.5 ppm (Figure S4). When the reaction was performed under near UV LED light (365 nm) and longer reaction times, minor signals were observed at −255.5 ppm and −261.6 ppm attributed to Bu_3GePH_2 and $(Bu_3Ge)_2PH$, respectively (Figures S5 and S6). Other attempts to achieve useful reactivity using Bu_3GeH also led to unsatisfactory results.

Representative procedure:

To a 10 mL, flat-bottomed, stoppered tube were added P_4 (0.01 mmol, as a stock solution in 84.3 µL PhH), PhMe (500 µL), and Bu_3GeH (46.5 µL, 0.18 mmol). The tube was sealed, placed in a water-cooled block to maintain near-ambient temperature, and irradiated with UV light (365 nm, 14 V, 700 mA, Osram OSLON SSL 80) for 3 days. Ph_3PO (0.02 mmol, stock solution in benzene) was subsequently added to act as an internal standard. The resulting mixture was analysed by $^{31}P\{^1H\}$ and ^{31}P NMR spectroscopy, as shown in Figures S4-6 below.

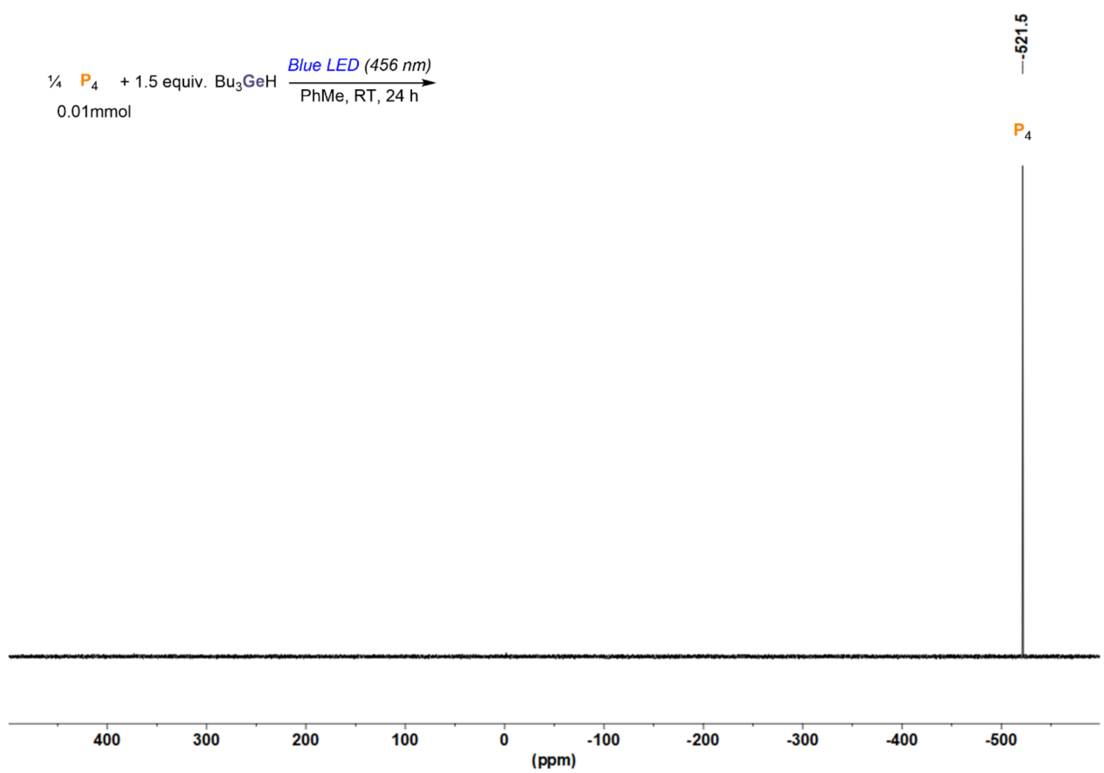


Figure S4. $^{31}P\{^1H\}$ NMR spectrum for the reaction of P_4 (0.01 mmol) with Bu_3GeH (0.06 mmol) in PhMe and driven by 456 nm LED irradiation for 24 h.

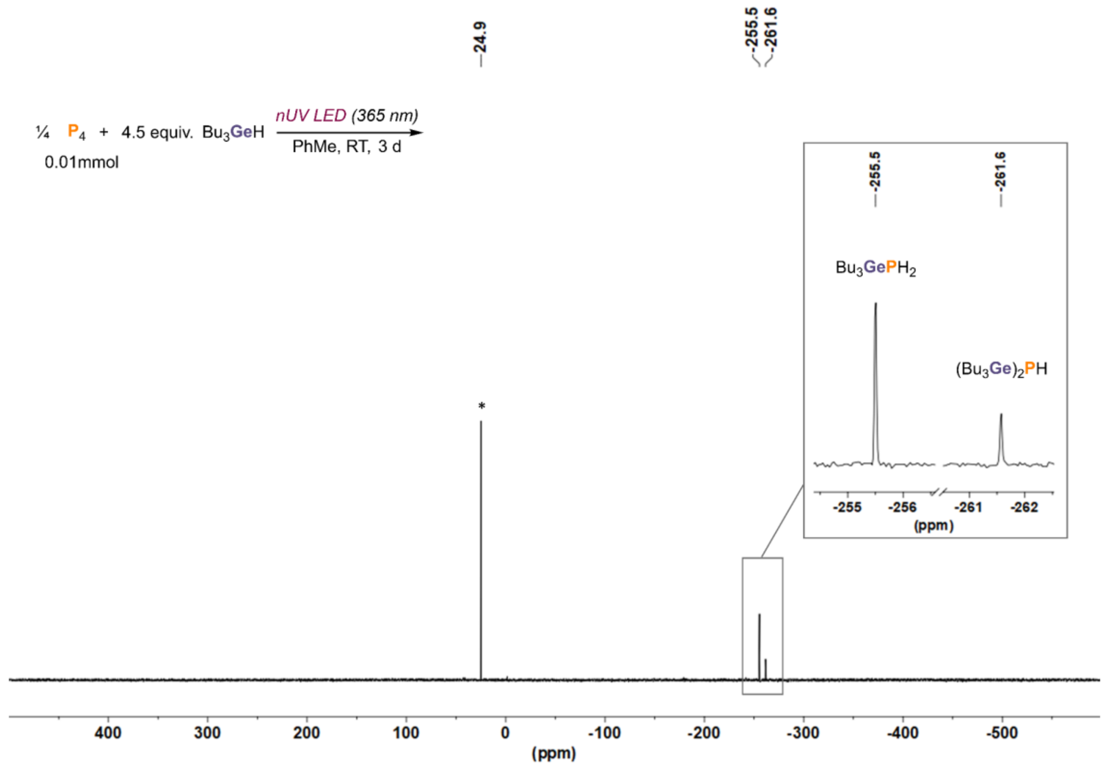


Figure S5. $^{31}P\{^{1}H\}$ NMR spectrum for the reaction of P_4 (0.01 mmol) with Bu_3GeH (0.18 mmol) in PhMe and driven by 356 nm, 10 W LED irradiation for 3 days. * marks the internal standard Ph_3PO.

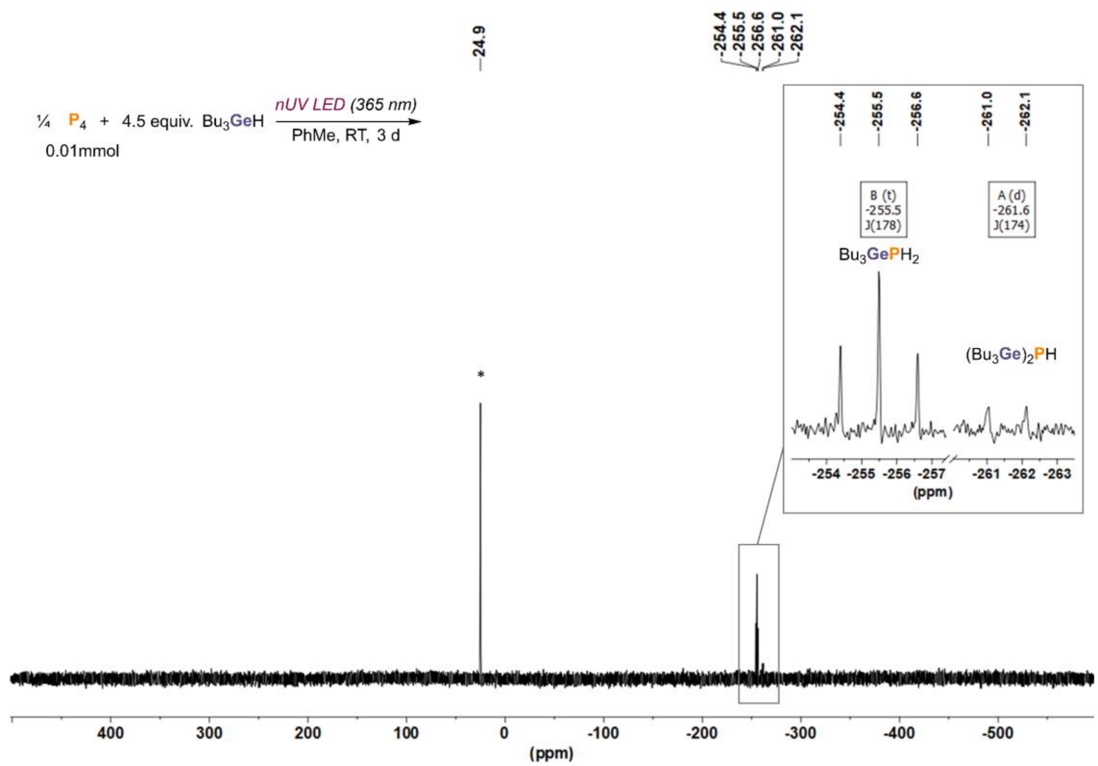
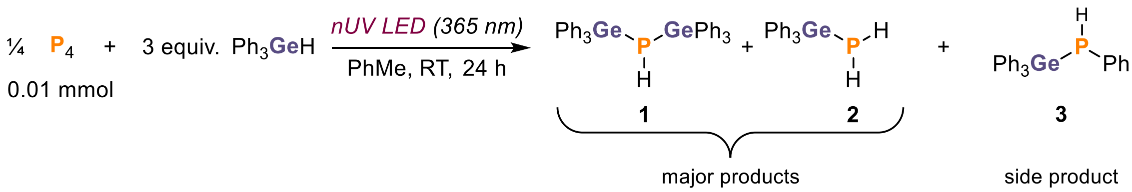


Figure S6. ^{31}P NMR spectrum for the reaction of P_4 (0.01 mmol)with Bu_3GeH (0.18 mmol) in PhMe and driven by 356 nm, 10 W LED irradiation for 3 days. The insets show expansions of the signals attributed to Bu_3GePH_2 and $(Bu_3Ge)_2PH$, highlighting their multiplicity due to $^{1}J(^{31}P\text{-}^{1}H)$ couplings. * marks the internal standard Ph_3PO.

3.2. General procedure and optimisation for the hydrogermylation of P_4 using Ph_3GeH and LED irradiation (0.01 mmol scale)



Representative procedure:

To a 10 mL, flat-bottomed, stoppered tube were added P_4 (0.01 mmol, as a stock solution in 84.3 µL PhH), PhMe (100 µL), and Ph_3GeH (36.6 mg, 0.12 mmol). The tube was sealed, placed in a water-cooled block to maintain near-ambient temperature, and irradiated with UV light (365 nm, 4.3 V, 700 mA, Osram OSLON SSL 80) for 24 hours. Ph_3PO (0.02 mmol, stock solution in benzene) was subsequently added to act as an internal standard. The resulting mixture was analysed by ^{1}H, $^{31}P\{^{1}H\}$, and ^{31}P NMR spectroscopy, as shown in Figures S7-9, below. Compounds **1-3** have not been reported previously. However, the observed NMR data are consistent with those reported for similar compounds such as $(Me_3Ge)_2PH$[32] and $R_3Ge_2P(H)Ph$ (R = Me, Et).[33]

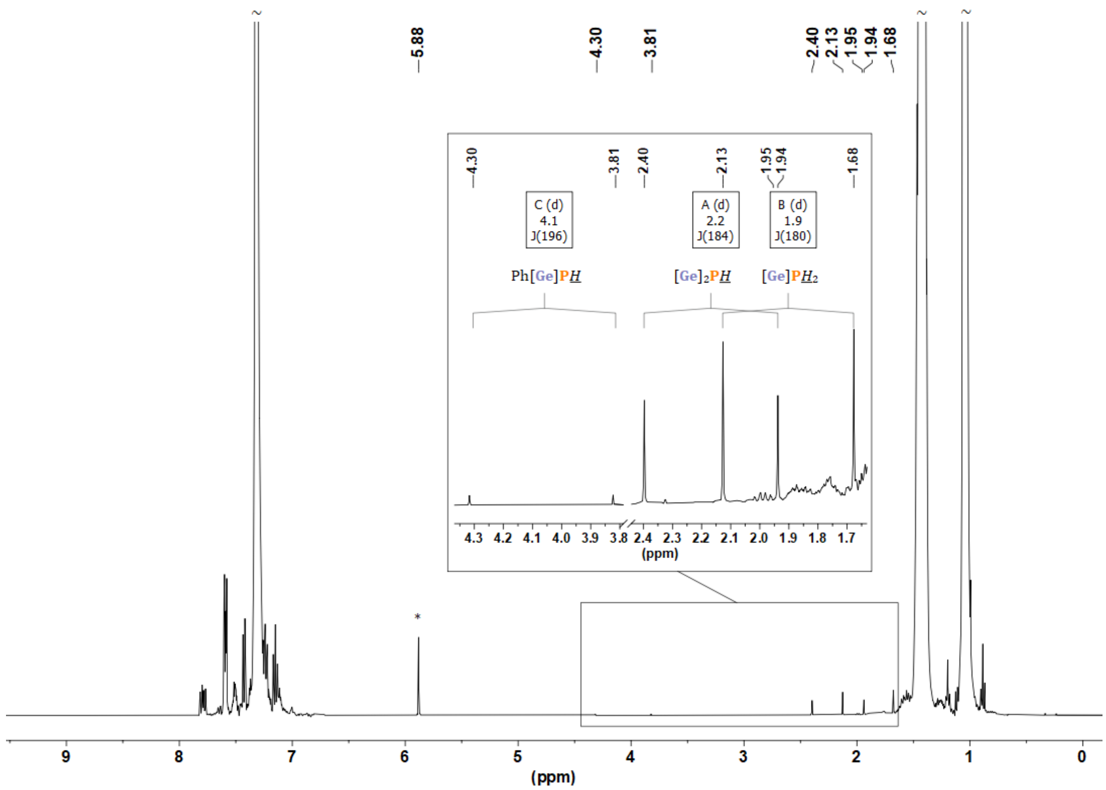


Figure S7. ^{1}H NMR spectrum for the reaction of P_4 with Ph_3GeH (0.12 mmol) in hexane and driven by 365 nm, 3 W LED irradiation for 3 d (Table S2, Entry 9). The inset shows expansions of the doublet resonances attributed to the P*H* moieties of $(Ph_3Ge)_2PH$ (**1**) and [Ge]P(H)Ph (**3**), and the PH_2 moiety of $(Ph_3Ge)PH_2$ (**2**). [Ge] = Ph_3Ge. * marks Ph_3GeH. ~ marks solvent resonances truncated for clarity.

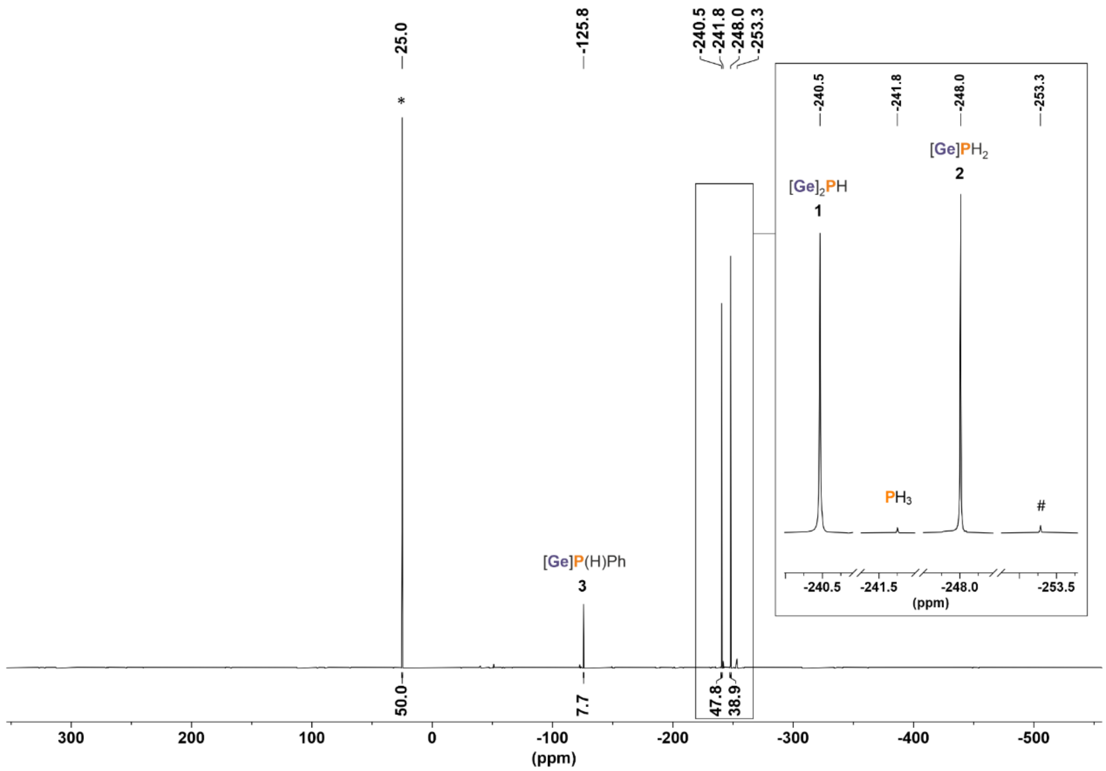


Figure S8. Quantitative $^{31}P\{^1H\}$ NMR spectrum (D1 = 40 s) for the reaction of P_4 with Ph_3GeH (0.12 mmol) in PhMe and driven by 365 nm, 3 W LED irradiation for 3 d (Table S2, Entry 9). [Ge] = Ph_3Ge. * marks the internal standard Ph_3PO (0.02 mmol). # marks an unknown side product.

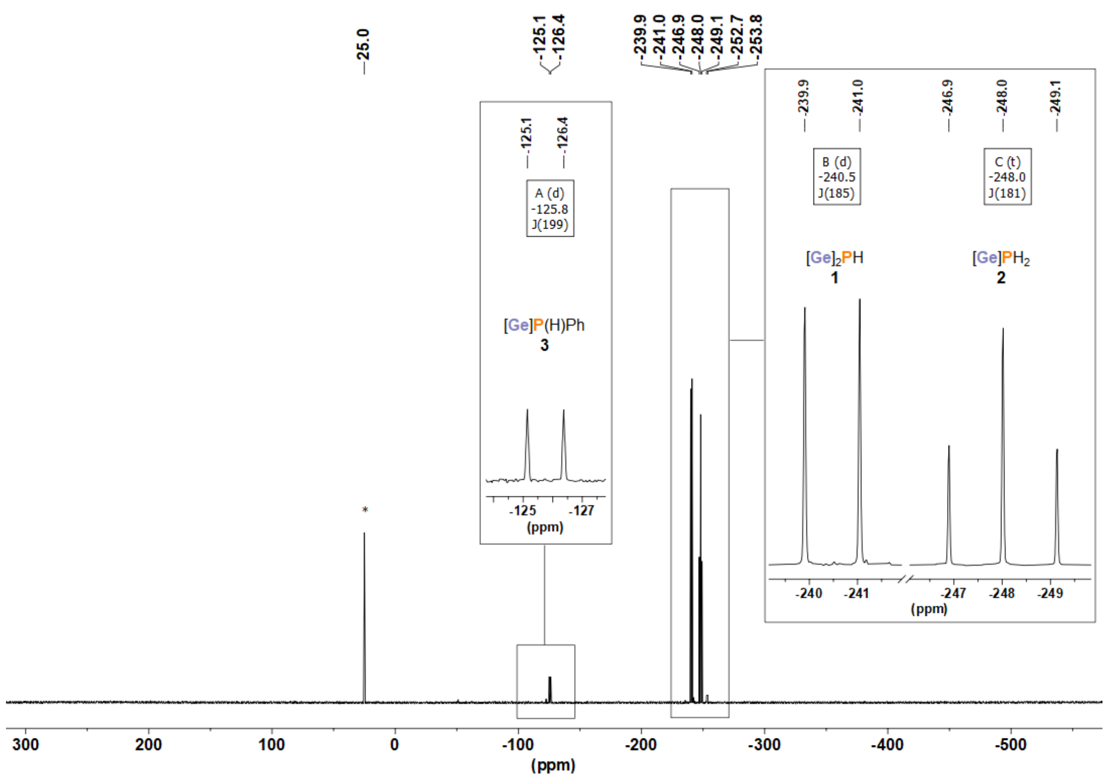
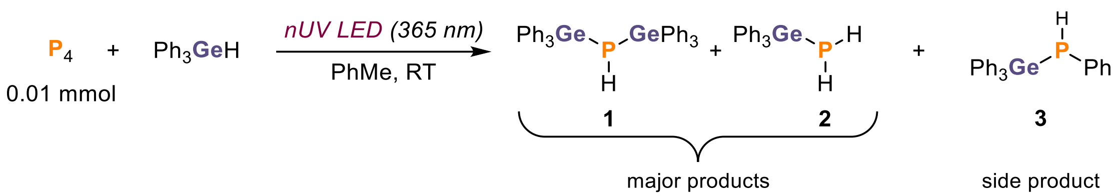


Figure S9. ^{31}P NMR spectrum for the reaction of P_4 with Ph_3GeH (0.12 mmol) in hexane and driven by 365 nm, 3 W LED irradiation for 3 d (Table S2, Entry 9). The insets show expansions of the signals attributed to $[Ge]_2PH$ (**1**), $[Ge]PH_2$ (**2**) and [Ge]P(H)Ph (**3**), highlighting their multiplicity due to $^1J(^{31}P\text{-}^1H)$ couplings. [Ge] = Ph_3Ge. * marks the internal standard Ph_3PO (0.02 mmol).

For reasons of experimental expediency, during the optimization of the hydrogermylation of P_4, non-quantitative $^{31}P\{^1H\}$ NMR spectra were recorded to analyse each experiment and to assess the relative total conversion to **1-3**. Although this did not provide precise, quantitative conversions directly it did allow for meaningful, qualitative comparisons between experiments. Under the conditions highlighted in Table S2, entry 9, a quantitative $^{31}P\{^1H\}$ NMR spectrum was recorded using an inverse-gated decoupled pulse sequence (D1 = 40 s, Figure S8), and the conversion of P_4 to products **1-3** was determined. Thus, for ease of interpretation, the integrals measured for **1-3** for all optimization experiments have been normalized relative to the value for this experiment (Table S2, entry 9) to provide the relative conversions indicated in Table S2.

Table S2. Optimization of hydrogermylation of P_4 using Ph_3GeH and near-UV LED irradiation(365 nm).[a]



Entry	Ph_3GeH (mmol)	PhMe (μL)	Time (days)	Full conv. of P_4?	Relative conv. to **1** and **2** (%)	Relative conv. to **3** (%)
1[c]	0.06	500	1	X	traces	-
2[c]	0.06	500	3	✓	9	-
3	0.06	500	3	✓	46.7	10.0
4	0.06	500 (hexane)	3	✓	54.1	8.9
5	0.06	500 (THF)	3	✓	49.0	11.9
6	0.06	500 (EtOH)	3	X	4.7	-
7	0.06	500 (CH_3CN)	3	✓	7.9	-
6	0.09	500	4	✓	75.6	12.8
7	0.09	500 (hexane)	3	✓	70.2	7.6
8	0.12	500 (hexane)	3	✓	81.9	4.8
9	**0.12**	**500**	**3**	**✓**	**86.7**	**7.7**
10	0.12	100	3	✓	57.7	13.3
11	0.12	100	2	✓	77.9	12.0
12	**0.12**	**100**	**1**	**✓**	**87.4**	**7.8**

[a] The general procedure described in this section was modified to use the indicated amount of reactants and solvent. [b] Conversions were calculated by integration of the ^{31}P resonances of **1-3** relative to an internal standard, which was then normalized relative to entry 9 as described in the text above. [c] Blue LED (455 nm).

Crystals of $(Ph_3Ge)_2PH$ (**1**) suitable for X-ray analysis were obtained by removing volatiles from the product mixture under vacuum, washing the solid residue with n-hexane, re-dissolving in a minimal amount of toluene and adding n-hexane by slow diffusion at ambient temperature (see Section 3.3).

3.3. Crystallographic characterisation of $(Ph_3Ge)_2PH$ (1)

Single crystal X-ray diffraction data for $(Ph_3Ge)_2PH$ (**1**) were recorded on a Rigaku XtaLAB Synergy DW R (DW system, HyPix-Arc 150) diffractometer with microfocus Cu-Kα radiation (λ = 1.54184 Å). The crystal was selected under mineral oil, mounted on a micromount loop and quench-cooled using an Oxford Cryosystems open flow N_2 cooling device. Data processing, reduction and multi-scan absorption correction[50,51] was performed with the program CrysAlisPro (Rigaku Oxford Diffraction, 2021). Using Olex2,[52] the structure was solved with the SHELXT[53] structure solution program using Intrinsic Phasing and refined using SHELXL using Squares refinements on F^2.[54] $(Ph_3Ge)_2PH$ crystallizes in the monoclinic space group $P2_1$ with two molecules in the asymmetric unit. All non-hydrogen atoms were refined using anisotropic displacement parameters. All hydrogen atoms but the P bound hydrogen atoms were located in idealized positions and refined isotropically with a riding model. The P bound hydrogen atoms were located from the electron density map and had its positions and isotropic displacement parameters refined freely. The disorder of the P bound hydrogen atom (H2 at P2) was treated with a geometrical restraint. Crystallographic data for this structure has been deposited with the Cambridge Crystallographic Data Centre, CCDC, 12 Union Road, Cambridge CB21EZ, UK. Copies of this data can be obtained free of charge on quoting the depository number: 2408662; E-mail: deposit@ccdc.cam.ac.uk, http://www.ccdc.cam.ac.uk.

Crystal and refinement data of $(Ph_3Ge)_2PH$ (**1**) are collected in Table S3, and the structure itself is illustrated in Figure S10. Selected bond lengths and angles are listed in the figure caption of the latter. The Ge–P distances (Ge1–P1 2.3325(7) Å, Ge2–P1 2.3269(7) Å) are slightly elongated compared to that observed in the phosphanylgermane $((F_5C_6)Ge)_3PH_2$ (2.307(1) Å),[55] while the P–H bond length (P1–H1 1.21(4) Å) is identical.

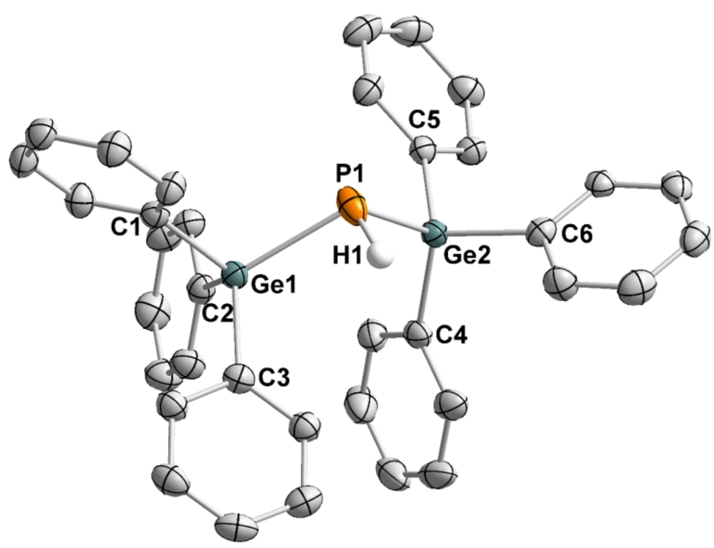
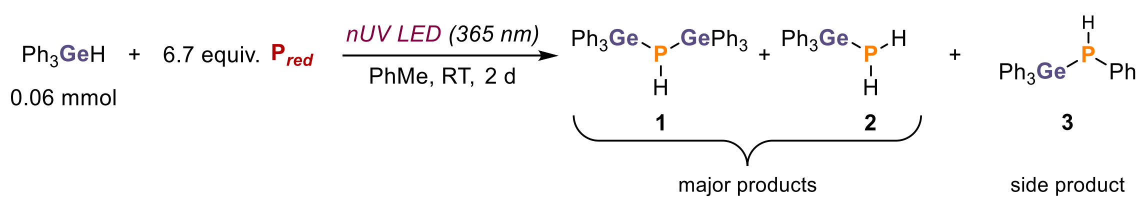


Figure S10. Single-crystal XRD structure of $(Ph_3Ge)_2PH$ (**1**). Thermal ellipsoids are shown at 50%. H atoms, except for the one bound directly to P, are omitted. C atoms are shown in grey, H in white, P in orange, and Ge in dark green. Selected bond lengths/Å and angles/°: P1–H1 1.21(4), Ge1–P1 2.3325(7), Ge2–P1 2.3269(7), Ge1–C1 1.956(2), Ge1–C2 1.951(2), Ge1–C3 1.953(2), Ge2–C4 1.957(2), Ge2–C5 1.956(2), Ge2–C6 1.964(2), Ge1–P1–Ge2 108.03(3), C1–Ge1–P1 105.04(7), C2–Ge1–P1 115.83(7), C3–Ge1–P1 111.24(7), C4–Ge2–P1 116.59(7), C5–Ge2–P1 108.74(7), C6–Ge2–P1 104.44(7).

Table S3. Crystal data and structure refinement of **$(Ph_3Ge)_2PH$ (1)**.

	$(Ph_3Ge)_2PH$ (1)
Formula	$C_{36}H_{31}Ge_2P$
Formula weight, g mol^{-1}	639.76
Crystal system	123.0(1)
Crystal size, mm	monoclinic
Space group	$P2_1$
a, Å	9.67692(3)
b, Å	18.31240(5)
c, Å	17.49013(6)
α, °	90
β, °	105.3799(3)
γ, °	90
V, Å^3	2988.388(17)
Z	4
ρ_{calcd}, Mg m^{-3}	1.422
μ (Mo *K*α), mm^{-1}	3.148
F(000)	1304.0
2θ range, deg	0.129 × 0.115 × 0.078
Index ranges	Cu Kα (λ = 1.54184)
	5.24 to 150.644
	$-12 \leq h \leq 11$, $-22 \leq k \leq 22$, $-21 \leq l \leq 21$
No. of reflns collected	174471
No. indep. Reflns	12237 [R_{int} = 0.0318, R_{sigma} = 0.0135]
No. refined params	12237/1/716
GooF (F^2)	1.040
R_1 (*F*) ($I > 2\sigma(I)$)	R_1 = 0.0168, wR_2 = 0.0426
wR_2 (F^2) (all data)	R_1 = 0.0172, wR_2 = 0.0427
Largest diff peak/hole, e Å^{-3}	0.25/-0.16
CCDC number	2408662

3.4. Hydrogermylation of P_{red} using Ph_3GeH and LED irradiation (0.06 mmol scale)



To a 10 mL, flat-bottomed, stoppered tube were added P_{red} (0.4 mmol, 12.4 mg), PhMe (250 μL), and Ph_3GeH (18.3 mg, 0.06 mmol). The tube was sealed, placed in a water-cooled block to maintain near-ambient temperature, and irradiated with UV light (365 nm, 14 V, 700 mA, Osram OSLON SSL 80) for 2 days. Ph_3PO (0.02 mmol, stock solution in benzene) was subsequently added to act as an internal standard. The resulting mixture was analysed by $^{31}P\{^1H\}$ NMR spectroscopy, as shown in Figure S11, below.

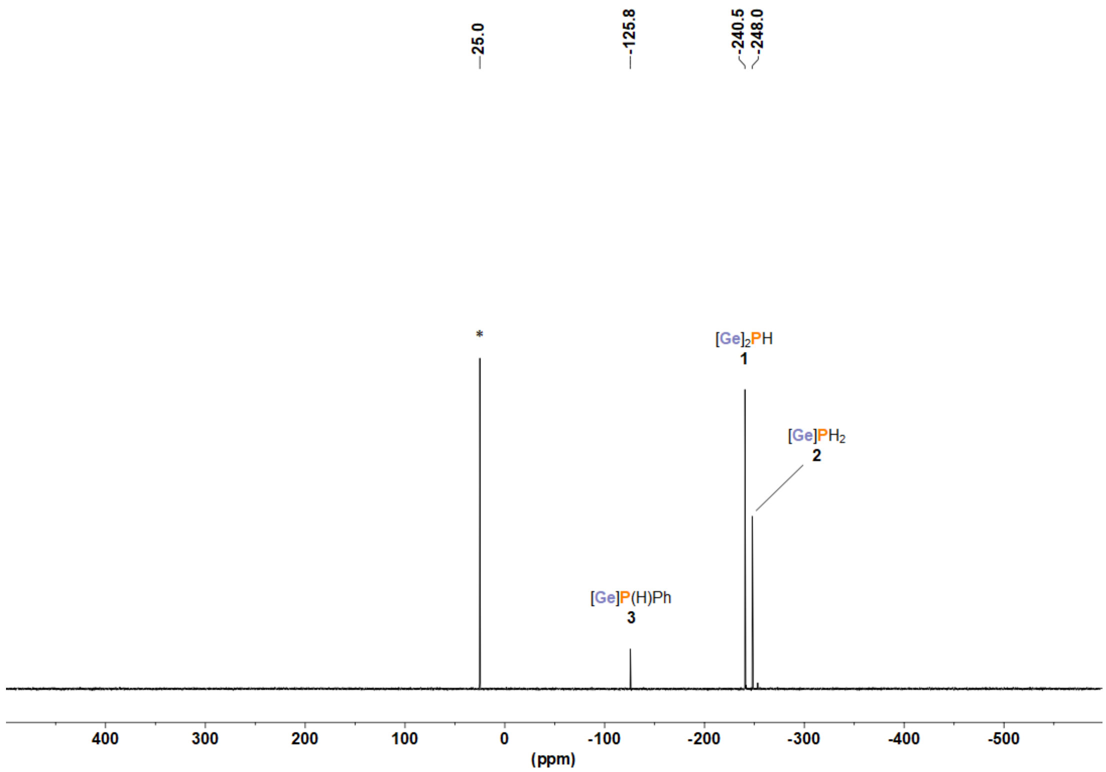
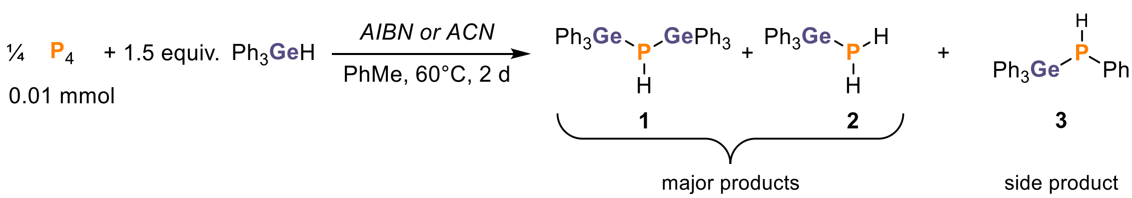


Figure S11. $^{31}P\{^{1}H\}$ NMR spectrum for the reaction of P_{red} with Ph_3GeH (0.06 mmol) in PhMe and driven by 356 nm, 10 W LED irradiation for 2 days. * marks the internal standard Ph_3PO. [Ge] = Ph_3Ge.

3.5. General procedure and optimization for the hydrogermylation of P_4 using Ph_3GeH and chemical radical initiators (0.01 mmol scale)



Representative procedure:

To a 10 mL, flat-bottomed, stoppered tube were added P_4 (0.01 mmol, as a stock solution in 84.3 µL PhH), PhMe (500 µL), AIBN (0.05 mmol, as a stock solution in PhH) and Ph_3GeH (18.3 mg, 0.06 mmol). The tube was sealed, wrapped in Al foil to exclude light, and heated to 60 °C for 2 days. Ph_3PO (14.0 mg, 0.0503 mmol) was subsequently added to act as an internal standard. The resulting mixture was analysed by $^{31}P\{^{1}H\}$ NMR spectroscopy, as shown in Figures S12 and 13, below.

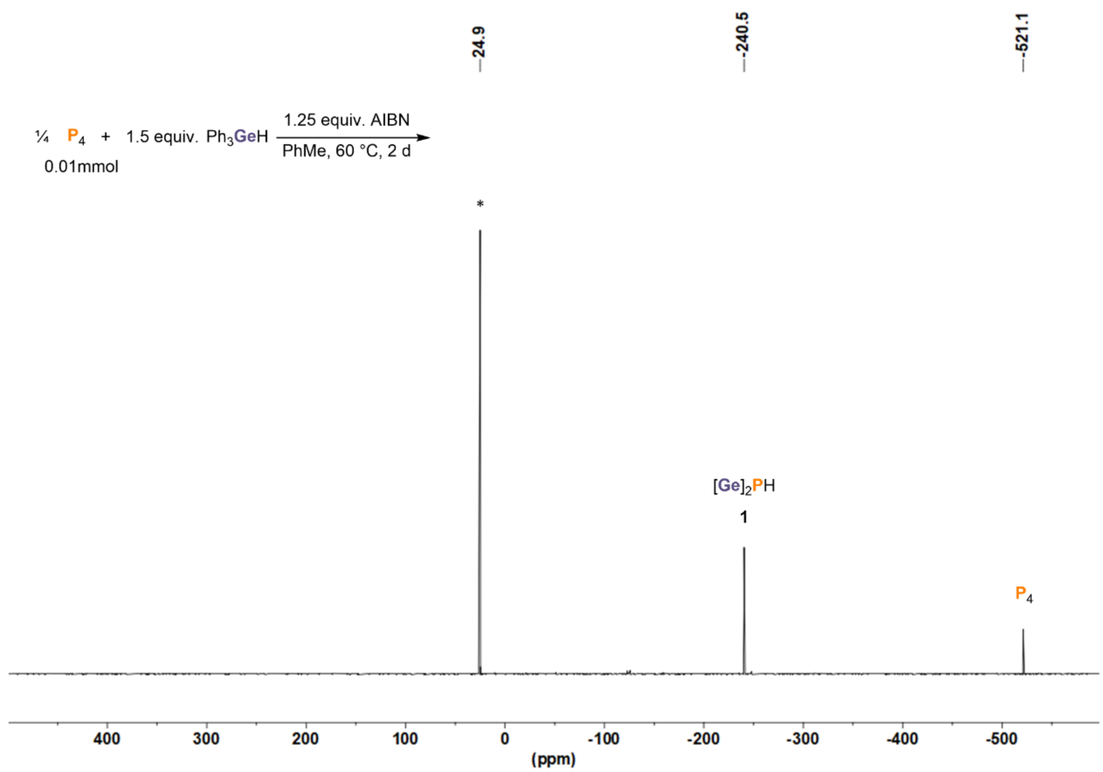


Figure S12. $^{31}P\{^{1}H\}$ NMR spectrum for the reaction of P_4 with Ph_3GeH (0.06 mmol) and AIBN (azobis(isobutyronitrile), 0.05 mmol) in PhMe, heated to 60 °C for 2 d (Table S4, Entry 4). * marks the internal standard Ph_3PO (0.0503 mmol). [Ge] = Ph_3Ge.

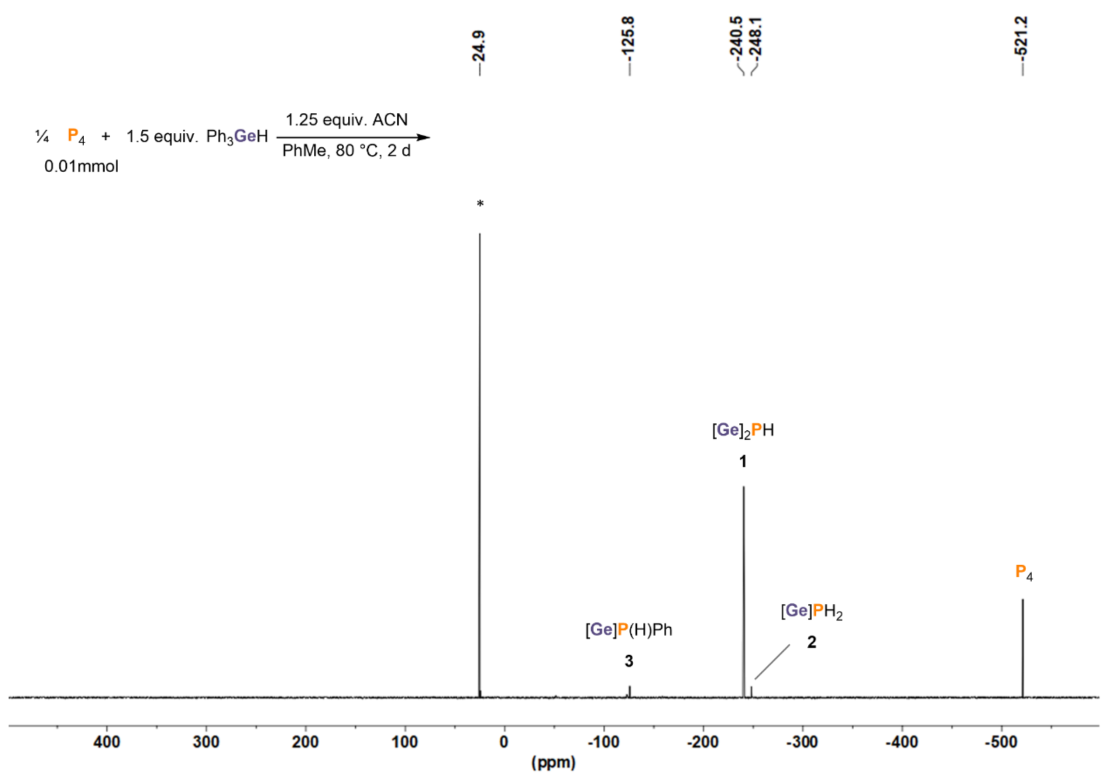
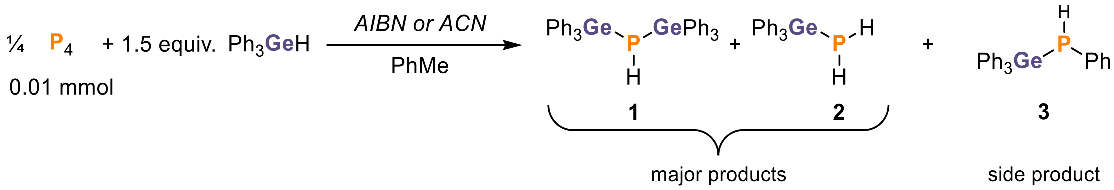


Figure S13. $^{31}P\{^{1}H\}$ NMR spectrum for the reaction of P_4 with Ph_3GeH (0.06 mmol) and ACN (1,1'-azobis(cyclohexanecarbonitrile), 0.05 mmol) in PhMe, heated to 80 °C for 2 d (Table S4, Entry 7). * marks the internal standard Ph_3PO (0.041 mmol). [Ge] = Ph_3Ge.

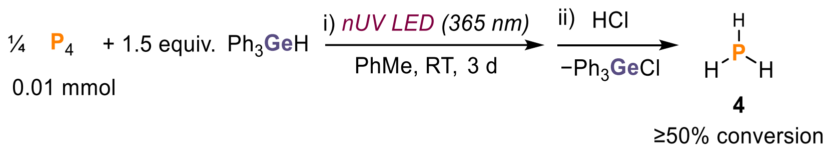
Table S4. Optimization of hydrogermylation of P_4 using Ph_3GeH and chemical radical initiators.[a]



Entry	Radical initiator (mmol)	Temperature (°C)	Time (days)	Full conv. of **P_4**?	Relative conv. to **1** and **2** (%)	Relative conv. to **3** (%)
1	AIBN (0.001)	60	1	X	traces	-
2	AIBN (0.001)	60	2	X	traces	-
3	AIBN (0.05)	60	1	X	<15	traces
4	AIBN (0.05)	60	2	X	27.6	traces
6	ACN (0.001)	80	1	X	traces	-
7	ACN (0.05)	80	2	X	21.7	traces
8	ACN (0.05)	100	2	X	<15	traces

[a] The general procedure described in this section was modified to use the indicated amount of reactant, temperature and time. [b] Conversions were calculated by integration of the ^{31}P resonances of **1**-**3** relative to an internal standard, which was then normalized relative to Table S2, entry 9 as described in Section 3.2. AIBN = azobis(isobutyronitrile)). ACN = 1,1'-azobis(cyclohexanecarbonitrile).

3.6. Synthesis and quantification of PH_3 (4) via hydrogermylation of P_4 (0.01 mmol scale)



To an NMR tube fitted with a J. Young valve were added PhMe (500 μL), P_4 (0.01 mmol, as a stock solution in 97.7 μL PhH), Ph_3PO (11.5 mg, 0.0413 mmol) and Ph_3GeH (18.3 mg, 0.06 mmol). The NMR tube was sealed, placed in thermal contact with a water-cooled block to maintain near-ambient temperature (by placing in a water-filled, flat-bottomed glass tube, which was in turn placed in the block and wrapped in Al foil), and irradiated with UV light (365 nm, 4.3 V, 700 mA, Osram OSLON SSL 80) for 3 days. The resulting yellow suspension was frozen by placing the NMR tube in a bath of liquid nitrogen, and HCl (0.4 mmol, 4.0 M in 1,4-dioxane) was added (while still maintaining an inert atmosphere). The NMR tube was sealed and its contents were then thawed, agitated briefly, and analysed by ^{1}H, $^{31}P\{^{1}H\}$ and ^{31}P NMR spectroscopy. The resulting spectra indicated clean conversion of **1** and **2** to PH_3,[20] and the formation of $PhPH_2$ from **3** as shown in Figures S14-16, below.[56]

In order to accurately quantify the amount of PH_3 in solution, a proton-coupled ^{31}P spectrum was acquired with a 20 s delay between scans (which was confirmed to be > 5 x T_1), and the intensity of the PH_3 resonance was integrated relative to that of Ph_3PO (which had been added specifically to act as an internal standard). This indicated 50% of the theoretical maximum conversion to PH_3 (Figure S17), which provides a lower bound for the actual conversion (this value does not include any PH_3 present in the NMR tube headspace).

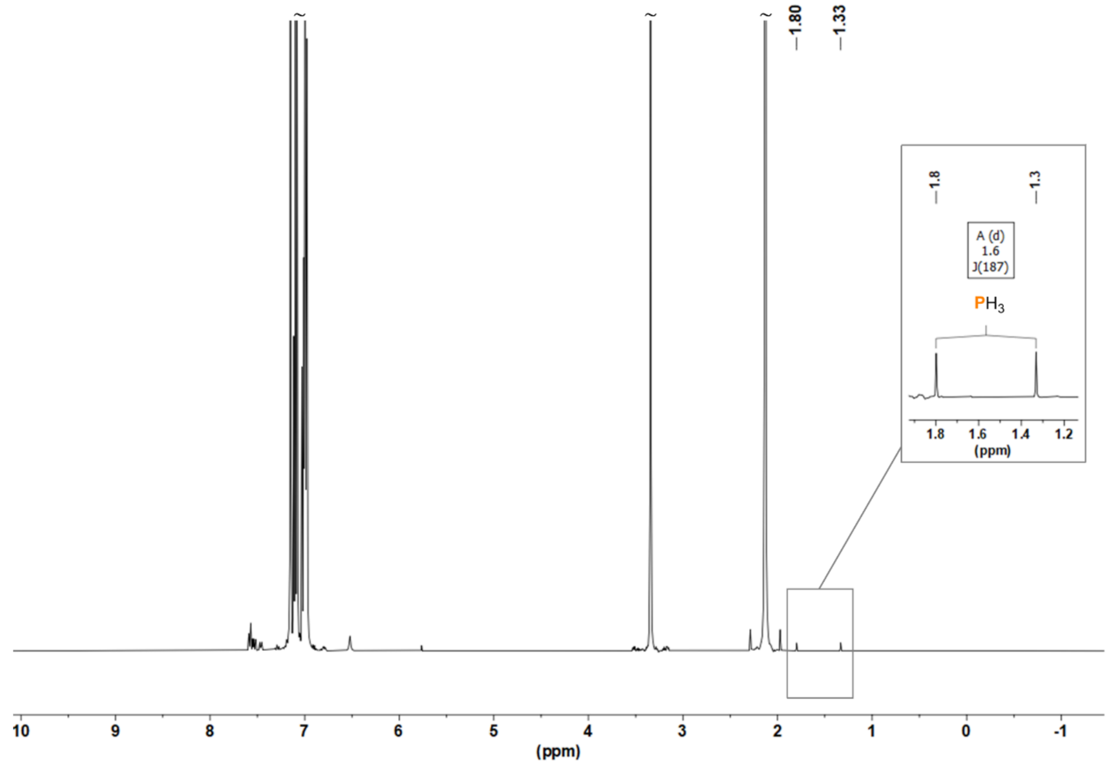


Figure S14. ^{1}H NMR spectrum of a solution of PH_3 (**4**) generated *via* hydrogermylation of P_4 in PhMe, followed by acidification. Solvent resonances (~) truncated for clarity.

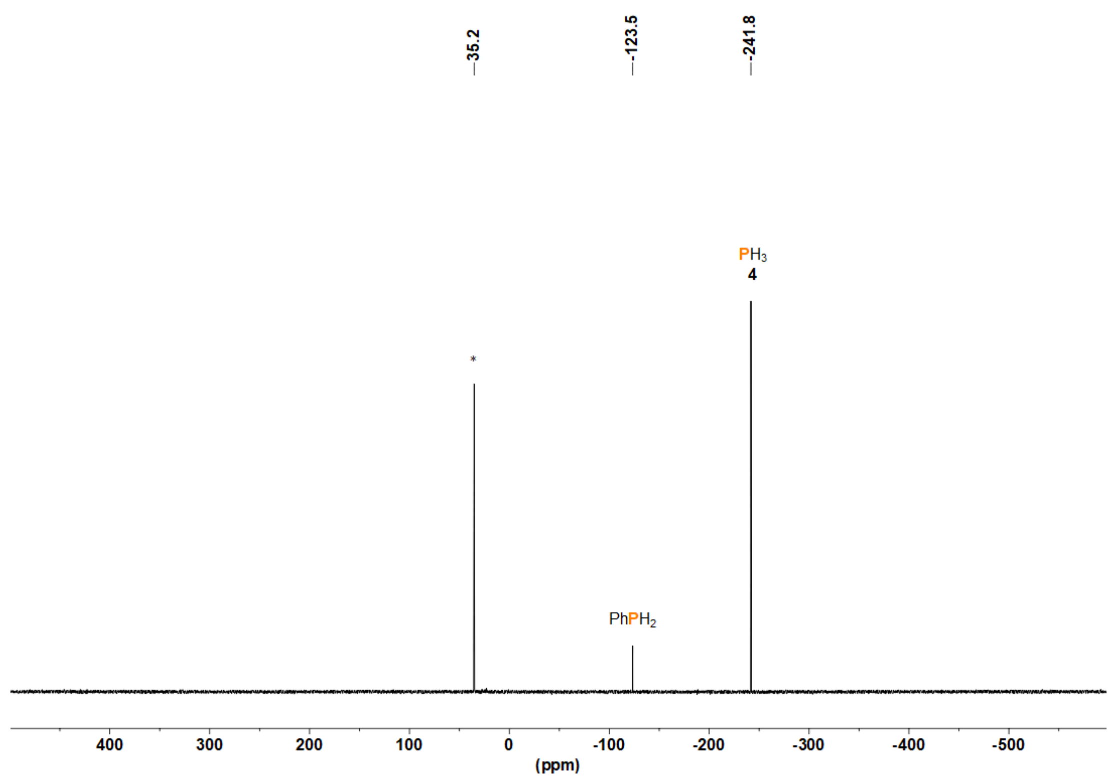


Figure S15. $^{31}P\{^{1}H\}$ NMR spectrum of PH_3 (**4**) generated *via* hydrogermylation of P_4 in PhMe, followed by acidification in the presence of Ph_3PO (*) as an internal standard.

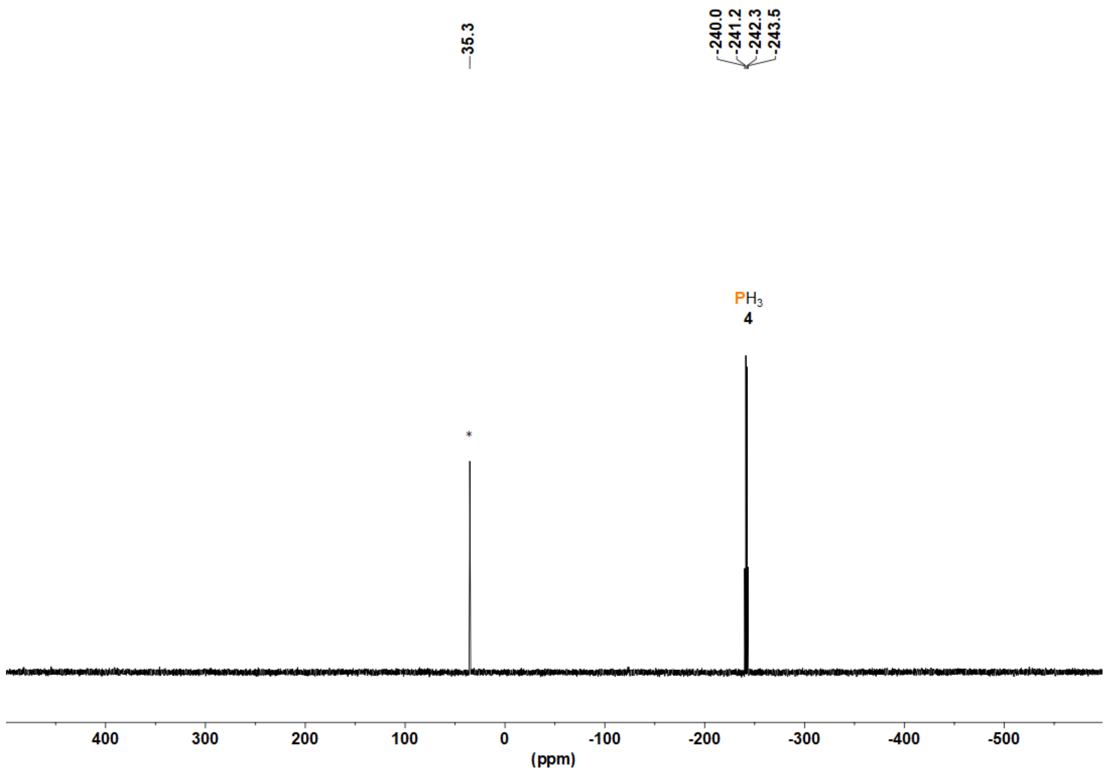


Figure S16. ^{31}P NMR spectrum of PH_3 (**4**) generated *via* hydrogermylation of P_4 in PhMe, followed by acidification in the presence of Ph_3PO (*) as an internal standard.

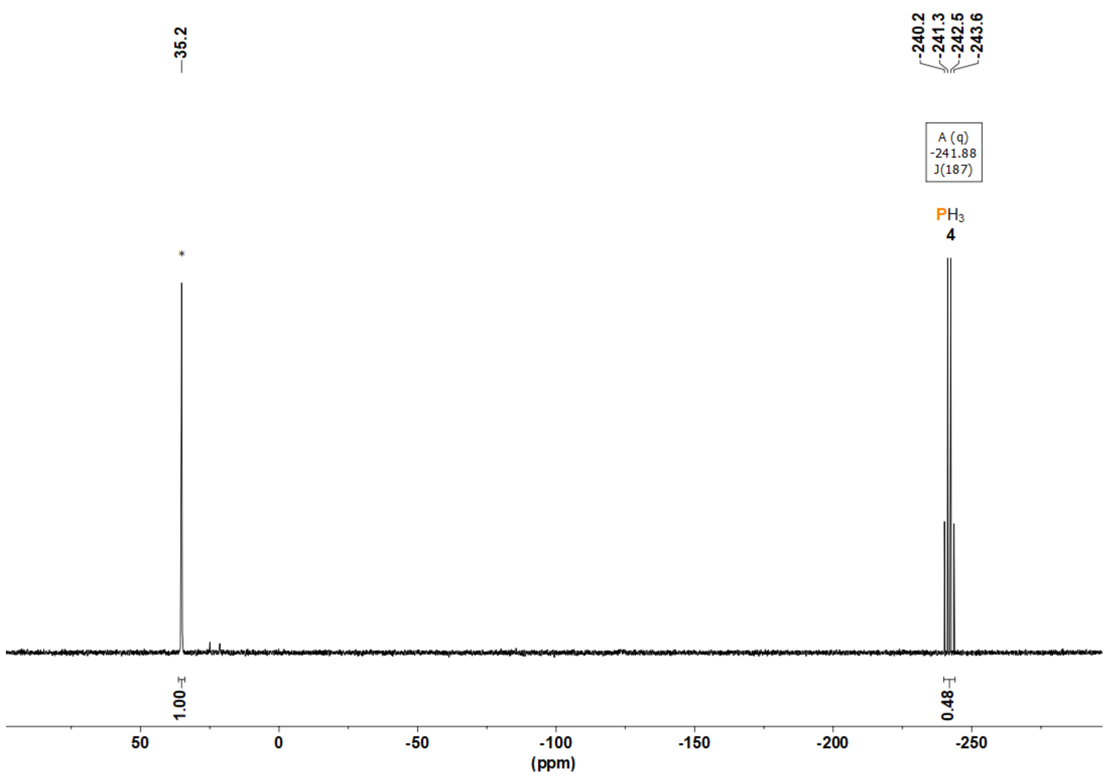


Figure S17. Quantitative ^{31}P NMR spectrum (D1 = 20 s) of PH_3 (**4**) generated *via* hydrogermylation of P_4 in PhMe, followed by acidification, in the presence of Ph_3PO (*) as an internal standard.

3.7. General procedure for the functionalisation of the mixture $(Ph_3Ge)_xPH_{3-x}$ (x = 1, 2)

The conversions of the products shown in this section were determined by a quantitative single scan inverse-gated $^{31}P\{^1H\}$ NMR (DS = 0, D1 = 2 s) methodology that we have described previously, and whose use to quantify tertiary phosphines and quaternary phosphonium salts has previously been validated.[16]

To a 10 mL, flat-bottomed, stoppered tube were added P_4 (0.01 mmol, as a stock solution in 84.3 µL PhH), PhMe (100 µL), and Ph_3GeH (36.6 mg, 0.12 mmol). The tube was sealed, placed in a water-cooled block to maintain near-ambient temperature, and irradiated with UV light (365 nm, 4.3 V, 700 mA, Osram OSLON SSL 80) for 24 hours (unless stated otherwise). The resulting clear yellowish solution was treated with the corresponding electrophiles as follows:

Reactivity towards benzyl bromide: Benzyl bromide (47.6 µL, 0.4 mmol) and KHMDS (19.9 mg, 0.1 mmol) were added to the yellowish solution, and heated to 100 °C with stirring for 3 days. After cooling to room temperature, Ph_3PO (0.02 mmol, stock solution in benzene) was subsequently added to act as an internal standard. Volatiles were removed under vacuum, and CH_3CN (0.5 mL) was then added. NMR analysis of the resulting mixture showed the formation of $[Bn_4P]Br$ (**5**) as the main product with 90 % conversion as shown in Figure S18.

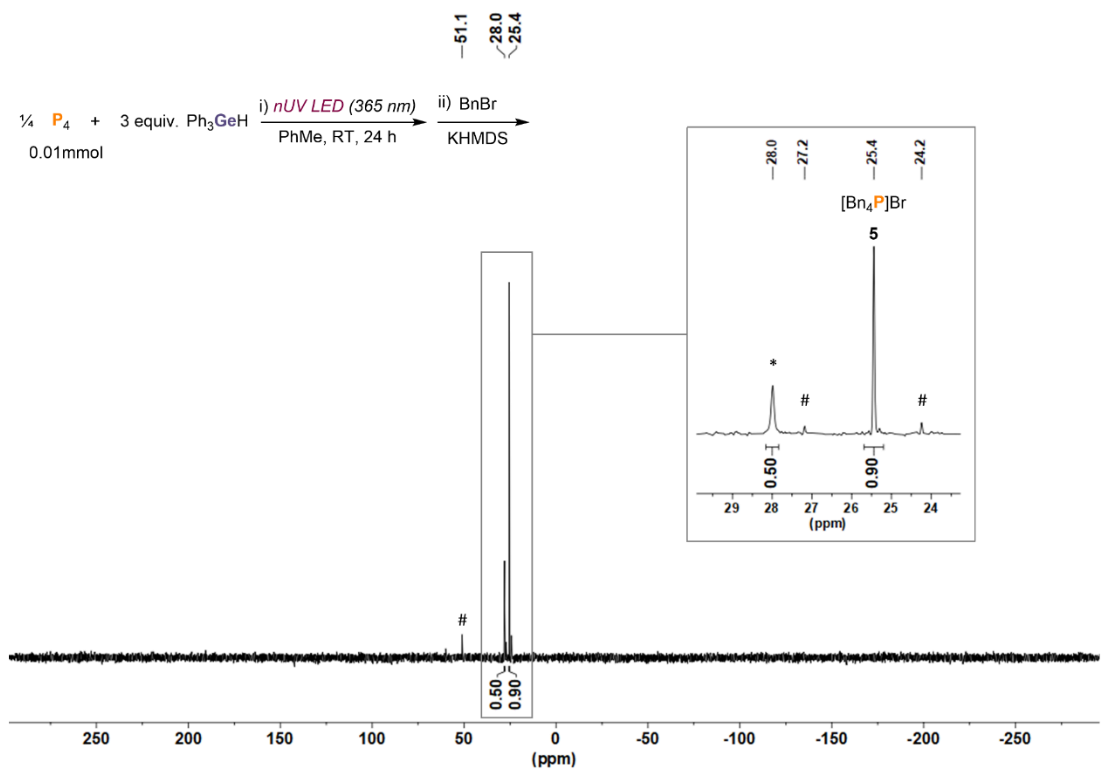


Figure S18. $^{31}P\{^1H\}$ NMR spectrum of $[Bn_4P]Br$ (**5**) generated *via* hydrogermylation of P_4 in PhMe, followed by treatment with benzyl bromide (0.4 mmol) and KHMDS (0.1 mmol), heated to 100 °C for 3 d. * marks the internal standard Ph_3PO (0.02 mmol). # marks unknown side products.

Reactivity towards bromoethane: Bromoethane (30 µL, 0.4 mmol) and KHMDS (19.9 mg, 0.1 mmol) were added to the yellowish solution, and heated to 100 °C with stirring for 3 days. After cooling to room temperature, Ph_3PO (0.02 mmol, stock solution in benzene) was subsequently added to act as an internal standard. Volatiles were removed under vacuum, and CH_3CN (0.5 mL) was then added. NMR analysis of the resulting mixture showed the formation of $[Et_4P]Br$ (**6**) as the main product with 42 % conversion as shown in Figure S19.

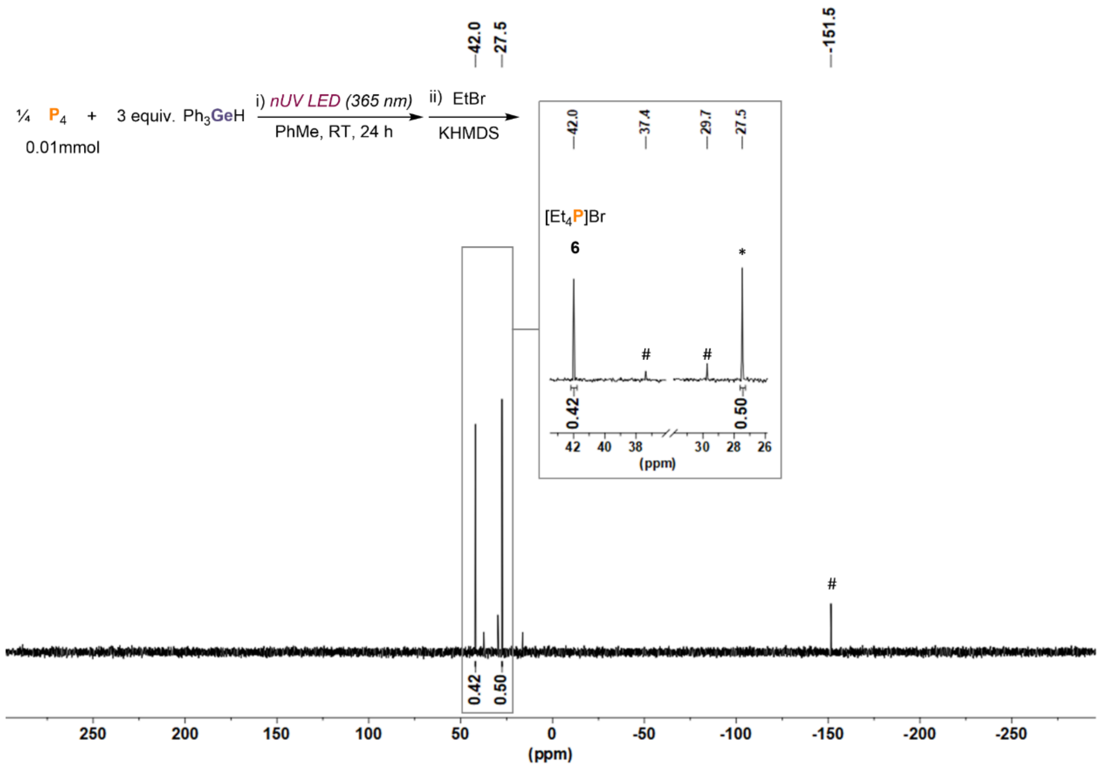


Figure S19. $^{31}P\{^1H\}$ NMR spectrum of $[Et_4P]Br$ (**6**) generated *via* hydrogermylation of P_4 in PhMe, followed by treatment with bromoethane (0.4 mmol) and KHMDS (0.1 mmol), heated to 100 °C for 3 d. * marks the internal standard Ph_3PO (0.02 mmol). # marks unknown side products.

Reactivity towards paraformaldehyde: Volatiles were removed under vacuum. EtOH (0.5 mL) and paraformaldehyde (15.0 mg, 0.5 mmol) were added to the oily solid residue, and the resulting suspension was heated to 50 °C with stirring for 2 days. After cooling to room temperature, the mixture was frozen in a liquid-nitrogen bath, and HCl (4.0 M in 1,4-dioxane, 100 µL, 0.4 mmol) was added. After thawing, the reaction mixture was stirred at room temperature for 2 hours. Ph_3PO (0.02 mmol, stock solution in benzene) was subsequently added to act as an internal standard. NMR analysis of the resulting mixture showed only traces of the desired product THPC (−27.6 ppm, <5% conversion), along with PH_3 (−242.7 ppm) and an unknown signal (−20.2 ppm), as shown in Figure S20.

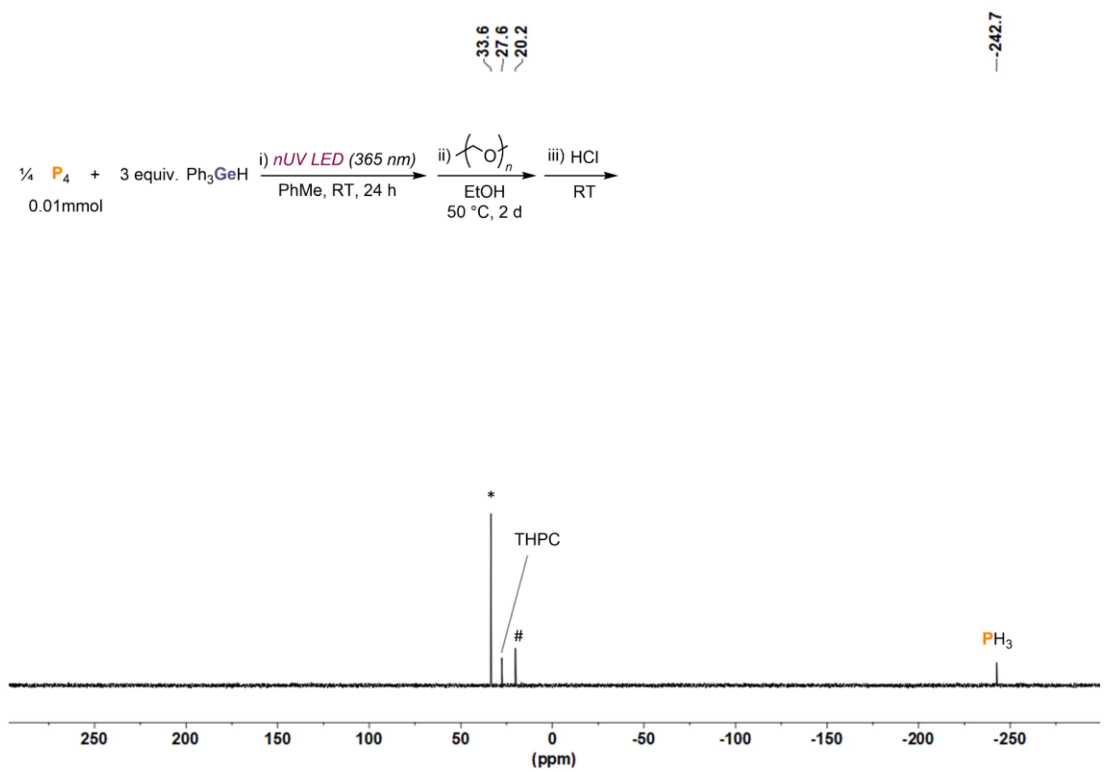


Figure S20. $^{31}P\{^1H\}$ NMR spectrum of THPC generated *via* hydrogermylation of P_4 in PhMe, followed by treatment with paraformaldehyde (0.5 mmol) in EtOH, heated to 50 °C for 2 d. Then, quenched with HCl (0.4 mmol).* marks the internal standard Ph_3PO (0.02 mmol). # marks unknown side products.

<u>*Reactivity towards benzoyl chloride:*</u> PhC(O)Cl (27.9 µL, 0.24 mmol) and KHMDS (19.9 mg, 0.1 mmol) were added to the yellowish solution, and stirred at room temperature for 24 hours. The resulting mixture was analysed by $^{31}P\{^1H\}$ and ^{31}P NMR spectroscopy as shown in Figure S21.

The spectra show the complete consumption of the crude **1**/**2** mixture and the formation of the desired product $P(C(O)Ph)_3$ at −54.1 ppm, albeit in trace amounts. Two other unidentified P-containing species were observed at −24.6 and −75.3 ppm, the latter being the main product of this reaction. Based on their chemical shifts and the absence of $^1J(^{31}P\text{-}^1H)$ splitting in the proton-coupled spectrum, these resonances are attributed to partially acylated species such as $Ph_3GeP(C(O)Ph)_2$ or $(Ph_3Ge)_2PC(O)Ph$ (or possibly $Ph_3GeP(Ph)C(O)Ph$, formed *via* acylation of side-product **3**). Similar outcomes were observed during experiments with higher temperatures and extended reaction times. Analogous experiments using fewer equivalents of PhC(O)Cl were also unsuccessful in our attempts to target these potential intermediates more selectively.

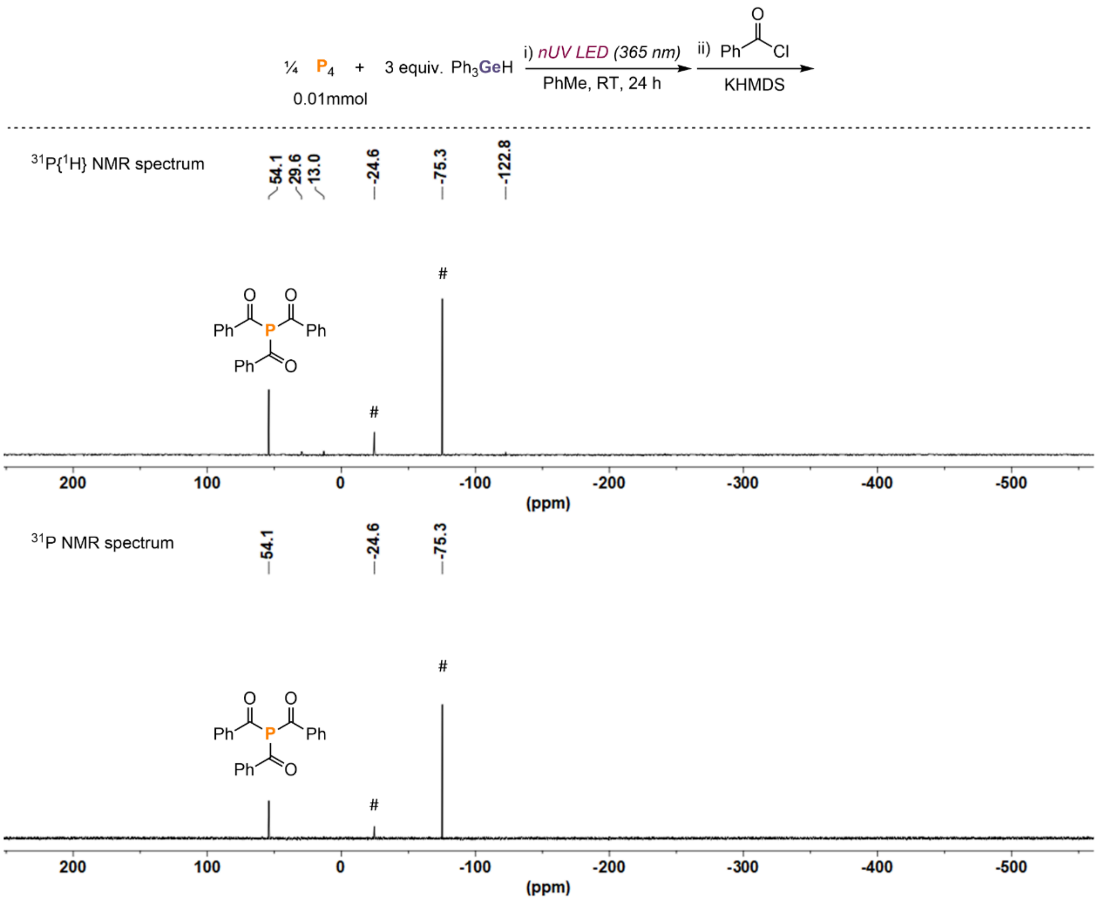


Figure S21. $^{31}P\{^1H\}$ and ^{31}P NMR spectra for the hydrogermylation of P_4 in PhMe, followed by treatment with benzoyl chloride (0.24 mmol) and KHMDS (0.1 mmol), stirred at room temperature for 24 h. # marks unknown species.

Reactivity towards pivaloyl chloride: *t*BuC(O)Cl (29.6 µL, 0.24 mmol) and KHMDS (19.9 mg, 0.1 mmol) were added to the yellowish solution, and heated to 60 °C with stirring for 24 hours. The resulting mixture was analysed by $^{31}P\{^1H\}$ and ^{31}P NMR spectroscopy as shown in Figure S22.

Similar to the reaction with benzoyl chloride, the $^{31}P\{^1H\}$ NMR spectrum shows only traces amounts of the desired product $P(C(O)tBu)_3$ (−51.9 ppm) along with a variety of other unknown species. The main product of this reaction appears as a singlet resonance at −117.1 ppm, which splits into a doublet in the ^{31}P spectrum ($^1J(^{31}P\text{-}^1H)$ = 200 Hz). Given the similarities on chemical shift and $^1J(^{31}P\text{-}^1H)$ coupling constant with analogous compounds ($Bu_3SnP(H)C(O)tBu$[20] and $Me_3SiP(H)C(O)tBu$[57]), this species was assigned as $Ph_3GeP(H)C(O)tBu$. Additional experiments using fewer equivalents of *t*BuC(O)Cl, in our attempts to target this potential intermediate more selectively, were unsuccessful. Moreover, similar outcomes were observed during experiments at higher temperatures and with longer reaction times.

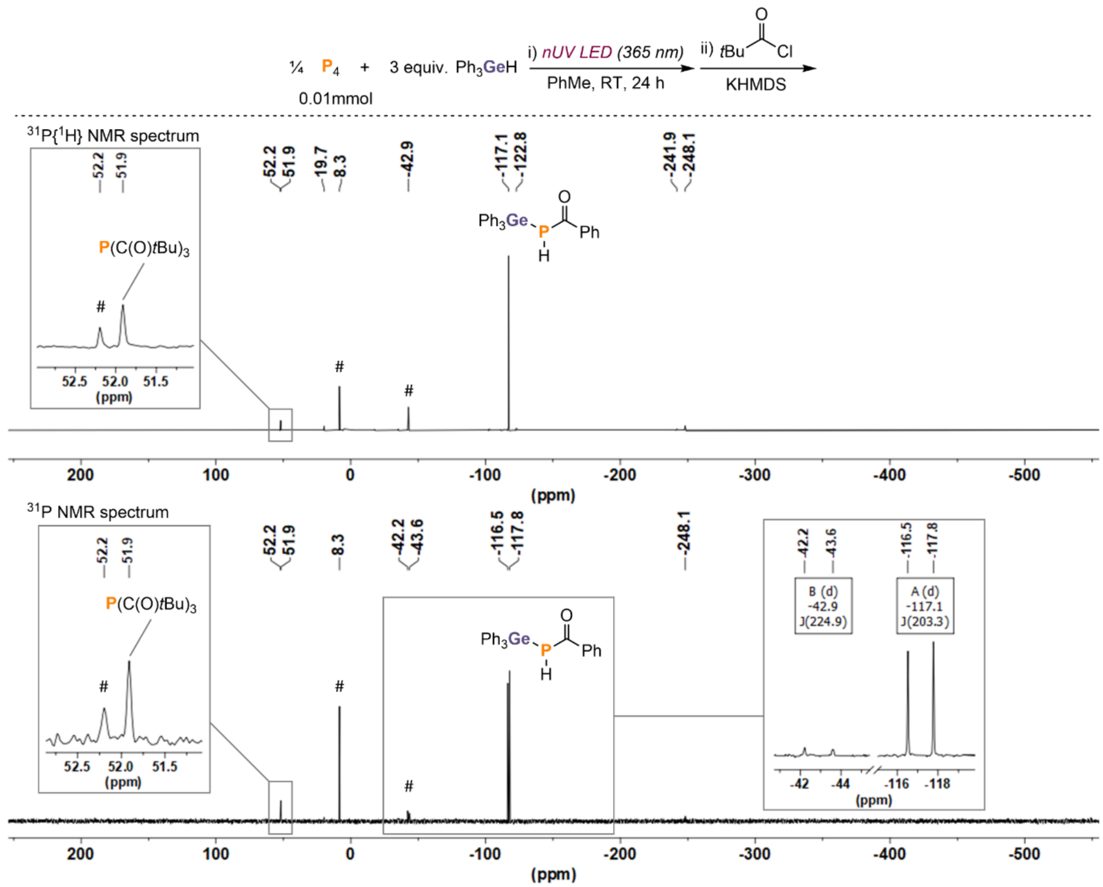
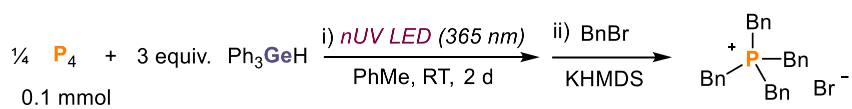


Figure S22. $^{31}P\{^1H\}$ and ^{31}P NMR spectra for the hydrogermylation of P_4 in PhMe, followed by treatment with benzoyl chloride (0.24 mmol) and KHMDS (0.1 mmol), heated to 60 °C for 24 h. # marks unknown species.

3.8. Synthesis and isolation of TBPB (5) via hydrogermylation of P_4 (0.1 mmol scale)



To a 50 mL, flat-bottomed, stoppered tube were added P_4 (12.4 mg, 0.1 mmol), PhMe (2.0 mL), and Ph_3GeH (366.0 mg, 1.2 mmol). After stirring to obtain a homogeneous solution, the tube was placed in a water-cooled block to maintain near-ambient temperature, and irradiated with UV light (365 nm, 14 V, 700 mA, Osram OSLON SSL 80) for 2 days. To the yellowish solution benzyl bromide (476 µl, 4.0 mmol) and KHMDS (120 mg, 0.6 mmol) were added and the reaction mixture heated to 100 °C with stirring for 3 days. After cooling to room temperature the pale yellow suspension was filtered, and the remaining solid was washed with PhMe (3 x 6 mL) and extracted into acetonitrile (3 x 10 mL). Removal of volatiles under vacuum yielded the target product as a white solid (146 mg, 77 %).

^{1}H NMR (400 MHz, 300 K, CD_3CN) : δ = 7.35 ppm (3H, m), 7.21 ppm (2H, m), 3.87 ppm (2H, d, $^2J(^{31}P-^1H)$ = 14.6 Hz). **^{31}P{^{1}H} NMR** (121 MHz, 300 K, CD_3CN) : δ = 25.8 ppm (s). **^{31}P NMR** (121 MHz, 300 K, CD_3CN) : δ = 25.8 ppm (m). NMR data are consistent with our previous report.[20]

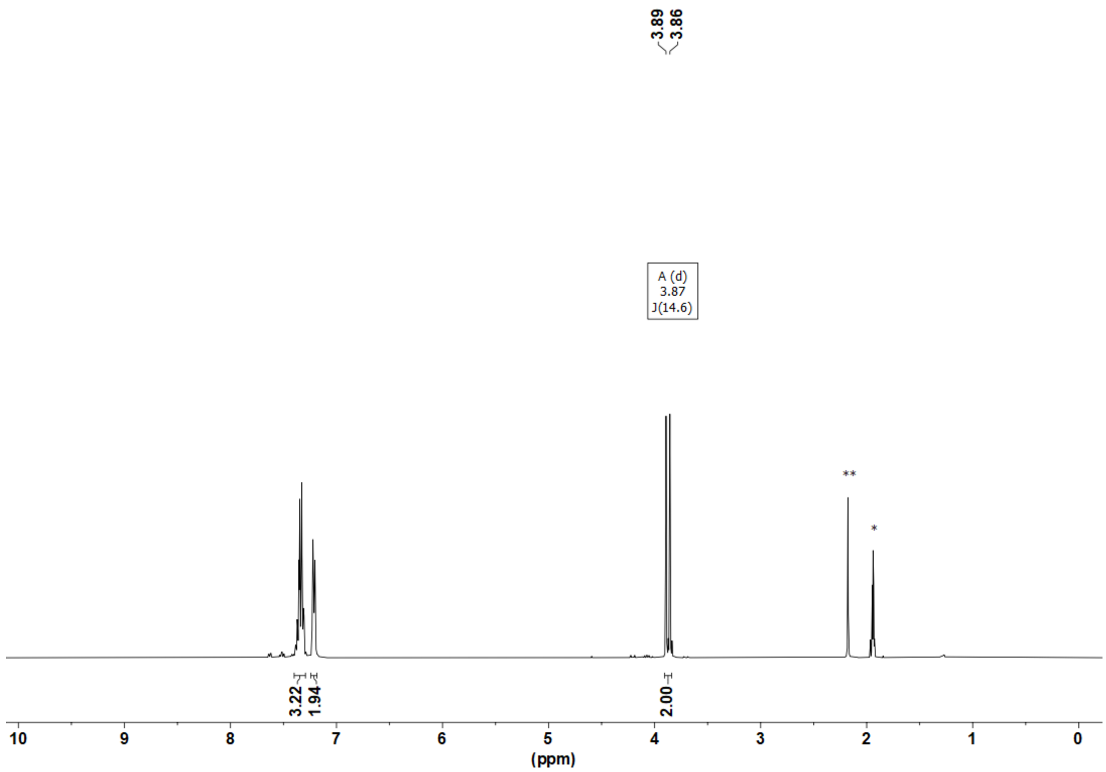


Figure S23. ^{1}H NMR spectrum of $[Bn_4P]Br$ (**5**) in CD_3CN (*solvent, **H_2O).

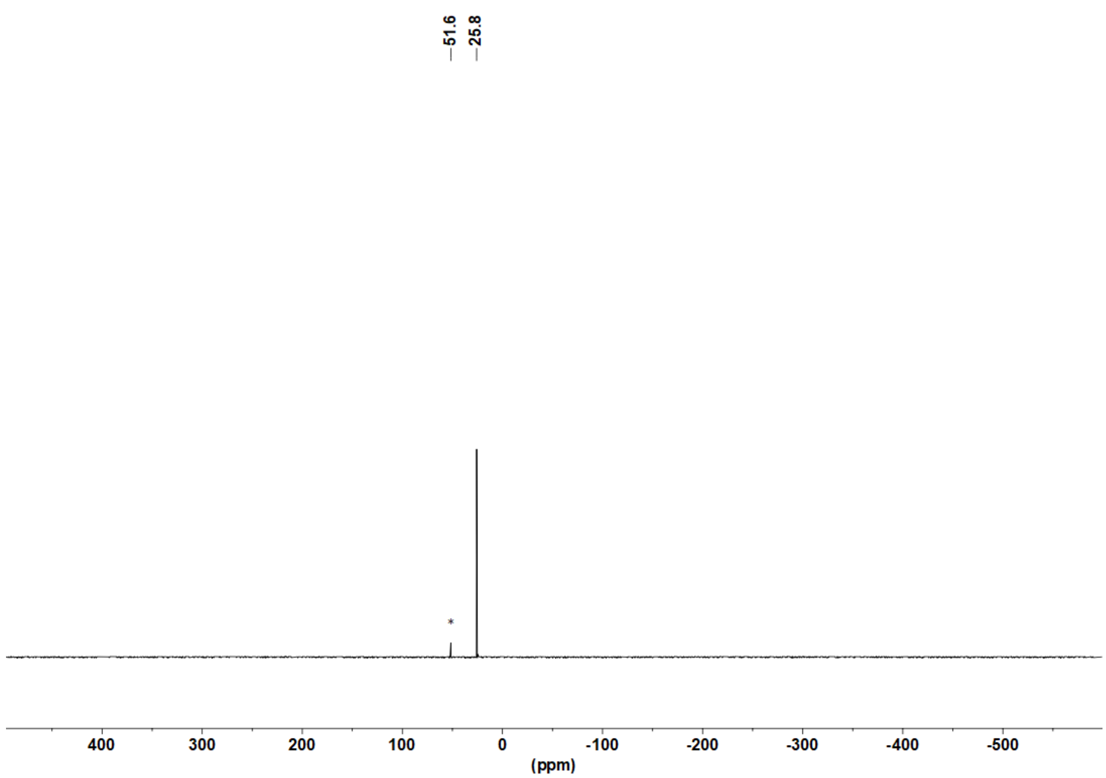


Figure S24. ^{31}P{^{1}H} NMR spectrum of $[Bn_4P]Br$ (**5**) in CD_3CN. * maks an unknown side product.

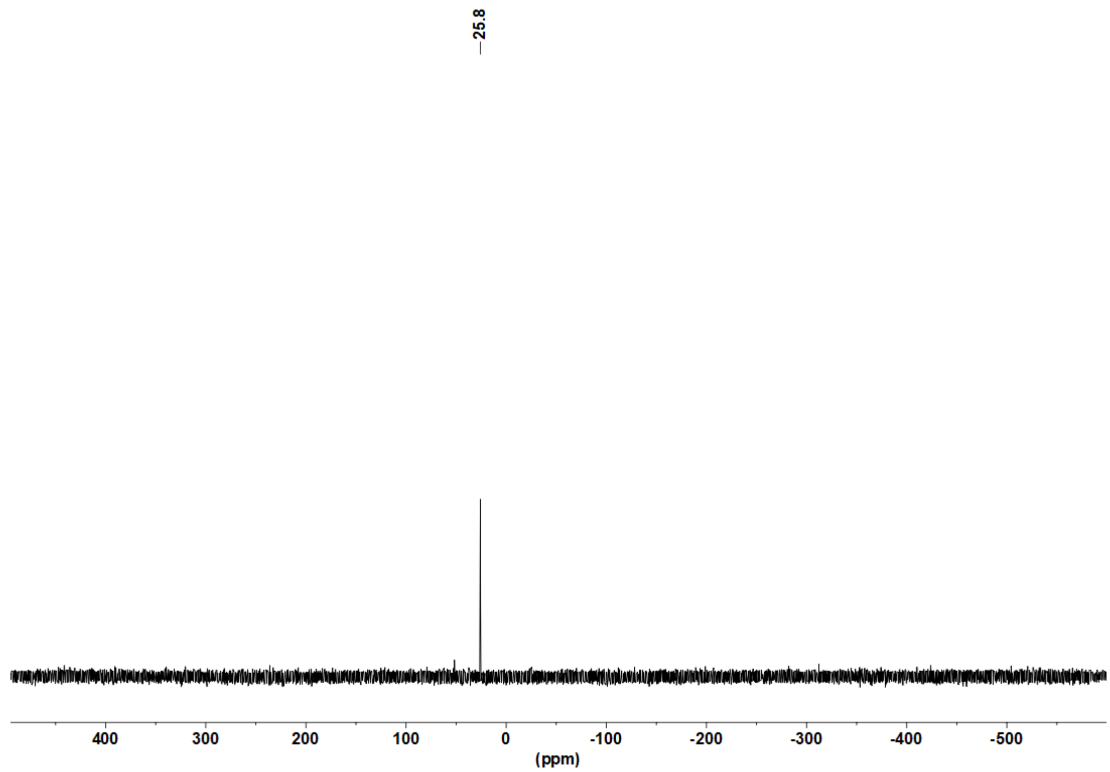
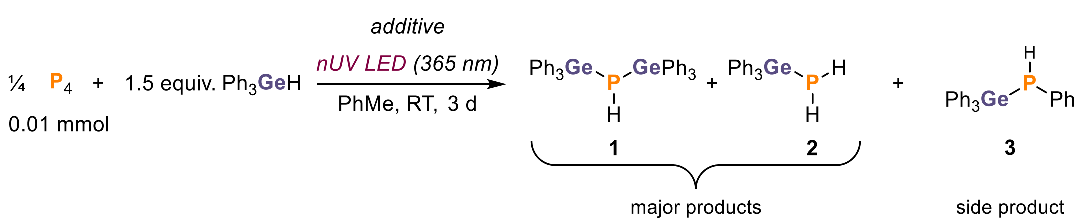


Figure S25. ^{31}P NMR spectrum of $[Bn_4P]Br$ (**5**) in CD_3CN.

3.9. Hydrogermylation of P_4 using Ph_3GeH and HAT donors (0.01 mmol scale): general procedure and optimization

The hydrogermylation of P_4 mediated by a HAT donor was also investigated. In summary, the outcomes of these reactions were found to be similar to those observed in the absence of additives, apart from different product distribution and the presence of PH_3 in the $^{31}P\{^1H\}$ and ^{31}P NMR spectra, in minor to considerable amounts. See Figures S26 and S27 for selected examples.



Representative procedure:

To a 10 mL, flat-bottomed, stoppered tube were added P_4 (0.01 mmol, as a stock solution in 84.3 µL PhH), PhMe (100 µL), Ph_3GeH (18.3 mg, 0.06 mmol) and 1,4-CHD (5.7 µL, 0.06 mmol). The tube was sealed, placed in a water-cooled block to maintain near-ambient temperature, and irradiated with UV light (365 nm, 4.3 V, 700 mA, Osram OSLON SSL 80) for 3 days (unless stated otherwise). Ph_3PO (0.02 mmol, stock solution in benzene) was subsequently added to act as an internal standard. The resulting mixture was analysed by ^1H, $^{31}P\{^1H\}$, and ^{31}P NMR spectroscopy.

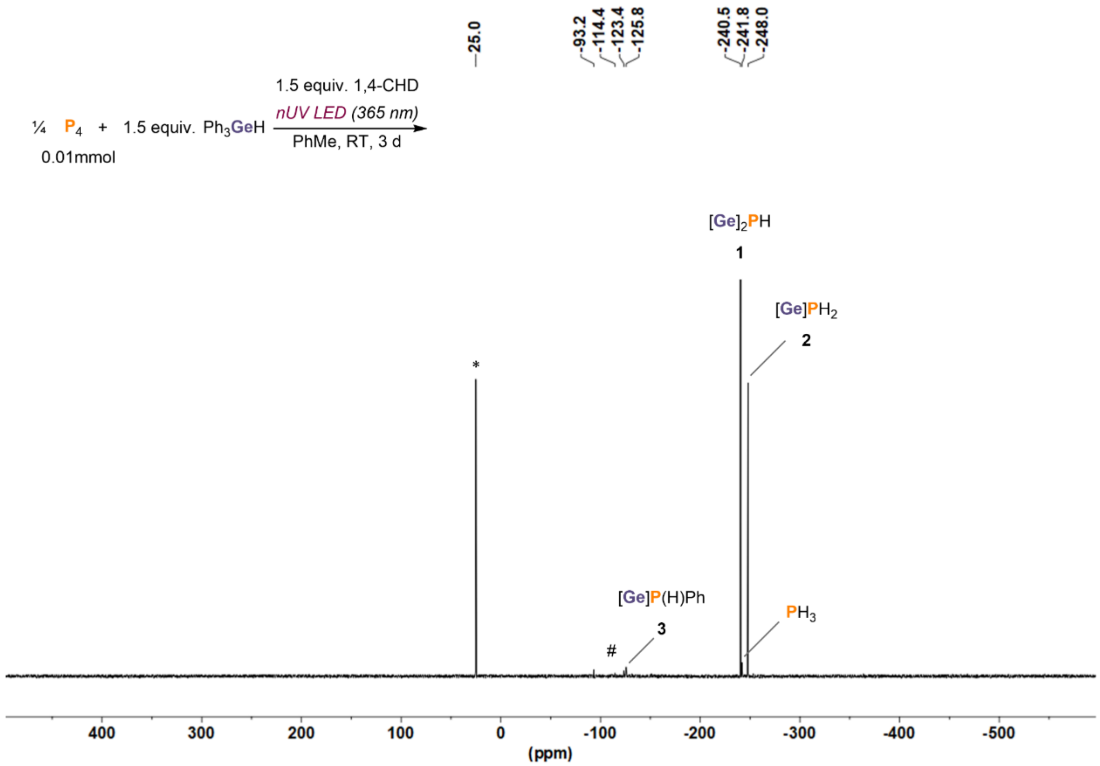


Figure S26. $^{31}P\{^{1}H\}$ NMR spectrum for the reaction of P_4 with Ph_3GeH (0.06 mmol) and 1,4-CHD (0.06 mmol) in PhMe and driven by 356 nm, 3 W LED irradiation for 3 d (Table S5, Entry 6). * marks the internal standard Ph_3PO. # marks unknown side products. [Ge] = Ph_3Ge.

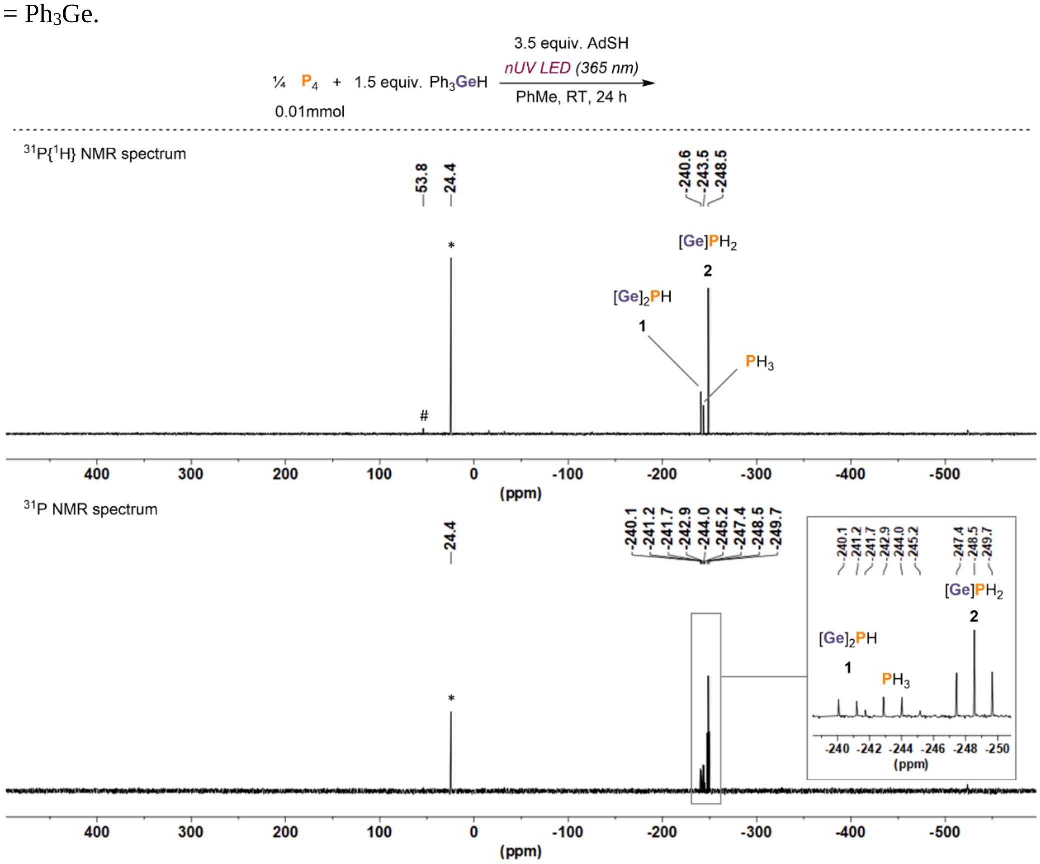
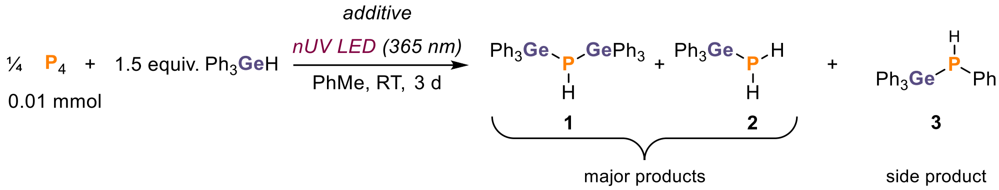


Figure S27. $^{31}P\{^{1}H\}$ and ^{31}P NMR spectra for the reaction of P_4 with Ph_3GeH (0.06 mmol) and AdSH (1-adamantanethiol, 0.14 mmol) in hexane and driven by 356 nm, 3 W LED irradiation for 3 d (Table S5, Entry 2). * marks the internal standard Ph_3PO. # marks unknown side products. [Ge] = Ph_3Ge.

Table S5. Optimization of hydrogermylation of P_4 using Ph_3GeH in the presence of a HAT donor.[a]

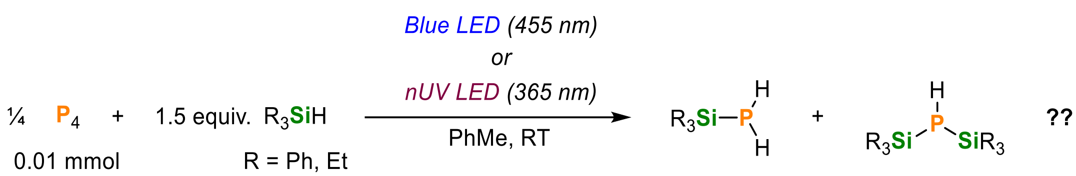


Entry	Additive (mmol)	PhMe (μL)	Time (days)	Full conv. of **P**$_4$?	Relative conv. to **1** and **2** (%)[b,c]	Relative conv. to **3** (%)
1	AdSH (0.06)	500 (hexane)	3	✓	23.6	traces
2	AdSH (0.14)	500 (hexane)	3	✓	26.1	-
3	PhSH (0.01)	500	3	✓	49.4	traces
4	PhSH (0.06)	500	3	✓	19.3	traces
5	1,4-CHD (0.01)	100	3	✓	54.9	12.7
6	1,4-CHD (0.06)	100	3	✓	62.1	traces
7	*i*Pr_3SiSH (0.06)	500 (hexane)	3	✓	60.1	7.1

[a] The general procedure described in this section was modified to use the indicated amount of reactant and solvent. [b] Conversions were calculated by integration of the ^{31}P resonances of **1**-**3** relative to an internal standard, which was then normalized relative to Table S2, entry 9 as described in Section 3.2. [c] The signal assigned to PH_3 was observed in the $^{31}P\{^1H\}$ and ^{31}P NMR spectra (see Figures S26 and S27 for selected examples).

4. Hydrosilylation of white phosphorus (P_4)

4.1. General procedure for reactivity studies of R_3SiH (R = Ph, Et) towards P_4 under LED irradiation (0.01 mmol scale)



To a 10 mL, flat-bottomed, stoppered tube were added P_4 (0.01 mmol, as a stock solution in 84.3 μL PhH), PhMe (100 μL) and Ph_3SiH (15.6, 0.06 mmol) or Et_3SiH (18.5 μL, 0.06 mmol). The tube was sealed, placed in a water-cooled block to maintain near-ambient temperature, and irradiated with blue light (455 nm, 3.2 V, 700 mA, Osram OSLON SSL 80) or UV light (365 nm, 4.3 V, 700 mA, Osram OSLON SSL 80) for 3 days (unless stated otherwise). The resulting mixture was analysed by ^1H, $^{31}P\{^1H\}$, and ^{31}P NMR spectroscopy.

The $^{31}P\{^1H\}$ NMR spectra for the reaction of P_4 with R_3SiH (R = Ph, Et) only showed uncomsumed P_4. Figure S28 displays the $^{31}P\{^1H\}$ NMR spectrum for the reaction of P_4 with Ph_3SiH (0.06 mmol) in PhMe driven by 365 nm LED irradiation for 3 days as a selected example.

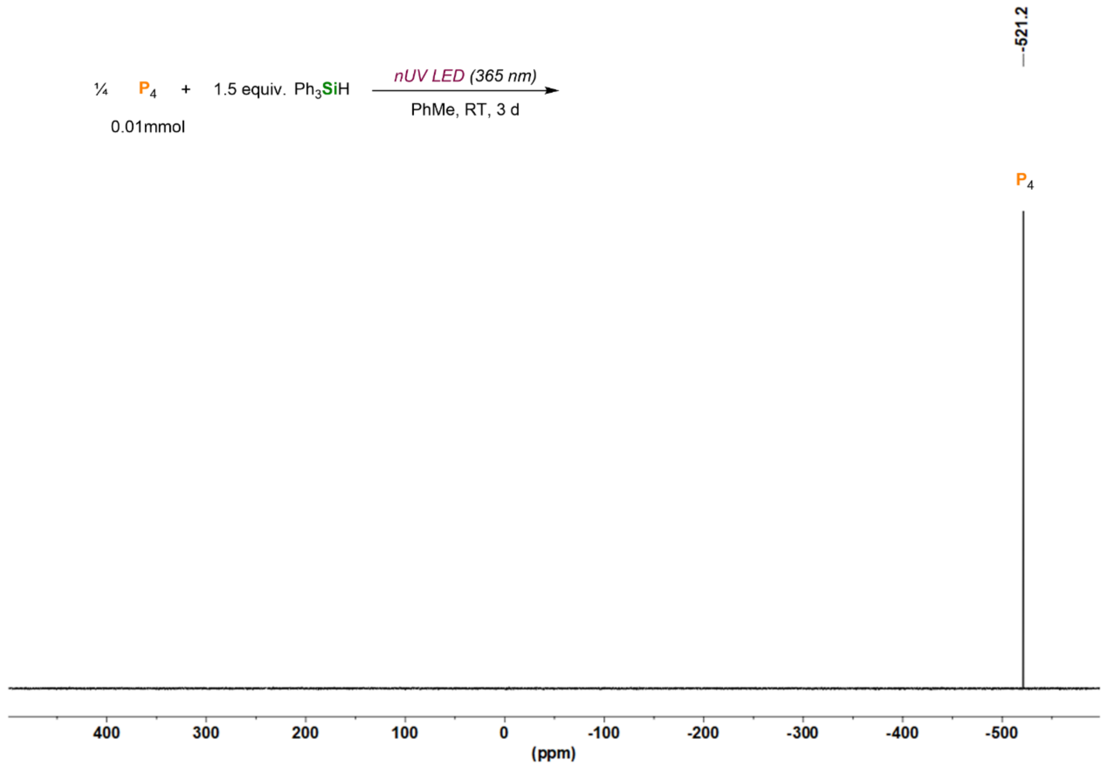
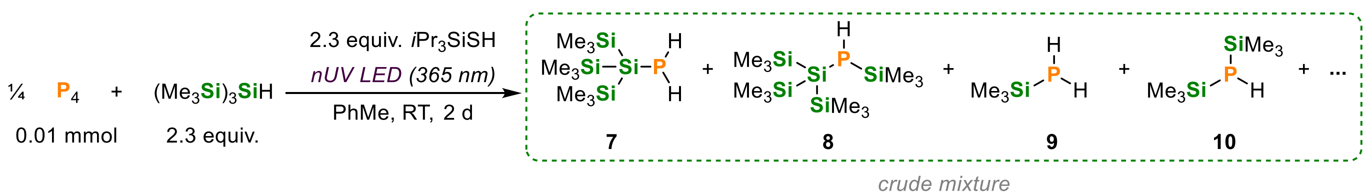


Figure S28. $^{31}P\{^1H\}$ NMR spectrum for the reaction of P_4 with Ph_3SiH (0.06 mmol) in PhMe and driven by 365 nm, 3 W LED irradiation for 3 d.

4.2. General procedure and optimisation for the hydrosilylation of P_4 using $(Me_3Si)_3SiH$ and *i*Pr_3SiSH, under LED irradiation (0.01 mmol scale)



To a 10 mL, flat-bottomed, stoppered tube were added P_4 (0.01 mmol, as a stock solution in 84.3 µL PhH), PhMe (100 µL), $(Me_3Si)_3SiH$ (27.9 µL, 0.09 mmol), and *i*Pr_3SiSH (19.3 µL, 0.09 mmol). The tube was sealed, placed in a water-cooled block to maintain near-ambient temperature, and irradiated with UV light (365 nm, 4.3 V, 700 mA, Osram OSLON SSL 80) for 2 days (unless stated otherwise). Ph_3PO (0.02 mmol, stock solution in benzene) was subsequently added to act as an internal standard. The resulting mixture was analysed by $^{31}P\{^1H\}$ and ^{31}P NMR spectroscopy, as shown in Figures S29-31, below.

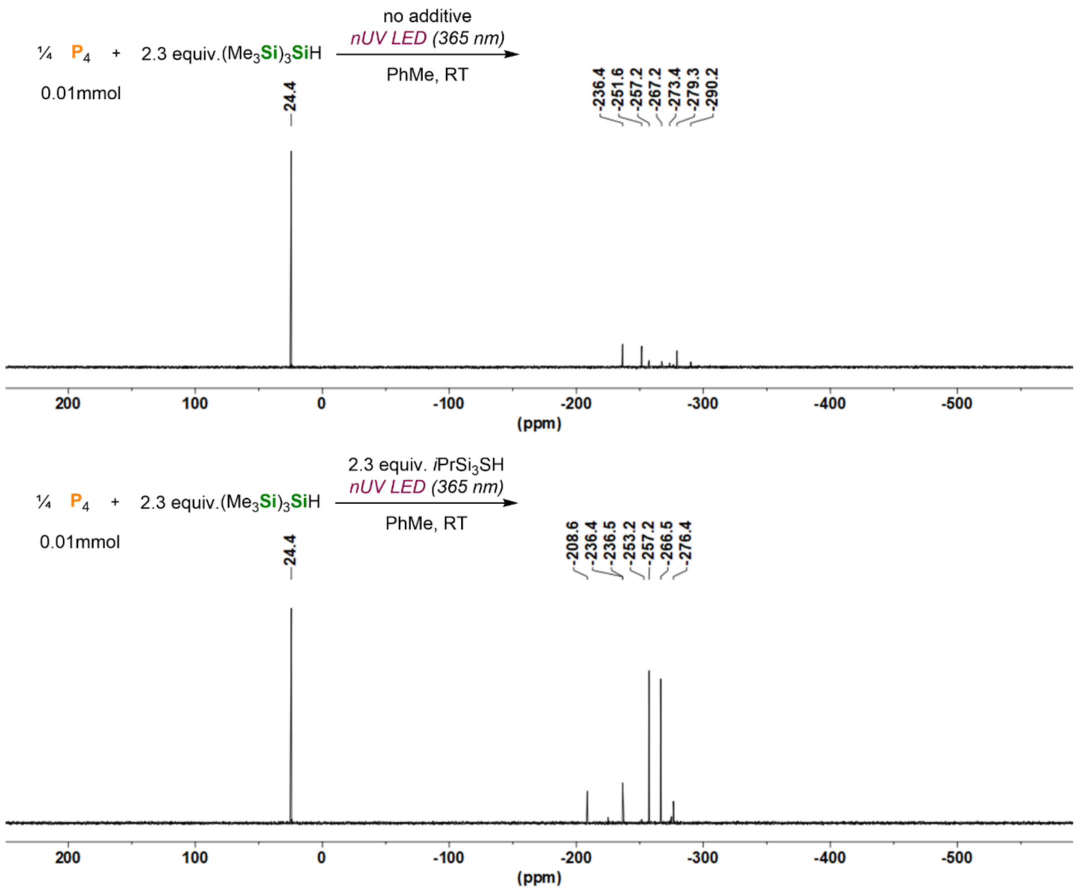


Figure S29. $^{31}P\{^{1}H\}$ NMR spectra for the reactions of P_4 with $(Me_3Si)_3SiH$ (0.14 mmol) and no additive (top) or in the presence of $i$$Pr_3SiSH$ (0.14 mmol) as additive (bottom), both in hexane and driven by 365 nm, 3 W LED irradiation for 3 or 1 days, respectively. * marks the internal standard Ph_3PO (0.02 mmol).

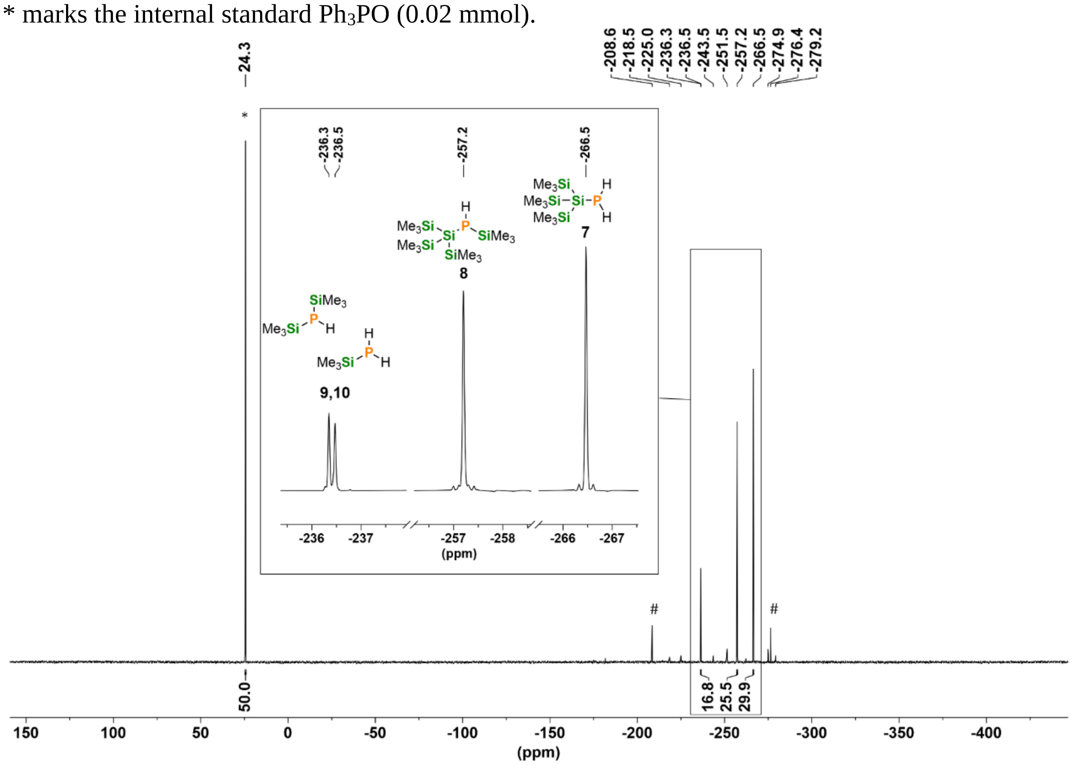


Figure S30. Quantitative $^{31}P\{^{1}H\}$ NMR spectrum (D1 = 40 s) for the reaction of P_4 with $(Me_3Si)_3SiH$ (0.14 mmol) and $i$$Pr_3SiSH$ (0.14 mmol) in hexane and driven by 390 nm, 40W LED irradiation for 24 h. * marks the internal standard Ph_3PO (0.02 mmol). # marks unknown side products. Assigments are consistent with previous reports.[39,40]

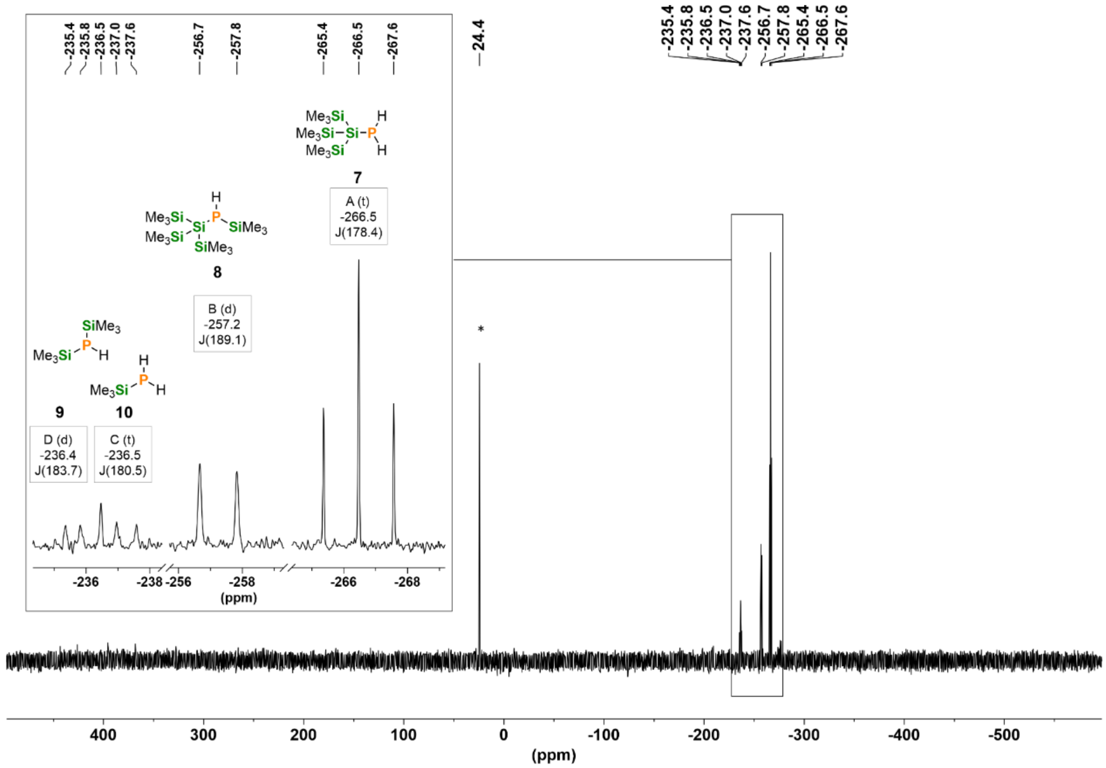
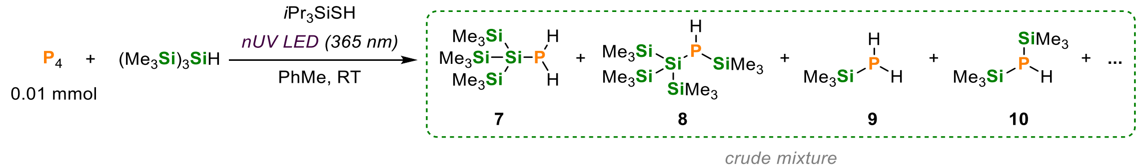


Figure S31. ^{31}P NMR spectrum for the reaction of P_4 with $(Me_3Si)_3SiH$ (0.14 mmol) and *i*Pr_3SiSH (0.14 mmol) in hexane and driven by 390 nm, 40W LED irradiation for 24 h. The insets show expansions of the signals attributed to $[(Me_3Si)_3Si]PH_2$ (**7**), $[(Me_3Si)_3Si]P(H)SiMe_3$ (**8**), Me_3SiPH_2 (**9**) and $(Me_3Si)_2PH$ (**10**), highlighting their multiplicity due to $^1J(^{31}P\text{-}^1H)$ couplings. * marks the internal standard Ph_3PO (0.02 mmol). Assigments are consistent with previous reports.[39,40]

For reasons of experimental expediency, during the optimization of the hydrosilylation of P_4, acquisition of quick but non-quantitative $^{31}P\{^1H\}$ NMR spectra was used to analyse each experiment and to assess the relative total conversion to **7-10**. Although this did not directly provide precise, quantitative conversions it did allow for meaningful, qualitative comparisons between experiments. Under the conditions highlighted in Table S6, entry 4 a quantitative $^{31}P\{^1H\}$ NMR spectrum was recorded using an inverse-gated decoupled pulse sequence (D1 = 40 s, Figure S30), and the conversion of P_4 to products **7-10** was determined. Thus, for ease of interpretation, the integrals measured for **7-10** for all optimization experiments have been normalized relative to the value for this experiment (Table S6, entry 4) to provide the relative conversions indicated in Table S6. However, additional integrations (of signals of as yet unidentified monophosphorus species) have not been taken into account, although they may contribute to the final yield in the formation of the desired end products (*e.g.* PH_3) after subsequent functionalization with electrophiles.

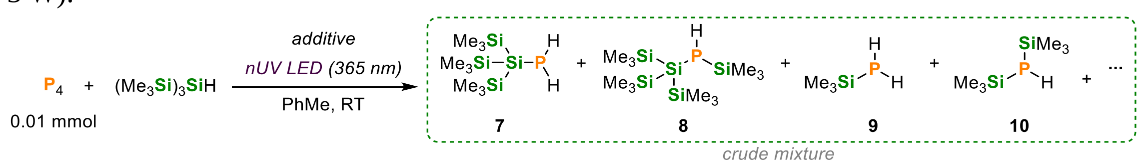
Table S6. Optimization of hydrosilylation of P_4 using $(Me_3Si)_3SiH$, $i$$Pr_3SiSH$, and near-UV LED irradiation (365 nm, 3 W).[a]



Entry	$(Me_3Si)_3SiH$ (mmol)	$i$$Pr_3SiSH$ (mmol)	PhMe (μL)	Time (days)	Full conv. of $\mathbf{P_4}$?	Relative conv. to **7-10** (%)[b]
1[c]	0.06	-	500	1	✓	traces
2[d]	0.06	-	500	3	✓	traces
3[e]	0.14	-	500 (hexane)	3	✓	6.1
4[e]	0.14	0.14	500 (hexane)	1	✓	72.2
5	0.14	0.14	500 (hexane)	1	✓	73.4
6	**0.14**	**0.14**	**500**	**1**	**✓**	**77.5**
7	0.14	0.06	500	3	✓	69.8
8	0.14	0.01	500	3	✓	8.9
9	0.06	0.06	500	1	✓	42.4
10	0.06	0.06	500	2	✓	44.3
11	0.06	0.06	500	3	✓	49.9
12	0.09	0.09	500	4	✓	72.7
13	0.09	0.09	100	3	✓	67.0
14	**0.09**	**0.09**	**100**	**2**	**✓**	**67.4**
15	0.09	0.09	100	1	✓	55.0

[a] The general procedure described in this section was modified to use the indicated amount of reactants and solvent. [b] Conversions were calculated by integration of the ^{31}P resonances of **7-10** relative to an internal standard, which was then normalized relative to entry 4 as described in the text above. [c] 455 nm. [d] 365 nm, 10 W.[e] 390nm 40 W.

Table S7. Screening of additive for the hydrosilylation of P_4 using $(Me_3Si)_3SiH$ and near-UV LED irradiation (365 nm, 3 W).[a]



Entry	$(Me_3Si)_3SiH$ (mmol)	*additive* (mmol)	PhMe (μL)	Time (days)	Full conv. of $\mathbf{P_4}$?	Relative conv. to **7-10** (%)
1	0.06	CySH (0.06)	500	4	✓	21.0
2	0.14	AdSH (0.14)	500 (hexane)	1	✓	71.9
3	0.06	AdSH (0.06)	500 (hexane)	1	✓	35.9
4	0.14	PhSH (0.14)	500	1	✓	67.8
5	0.14	4-MePhSH (0.14)	500	1	✓	76.5
6	0.14	4-MePhSH (0.06)	500	1	✓	26.8
7	0.09	1,4-CHD (0.09)	100	3	✓	71.0
8[c]	0.09	1,4-CHD (0.09)	100	3	✓	50.3

[a] The general procedure described in this section was modified to use the indicated amount of reactants and solvent. [b] Conversions were calculated by integration of the ^{31}P resonances of **7-10** relative to an internal standard, which was then normalized relative to Table S6, entry 4 as described in the text above. [c] 455 nm.

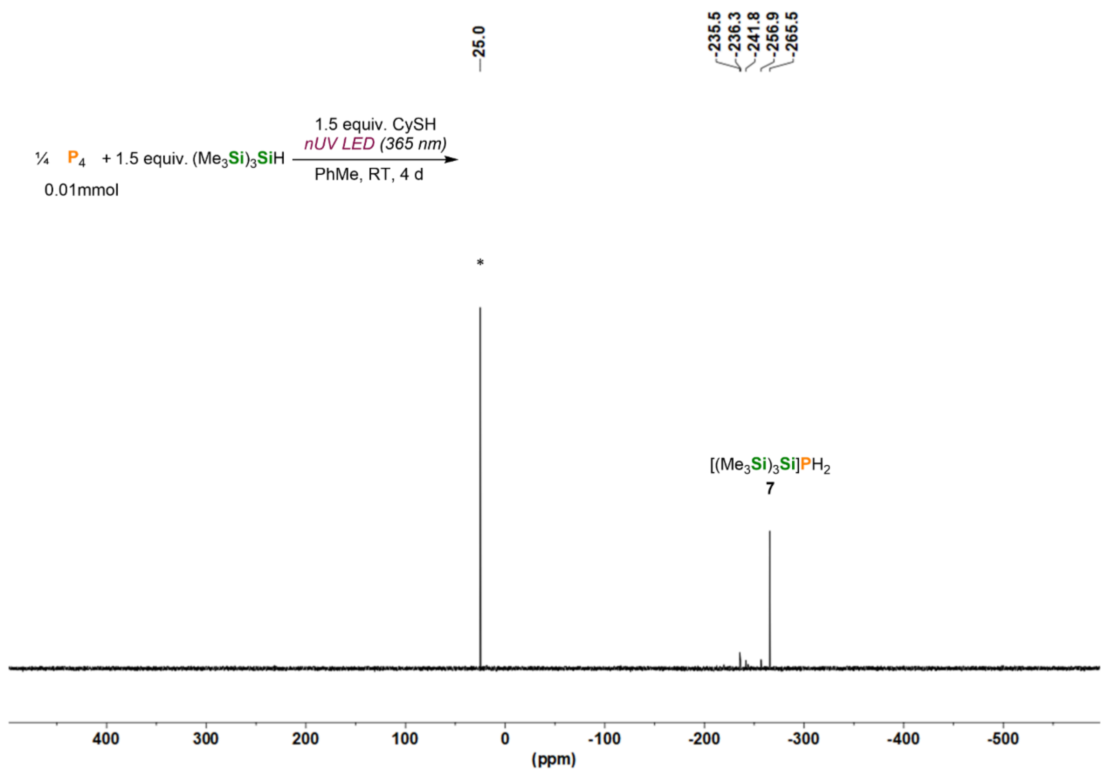


Figure S32. $^{31}P\{^{1}H\}$ NMR spectrum for the reaction of P_4 with $(Me_3Si)_3SiH$ (0.06 mmol) and CySH (0.06 mmol) in PhMe and driven by 365 nm, 3 W LED irradiation for 4 d (Table S7, Entry 1). * marks the internal standard Ph_3PO (0.02 mmol).

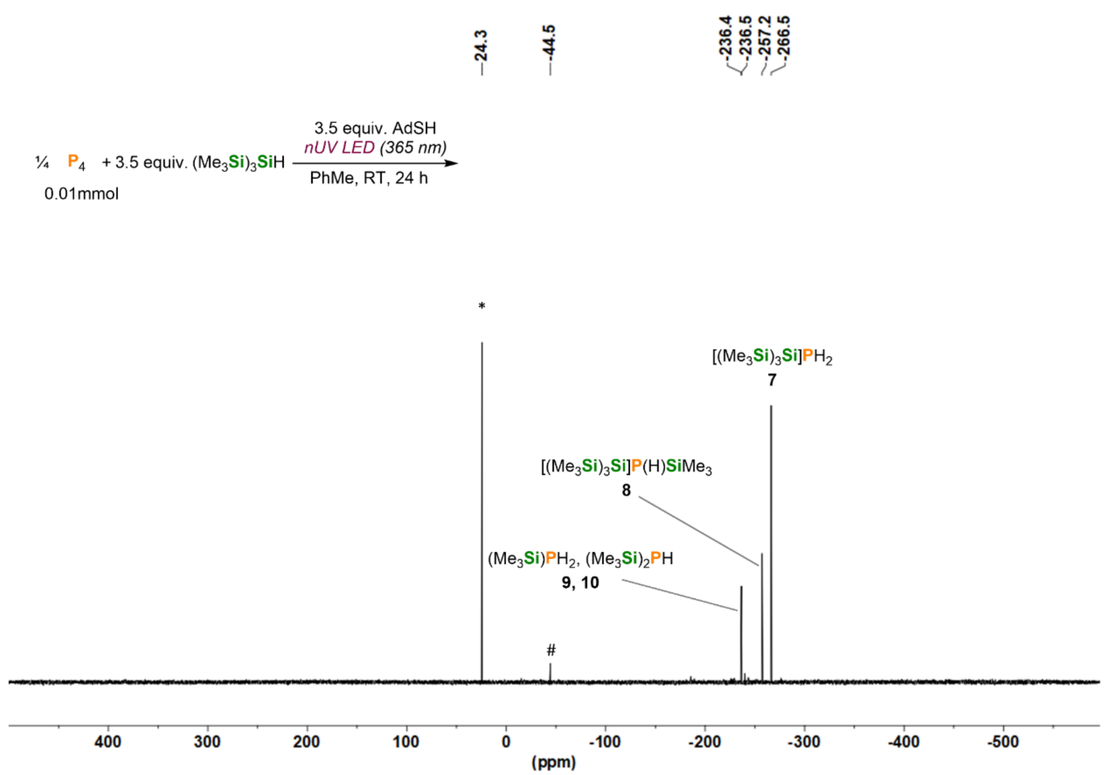


Figure S33. $^{31}P\{^{1}H\}$ NMR spectrum for the reaction of P_4 with $(Me_3Si)_3SiH$ (0.14 mmol) and AdSH (0.14 mmol) in hexane and driven by 365 nm, 3 W LED irradiation for 24 h (Table S7, Entry 2). * marks the internal standard Ph_3PO (0.02 mmol). # marks an unknown side product.

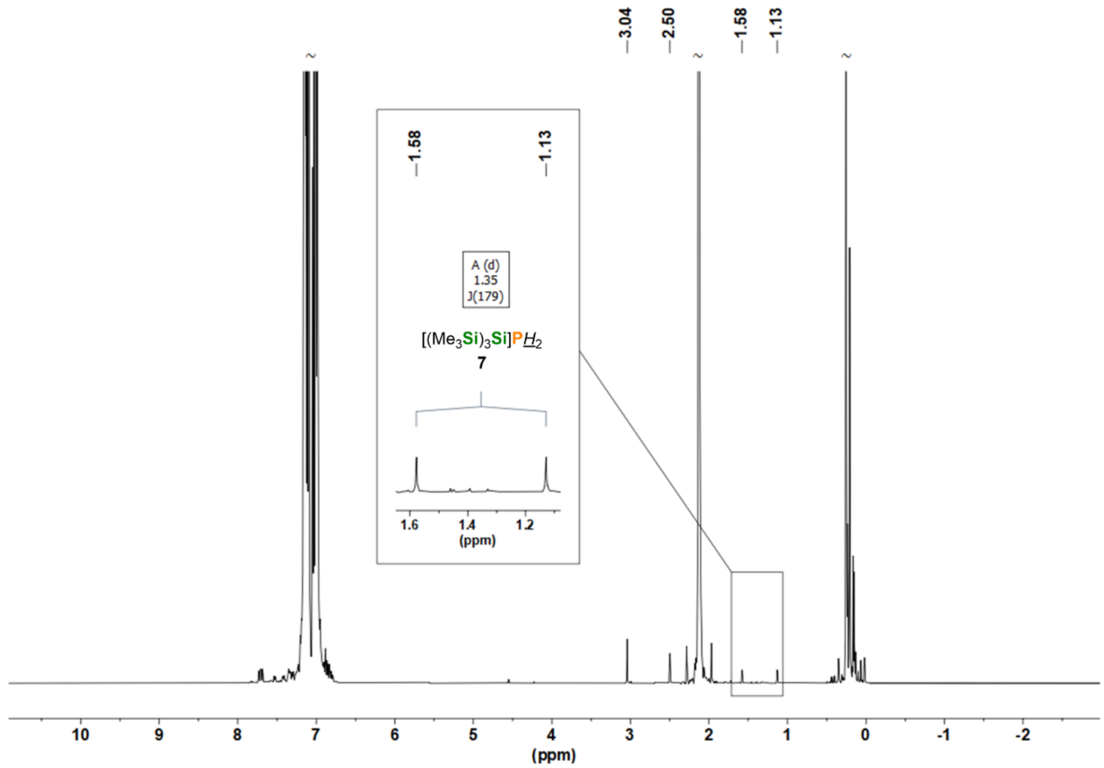


Figure S34. ^{1}H NMR spectrum for the reaction of P_4 with $(Me_3Si)_3SiH$ (0.14 mmol) and PhSH (0.14 mmol) in PhMe and driven by 365 nm, 3 W LED irradiation for 24 h (Table S7, Entry 4). The inset shows expansion of the doublet resonances attributed to the PH_2 moiety of $[(Me_3Si)_3Si]PH_2$ (**7**).~ marks solvent resonances truncated for clarity.

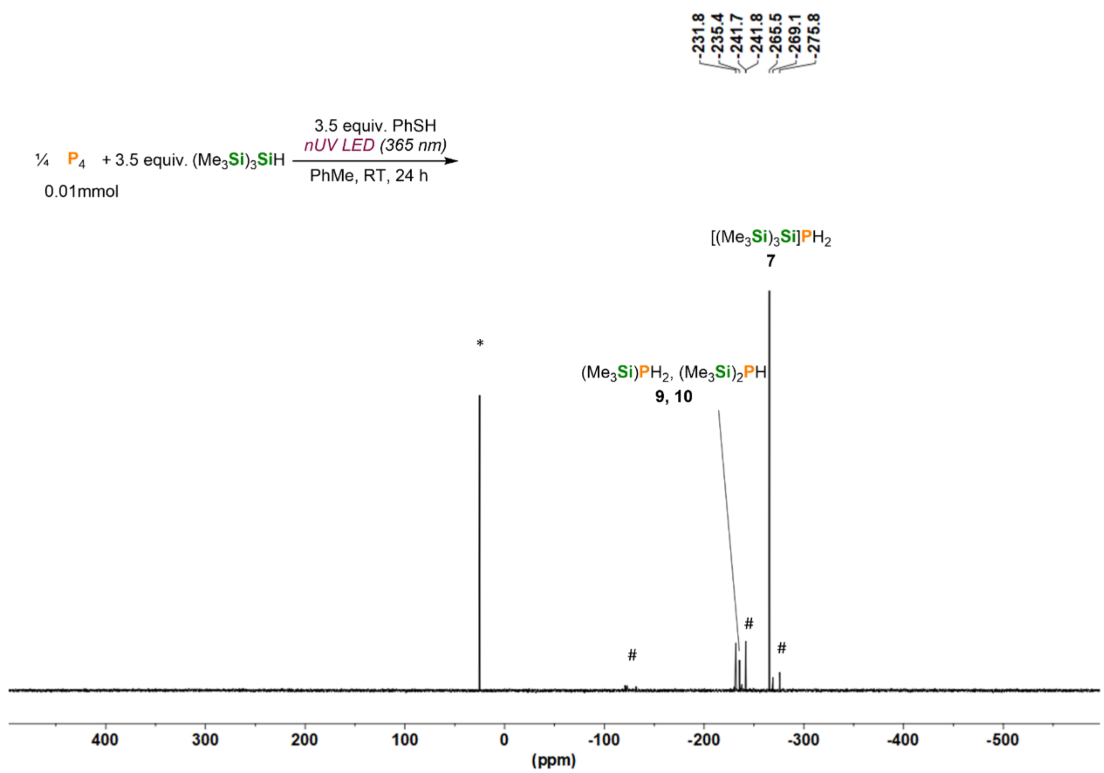


Figure S35. $^{31}P\{^{1}H\}$ NMR spectrum for the reaction of P_4 with $(Me_3Si)_3SiH$ (0.14 mmol) and PhSH (0.14 mmol) in PhMe and driven by 365 nm, 3 W LED irradiation for 24 h (Table S7, Entry 4). * marks the internal standard Ph_3PO (0.02 mmol). # marks unknown side products.

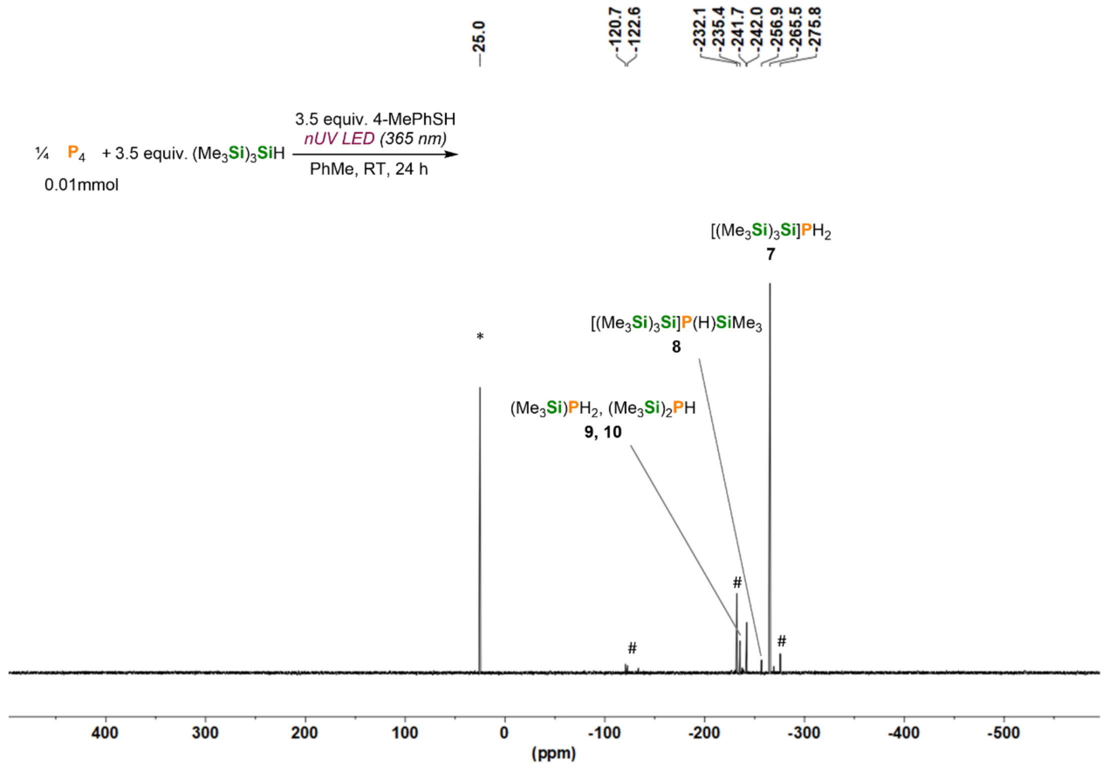


Figure S36. $^{31}P\{^{1}H\}$ NMR spectrum for the reaction of P_4 with $(Me_3Si)_3SiH$ (0.14 mmol) and 4-MePhSH (4-methylbenzenethiol, 0.14 mmol) in PhMe and driven by 365 nm, 3 W LED irradiation for 24 h (Table S7, Entry 5). * marks the internal standard Ph_3PO (0.02 mmol). # marks unknown side products.

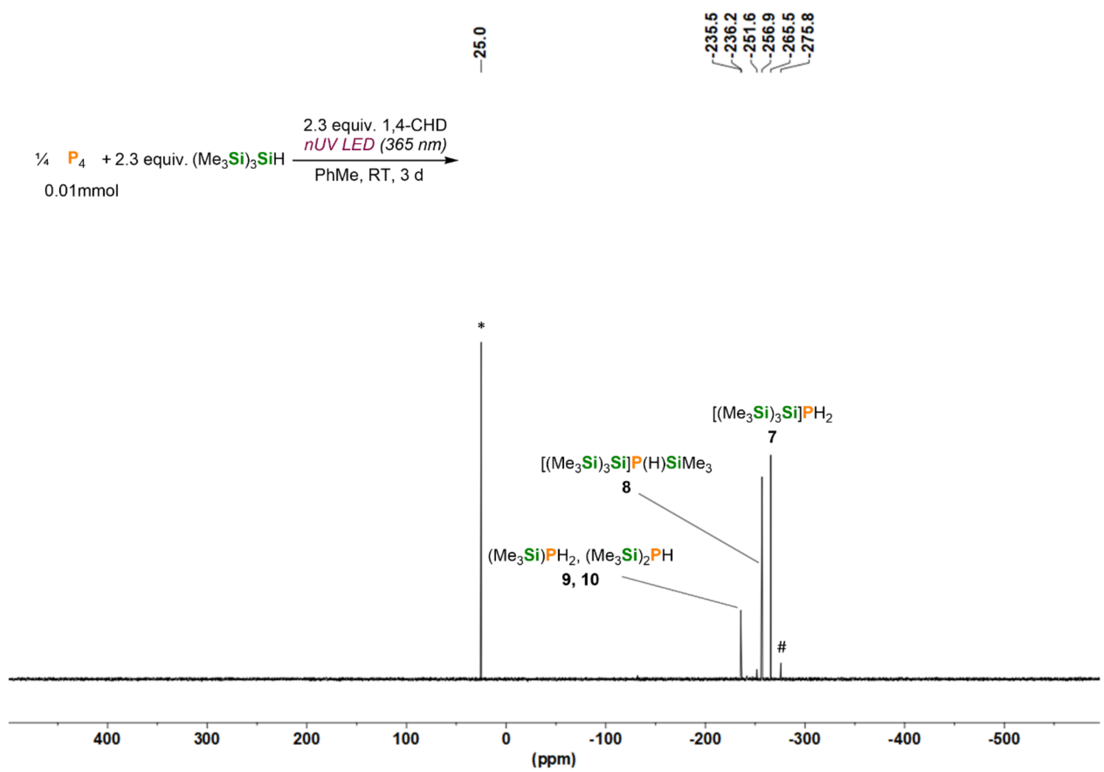


Figure S37. $^{31}P\{^{1}H\}$ NMR spectrum for the reaction of P_4 with $(Me_3Si)_3SiH$ (0.09 mmol) and 1,4-CHD (0.09 mmol) in PhMe and driven by 365 nm, 3 W LED irradiation for 3 d (Table S7, Entry 7). * marks the internal standard Ph_3PO (0.02 mmol). # marks unknown side products. Relative conversion to **7**: 32.5%; **8**: 23.2%; **9**,**10**: 15.3%.

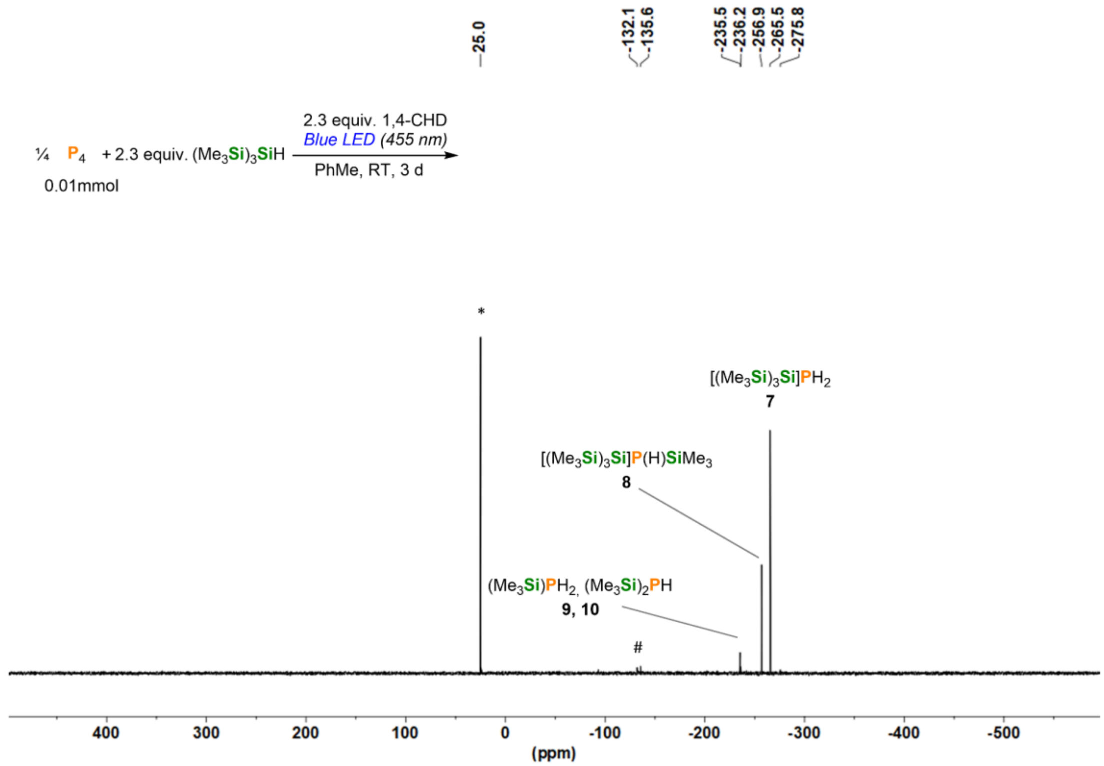
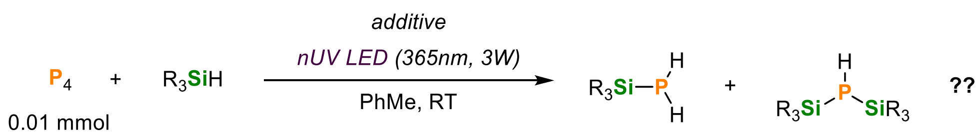


Figure S38. $^{31}P\{^1H\}$ NMR spectrum for the reaction of P_4 with $(Me_3Si)_3SiH$ (0.09 mmol) and 1,4-CHD (0.09 mmol) in PhMe and driven by 455 nm, 3 W LED irradiation for 3 d (Table S7, Entry 8). * marks the internal standard Ph_3PO (0.02 mmol). # marks unknown side products. Relative conversion to **7**: 34.1%; **8**: 12.1%; **9**,**10**: 4.1%.

Table S8. Screening of silanes for the hydrosilylation of P_4 using near-UV LED irradiation (365 nm, 3 W).[a]



Entry	R_3SiH (mmol)	*additive* (mmol)	PhMe (μL)	Time (days)	Full conv. of **P_4**?	Relative conv. to **P_1** compounds
1		-	500	3	X	-
2	Ph_3SiH	*i*Pr_3SiSH (0.14)	500	3	X	-
3	0.14	PhSH (0.14)	500	3	X	-[b]
4[c]		1,4-CHD (0.14)	100	2	X	-[b]
5		-	500	3	X	-
6	Et_3SiH	*i*Pr_3SiSH (0.14)	500	3	X	-
7	0.14	PhSH (0.14)	500	3	X	-[b]
8[c]		1,4-CHD (0.14)	100	2	X	-[b]
9[c]	$(Me_3SiO)_3SiH$	-	500	1	X	-
10[c]	0.09	*i*Pr_3SiSH (0.09)	500	1	X	-

[a] The general procedure described in this section was modified to use the indicated amount of reactants and solvent. [b] A small signal assigned to PH_3 was observed in the $^{31}P\{^1H\}$ and ^{31}P NMR spectra (see Figure S39 for a selected example). [c] 365 nm, 10 W.

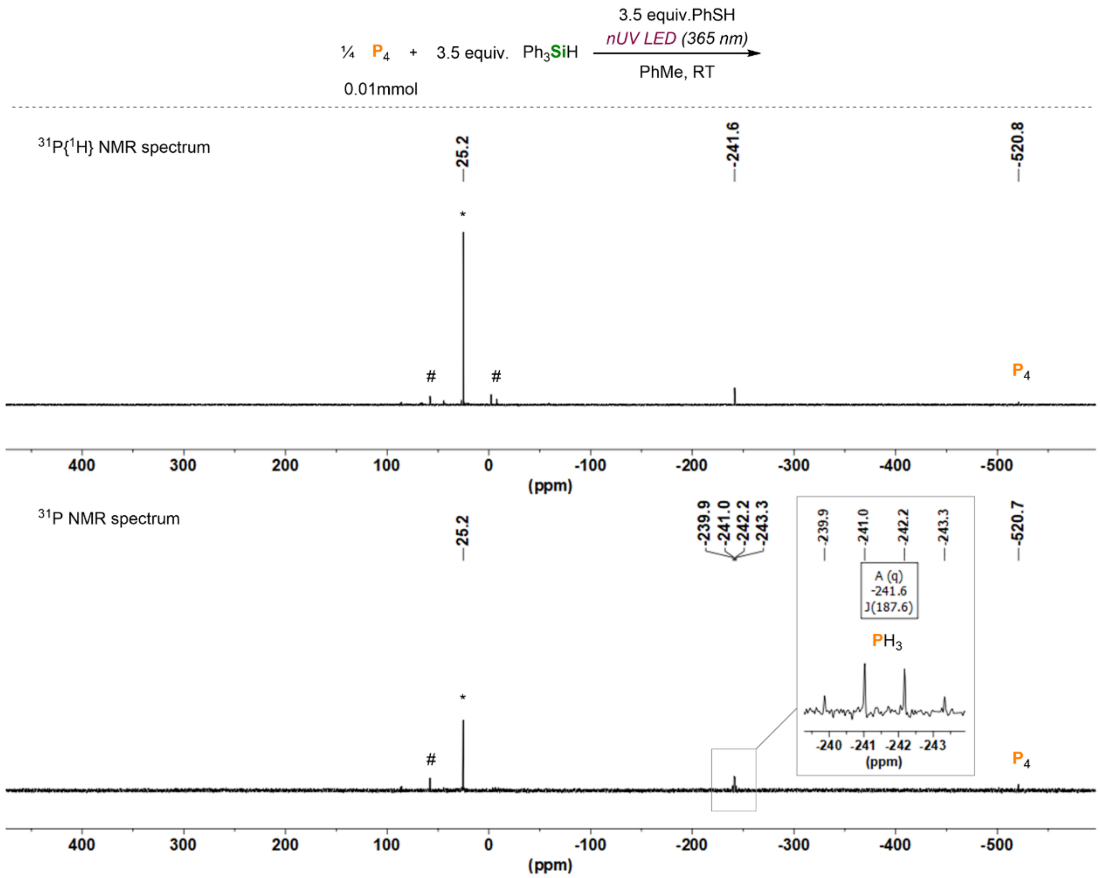


Figure S39. $^{31}P\{^1H\}$ and ^{31}P NMR spectra for the reaction of P_4 with Ph_3SiH (0.14 mmol) and PhSH (0.14 mmol) in PhMe and driven by 365 nm, 3 W LED irradiation for 3 d (Table S8, Entry 3). * marks the internal standard Ph_3PO (0.02 mmol). # marks unknown side products.

4.3. General procedure for the functionalisation of the hydrosilylphosphine mixture

The conversions of the products shown in this section were determined by a quantitative single-scan inverse-gated $^{31}P\{^1H\}$ NMR (DS = 0, D1 = 2 s) methodology that we have described previously, and whose use to quantify tertiary phosphines and quaternary phosphonium salts has previously been validated.[16]

To a 10 mL, flat-bottomed, stoppered tube were added P_4 (0.01 mmol, as a stock solution in 84.3 µL PhH), PhMe (100 µL), $(Me_3Si)_3SiH$ (27.9 µL, 0.09 mmol), and $i$$Pr_3SiSH$ (19.3 µL, 0.09 mmol). The tube was sealed, placed in a water-cooled block to maintain near-ambient temperature, and irradiated with UV light (365 nm, 4.3 V, 700 mA, Osram OSLON SSL 80) for 2 days (unless stated otherwise). The resulting clear colourless solution mixture was treated with the corresponding electrophiles as follows:

<u>*Reactivity towards benzyl bromide:*</u> Benzyl bromide (47.6 µL, 0.4 mmol) and KHMDS (19.9 mg, 0.1 mmol) were added to the colourless solution, and heated to 100 °C with stirring for 3 days. After cooling to room temperature, Ph_3PO (0.02 mmol, stock solution in benzene) was subsequently added to act as an internal standard. Volatiles were removed under vacuum, and CH_3CN (0.5 mL) was then added. NMR analysis of the resulting mixture showed the formation of $[Bn_4P]Br$ (**5**) as the main product with 73 % conversion as shown in Figure S40.

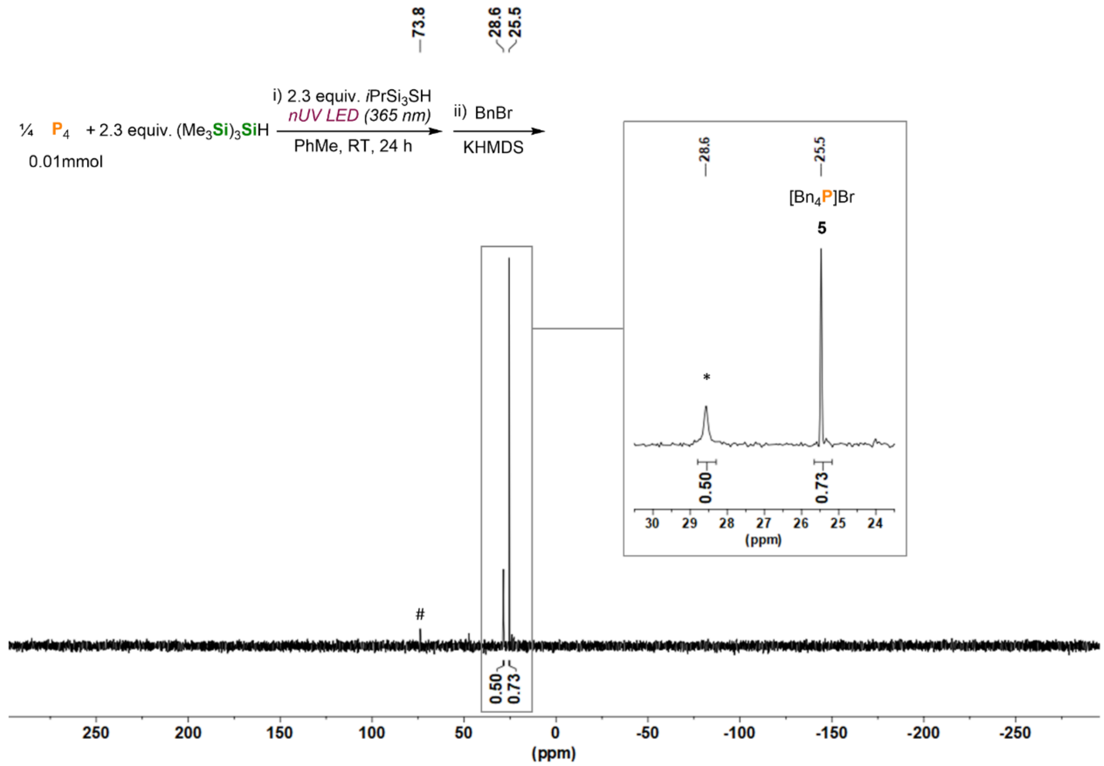


Figure S40. $^{31}P\{^{1}H\}$ NMR spectrum of [Bn_4P]Br (**5**) generated *via* hydrosilylation of P_4 in PhMe, followed by treatment with benzyl bromide (0.4 mmol) and KHMDS (0.1 mmol), heated to 100 °C for 3 d. * marks the internal standard Ph_3PO (0.02 mmol). # marks an unknown side product.

<u>*Reactivity towards bromoethane:*</u> Bromoethane (30 μL, 0.4 mmol) and KHMDS (19.9 mg, 0.1 mmol) were added to the colourless solution, and heated to 100 °C with stirring for 3 days. After cooling to room temperature, Ph_3PO (0.02 mmol, stock solution in benzene) was subsequently added to act as an internal standard. Volatiles were removed under vacuum, and CH_3CN (0.5 mL) was then added. NMR analysis of the resulting mixture showed the formation of [Et_4P]Br (**6**) as the main product with 54 % conversion as shown in Figure S41.

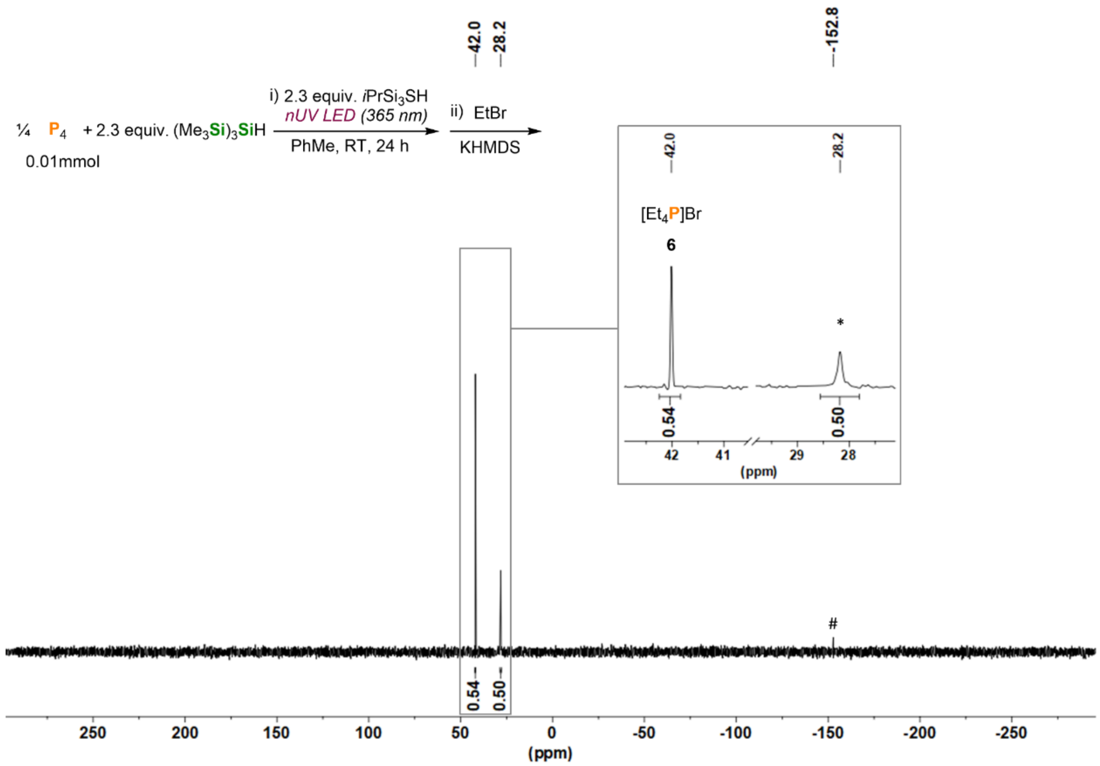


Figure S41. $^{31}P\{^{1}H\}$ NMR spectrum of [Et$_4$P]Br (**6**) generated *via* hydrosilylation of P_4 in PhMe, followed by treatment with bromoethane (0.4 mmol) and KHMDS (0.1 mmol), heated to 100 °C for 3 d. * marks the internal standard Ph_3PO (0.02 mmol). # marks an unknown side product.

<u>*Reactivity towards 1-bromobutane:*</u> 1-bromobutane (43.2 μL, 0.4 mmol) and KHMDS (19.9 mg, 0.1 mmol) were added to the colourless solution, and heated to 100 °C with stirring for 3 days. After cooling to room temperature, Ph_3PO (0.02 mmol, stock solution in benzene) was subsequently added to act as an internal standard. Volatiles were removed under vacuum, and CH_3CN (0.5 mL) was then added. NMR analysis of the resulting mixture showed the formation of [Bu$_4$P]Br (**11**) as the main product with 40 % conversion as shown in Figure S42.

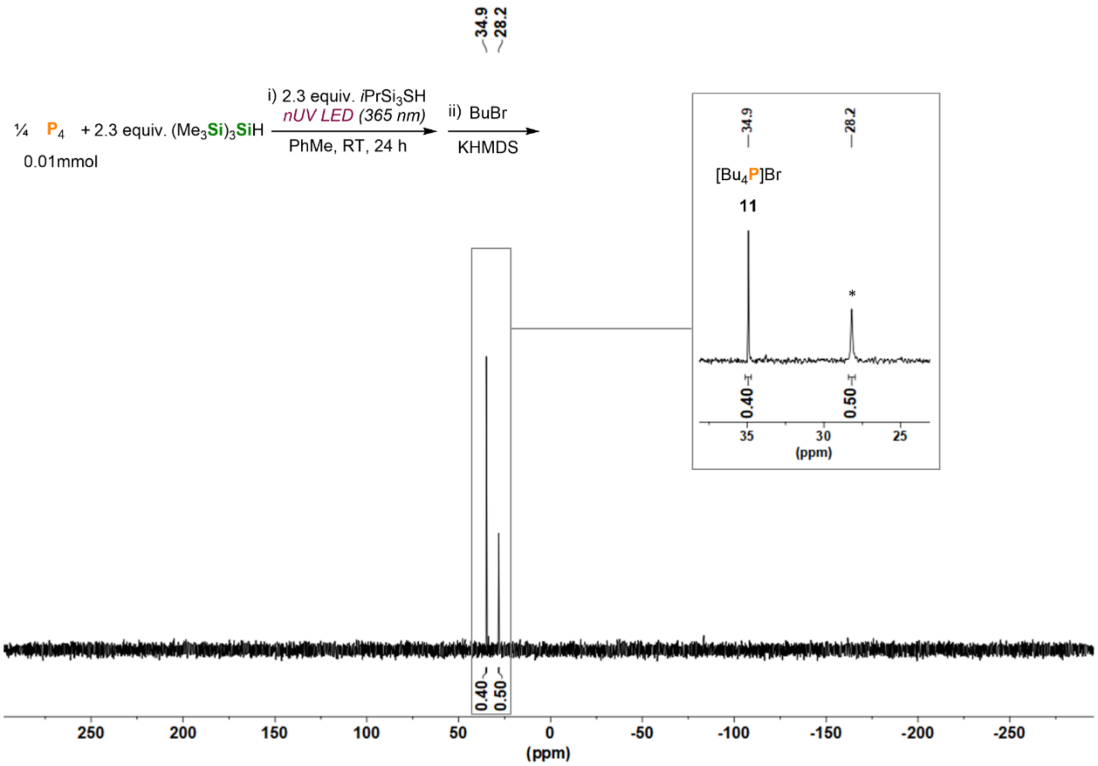


Figure S42. $^{31}P\{^1H\}$ NMR spectrum of $[Bu_4P]Br$ (**11**) generated *via* hydrosilylation of P_4 in PhMe, followed by treatment with 1-bromobutane (0.4 mmol) and KHMDS (0.1 mmol), heated to 100 °C for 3 d. * marks the internal standard Ph_3PO (0.02 mmol).

Reactivity towards paraformaldehyde: Volatiles were removed under vacuum. EtOH (0.5 mL) and paraformaldehyde (15.0 mg, 0.5 mmol) were added to the oily residue, and heated to 50 °C with stirring for 2 days. After cooling to room temperature, the mixture was frozen in a liquid nitrogen bath, and HCl (4.0 M in 1,4-dioxane, 100 µL, 0.4 mmol) was added. After thawing, the reaction mixture was stirred at room temperature for 2 hours. Ph_3PO (0.02 mmol, stock solution in benzene) was subsequently added to act as an internal standard. NMR analysis of the resulting mixture showed the formation of THPC (**12**) as the main product with 27% conversion, along with other unknown side products (<12%). Nevertheless, analogous reactivity studies of the crude $[Si]_nPH_{3-n}$ mixture generated in the presence of 1,4-CHD instead of iPr$_3$SiSH, resulted in the exclusive formation of THPC (**12**) with 48% conversion as shown in Figure S43.

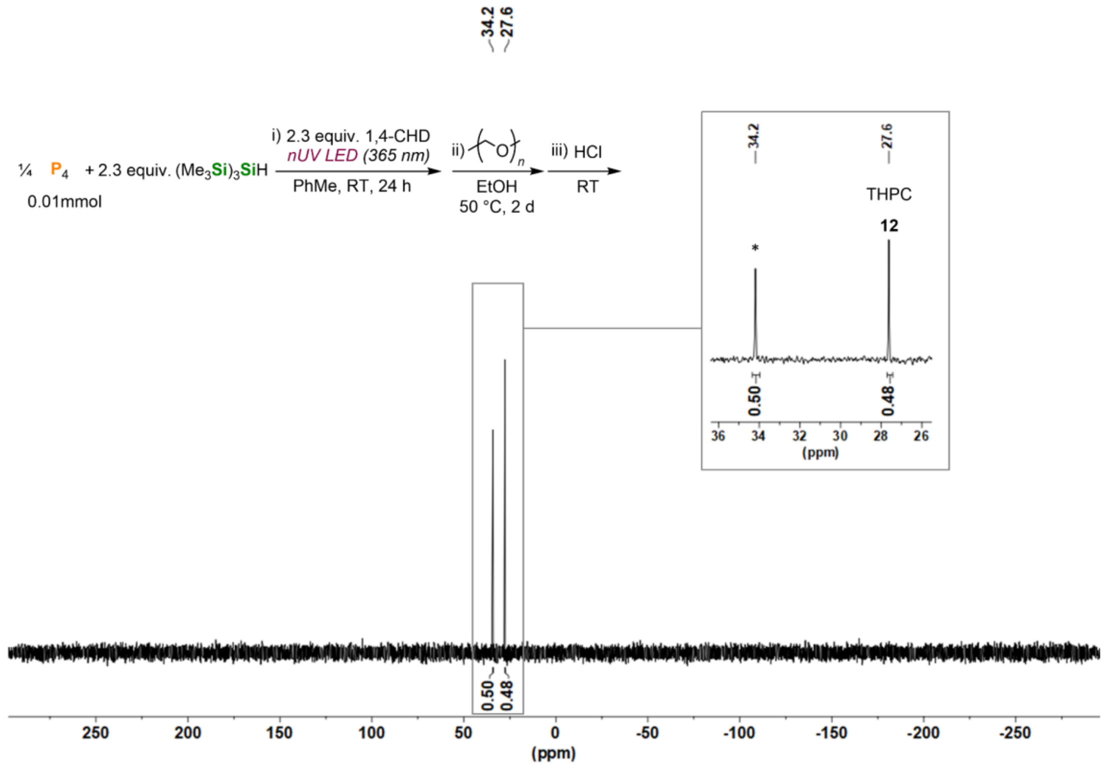


Figure S43. $^{31}P\{^1H\}$ NMR spectrum of THPC generated *via* hydrosilylation of P_4 in PhMe, followed by treatment with paraformaldehyde (0.5 mmol) in EtOH, heated to 50 °C for 2 d. Then, quenched with HCl (0.4 mmol).* marks the internal standard Ph_3PO (0.02 mmol).

<u>*Reactivity towards benzoyl chloride:*</u> PhC(O)Cl (27.9 µL, 0.24 mmol) and KHMDS (19.9 mg, 0.1 mmol) were added to the colourless solution, and stirred at room temperature for 24 hours. The resulting mixture was analysed by $^{31}P\{^1H\}$ and ^{31}P NMR spectroscopy as shown in Figure S44.

The $^{31}P\{^1H\}$ NMR spectrum showed only traces amounts of the desired product $P(C(O)tBu)_3$ (−54.1 ppm) along with a variety of other unknown species. The main product of this reaction appears as a singlet resonance at −114.6 ppm, which splits into a doublet in the ^{31}P spectrum ($^1J(^{31}P\text{-}^1H)$ = 208 Hz). Given the similarities on chemical shift and $^1J(^{31}P\text{-}^1H)$ coupling constant with analogous compounds ($Bu_3SnP(H)C(O)tBu$[20] and $Me_3SiP(H)C(O)tBu$[57]), this species was assigned to $R_3SiP(H)C(O)Ph$ (R = $SiMe_3$ or Me). Additional experiments using fewer equivalents of PhC(O)Cl, in our attempts to target this potential intermediate more selectively, were unsuccessful. Moreover, similar outcomes were observed during experiments at higher temperatures and longer reaction times.

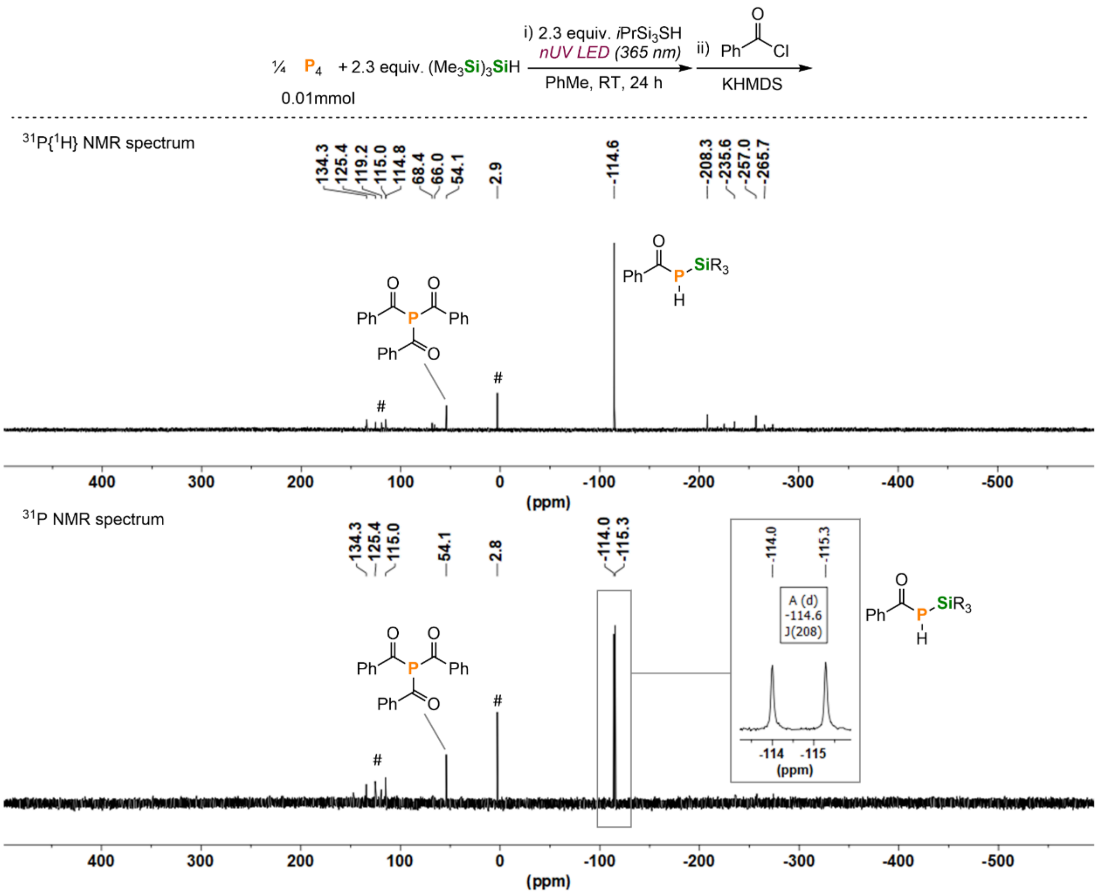


Figure S44. $^{31}P\{^1H\}$ and ^{31}P NMR spectra for the hydrosilylation of P_4 in PhMe, followed by treatment with benzoyl chloride (0.24 mmol) and KHMDS (0.1 mmol), stirred at room temperature for 24 h. # marks unknown species. R = $SiMe_3$, Me.

<u>*Reactivity towards pivaloyl chloride:*</u> *t*BuC(O)Cl (29.6 µL, 0.24 mmol) and KHMDS (19.9 mg, 0.1 mmol) were added to the colourless solution, and stirred at room temperature for 24 hours. The resulting mixture was analysed by $^{31}P\{^1H\}$ and ^{31}P NMR spectroscopy as shown in Figure S45.

Similar to the reaction with benzoyl chloride, the $^{31}P\{^1H\}$ NMR spectrum showed only trace amounts of the desired product $P(C(O)tBu)_3$ (−52.0 ppm) along with a variety of other unknown species. The main product of this reaction appears as a singlet resonance at −128.4 ppm, which splits into a doublet in the ^{31}P spectrum ($^1J(^{31}P\text{-}^1H)$ = 210 Hz). Given the similarities on chemical shift and $^1J(^{31}P\text{-}^1H)$ coupling constant with analogous compounds ($Bu_3SnP(H)C(O)tBu$[20] and $Me_3SiP(H)C(O)tBu$[57]), this species was assigned to $R_3SiP(H)C(O)tBu$ (R = $SiMe_3$ or Me). Aditional experiments using fewer equivalents of *t*BuC(O)Cl, in our attempts to target this potential intermediate more selectively, were unsuccessful. Moreover, similar outcomes were observed during experiments at higher temperatures and with longer reaction times.

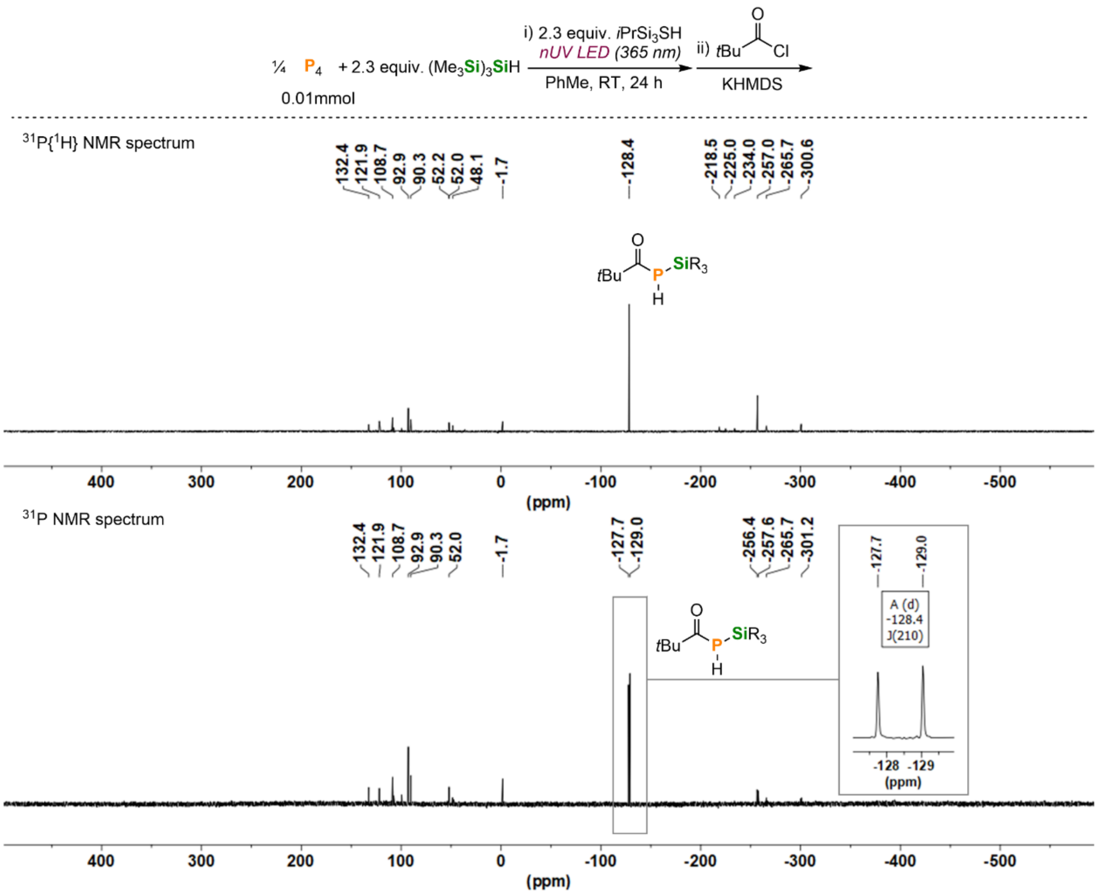
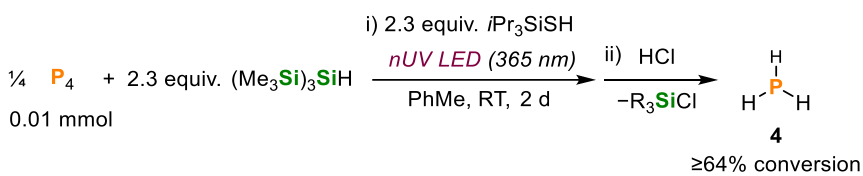


Figure S45. $^{31}P\{^{1}H\}$ and ^{31}P NMR spectra for the hydrosilylation of P_4 in PhMe, followed by treatment with pivaloyl chloride (0.24 mmol) and KHMDS (0.1 mmol), stirred at room temperature for 2 d. R = $SiMe_3$, Me.

4.4. Synthesis and quantification of PH_3 (4) via hydrosilylation of P_4 (0.01 mmol scale)



To a 10 mL, flat-bottomed, stoppered tube were added P_4 (0.01 mmol, as a stock solution in 84.3 µL PhH), PhMe (100 µL), $(Me_3Si)_3SiH$ (27.9 µL, 0.09 mmol), and $i$$Pr_3SiSH$ (19.3 µL, 0.09 mmol). The tube was sealed, placed in a water-cooled block to maintain near-ambient temperature, and irradiated with UV light (365 nm, 4.3 V, 700 mA, Osram OSLON SSL 80) for 2 days. Ph_3PO (0.02 mmol, stock solution in benzene) was subsequently added to act as an internal standard to the resulting clear colourless solution mixture and transferred to an NMR tube fitted with a J. Young valve. The mixture was frozen by placing the NMR tube in a bath of liquid nitrogen, and HCl (0.4 mmol, 4.0 M in 1,4-dioxane) was added (while still maintaining an inert atmosphere). The NMR tube was sealed and its contents were then thawed, agitated briefly, and analysed by ^{1}H, $^{31}P\{^{1}H\}$, and ^{31}P NMR spectroscopy. The resulting spectra indicated clean conversion to PH_3,[20] as shown in Figures S46-48, below.

In order to accurately quantify the amount of PH_3 in solution, a proton-coupled ^{31}P spectrum was acquired with a 20 s delay between scans (which was confirmed to be > 5 x T_1), and the intensity of the PH_3 resonance was integrated relative to that of Ph_3PO. This indicated 64% of the theoretical maximum conversion to PH_3 (Figure S49), which provides a lower bound for the actual conversion (this value does not include any PH_3 present in the NMR tube headspace).

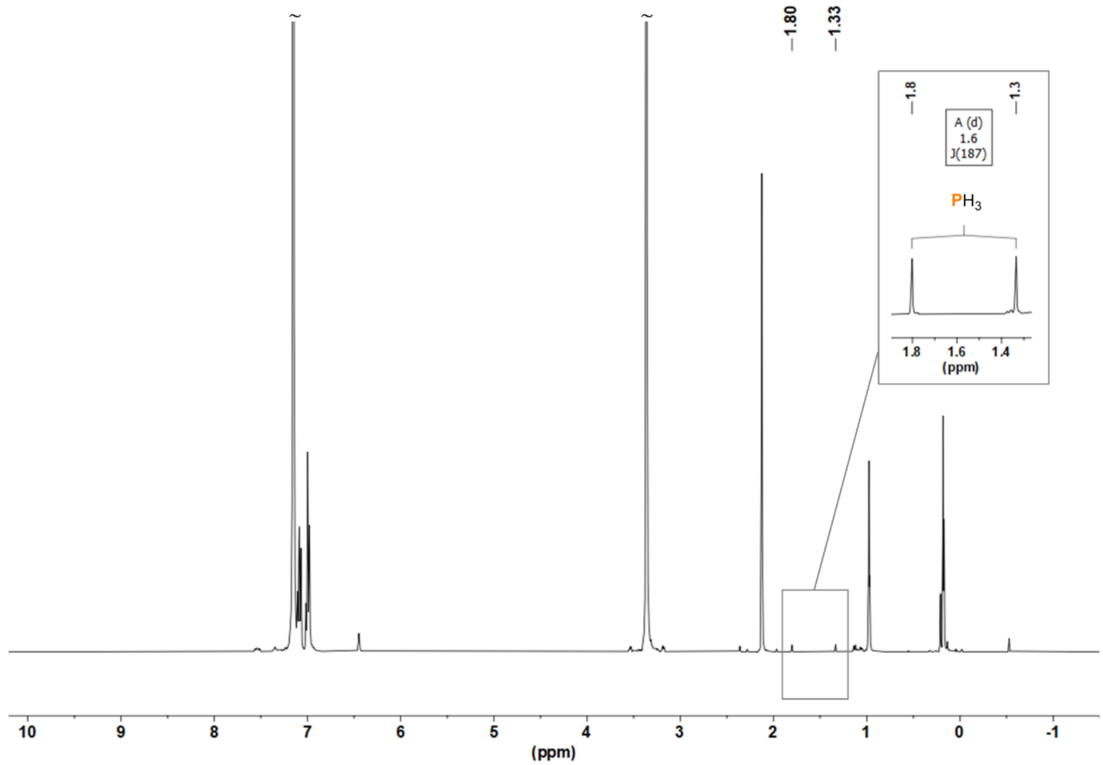


Figure S46. ^{1}H NMR spectrum of a solution of PH_3 (**4**) generated *via* hydrosilylation of P_4 in PhMe, followed by acidification. Solvent resonances (~) truncated for clarity.

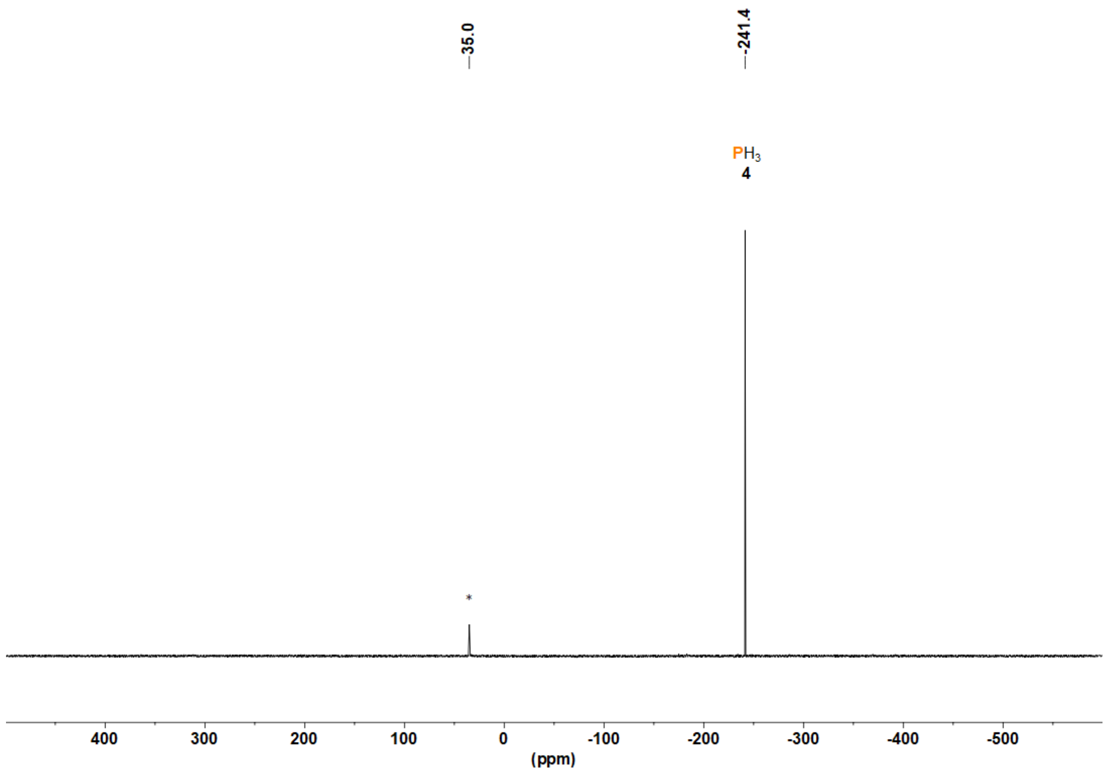


Figure S47. $^{31}P\{^1H\}$ NMR spectrum of PH_3 (**4**) generated *via* hydrosilylation of P_4 in PhMe, followed by acidification in the presence of Ph_3PO (*) as an internal standard.

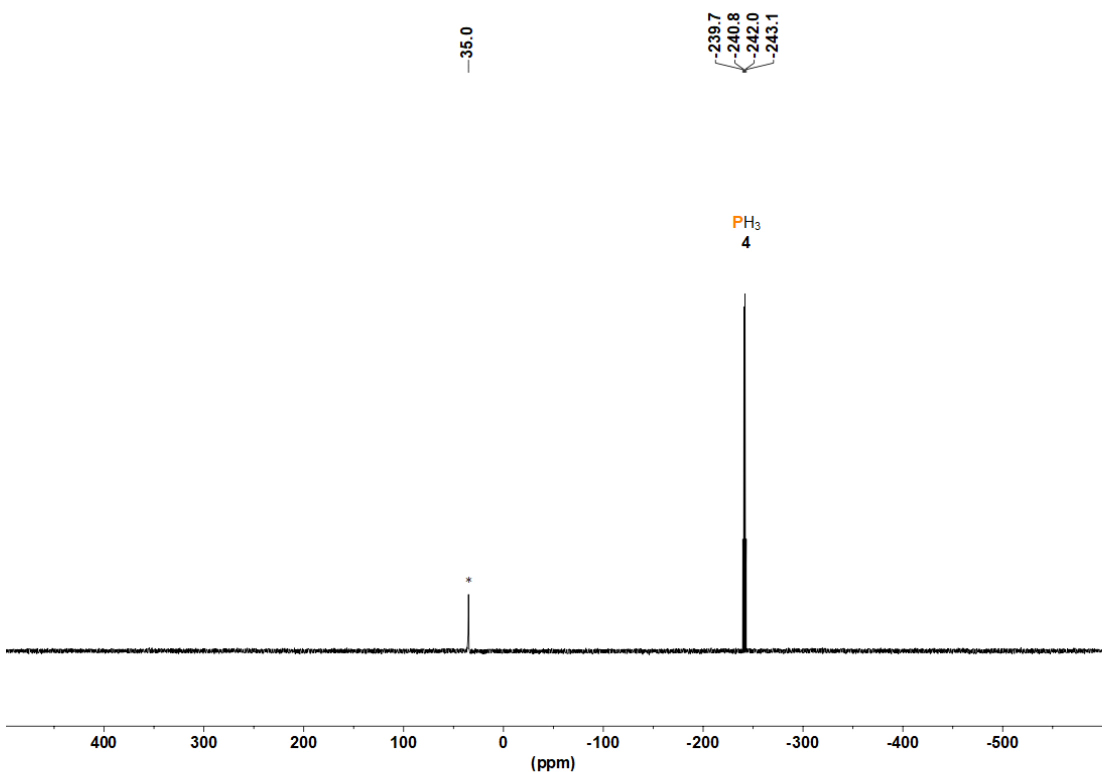


Figure S48. ^{31}P NMR spectrum of PH_3 (**4**) generated *via* hydrosilylation of P_4 in PhMe, followed by acidification in the presence of Ph_3PO (*) as an internal standard.

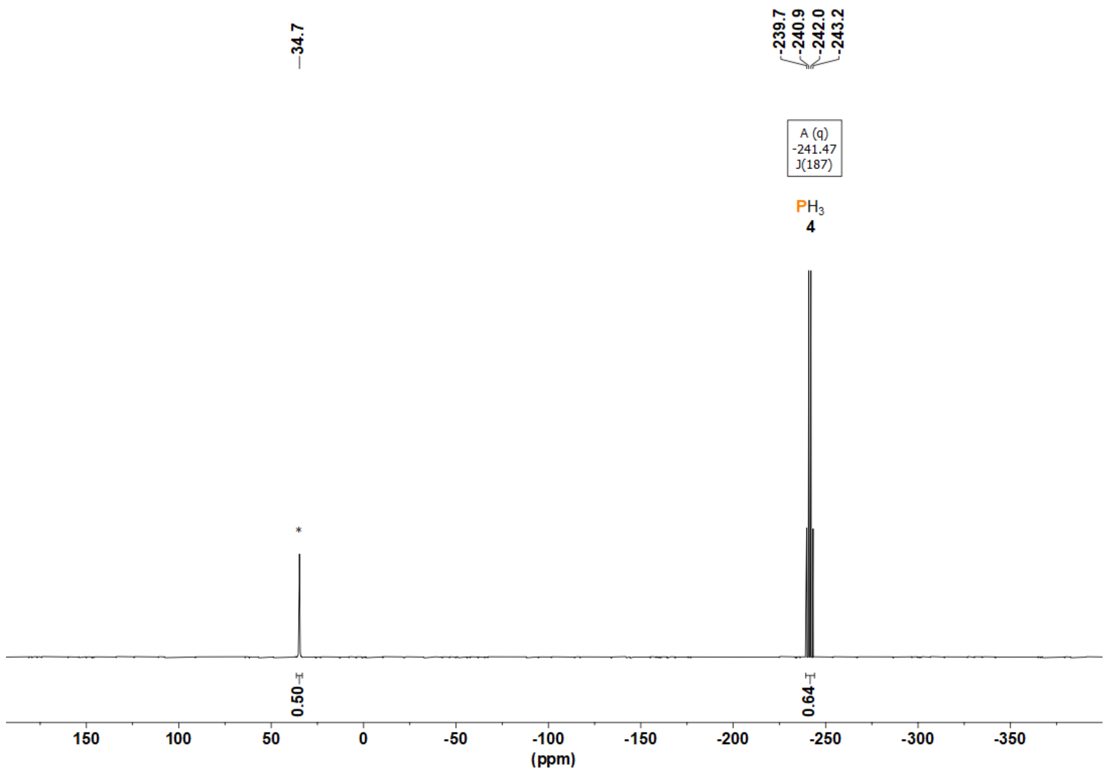
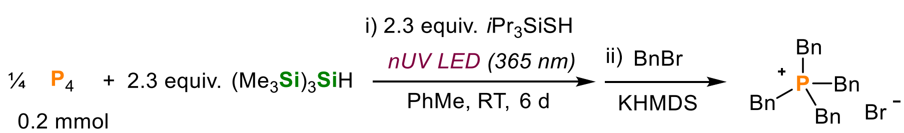


Figure S49. Quantitative ^{31}P NMR spectrum (D1 = 20 s) of PH_3 (**4**) generated *via* hydrosilylation of P_4 in PhMe, followed by acidification, in the presence of Ph_3PO (*) as an internal standard.

4.5. Synthesis and isolation of TBPB (5) via hydrosilylation of P_4 (0.2 mmol scale)



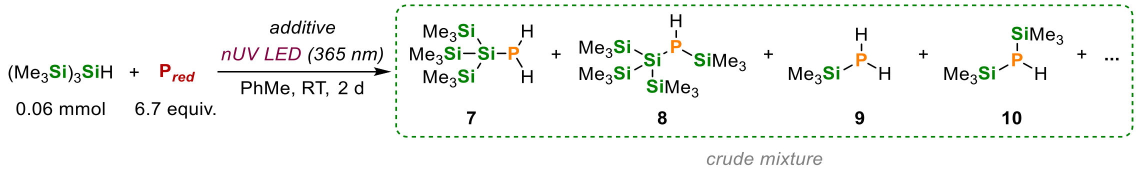
5

70% yield

To a 50 mL, flat-bottomed, stoppered tube were added P_4 (24.8 mg, 0.2 mmol), PhMe (2.0 mL), $(Me_3Si)_3SiH$ (555.3 µL, 1.8 mmol), and $i$$Pr_3SiSH$ (386.4 µL, 1.8 mmol). After stirring to obtain a homogeneous solution, the tube was placed in a water-cooled block to maintain near-ambient temperature, and irradiated with UV light (365 nm, 14 V, 700 mA, Osram OSLON SSL 80) for 6 days. To the colorless solution benzyl bromide (951.5 µl, 8.0 mmol) and KHMDS (398.9 mg, 2.0 mmol) were added and the reaction mixture heated to 100 °C with stirring for 3 days. After cooling to room temperature the pale yellow suspension was filtered, and the remaining solid was washed with PhMe (3 x 6 mL) and extracted into acetonitrile (3 x 10 mL). Removal of volatiles under vacuum yielded the target product as a white solid (266 mg, 70 %).

For characterisation data, see Section 3.8.

4.6. Hydrosilylation of P$_{red}$ using using $(Me_3Si)_3SiH$, *i*Pr_3SiSH or 1,4-CHD and LED irradiation (0.06 mmol scale)



To a 10 mL, flat-bottomed, stoppered tube were added P$_{red}$ (0.4 mmol, 12.4 mg), PhMe (250 µL), $(Me_3Si)_3SiH$ (18.5 µL, 0.06 mmol), and *i*Pr_3SiSH (12.9 µL, 0.06 mmol) or 1,4-CHD (5.7 µL, 0.06 mmol). The tube was sealed, placed in a water-cooled block to maintain near-ambient temperature, and irradiated with UV light (365 nm, 14 V, 700 mA, Osram OSLON SSL 80) for 2 days. Ph_3PO (0.02 mmol, stock solution in benzene) was subsequently added to act as an internal standard. The resulting mixture was analysed by $^{31}P\{^1H\}$ NMR spectroscopy, as shown in Figures S50 and S51, below.

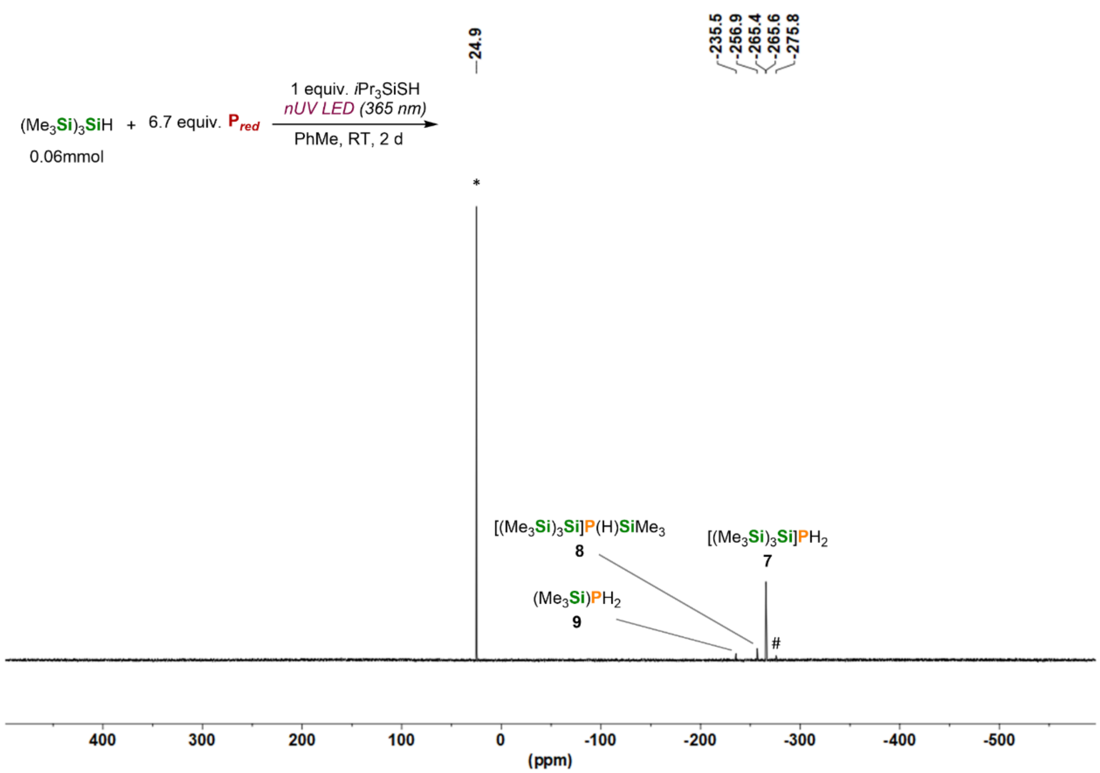


Figure S50. $^{31}P\{^1H\}$ NMR spectrum for the reaction of P$_{red}$ with $(Me_3Si)_3SiH$ (0.06 mmol) and *i*Pr_3SiSH (0.06 mmol) in PhMe and driven by 365 nm, 10 W LED irradiation for 2 d. * marks the internal standard Ph_3PO.

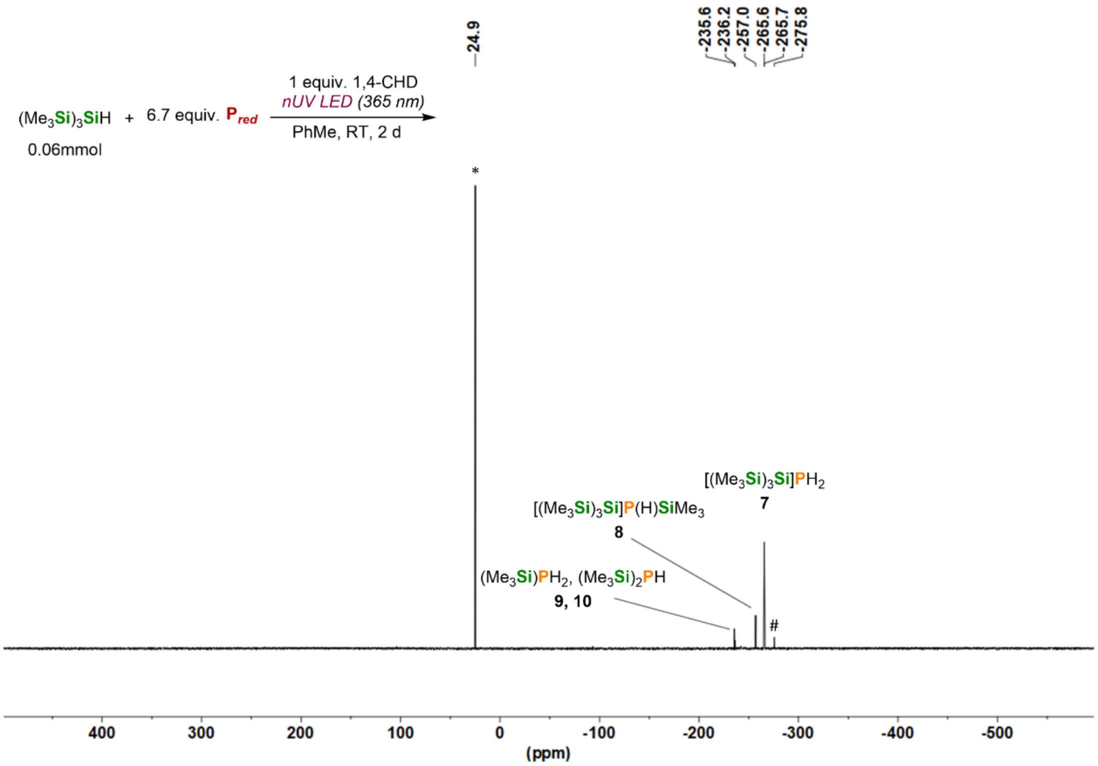
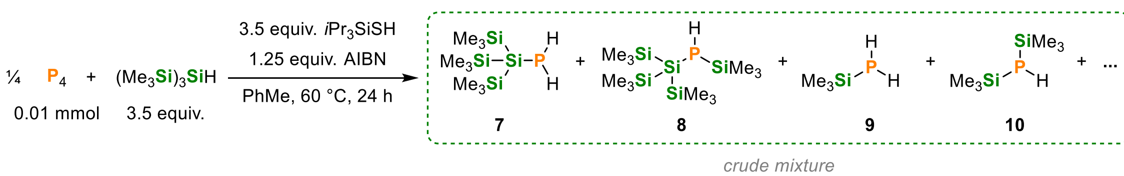


Figure S51. $^{31}P\{^{1}H\}$ NMR spectrum for the reaction of P_{red} with $(Me_3Si)_3SiH$ (0.06 mmol) and 1,4-CHD (0.06 mmol) in PhMe and driven by 365 nm, 10 W LED irradiation for 2 d. * marks the internal standard Ph_3PO.

4.7. General procedure for the hydrosilylation of P_4 using $(Me_3Si)_3SiH$, *i*Pr_3SiSH and chemical radical initiators (0.01 mmol scale)



To a 10 mL, flat-bottomed, stoppered tube were added P_4 (0.01 mmol, as a stock solution in 84.3 µL PhH), PhMe (500 µL), AIBN (0.05 mmol, as a stock solution in PhH), $(Me_3Si)_3SiH$ (43.2 µL, 0.14 mmol), and *i*Pr_3SiSH (30 µL, 0.14 mmol). The tube was sealed, wrapped in Al foil to exclude light, and heated to 60 °C for 24 hours (unless stated otherwise). Ph_3PO (0.02 mmol, stock solution in benzene) was subsequently added to act as an internal standard. The resulting mixture was analysed by $^{31}P\{^{1}H\}$ NMR spectroscopy, as shown in Figure S52, below.

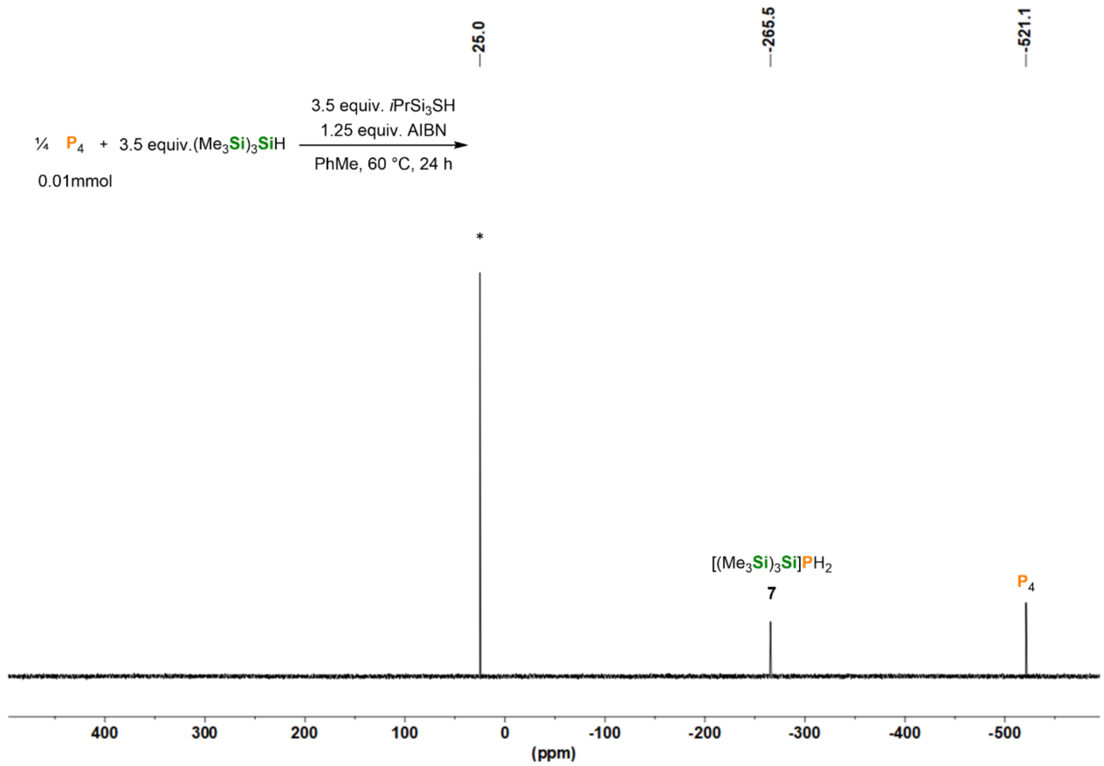
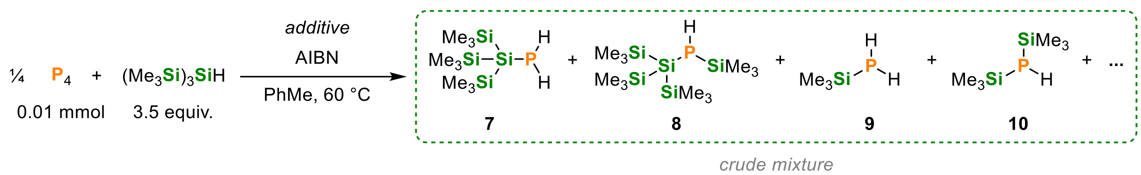


Figure S52. $^{31}P\{^1H\}$ NMR spectrum for the reaction of P_4 with $(Me_3Si)_3SiH$ (0.14 mmol), $i$$Pr_3SiSH$ (0.14 mmol) and AIBN (0.05 mmol) in PhMe, heated to 60 °C for 24 h (Table S9, Entry 2). * marks the internal standard Ph_3PO (0.02 mmol).

Table S9. Optimization of hydrosilylation of P_4 using $(Me_3Si)_3SiH$, HAT donor and chemical radical initiators.[a]



Entry	Additive (mmol)	Radical initiator (mmol)	Temperature (°C)	Time (days)	Full conv. of **P**$_4$?	Relative conv. to **7-10** (%)
1	AdSH (0.14)	AIBN (0.05)	60	1	X	traces
2	$i$$Pr_3SiSH$ (0.14)	AIBN (0.05)	60	1	X	traces
3	$i$$Pr_3SiSH$ (0.14)	AIBN (0.14)	60	2	X	traces
4	1,4-CHD (0.14)	AIBN (0.14)	60	2	X	traces

[a] The general procedure described in this section was modified to use the indicated amount of reactant, temperature and time. [b] Conversions were calculated by integration of the ^{31}P resonances of **7-10** relative to an internal standard.

5. References for supplementary information

For references [1]-[42] please refer to the main manuscript.

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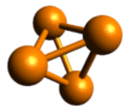
6. Cartesian coordinates of optimized structures

P_4
E= -1365.03900477 Eh



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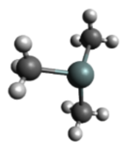
P	-6.96619533814420	0.33677370507047	0.79516442354124
P	-8.68358341986195	0.14155911530574	-0.53970683749054

$Me_3Sn^{\bullet}$
E= -333.83773926 Eh
H= -333.79419951 Eh



0 2

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C	0.01624841845516	-0.03766963620385	0.02408622563928
C	1.95707088074064	-0.56728058815974	2.88224279632402
C	-0.55523065397075	1.85612096675477	2.90912231806715
H	0.34106820462594	-0.99425367785191	-0.38489706900594
H	0.72681657543460	0.73715997838795	-0.27485231550035
H	-0.96671998773747	0.20757913395128	-0.37752448186928
H	-1.54006851800091	2.15245397070418	2.54845420629491
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H	-0.55323100757316	1.87485945633416	3.99882489447740
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$(Me_3Sn)P_4^{\bullet}$
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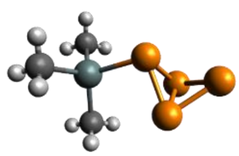

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Sn	-0.07502888407850	-0.06570514227185	2.04485724530151
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C	1.74654435191822	-0.82572726558248	2.88612211424798
C	-0.48175123769149	1.90665066206422	2.77896956639695
H	0.83447392423197	0.56515094414195	-0.43235579842360
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H	0.16242055058868	-1.07789405977524	-0.47240897596584
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H	-0.44879161676758	1.91659140180575	3.86818390953441
H	2.58342993775571	-0.19270279932788	2.58655002116582
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Me_3SnH
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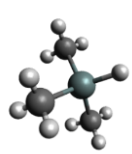
H= -334.41002696 Eh



0 1

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H	-8.06703535137819	-1.48923307853153	0.28038348036314
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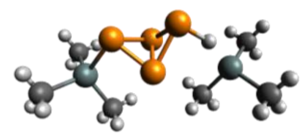
H	-3.61978984365241	-0.41541993363825	-0.60385958039123
H	-4.84474622633764	-1.58366861053805	-1.13017019072076
H	-4.20148444456054	-1.65639892611004	0.51961102706190
C	-5.30862551989089	1.54303464840539	1.99503785789955
H	-6.07816567053497	2.23852704188395	2.33151435304507
H	-4.43742575389723	2.11525142695790	1.67425342800372
H	-5.02041604962666	0.90799357813743	2.83410633460966
H	-6.54115813721747	1.34597608274776	-0.91038483357233

TS($(Me_3Sn)P_4^{\bullet}$→$(Me_3Sn)P_4H$)
E= -2033.30911684 Eh
im. freq. = 771.71 *i*



0 2

H	0.06423181035575	-1.73612866467063	3.30241068825383
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P	2.36010497775788	-1.65044831208672	4.81973330963943
P	0.56817678001534	-1.31073628529748	5.97583112593764
Sn	3.39345664481709	-0.82075258000473	8.10313762842307
C	2.67156601350831	1.12652783338235	7.55877446665433
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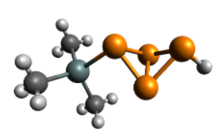

0 1

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P	4.83618138677669	0.90114854014262	3.61294963869152

P	2.72930937079770	0.66783647939390	4.25216617051788
P	3.17430640760397	1.85064563304859	2.50069754164659
Sn	0.11767835233257	0.08158718528474	1.89492329543462
C	-0.47884956851307	2.02029042606585	2.58867641859464
C	-0.90658708668548	-1.44399803208477	3.00011104950728
C	-0.26247665066296	-0.12429133016896	-0.20608062449968
H	-0.15551634111142	2.16966592351333	3.61877548901145
H	-1.56665037597744	2.09482322070214	2.54211007348659
H	-0.04123314402378	2.79952592334858	1.96503170424256
H	0.24993368701561	0.66368396790055	-0.75828784086817
H	-1.33420845352469	-0.05088767232442	-0.39675450940367
H	0.09295656157647	-1.09217111849208	-0.56034463311294
H	-0.70608613549304	-1.32503104317873	4.06516545889515
H	-0.57060112492773	-2.43215906141740	2.68557342335666
H	-1.98166070287450	-1.36523508574272	2.83138429056076
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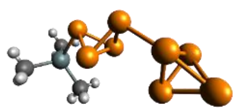
TS((Me$_3$Sn)P$_4^{\bullet}$→(Me$_3$Sn)P$_8^{\bullet}$)



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0 2

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C	-1.37905785297348	1.86449818948982	2.77895834461659
H	0.70917817633123	0.79000707172598	-0.10314331799110
H	-0.92118095409734	0.21541307134253	-0.50589343086431
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H	-2.18760556060772	2.14732861144434	2.10486998832881
H	-0.60449492123789	2.63279506678443	2.74972183110074
H	-1.77338431752628	1.79515187424043	3.79274854344711
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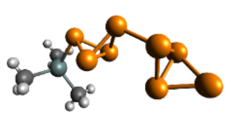
(Me$_3$Sn)P$_8^{\bullet}$



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P	6.60537008018981	1.87548728955946	5.87402903164898
P	5.60202515492911	2.87315991350147	4.20956242397067
H	0.59365150584319	-0.04102484416759	0.46132195844439
P	3.85730307874197	0.19196847501584	2.49459688656549
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P	5.42151872582528	-0.62804985648977	3.81986823078707
P	2.71200534542806	-1.42837409495145	3.47443499090614
C	0.44180369728059	1.69160070601011	3.67401733408055
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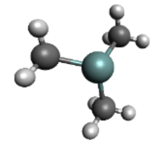
Me$_3$Ge$^{\bullet}$



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H= -2196.23749239 Eh

0 2

Ge	-6.03032719953612	0.30323244649022	0.42012632065943
C	-7.56354208901077	-0.75674867757626	1.04723080471239
H	-7.24933695643939	-1.38107096967147	1.88951262736187
H	-7.93662642644507	-1.40616646153573	0.25479950545397
H	-8.37416473998071	-0.10747445879040	1.37956270969865
C	-4.60513250651833	-0.90579213259089	-0.19168912386877
H	-3.73427082111365	-0.33926970587033	-0.52351139490647
H	-4.95224651126682	-1.52993975938974	-1.01570534938295
H	-4.30207077507694	-1.55690209854285	0.63399744024195
C	-5.35615022289328	1.41182021757530	1.89830815822001
H	-6.12802301586116	2.09476120984888	2.25461408455449
H	-4.49206497119805	1.99654398672809	1.58078173470203
H	-5.05388376465968	0.76516640332518	2.72789248255340

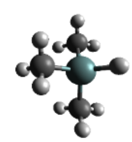
(Me$_3$Ge)P$_4^{\bullet}$

E= -3561.32408927 Eh

0 2

P	2.42558728149884	-0.25550882448982	2.25217185967132
P	4.69195391212326	0.81330550677054	3.49670748627093
P	2.63197416426256	0.71268616632875	4.23511882842292
P	3.08166274136950	1.85352097923624	2.43897677673396
Ge	0.10328307905216	0.09952894969010	1.92105057049387
C	-0.46483480968926	1.86201123697519	2.54411360513092
C	-0.82669753892190	-1.30562996086839	2.91513543784380
C	-0.20469542455597	-0.08657053815520	-0.00277063460256
H	-0.19325250271151	2.01291957199252	3.58950113476215
H	-1.55068735354438	1.93786972968373	2.45094655431498
H	-0.00678864274470	2.65212541985503	1.94834210179275
H	0.32876090456159	0.69218788954658	-0.54938505317920
H	-1.27109879630000	0.00186470871274	-0.22108971582520
H	0.14243146490425	-1.05892232541339	-0.35495518001395
H	-0.64262370331514	-1.19523232521587	3.98462620977393
H	-0.48489001304776	-2.29296233469123	2.60214960256393
H	-1.90207476294154	-1.23618384995752	2.73712041584547

Me$_3$GeH



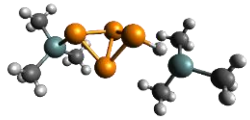
E= -2196.90908050 Eh
H= -2196.86847032 Eh

0 1

Ge	-6.02484253113286	0.29233964428955	0.43396098170902
C	-7.55719281423406	-0.75637268264983	1.04819142270586
H	-7.26196208628080	-1.39314114038797	1.88474157459735
H	-7.93617358861047	-1.39366064841813	0.24789562918773
H	-8.36477764511334	-0.10227260916580	1.38052134201254
C	-4.60770933278757	-0.90502515072871	-0.18471008958487
H	-3.74256006393516	-0.33454914742391	-0.52649969814145
H	-4.95887208925337	-1.52724206900824	-1.00928455697813
H	-4.28851252301713	-1.55944994243157	0.62889604477255
C	-5.35708030830475	1.40540636350897	1.89709719798970

H	-6.13100446358158	2.09094513034933	2.24575906178828
H	-4.49696621901376	1.99386348362322	1.57364924913678
H	-5.04989046190243	0.77715012402210	2.73568934391907
H	-6.46789587283271	1.20298864442097	-0.73605750311443

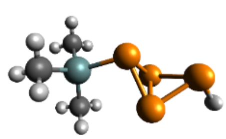
TS((Me$_3$Ge)P$_4^{\bullet}$→(Me$_3$Ge)P$_4$H)
E= -5758.20342573 Eh
im. freq. = 131.50 *i*



0 2

P	3.07428885917582	-0.74811432365135	2.38897500515331
P	5.87863377854958	-0.48088139672441	2.88813527627351
P	4.14675247253712	0.24456213208272	4.05381155632408
P	4.43729399931663	0.96017919753545	2.03490202693636
Ge	1.04167121721564	0.44393401149729	2.45488143244306
C	1.17536634259464	2.11363278448522	3.46465002921999
C	-0.28241490125267	-0.73764477532669	3.27888298229168
C	0.55434516586656	0.81589047123786	0.59548662548154
H	1.39127140644483	1.91423217158455	4.51508969437364
H	0.22485915055828	2.64777377301852	3.39822698677184
H	1.96274991879479	2.75224380268855	3.06252568634665
H	1.29775208569062	1.46688296603921	0.13294654727026
H	-0.41763914819513	1.31250541535305	0.55487362491448
H	0.49669660076966	-0.10904624573060	0.02052988245954
H	-0.01688854493263	-0.94118076313201	4.31704506349240
H	-0.33682320556515	-1.68543029638552	2.74139738023884
H	-1.26768954668244	-0.26747745364713	3.25639811612034
H	9.58192282346799	2.79850619622769	3.02069792535177
H	6.62826990268200	4.09090113524281	2.44192558023745
H	9.62997168235085	3.68074142138670	4.55801439023358
C	9.31929008916926	2.74797814258621	4.07798924741110
H	6.68231140539183	4.93532279833854	4.00231224659700
C	6.40042196965027	4.00261942813594	3.50462040285360
H	9.86773265784496	1.92350108349798	4.53508885874602
Ge	7.38279707050351	2.50164224535820	4.30369222154366
H	5.32636294216179	3.85310034594753	3.61904956162050
H	6.77219515718480	0.63721867706682	3.41730593648693
H	7.26987634641221	3.21916650639399	6.74967968709026
C	6.93450782233008	2.32992703990926	6.20816631175023
H	7.42083566188356	1.45547496052001	6.64219226928830
H	5.85598881808050	2.22870854846354	6.33489744467788

(Me$_3$Ge)P$_4$H
E= -3561.93766778 Eh

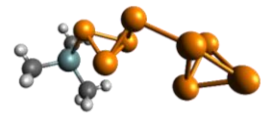


0 1

P	2.41563134296158	-0.26310839398710	2.24078466387278
P	4.72410392445625	0.83367398481781	3.53158072244176
P	2.62479335240054	0.69871237925066	4.22499226513485
P	3.07829127033371	1.84065502673889	2.44568038027192
Ge	0.11191151540641	0.09934371392732	1.91889951575956
C	-0.46369437886685	1.86132248306837	2.54061581801322
C	-0.82258931115185	-1.30186997044448	2.91395552651133
C	-0.21086017235406	-0.08644506589942	-0.00196955182881
H	-0.19850098744781	2.01294634753757	3.58749887879574
H	-1.54918773787919	1.93340562071945	2.44133057769182
H	-0.00553851058479	2.65369487638344	1.94782947428334
H	0.31565812967733	0.69379524673330	-0.55331247534835
H	-1.27910398700370	-0.00108292256902	-0.21154074107830
H	0.13626464313080	-1.05757519505045	-0.35767283455303
H	-0.63609509234976	-1.19324126323113	3.98329116840890
H	-0.48559078236904	-2.29068591184082	2.60022988773978
H	-1.89789425725815	-1.22791719049873	2.73831393414492

H	5.06575103889859	1.96559623434434	4.34157278973857

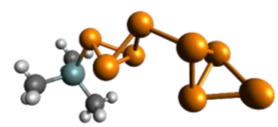
TS((Me$_3$Ge)P$_4^{\bullet}$→(Me$_3$Ge)P$_8^{\bullet}$)
E= -4926.35020504 Eh
im. freq. = 105.96 *i*



0 2

P	2.57634092669917	-0.81423067389992	1.98602568749661
P	5.25389759013495	-0.25613965147818	2.64717775310880
P	3.41768201003514	0.27450514660820	3.72755337800731
P	3.74182072660894	1.05049385911874	1.72877460793962
Ge	0.40021362297731	0.11240610416707	2.01072641686715
C	0.39756936485301	1.95895825061705	2.64916071049511
C	-0.68119962661830	-1.02638861758345	3.17768525411737
C	-0.24541535472015	0.02254692931608	0.16641914406077
H	0.80397945591060	2.02593744563693	3.65886324476367
H	-0.62968670702691	2.33038133206199	2.66065161785609
H	0.99062807905314	2.59827100450931	1.99408995739302
H	0.37882076172339	0.63623230236875	-0.48463718542041
H	-1.27197185231062	0.39135429228312	0.11372829008988
H	-0.22565192117025	-1.00468989914829	-0.19973187509362
H	-0.30951852855707	-0.98368100351094	4.20215570882302
H	-0.65124964271932	-2.06236569568178	2.83800524766375
H	-1.71891187951537	-0.68631667099352	3.16810398251698
P	6.79413112139291	1.51268945117876	3.46679280841243
P	7.48573427633859	3.28588713985482	4.88594536382307
P	6.28284937025999	1.59538760380395	5.58889371219812
P	5.41738820665069	3.04364135077122	4.20832617488097

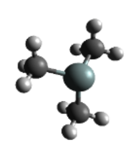
(Me$_3$Ge)P$_8^{\bullet}$
E= -4926.35080109 Eh



0 2

P	6.80794242672950	1.06336545571780	3.82513987519387
P	7.53860675230855	3.48454635334003	4.92610458823482
P	6.54063355107072	1.79646930323166	5.89180746817471
P	5.56033839030261	2.84428484877948	4.24334200605638
H	0.61080287841661	-0.02392590635154	0.61462616175226
P	3.75944467506537	0.27356468247069	2.48494211902891
C	-0.06258855160350	-0.59242209466097	1.25753287674895
H	1.17927088067082	2.09600938840511	3.03113808266267
H	-1.08306055858059	-0.24002590775149	1.09265516027423
H	-0.00861030785828	-1.64465404704312	0.97557100779901
P	5.29891002146424	-0.64163323232548	3.77780070391777
P	2.55650325964176	-1.33564521672988	3.40767448836278
C	0.42140672643137	1.55128799045201	3.59539974196802
Ge	0.42815437622619	-0.34921879013893	3.13608196193534
H	-0.55899182340478	1.96887897755684	3.35449859836052
P	3.48063638338620	0.27009353847783	4.63425579885958
H	0.60921269394913	1.69634387014246	4.65969910243827
C	-0.78355359192414	-1.34536967055900	4.30561501293049
H	-1.79925245259154	-0.95608559926557	4.20942060305677
H	-0.79023481857926	-2.40307301033589	4.03888638431218
H	-0.47241091112098	-1.25156093341202	5.34687825793238

Me$_3$Si$^{\bullet}$
E= -408.91880037 Eh
H= -408.87946501 Eh



0 2

Si	-6.01402051526227	0.27061830776064	0.46188261231549
C	-7.49572177038263	-0.72928209931292	1.03987549331333
H	-7.20999313844297	-1.37485409559983	1.87868838845208

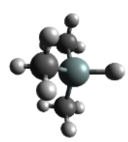
H	-7.88105082580489	-1.36723195801090	0.24179892912929
H	-8.30677872666042	-0.07987656429112	1.37610169639179
C	-4.65423753233380	-0.87250476273634	-0.14792647301809
H	-3.78453929170950	-0.30664987918378	-0.48886379525873
H	-4.99982067671912	-1.49485790967117	-0.97610006086427
H	-4.32757881798652	-1.53784494558140	0.65971261201179
C	-5.37642272184734	1.35504288780905	1.85706718820993
H	-6.14718924291025	2.04408102100073	2.20895832536620
H	-4.51508275436684	1.94608197754458	1.53842619346284
H	-5.06540398557342	0.73543802027247	2.70629889048834

$(Me_3Si)P_4^{\bullet}$
E= -1773.97201212 Eh

0 2

P	2.34947013291138	-0.25875155855258	2.23203374798272
P	4.64287752089734	0.78988328280609	3.47698857756903
P	2.57991826824500	0.71029281573002	4.21321975843626
P	3.04084471625620	1.84069561489277	2.41454919478782
Si	0.09881176169652	0.10820645615874	1.92403562195825
C	-0.44959584157801	1.79310502271836	2.51962980030735
C	-0.78369804831968	-1.24073493583690	2.87594868279375
C	-0.19613165027979	-0.07319651712265	0.08369236205008
H	-0.21188018917704	1.94712128585575	3.57432363818549
H	-1.53408198986518	1.88160839835441	2.40159761026664
H	0.01914472369145	2.59604138490059	1.94703611984932
H	0.33614146760016	0.69834725672018	-0.47731405548138
H	-1.26235300450979	0.01749805889459	-0.14383744056271
H	0.14325925229600	-1.04717535967083	-0.27668022604903
H	-0.60431711280528	-1.14120020242494	3.94894059158311
H	-0.44744780490449	-2.23313860554600	2.56720247948578
H	-1.86296220215478	-1.18161239787760	2.70638353683752

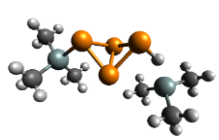
Me_3SiH
E= -409.55922044 Eh
H= -409.52053043 Eh



0 1

Si	-6.01248331123423	0.26782889926965	0.46602798014279
C	-7.48855346046404	-0.73013459568590	1.04317364315214
H	-7.21259431195311	-1.37615306499274	1.88145080794240
H	-7.87375211982764	-1.36659962297267	0.24299268093057
H	-8.30081103755454	-0.07865747686688	1.37451537814760
C	-4.65690432196795	-0.87231024808338	-0.14127140546444
H	-3.78993052399976	-0.30468265685610	-0.48809688973143
H	-5.00495791262431	-1.49410340890456	-0.96964936335428
H	-4.32287928502732	-1.53771482366907	0.65971170322898
C	-5.37642313512936	1.34689306923911	1.85838846524285
H	-6.14748471167042	2.03882721315529	2.20585674630476
H	-4.51544827212018	1.93879592575456	1.53823551534058
H	-5.06576273840850	0.73579668618106	2.71050594586001
H	-6.44049485801863	1.14703410443163	-0.66389120774251

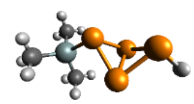
TS($(Me_3Si)P_4^{\bullet}$→$(Me_3Si)P_4H$)
E= -2183.49388392 Eh
im. freq. = 187.56 *i*



0 2

H	1.76785332166208	1.73192075453450	-0.74352556675964
P	5.26548175904519	1.57400204163037	0.44593987257250
C	1.41888243281266	0.69764885679241	-0.69952391982808
H	1.48794077398493	0.27571723064116	-1.70493255822981
H	0.36435626740824	0.70751884057105	-0.40914881547324
H	2.72152173980685	1.50289981516152	2.21905679621848
P	7.23129372702742	0.58670560754539	0.22214101631096
P	4.55784810420592	-0.38260342904176	-0.30988831320128
C	2.33596696123415	0.48106480099930	2.22410501193292
Si	2.42811498512531	-0.29885069111586	0.52488983724384
H	1.29236120083102	0.51412557799601	2.55164245033094
P	5.68723751237105	-0.20739785982348	1.59010784589570
H	2.90395935766787	-0.08961000730645	2.96184139407352
C	1.81822306163252	-2.06845147414236	0.58891405261393
H	1.86435931048357	-2.53644237214456	-0.39730456909300
H	0.78024959314093	-2.10508457569791	0.93176399347354
H	2.42242853207219	-2.66773520507423	1.27411865095924
H	6.17008741009510	3.38899185956549	4.89365058507193
H	7.57656389432358	5.26897175153512	2.71809265822366
H	9.31947205848223	3.56084754252580	4.76083998657407
C	6.20948089969268	2.58988308109948	4.14418273431479
C	7.58993419436337	4.40128785862589	2.04912459921795
C	9.29818664978982	2.74809728620655	4.02578344267518
Si	7.70567293573662	2.80847091729087	3.03321330045283
H	10.17178029613813	2.85788197386182	3.37948529956272
H	5.28669145814389	2.61892456426778	3.56161394670775
H	6.67675184458759	4.42334186137115	1.45008345834602
H	8.44100918080324	4.51033654357462	1.37319287737545
H	6.24348301988100	1.63349018813402	4.66993747500349
H	9.39315004821745	1.80418652680018	4.56672910774082
H	7.80266746923170	1.42645013361575	1.34539334969225

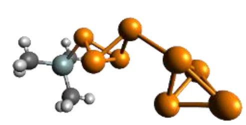
$(Me_3Si)P_4H$
E= -1774.58612818 Eh



0 1

P	2.34160725142255	-0.26015142346776	2.22923655084666
P	4.67547418971061	0.80810515159025	3.50735562410747
P	2.57584724317160	0.70686302135387	4.20876956630948
P	3.03865988421143	1.83428241275955	2.42393381692182
Si	0.10626585786440	0.10933683803006	1.92450299394151
C	-0.45041090319057	1.79363722083104	2.51817962649802
C	-0.77944640028840	-1.23813433873107	2.87609299102146
C	-0.19647533154646	-0.07172476442247	0.08538540143955
H	-0.21863712782384	1.94814933742902	3.57412194755100
H	-1.53435347360124	1.87900689486086	2.39394772161822
H	0.01920275572997	2.59825637155943	1.94849654654072
H	0.33243725914831	0.70070708103751	-0.47772598479367
H	-1.26343848267232	0.01693208127468	-0.13853387173446
H	0.14394225102503	-1.04493569207092	-0.27625274639312
H	-0.59992800326494	-1.13903226224294	3.94918743423886
H	-0.44334683818464	-2.23072034223980	2.56755911008737
H	-1.85852546944850	-1.17850552334198	2.70670624120257
H	5.03445533773700	1.93913793579068	4.31110703059651

TS($(Me_3Si)P_4^{\bullet}$→$(Me_3Si)P_8^{\bullet}$)
E= -3138.99921989 Eh
im. freq. = 101.26 *i*

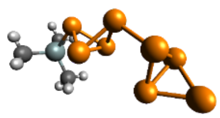


0 2

P	6.80930377065385	1.31257592157288	3.97650312244923
P	7.58148297273131	3.23878324693308	5.06573963322217
P	6.57453563818840	1.60792622097576	6.12593314380650
P	5.45142484967171	2.85191127235550	4.73130573080480
H	0.39469323040173	-0.18143663740558	0.56769085214903
P	3.70432564299016	0.51068575614294	2.48605309822503
C	-0.21047792634541	-0.68460084278552	1.32519659425797
H	1.03213929355579	2.05778989538455	2.63848419472026
H	-1.24202384960440	-0.33490930682332	1.22362864293390
H	-0.19534287549680	-1.75629529070821	1.11343749462599

P	5.24411332885430	-0.61815003062887	3.57819949468350
P	2.53061970644032	-1.25348673862987	3.12828395731171
C	0.43405488835684	1.51646546580289	3.37449297677182
Si	0.43176079306204	-0.32504733803216	3.04651373989537
H	-0.59233918735693	1.89212857896968	3.31715671746463
P	3.45057248842806	0.12892113693711	4.60403926202759
H	0.82442533892916	1.75349680539972	4.36632367083483
C	-0.58585641784556	-1.22514254059766	4.33449897371637
H	-1.62575210341447	-0.88697973447153	4.30247023004516
H	-0.57722206477507	-2.30398366168832	4.16315160451386
H	-0.20127751742521	-1.03943217870310	5.33997686553992

$(Me_3Si)P_8^{\bullet}$

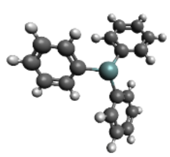


E= -3138.99919594 Eh

0 2

P	6.77027283155221	1.04974892229513	3.82668057190752
P	7.51090745474446	3.45862374009500	4.95528289769527
P	6.50554709174998	1.76314066105081	5.90104793902137
P	5.53165674734286	2.83346854494524	4.26302514278594
H	0.61662664890327	-0.02195070932587	0.67430379695746
P	3.71442836007537	0.31026000653690	2.48370763597252
C	-0.04709260996760	-0.58251204792616	1.33660665746047
H	1.14424278198834	2.04932681993334	2.96390790671796
H	-1.06991566222461	-0.23407077212283	1.16600643453481
H	0.00194148537523	-1.63610446168719	1.05231969895078
P	5.25129763455232	-0.64444229818586	3.75200124017370
P	2.49608893259533	-1.30640309172119	3.37405978315460
C	0.42376815087547	1.48520820304494	3.56009919945864
Si	0.43342710187942	-0.33525680302538	3.12940222397278
H	-0.57170680933178	1.89498808805727	3.36251264897932
P	3.44134907416976	0.26352114068074	4.63265001756066
H	0.65303374410620	1.65297473603823	4.61445933207992
C	-0.71210869741062	-1.28743409539801	4.26363999847774
H	-1.73663011623462	-0.91527954756804	4.17291911999094
H	-0.71684815688385	-2.35163904874104	4.01680660099509
H	-0.40712598785745	-1.18494798697608	5.30764115315196

$Ph_3Ge^{\bullet}$



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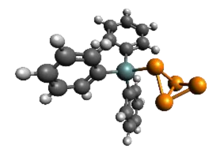
H= -2770.81938847 Eh

0 2

Ge	-4.43429441611669	0.48085306309191	-0.04362897639998
C	-5.52853984518282	-1.04737842430767	0.46257211683583
C	-5.43425524229980	-2.24687735391876	-0.24712099461443
C	-6.43799272769615	-0.96745045736590	1.51821933781657
C	-4.84562756039471	2.04329351722765	1.04230130691164
C	-6.14149535358907	2.56362630955382	1.06318803384841
C	-3.85868925693875	2.68078418473039	1.79589927936165
H	-0.40023544086488	-2.44321793200358	0.88923722067853
C	-0.73323557226290	-1.48268186470829	0.51207710231647
C	-2.08756056048989	-1.18330087215191	0.48850251082749
H	-2.80211553471523	-1.91368249853984	0.85316517775897
C	-2.53613853705564	0.05003078980254	0.01346371973393
C	-1.59232553520503	0.97175469923824	-0.44514996794701
H	-1.91774322617305	1.93352371910070	-0.82948312210057
C	-0.23884207968209	0.67459094269692	-0.41880466185993
H	0.48140024738365	1.40212176716357	-0.77588004828020
C	0.19332313818814	-0.55524569055854	0.05823454365210
H	1.25132268848450	-0.79048815085035	0.07471233665122
C	-6.44661756215418	3.67850232055406	1.82784223670115
C	-4.16234125100168	3.80012160759954	2.55691419635230
C	-5.45594026596202	4.30056508210357	2.57522214970643
H	-5.69241471429284	5.17508256621039	3.17040408219489
H	-7.45885475474650	4.06685186008708	1.83651173967769
H	-2.84536970803399	2.29313218895267	1.79788959848158
H	-3.38606011036793	4.28139272084791	3.14141648670070
H	-6.92297872442399	2.09268334705929	0.47472673846896
C	-6.21496448387858	-3.33886526739942	0.09785057127724
C	-7.22302213727381	-2.05850169710698	1.86089851373550
C	-7.11298997058653	-3.24599011556876	1.15218642213338
H	-6.12641186940662	-4.26421781275303	-0.46021174127010
H	-6.52609030200614	-0.04767593302464	2.08654539770266
H	-4.74248171744768	-2.33055338955633	-1.07970639279192
H	-7.72649957802238	-4.09860583964969	1.41966486272370
H	-7.92065803578455	-1.98139738655658	2.68738022301509

$(Ph_3Ge)P_4^{\bullet}$



E= -4135.92468393 Eh

0 2

P	-6.78111348136322	-3.69311545219836	-0.35059140525359
P	-5.80827922024736	-2.93427722491734	2.12313874443235
P	-7.65446287371033	-2.29599783723228	1.13036645233739
P	-5.73669194264887	-1.83128615435831	0.22774808501138
H	-11.39224235788280	-5.82066421317482	-4.5938136877222
H	-11.09388334815745	0.91096304483060	-1.2064929037209
H	-6.02366361440199	-1.73064483011601	-6.77666553870203
C	-11.07767991989609	-5.41815886896582	-3.6374729326752
C	-10.08027835323801	0.64149159362262	-1.4806846024381
C	-6.03932996265480	-2.46709430684567	-5.98119161885324
H	-9.41126204408754	-4.36237426600030	-4.47168553422268
H	-9.36812731685237	2.66601139576133	-1.45522494331422
H	-10.51488414854629	-1.45351455416448	-1.5809166139191
H	-12.65120137089670	-6.37978522428943	-2.5393248114501
C	-9.96402269017787	-4.59356793893319	-3.56681555632038
H	-4.65845922839166	-3.78395283924399	-6.96173047257012
H	-7.41925561230989	-1.34874373782195	-4.78607571216568
C	-9.11276408348076	1.62576608518142	-1.62146462688752
C	-11.78401576068920	-5.73158335580370	-2.4852993109930
C	-9.75190282135752	-0.68971353981036	-1.69065394311341
C	-5.27455384190712	-3.61901297385262	-6.08528139943220
C	-6.82533416038348	-2.25387533562693	-4.85735898915292
C	-7.81788738443464	1.27752290287931	-1.97719797737805
C	-5.29906973173829	-4.56025135516429	-5.06556733004458
C	-8.45433495754315	-1.05248969608856	-2.04614377865156
C	-9.54567765993090	-4.06979830866155	-2.34510263853013
C	-6.85669074074220	-3.19053248822977	-3.82615020358016
C	-11.37463069223024	-5.21973211248198	-1.2624385849683
C	-6.08492560141626	-4.34549700055632	-3.94410924552678
C	-7.49089757302985	-0.05343263630072	-2.18693932268138
C	-10.26137453881250	-4.39523364017455	-1.1940931295382
Ge	-7.97328611313903	-2.92270874873984	-2.25511061167011
H	-4.70235484341569	-5.46198602006285	-5.14239593094277
H	-7.05940280538349	2.04398292018752	-2.08802539210039
H	-11.91981434248225	-5.46777428066903	-0.3588771639139
H	-6.09395069058595	-5.08863507569929	-3.15254532562799
H	-6.47480201207214	-0.31276050294831	-2.46598822340866
H	-9.94371215976186	-4.00985342333010	-0.22992382031100

Ph_3GeH
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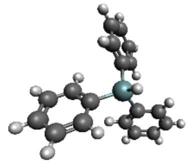
H= -2771.44522483 Eh



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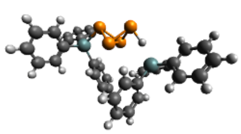
Ge	-4.46080381737895	0.79792562282311	-0.12917702870032
C	-5.61433443005909	-0.75801504254840	0.07677011735454
C	-5.13113840232917	-1.90666262086566	0.70006731755576
C	-6.93916865734013	-0.73957736364770	-0.35565401159216
C	-4.75630600929185	2.02819337826207	1.35378995008287
C	-5.64652911244021	1.71025928054385	2.37610602671997
C	-4.05363405328400	3.23063330326134	1.42967917551922
H	0.09165617948816	0.08982741857059	1.96339955888669
C	-0.50621868432775	-0.05778195674465	1.07101951851871
C	-1.81665562774281	0.39891822704865	1.03316146025969
H	-2.23178063635858	0.90323960156014	1.89980387204245
C	-2.60084678159252	0.21982594836608	-0.10405771823770
C	-2.04183319629545	-0.42823243237058	-1.20465798582254
H	-2.63344043896233	-0.58214917146808	-2.10197353287615
C	-0.73310015091298	-0.88493556272095	-1.17090575233572
H	-0.31186429331302	-1.38570070583230	-2.03543214653385
C	0.03711690243150	-0.69958758498039	-0.03117308224065
H	1.06102185496935	-1.05463099151073	-0.00405566761114
H	-4.77716531314581	1.48973331918451	-1.47228780241235
C	-5.83066275722824	2.57072027681174	3.45010469170566
C	-4.23367045049807	4.09170172133629	2.50163771571336
C	-5.12358159754993	3.76162504854214	3.51430243649975
H	-5.26487014740409	4.43395674775633	4.35291968488151
H	-6.52685049526696	2.30860565958960	4.23888729379529
H	-3.35056423896404	3.49952804913173	0.64710259986037
H	-3.67962377046162	5.02254372467632	2.54806864263096
H	-6.20141606330293	0.77845025046001	2.33552529647391
C	-5.95152798313789	-3.00920015379655	0.89104388528395
C	-7.76237890295225	-1.84039317224079	-0.16741902407185
C	-7.26852389359227	-2.97673039726279	0.45706977802390
H	-5.56054017532929	-3.89606267611235	1.37699966391414
H	-7.33749274413619	0.14261806560346	-0.84745315953141
H	-4.09914648260255	-1.94443247644502	1.03440028897724
H	-7.91042197483451	-3.83795992673060	0.60346691596755
H	-8.79072365485317	-1.81232340825048	-0.50988897870171

TS($(Ph_3Ge)P_4^{\bullet}$→$(Ph_3Ge)P_4H$)
E= -6907.41123410 Eh
im. freq. = 595.25 *i*



0 2

P	-7.13763354625216	-4.72204246910222	0.45267989337738
P	-6.16597148154660	-4.88601553035032	3.16794546162277
P	-7.46202171918178	-3.38399135418784	2.19264433062941
P	-5.45929088333216	-3.69210576706328	1.45080463438696
H	-10.88319219461299	-3.15442867867250	-4.9343740308220
H	-9.41822096730279	1.16329274496098	0.76684912274778
H	-4.18043918195000	-1.40659482429811	-4.66668285883142
C	-10.72551594189463	-3.32233226972200	-3.8749209297523
C	-8.50090901130924	0.63214114821399	0.53791472154244
C	-4.58922610601068	-2.28562059067630	-4.18107108581958
H	-8.63727967656281	-2.85647417723866	-3.96944067832121
H	-7.22979238056711	2.13337934961345	1.39933404744303
H	-9.52023633440864	-1.01913428866281	-0.36948586476173
H	-12.77172030195608	-3.84600740551157	-3.4936256925250
C	-9.46185112530200	-3.15215317867893	-3.32844599226435
H	-3.38316945379655	-3.65916637610719	-5.30516974314035
H	-5.89971939695860	-1.15251258640672	-2.92177551140079
C	-7.27397395321511	1.17912568726138	0.88640767158904
C	-11.78468365858694	-3.70968365750075	-3.0666834314903
C	-8.55654652866684	-0.59734238100244	-0.10275532828964
C	-4.14236566856533	-3.54850236796592	-4.53935937349212
C	-5.55954542139662	-2.14511488041193	-3.19844383933599
C	-6.10231155845773	0.50015334770237	0.58348015907891
C	-4.66714106645866	-4.67085608011569	-3.91406619770465
C	-7.38748483630814	-1.29111383737672	-0.41077807063369
C	-9.24213997529557	-3.36345108755681	-1.96905763943197
C	-6.09448623435736	-3.26413150159894	-2.56309961693647
C	-11.57772190839616	-3.92766493424879	-1.7123669237793
C	-5.63583461892667	-4.52762116740076	-2.93222443605120
C	-6.16074151625306	-0.72451850584723	-0.06353749454313
C	-10.31286819562667	-3.75612623409544	-1.1682671092691
Ge	-7.47541872777959	-3.06930854576905	-1.20323786968322
H	-4.31806278482174	-5.65944005888370	-4.19036857349809
H	-5.14202199105456	0.91428927248509	0.86594269513090
H	-12.40192461922273	-4.23596740474225	-1.0791192757738
H	-6.03490455619558	-5.41332904754260	-2.44723381367502
H	-5.23586614693813	-1.24277339495475	-0.29286882855549
H	-10.16114784531550	-3.93605571369004	-0.1079189582994
H	-5.62111939671328	-3.74497652934979	4.12207074211036
H	-7.18849676862857	-0.43260919654590	3.26189039944711
H	-5.66963193058612	-3.90606814423901	7.17513983700903
H	-2.97616152537254	-2.28821245406684	2.81949801721282
Ge	-5.20363191646079	-1.97817086094486	4.87850200844610
C	-7.61752347463162	-0.50929229070164	4.25542449918821
C	-4.71462838367769	-3.42710391575661	7.36837993965370
C	-3.15969412180767	-1.22310129911635	2.91261815361886
H	-9.38437693890634	0.55859452986697	3.69421112694566
H	-4.40222667901034	-4.51156314305453	9.19155569164946
C	-8.86040818608266	0.05275921419366	4.49750522939357
C	-3.99964334966915	-3.77631006862525	8.50398513297424
C	-4.14929886190554	-0.75992200985161	3.77807983493357
C	-4.21476917407718	-2.47741484435536	6.47615638479014
C	-6.92187001676654	-1.16499275114366	5.27415493426494
H	-1.64429345228663	-0.71478930485922	1.48368649802392
C	-2.40532341292997	-0.33758626519745	2.15729063319998
C	-4.36418185615493	0.61542052442628	3.87171265661902
C	-2.62438070595051	1.02875652925331	2.26486333892213
C	-2.76727431365360	-3.19024913742527	8.75699794206532
C	-2.96934185840096	-1.90578359332232	6.73559056672402
C	-9.43213469092276	-0.03940414297571	5.75909644324997
C	-7.50537459865233	-1.24882139108236	6.53808833554634
C	-3.60253016109807	1.50412539619025	3.12663907555768
H	-5.13330047243342	0.99847511007734	4.53385771316807
C	-2.25123017792999	-2.25824926621782	7.86854372896648
H	-2.03356187359895	1.72190838944685	1.67682073346189
H	-2.20729728229394	-3.46433514687082	9.64368800990892
C	-8.75193314082561	-0.68993026474324	6.77887528660587
H	-2.55928864521867	-1.17300556075051	6.04837921418234
H	-10.40661646212584	0.39646157180916	5.94787663155210
H	-6.97723252321430	-1.74079192388278	7.34815270995740
H	-3.77682199743832	2.57065244382625	3.21651250742998
H	-1.28659634360605	-1.80137494739822	8.05918291969744
H	-9.19202379218119	-0.75961650946652	7.76734955405512

$(Ph_3Ge)P_4H$
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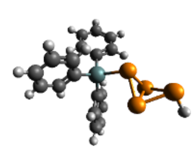

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P	-6.78608463988543	-3.70970158730422	-0.36008176534194
P	-5.81593152733154	-2.88176943471731	2.19142476056753
P	-7.67316962582306	-2.31907255539952	1.12138240847374

P	-5.76702689539123	-1.83594153249058	0.23444302272974
H	-5.74901004693786	-1.68489977022604	2.97662736666882
H	-11.43662721681040	-5.75217583407766	-4.6081137829266
H	-11.08093218746120	0.90698092017580	-1.2068953128698
H	-6.08154891835011	-1.75421829612744	-6.79226616752881
C	-11.10580286615460	-5.37615583211330	-3.6464889499945
C	-10.06873523312439	0.63545732459705	-1.4843118027728
C	-6.07049702288875	-2.48072835420275	-5.98762120199891
H	-9.44418044192762	-4.31006095987341	-4.47705783405182
H	-9.35605099836507	2.65990706137127	-1.47574585458634
H	-10.50413351992774	-1.46035979598374	-1.5687050499585
H	-12.66980323395835	-6.35616377099857	-2.5508525427501
C	-9.98575411412675	-4.56065988130059	-3.57050392241337
H	-4.66031503851114	-3.77029876463985	-6.96250906162507
H	-7.47120065774835	-1.38616419263633	-4.79492351846093
C	-9.10178254556665	1.61845354796581	-1.63613741779612
C	-11.79755937811418	-5.71512302836129	-2.4926367667206
C	-9.74155173591957	-0.69741723152511	-1.68723323978934
C	-5.27411595819435	-3.61168527397483	-6.08326862122353
C	-6.85344706380650	-2.27572147642226	-4.86014286410813
C	-7.80875259596718	1.26727880164115	-1.99591315838104
C	-5.26397020364339	-4.53978136608385	-5.05142161268956
C	-8.44602928889220	-1.06294681671491	-2.04570543251346
C	-9.54537685092426	-4.07256762276023	-2.34201091631001
C	-6.84980873678596	-3.19873265121006	-3.81632847288873
C	-11.36704905501515	-5.23816334003687	-1.2630973193222
C	-6.04683432776172	-4.33280576201781	-3.92623504294584
C	-7.48334302640826	-0.06525443704010	-2.19817456281652
C	-10.24705993302226	-4.42310139404426	-1.1898026667167
Ge	-7.96443812345173	-2.93672677961076	-2.24207642294752
H	-4.64242285281302	-5.42515417078599	-5.12164843423954
H	-7.05062465586275	2.03275167794353	-2.11600316992028
H	-11.90069127161542	-5.50635185441257	-0.3583541682993
H	-6.02811459527083	-5.06535664851755	-3.12504415826089
H	-6.46872973692354	-0.32683941792819	-2.48077984983580
H	-9.91305387931721	-4.06524950015655	-0.22055649343473

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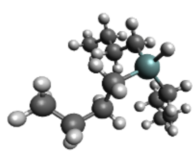
H= -2550.11498566 Eh



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Ge	-6.22940188625121	0.46944007030593	0.18105126649801
C	-7.69609152234307	-0.77566784203155	0.60164375400941
C	-7.62722810909431	-1.41513482660083	1.98152650273729
H	-7.71609892231484	-1.54918132296315	-0.17397260723460
H	-8.63417411888824	-0.22013816946886	0.49871121223362
C	-4.63804567681966	-0.49989519934769	-0.45837067193687
H	-3.78017561494736	0.16802188363432	-0.33527573815885
H	-4.75708304935970	-0.64953048977633	-1.53681421897686
C	-4.38397025775282	-1.84059107185614	0.21975199087210
C	-5.77942098478222	1.58330741838112	1.74161541082279
H	-6.71284038075762	1.84974081441080	2.24951514309487
H	-5.36153534351695	2.52189733170752	1.36283526893528
C	-4.80604331226130	0.94634888064472	2.72363090067723
H	-6.70988881904795	1.40628733792304	-0.95626542412665
C	-3.16433152516355	-2.58473747080527	-0.31452646593230
H	-5.26520691798222	-2.47945882965091	0.09783265368572
H	-4.26297272880298	-1.69814904183750	1.30030081088821
H	-6.68708711452224	-1.96653489305924	2.09787427873706
C	-8.78748232571183	-2.35789076851140	2.26410473372413
H	-7.61057340459447	-0.63412943722974	2.75134453707626
H	-3.88030565928199	0.67343558493089	2.20285381034207
H	-5.21828874182587	0.00670912145194	3.10951797590793
C	-4.45850314590047	1.84976494240165	3.89691471052562
H	-4.04974275611404	2.79122474633420	3.51207619776808
C	-3.47179353020056	1.21605284079119	4.86184602510909
H	-5.37979777003143	2.11535737946721	4.42799278238494
H	-8.80474333843355	-3.14204969247484	1.49850196192181
H	-9.72931800861436	-1.80823386521526	2.15353908678821
C	-8.71629742606288	-2.98752215636241	3.64386839167554
H	-3.27950429510108	-2.72851506509766	-1.39522255210084
H	-3.14152346606449	-3.58725011290922	0.12604019335802
C	-1.84644112677455	-1.88426679594762	-0.02947486967370
H	-7.79534710415382	-3.56481083593978	3.76498197362383
H	-9.55673012512172	-3.66140922541318	3.82440738898503
H	-8.72901407009648	-2.22322604396552	4.42613497117795
H	-1.79455507033457	-0.90688023392785	-0.51431067169856
H	-0.99875808725943	-2.47209160110158	-0.38842542192144
H	-1.71154470075150	-1.72842502758961	1.04510498451483
H	-2.52958212488097	0.97713721013927	4.36042118988955
H	-3.86800683342044	0.28406324202826	5.27476487366027
H	-3.24352060466111	1.87956121453113	5.69900366013587

Bu$_3$Ge$^•$
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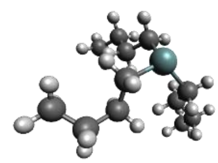
H= -2549.48491092 Eh



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Ge	-6.23673852680420	0.47719635488392	0.17154501746155
C	-7.69986457518610	-0.79342248169558	0.58850176103242
C	-7.63137554387525	-1.41036291887884	1.98088387174670
H	-7.68853021236536	-1.57504130676648	-0.17836784715439
H	-8.64802364119721	-0.26023772483997	0.46751831825022
C	-4.62181227265649	-0.48465807956713	-0.45797100916761
H	-3.77241884904736	0.18446514864900	-0.29359206224339
H	-4.70786025513007	-0.61422966967694	-1.54158585707913
C	-4.39251843297480	-1.83968799678922	0.20405230491756
C	-5.79881605104797	1.58757021672554	1.75412484562704
H	-6.73787156490821	1.81878309862540	2.26780424235363
H	-5.40341576892163	2.54229379492271	1.39363544240253
C	-4.80414726258479	0.94879746288584	2.71623486781267
C	-3.16827937513714	-2.58334272761032	-0.32294659066698
H	-5.27601571610537	-2.46930081583949	0.05490200907536
H	-4.28952385458708	-1.71429525967646	1.28824892917182
H	-6.68660283484580	-1.95037244568009	2.10944041885266
C	-8.78564234040064	-2.36075691373024	2.26823462903409
H	-7.62849053366005	-0.61777896492381	2.73856547075845
H	-3.88080204895696	0.69582420516817	2.18190449554289
H	-5.20128221066648	-0.00009341617774	3.09438757672693
C	-4.45632356171336	1.84474654215146	3.89647823432096
H	-4.06024554056251	2.79384535739120	3.51757732087697
C	-3.45480218893762	1.21003129853081	4.84568317508768
H	-5.37569969650089	2.09472893642918	4.43803286836998
H	-8.79070375773693	-3.15466802706265	1.51279347365692
H	-9.73146550696102	-1.82087499916748	2.14569368193787
C	-8.71544692191652	-2.97177022238535	3.65665917422361
H	-3.26799262303966	-2.71030917045384	-1.40714385031775
H	-3.15921048803923	-3.59227262039309	0.10358106309819
C	-1.85119411496938	-1.89484076415835	-0.00722694463940
H	-7.79007142125952	-3.53920409245540	3.78958515265063
H	-9.55083550114103	-3.65088883149424	3.84132115440578
H	-8.73918539376105	-2.19759157553513	4.42881179939040
H	-1.78567286373139	-0.91193841824861	-0.47903260594803
H	-1.00149765777126	-2.48372217652979	-0.35957188483736
H	-1.73333741411343	-1.75314645697505	1.07128609587228
H	-2.51532702274018	0.98464389149962	4.33309523927467
H	-3.83913539387584	0.27067567915988	5.25296689237298
H	-3.22489106017014	1.86753608968856	5.68717912574856

$Ph_3Si^{\bullet}$
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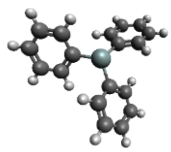
H= -983.46200346 Eh



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Si	-4.41032569756071	0.45595615782670	0.06408974815872
C	-5.48101405677812	-1.00335079736144	0.50799828061494
C	-5.39279075541156	-2.19115420331708	-0.22907781515098
C	-6.40760120041013	-0.94847521078254	1.55448079027604
C	-4.81092290817044	1.97713905239426	1.06398378942369
C	-6.10532084336759	2.51123641907614	1.04507762406451
C	-3.84192258057081	2.63176401657639	1.83176436250787
H	-0.40630349163571	-2.42940073378369	0.89501593445080
C	-0.75738922836073	-1.47449896144764	0.52011574315725
C	-2.11251586514806	-1.18169362094790	0.54098895308516
H	-2.80906962627426	-1.91260138594100	0.93748199391323
C	-2.59161714720357	0.04475752195551	0.06853728271252
C	-1.66137430967921	0.96546393793429	-0.42947687174117
H	-2.00473051363220	1.92168763361422	-0.81258681463486
C	-0.30714187624384	0.67667927000733	-0.44642921068024
H	0.39624210664868	1.40448546176772	-0.83497525536369
C	0.14823244725828	-0.54683429182095	0.02652365557005
H	1.20747103328479	-0.77649995009655	0.00879487598269
C	-6.42259826365598	3.64440853667232	1.77491041822495
C	-4.15640196603583	3.77055977960827	2.55756266535161
C	-5.44668492209046	4.27891257229629	2.53200833653414
H	-5.69230975016013	5.16881058512366	3.10012113524489
H	-7.43201683449449	4.03905160859413	1.74829944172453
H	-2.83132782848617	2.23923930569308	1.86865792969106
H	-3.39190537250074	4.26076778469362	3.14999524534512
H	-6.87528709421335	2.03204860379486	0.44790467862823
C	-6.18792966992568	-3.28311565173471	0.07543144695430
C	-7.20915768652420	-2.03872137197992	1.85642164281729
C	-7.10123124421985	-3.20845486629849	1.11857214642433
H	-6.10082072509784	-4.19413038915280	-0.50583422824890
H	-6.49496046865493	-0.04374135100388	2.14628457458996
H	-4.69081635829468	-2.26035840350339	-1.05463846046741
H	-7.72745484519309	-4.06120181590457	1.35434846657989
H	-7.91775245719733	-1.97600524255225	2.67468749425950

$(Ph_3Si)P_4^{\bullet}$
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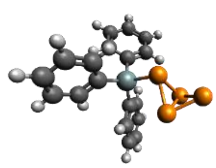

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P	-6.82672586411737	-3.68507073275573	-0.43127473901281
P	-5.79217735784035	-2.92426702375885	2.05029332568545
P	-7.63634727705684	-2.26287512227104	1.06562379940184
P	-5.71936487423000	-1.85302708326720	0.13564890505891
H	-11.35115647100554	-5.75564100745031	-4.6157882719612
H	-11.09123587875939	0.84570503688750	-1.2069928289724
H	-6.09192365218630	-1.75225178599243	-6.75069287748673
C	-11.03543080562803	-5.35923503497851	-3.6573411345007
C	-10.07823110873145	0.57730394623993	-1.4842418934390
C	-6.09669816480280	-2.47495990387558	-5.94262111533781
H	-9.36368496525519	-4.31013153654901	-4.48498993819837
H	-9.36480274504367	2.60130133832070	-1.44804011957854
H	-10.51537172417600	-1.51455186991227	-1.5966268431457
H	-12.61517558958097	-6.31778731877815	-2.5652406386744
C	-9.91790076274926	-4.54127518209914	-3.58119125204774
H	-4.70117462333371	-3.79094211328001	-6.90355736706820
H	-7.48753307599550	-1.35422283468848	-4.76566631558184
C	-9.11063137621801	1.56178819952874	-1.62093508119950
C	-11.74465762563434	-5.67428130172749	-2.5075192490818
C	-9.75085955046135	-0.75220036454416	-1.70320023254328
C	-5.31771632143139	-3.61873559357858	-6.02875230587412
C	-6.88257768317189	-2.25290949545762	-4.82110099234003
C	-7.81690077088037	1.21437811874871	-1.98225862103155
C	-5.32883810307551	-4.54268967866358	-4.99295185567797
C	-8.45346300697219	-1.12152383409790	-2.06357591502298
C	-9.49161847772199	-4.02147107977693	-2.35733708432666
C	-6.90331177215019	-3.16904250029507	-3.76784645778188
C	-11.33317166330665	-5.17057922601593	-1.2818105227506
C	-6.11457145783948	-4.31721958325457	-3.87448180654995
C	-7.49263046926715	-0.11489936292945	-2.20065342775681
C	-10.21575354616943	-4.35353438728055	-1.2096555819455
Si	-7.98623120214506	-2.91508385880994	-2.26687522241581
H	-4.72156660035762	-5.43838646679919	-5.05555656144912
H	-7.05804910061729	1.98070731866586	-2.09096554619713
H	-11.87994440711372	-5.42032421121082	-0.3797355321075
H	-6.11255307391405	-5.04803974924094	-3.07122984996961
H	-6.47771173380458	-0.37152804632140	-2.48629635664140
H	-9.89852711725521	-3.97480666873051	-0.24266249247711

Ph_3SiH
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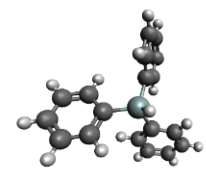
H= -984.09685731 Eh



0 1

Si	-4.42831323129758	0.76750287446236	-0.07579179214989
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C	-5.07924770842881	-1.91923138231690	0.62384045622924
C	-6.89486869714937	-0.64561984367191	-0.28300915506470
C	-4.74379458151755	1.96504491257608	1.32665870462704
C	-5.53842296065831	1.61131315141140	2.41694806155777
C	-4.15037436365972	3.23030558476835	1.32489363856540
H	0.06536465260139	0.09440796059126	2.01205412611709
C	-0.53763178716712	-0.05961702207763	1.12426927325144
C	-1.84559842016235	0.40309857198139	1.08697123458516
H	-2.25398927900038	0.91875315635064	1.94999655626022
C	-2.64116077146543	0.21723323615443	-0.04389409821318
C	-2.08440214952483	-0.44558997542354	-1.14042467255969
H	-2.68107110535829	-0.60569725166107	-2.03361131789217
C	-0.77852765239092	-0.90822746183579	-1.10875202509331
H	-0.36293254442941	-1.41902453668063	-1.97008838802448
C	-0.00267711504802	-0.71543110599835	0.02631004832445
H	1.01965554997915	-1.07526257411199	0.05253341953599
C	-5.73254538393887	2.48916969986892	3.47444971002328
C	-4.34009669236940	4.11005811801522	2.37876910233044
C	-5.13245493373319	3.73886626962437	3.45675968742158
H	-5.28230179618927	4.42616028974359	4.28169041725238
H	-6.35386946804246	2.19588287651369	4.31316865106060
H	-3.52605123209238	3.53262228510492	0.48915072152316
H	-3.87166813863718	5.08766313222014	2.36072163039073
H	-6.01243462354775	0.63547949729871	2.43901414826937
C	-5.92329315831970	-3.00768439661646	0.79096024220041
C	-7.74230732398696	-1.73032271536450	-0.11842108266959
C	-7.25620623201118	-2.91376178965929	0.42000636072876
H	-5.53895887987802	-3.93105635329868	1.20945195362580
H	-7.28750217661378	0.27407340952409	-0.70651296021682
H	-4.03602855983704	-2.00439589591404	0.91055672591961
H	-7.91718901514088	-3.76354918578416	0.54768878826852
H	-8.78335644419589	-1.65451963198120	-0.41163350410572
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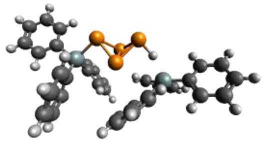

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P	-7.26120559919295	-3.75447193030393	2.36178764874369
P	-5.35515656602108	-3.34626216663464	1.42563879140475
H	-9.88959419116965	-3.14849789300153	-5.33153460280700
H	-11.68342929860889	-1.00003383388376	1.1966911697981
H	-5.20205733906855	0.94471254706919	-2.91449312651461
C	-9.78425363032760	-3.62519890823358	-4.36350510043062
C	-10.60561865934469	-0.92562028027437	1.1070722661255
C	-5.14007135462800	-0.11135079306182	-2.67667573921711
H	-8.30937158985026	-2.23292787814480	-3.68309238692992
H	-10.45042530406952	0.73234848480410	2.46267468336630
H	-10.47060666980272	-2.54687761344960	-0.2825355379780
H	-11.22649979250594	-5.15732499138301	-4.7884084513154
C	-8.89729535041874	-3.10976861063499	-3.43107122757354
H	-3.15823059891036	-0.33403834063805	-3.47012070949377
H	-7.09315649879751	-0.16979678455177	-1.80744408404943
C	-9.91413254171475	0.04525790571947	1.81756800229273
C	-10.53434713130765	-4.75228391237013	-4.0589479156976
C	-9.91890109292938	-1.79746746750844	0.27573679890444
C	-3.99476807776549	-0.82800429782877	-2.98873763532292
C	-6.20696820866143	-0.74474599551523	-2.05516459178194
C	-8.53537135712546	0.13944488080975	1.69525455398220
C	-3.92218299535582	-2.17971443615088	-2.68260076658314
C	-8.53130567069980	-1.71989443326892	0.14172096426508
C	-8.74373221476322	-3.70869104236385	-2.17928042172269
C	-6.15005531088719	-2.10225798204343	-1.73371089554670
C	-10.39145936509889	-5.36386028441042	-2.8224731785357
C	-4.99031135883698	-2.80689232998703	-2.06217668161016
C	-7.85093785155878	-0.73742874100902	0.86795436492993
C	-9.50153704517715	-4.84533598951537	-1.89320665085049
Si	-7.59826384076503	-2.95899279957151	-0.90504161424202
H	-3.02932082472286	-2.74509589727825	-2.92405067676398
H	-7.99211260409447	0.89464796675566	2.25214415967423
H	-10.97031760667052	-6.24872527643471	-2.5834253678554
H	-4.91352592899524	-3.86203290257892	-1.81839844296736
H	-6.77197649696117	-0.66016730458102	0.79042740341304
H	-9.39182789996765	-5.33950760963715	-0.93215656528367
H	-0.83339316100579	-3.58787300061938	8.96453962861490
C	-1.55459042416917	-3.30207561030622	8.20748332366871
H	-0.20361121582185	-1.97430565092670	7.19891079008105
C	-1.20089333011965	-2.39936333335459	7.21555246951176
H	-3.11497619713018	-4.54786471478797	8.99841869668442
C	-2.83446534386057	-3.83945840746888	8.22719307975040
C	-2.12322567526531	-2.03376872927898	6.24659247430735
C	-3.75266028434270	-3.47548631316429	7.25628923065054
H	-1.83681972110084	-1.31963861415279	5.48210338323964
C	-3.41737614215595	-2.56187885360995	6.25051155586867
H	-2.30426285389782	-2.57456053443638	3.31424171888311
H	-1.52214598335280	-1.65823787342806	1.17689595027384
H	-4.74871085352214	-3.90748709717734	7.27906701342310
C	-2.84130205426522	-1.74648521134919	2.86214410198126
C	-2.40143666541602	-1.23798743886761	1.65162881492647
Si	-4.69160783827567	-2.10295347429031	4.97317004990166
C	-3.98649719439587	-1.23628800163371	3.48889179401616
C	-3.10186676142114	-0.21237848867849	1.03200403334523
H	-2.77968149880981	0.16308873748354	0.06800009585520
H	-5.15959624746256	-3.86123426553823	4.09823369671375
H	-5.25935385803876	-0.95063633859714	7.64337579687940
C	-4.65879542415238	-0.18020588749939	2.86356914401126
C	-4.22307624328407	0.32423979243952	1.64908265456034
C	-6.15123127260687	-0.80806236405526	7.04251142610603
C	-6.17245842055650	-1.25651663691865	5.71746909575111
H	-5.54529233239805	0.23781012088659	3.32802827019575
H	-4.76717078068528	1.13262932838108	1.17314132141603
C	-7.25280278497664	-0.17687827149646	7.59897342786840
H	-7.21515989867503	0.16645298710583	8.62673870870153
C	-7.34186986549158	-1.05969734401464	4.97359910785447
H	-7.40137091743643	-1.41447603424706	3.94944949307407
C	-8.39918166148209	0.01866723038913	6.84205613772749
C	-8.44106147533563	-0.42486757838476	5.52741731685716
H	-9.26078860769509	0.51119478649817	7.27840084216400
H	-9.33496031478610	-0.28567033299197	4.92989210474838

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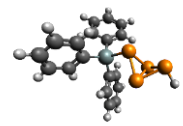

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P	-5.81287331415318	-2.88893764377429	2.11599697057789
P	-7.66318970903780	-2.26856739914395	1.06334287026523
P	-5.75271773454423	-1.84917594946698	0.15504114174207
H	-5.70070056343337	-1.69185436256907	2.89583401066333
H	-11.38419162984009	-5.69566475964680	-4.6352750554490
H	-11.07582236731079	0.84279510149210	-1.1886660643111
H	-6.15252109934803	-1.78376432642864	-6.76591583922090
C	-11.05779891176656	-5.32239516666793	-3.6711242172495
C	-10.06605080787216	0.57236006080876	-1.4756219762410
C	-6.12893771253603	-2.49377042773858	-5.94697999054045
H	-9.38559931630019	-4.26673655881098	-4.48953290828632
H	-9.35141071233573	2.59618846699314	-1.45904805505198
H	-10.50500387763701	-1.52032657465342	-1.5709235209286
H	-12.63465243505806	-6.29467878853493	-2.5868715422878
C	-9.93406928257085	-4.51376806869602	-3.58633807424933
H	-4.70046062633154	-3.78065339742608	-6.89871849734220
H	-7.54312091759822	-1.39735065204021	-4.77509948872100
C	-9.09967193572547	1.55550691453720	-1.62854513274092
C	-11.75921825986667	-5.65850298432119	-2.5224149042582
C	-9.74154097531480	-0.75877131304870	-1.69053946604011
C	-5.31535897246830	-3.61398175091338	-6.02167198226414
C	-6.91234363570237	-2.27868619597028	-4.82243442762213
C	-7.81017704748203	1.20513370467307	-2.00221721863529
C	-5.28961892651197	-4.52100753111669	-4.97136568706283
C	-8.44849334293159	-1.13091739312528	-2.06218032280234
C	-9.49300398147011	-4.02497079228896	-2.35516878646455
C	-6.89639213139485	-3.17773295778998	-3.75449737173860
C	-11.33345302177774	-5.18547846268760	-1.2895143641168
C	-6.07335614038542	-4.30228993849961	-3.84991832495823
C	-7.48913292209742	-0.12566781327865	-2.21612649323959
C	-10.20966549857859	-4.37781388906026	-1.2091132160706
Si	-7.98051238656555	-2.92788842283744	-2.25265950850389
H	-4.65506360864566	-5.39821120489045	-5.02489415702040
H	-7.05221795047120	1.97038278977885	-2.12431548083549
H	-11.87381566829858	-5.45194986277711	-0.3883212261232
H	-6.04189226550898	-5.01942320045929	-3.03507580151886
H	-6.47761120600388	-0.38476404966466	-2.51183881887872
H	-9.88138331509812	-4.02329610655622	-0.23665275226347

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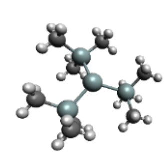

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Si	-5.99809376645207	0.22318408829073	0.51233391427571
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Si	-4.36479984871589	-1.15595592246039	-0.43120975559348
Si	-5.17606475496720	1.73459356175833	2.09209727422485
C	-4.91667374949453	-1.76612593970766	-2.12089112426272
C	-4.06866663682027	-2.64463249995235	0.68436016153496
C	-2.75280398740618	-0.20400202814064	-0.61202261347941
C	-4.14114556390797	3.06183197257178	1.25676279699172
C	-4.09500660215436	0.80375259457411	3.32221101841580
C	-6.59166249981878	2.55094575156452	3.02237117239630
C	-8.37901711330327	-2.22740176582971	-0.10094282720872
C	-9.40394757509104	0.37528354584717	1.15551996339560
C	-7.78076293323728	-1.60733654602097	2.83227644404270
H	-2.87762363179439	0.66423847577050	-1.26318293146657
H	-1.97970912581042	-0.84470205794883	-1.04720624681166
H	-2.38806909592474	0.15022498609962	0.35506492978836
H	-5.85081351474327	-2.32816261702695	-2.05163099696704
H	-4.15885589469533	-2.42322931017569	-2.55838103997067
H	-5.07899955613315	-0.93067122839378	-2.80555881638373
H	-3.31066837896532	2.62111293303827	0.70062834033168
H	-3.72430324811806	3.74808965034986	2.00012141964629
H	-4.74220161435342	3.64470651414022	0.55526750997075
H	-7.24635497601642	3.10112336931102	2.34278500436716
H	-6.20124986044438	3.25686512101604	3.76164621767117
H	-7.19883566356147	1.81283148747589	3.55176434432324
H	-9.55579824229194	0.82905583970258	0.17349531085331
H	-9.21269007490024	1.17890813361547	1.87030184487460
H	-10.33362211291874	-0.12269664500860	1.4472515070452
H	-8.53141019662511	-1.83343159976794	-1.10845446151544
H	-9.29283924085474	-2.74881258969207	0.19988098152401
H	-7.57274280273208	-2.96377914179094	-0.14507737543130
H	-3.24166774207750	0.33764444239564	2.82376273052997
H	-4.65992613005323	0.01459042089402	3.82396682368679
H	-3.70768212154066	1.48347999810806	4.08763524277661
H	-6.96791747968693	-2.33732926947959	2.84792633377569
H	-8.70063646304298	-2.11615127488288	3.13740525311029
H	-7.55640491554267	-0.84050672012076	3.57764403741111
H	-4.98535415109791	-3.22319481491714	0.82227337832150
H	-3.71797734346551	-2.33400684038727	1.67136871003788
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$((Me_3Si)_3Si)P_4^{\bullet}$
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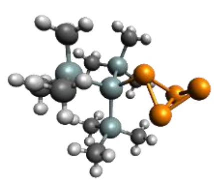

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P	1.44415818522012	0.47039235019247	1.11975640854554
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P	1.69877650436783	-0.62813318944975	3.02856694128274
P	1.65555309764277	1.54822742867641	3.04225241759852
H	1.07302897527928	-2.36700399458105	-0.36326931728181
H	-0.69887409303790	-2.89742770817159	2.15518952650472
C	0.16509954405678	-2.32257041152180	-0.96980473036907
H	-0.78424516251103	0.26237967409524	4.64123215123212
H	-0.03066239473597	-3.32601116795264	-1.35963036260180
C	-1.56854440154168	-2.88238586687456	1.49362107072188
H	-1.74016999010887	-3.90283742468311	1.13801651131972
H	-1.70341671975062	-1.11277173073100	4.02602336334659
C	-1.75082726533997	-0.04268944356566	4.23668863155689
H	0.36235880764151	-1.66208848179373	-1.81712623464698
Si	-1.29476041317919	-1.71791956725420	0.04349043071336
H	-2.43665142264026	-2.58503179190087	2.08622625093701
Si	-0.83887488545709	0.44204772300350	0.84915786927928
H	-2.51150298054651	0.11848801209509	5.00711578548427
H	0.78152835067185	1.18465890314094	-2.25014399967580
H	0.86524490495218	3.45058366726755	-0.13645115619993
Si	-2.19417156055202	0.94566423186531	2.70434995890658
H	-1.11390492440806	3.09777750473852	3.34285929904688
C	-0.26892522217917	1.43406483657269	-2.41931823254161
C	-0.20023132860090	3.63332716693078	-0.29721213629007
C	-2.12995994858131	2.78070248958459	3.09804729252957
Si	-1.07199913493469	2.06013720849296	-0.83973808058859
C	-2.83699187495024	-1.69006320072478	-1.03293005471181
H	-0.77070270879320	0.54067467180746	-2.79835310294404
H	-0.61633780367870	4.02155598630399	0.63496381710745
H	-3.07144096267144	-2.69837728367348	-1.38754004380799
H	-2.77049649211562	3.00415725141650	3.95657052588750
H	-4.03842489820987	-0.58490524807888	2.00893270609469
H	-0.29739589913130	4.40917598911730	-1.06247730597556
H	-0.31135087445359	2.20013695356509	-3.19931649140187
C	-3.94488626650718	0.48979753192722	2.18194924065921
H	-2.69542365757898	-1.05202626994786	-1.90851390741611
H	-3.70340944701722	-1.31708892102972	-0.48205377922481
H	-2.47927255557269	3.38077851245243	2.25457348272761
H	-4.65435744979183	0.76287270579609	2.96918123689083
C	-2.88973820982063	2.41954226506471	-1.15643635419371
H	-4.24325632154144	1.00483887845571	1.26621043760423
H	-3.43247054450836	1.51368342122112	-1.43639270055268
H	-3.37035568414509	2.84092771779800	-0.27035404125281
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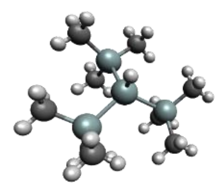

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Si	-4.39912711118081	-1.09428124977797	-0.45157737987403
Si	-5.20988077464873	1.72485571557291	2.04649171188940
H	-6.49497192938092	1.23105898264537	-0.79637207822122
C	-4.89761026846819	-1.76595824214982	-2.13522100525988
C	-4.17455523985166	-2.52716477604810	0.74753505382116
C	-2.75764758344452	-0.18937334730762	-0.61860641320577
C	-4.07971553624666	3.03408303112433	1.31005839765808
C	-4.22393340927585	0.65830642883358	3.24308476901186
C	-6.59329122318872	2.57882375275473	2.99303629140987
C	-8.35335714203179	-2.25696434712668	-0.06693224265418
C	-9.43091633799955	0.32363350400211	1.17664753414481
C	-7.61149998409573	-1.52731679092072	2.80755001340736
H	-2.84082343955077	0.65978575569174	-1.30114859357063
H	-1.98932653185823	-0.86304345616525	-1.01042802037143
H	-2.41001662273439	0.18811759826036	0.34596728500742
H	-5.83770860473799	-2.31933721738411	-2.07881251518451
H	-4.13024360308341	-2.44180910142128	-2.52477263159112
H	-5.03080807287058	-0.95386884270560	-2.85387186837471
H	-3.25598235642962	2.57952584141834	0.75536267966478
H	-3.65187714166277	3.66038383257846	2.09873422440197
H	-4.62811059773431	3.68298844303648	0.62322383288921
H	-7.21605809994148	3.17969484834185	2.32615558346797
H	-6.17953053181535	3.24274026228053	3.75803697100835
H	-7.23955471227210	1.85349172199384	3.49303831548808
H	-9.64859560763746	0.75134739515134	0.19510224904985
H	-9.24996028791924	1.14926591787477	1.86873511019474
H	-10.32091903336771	-0.21455641392854	1.5164668331612
H	-8.57700329198543	-1.89724814695215	-1.07419559265695
H	-9.22624067866320	-2.80842144318289	0.29552960367998

H	-7.51961197508138	-2.95971998225402	-0.13892987223593
H	-3.36076101898305	0.20398461239586	2.75055712327762
H	-4.83572138998791	-0.14750934969425	3.65529781505537
H	-3.85306173791902	1.25938114910127	4.07853734709480
H	-6.73729221897098	-2.18306602145917	2.80771810638647
H	-8.46820804417514	-2.10989938813236	3.15886230670757
H	-7.43120920573297	-0.72845891331720	3.53092822125382
H	-5.09572410869021	-3.10455630184158	0.85711702005033
H	-3.88124339747231	-2.17419196686576	1.73905685825880
H	-3.39498234371527	-3.20587510491190	0.38870607079843

TS(((Me$_3$Si)$_3$Si)P$_4^{\bullet}$→((Me$_3$Si)$_3$Si)P$_4$H)
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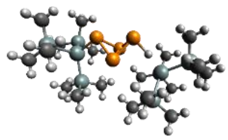

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P	2.12283083745918	-0.28702679406406	1.29907067015478
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P	2.46609117554004	-1.02113266383908	3.35622154138879
P	3.17754450021704	0.94271375785880	2.80107104615806
H	0.38602364059021	-2.96438543456301	0.80231647268159
H	-0.63767956738901	-2.15731533286324	3.69846880208896
C	-0.60292567491091	-2.69899034057841	0.42077447560761
H	0.92429077816638	0.94779107437928	5.01533911157888
H	-1.22296297840405	-3.60044031566973	0.43069401905397
C	-1.60521731398299	-1.98021629852095	3.22268968460451
H	-2.16227015507677	-2.92195984520475	3.22649272261063
H	-0.70686223418973	0.28554638966266	5.06840049673761
C	-0.13175313864383	1.20182387687216	4.92129588289074
H	-0.48505372114202	-2.37964209001420	-0.61702863841043
Si	-1.39269843905536	-1.35227162991241	1.46361254651682
H	-2.15573159038471	-1.26311032276357	3.83605264712103
Si	-0.01067112672349	0.54793344840429	1.45714517169740
H	-0.38898957791210	1.89850270644841	5.72517411683345
H	0.77354956068720	-0.20630949211609	-1.92146220871562
H	2.27895734288725	2.24849629514894	-0.66907563650671
Si	-0.50831411817414	1.97966887445719	3.25726783610157
H	1.49228117597322	3.46238793787521	3.06568936207285
C	-0.10911722573062	0.43404728047860	-1.99259109770745
C	1.34907482565345	2.81856551535638	-0.73926234660006
C	0.41062342905168	3.60948033565743	3.08811222851790
Si	-0.14359933571555	1.68670966926851	-0.59129506409433
C	-3.07937152247155	-0.91687156175752	0.75315991382080
H	-0.99388700585673	-0.20668643169434	-1.97619607118171
H	1.35805333209479	3.56768277833083	0.05577998401816
H	-3.74687282403989	-1.78306275867534	0.78831902943922
H	0.17469804353350	4.26185047340617	3.93444568388182
H	-2.93667849485432	1.41022621132231	3.33161910175029
H	1.34569411389383	3.34217822566631	-1.69989809979601
H	-0.07988071855922	0.94183649980542	-2.96134637967849
C	-2.35770430348859	2.32271517625416	3.17000796805269
H	-2.99687256040501	-0.59992415778641	-0.28934273256115
H	-3.55061031916967	-0.10530740377928	1.31256151758255
H	0.12089747271768	4.12999668270603	2.17211514834466
H	-2.64051841270679	3.03911880963409	3.94759395688603
C	-1.71810056657663	2.70953979036111	-0.69573424124463
H	-2.64992720890443	2.74062424234390	2.20455479196280
H	-2.60632145414806	2.09593024584534	-0.52836742241551
H	-1.71659402642514	3.51049527715233	0.04754248840055
H	-1.80835145834819	3.17136209152864	-1.68354389370906
H	4.99290339702516	-0.45837344679180	4.30773294733710
H	1.74974637451482	-1.34376526193984	6.14884730827343
H	7.47197322801252	-2.04159893928664	4.12738592703994
H	5.31230335516983	2.96317758482844	3.90298379897498
C	2.05097853835850	-1.04132835996705	7.15321648816000
C	7.72580231106688	-2.20024682499318	5.17846848211271
C	5.77173374408923	3.24018480992418	4.85466994096208
H	8.30937774123413	0.93857706535397	4.40171816536474
H	2.61950244989818	2.52343895147816	5.45149131464226
H	4.12333116093461	-3.39374754219886	6.09250997827161
Si	5.23312210189049	0.01695493730217	6.04100607425798
H	1.77286810541818	0.00685381808173	7.27996429944667
H	7.09192825957560	-3.00587427354534	5.55570753579695
H	6.83777563537350	3.01404356153053	4.79342285609245
H	1.47797372801815	-1.63244645110077	7.87452349847840
H	8.76612805746366	-2.53560659780760	5.22784793147006
H	5.66105839803531	4.32153967468503	4.98076276073740
C	8.59114754548968	0.71551501813982	5.43345292299044
C	3.14514101269413	2.82350984043100	6.35968220706190
C	4.29828268668963	-3.12002040193126	7.13594235801830
Si	3.88660935360462	-1.31000064196968	7.43395315463484
Si	4.95592440443100	2.33429354492551	6.28367850669152
Si	7.49011423418678	-0.61994841785517	6.16741060322575
H	3.05786821573000	3.91008989923885	6.45663312720521
H	9.63412607235674	0.38432632560246	5.43397836039838
H	3.67487715672467	-3.76374985524301	7.76357041085211
H	8.53503622747543	1.64308743634702	6.00785420793807
H	2.63704212151521	2.36634576023808	7.21176544687950
H	5.34396657659817	-3.33475825874749	7.36838927419871
C	4.27395370557107	-0.86149504499945	9.22157384400027
C	8.01046328616688	-0.91485539335872	7.95175908239751
C	5.78708079406650	2.83888613506603	7.89651246548493
H	3.99162466221621	0.17302597248279	9.43220819003118
H	6.85363119197546	2.60167931327059	7.88343633612456
H	7.46027428709568	-1.74945985053300	8.39269796332237
H	9.07764454825024	-1.15233254448467	8.00181586977803
H	3.71181431419916	-1.50717352774970	9.90362792634726
H	5.68240069607653	3.91578321847796	8.06186475644880
H	5.34086091053981	2.32114703176857	8.74883476748117
H	5.33640991776216	-0.97020531103895	9.44783159398127
H	7.83188427354953	-0.03118597619793	8.56893814062541

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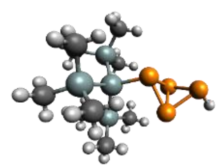

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P	1.43856599373669	0.46928363346328	1.11641493753588
P	3.60493808506801	0.51682669825966	2.99429617329620
P	1.69694023103359	-0.60804277287878	3.03384530397901
P	1.64898006988100	1.55470159372355	3.03155813994813
H	3.78813129287491	0.51877205348372	4.41507507027265
H	1.07182787010939	-2.37312574563885	-0.35916028311336
H	-0.70345328815629	-2.90034591355881	2.15293357744638
C	0.16533774139957	-2.32484560562934	-0.96755259432519
H	-0.78842113454936	0.26231011894136	4.64592545023013
H	-0.03395139433502	-3.32730127253673	-1.35820734114727
C	-1.57335283302368	-2.88079789889780	1.49168105017706
H	-1.74912077373769	-3.90004503400458	1.13460875887135
H	-1.70050384999155	-1.11548639496120	4.02609550647496
C	-1.75256284690963	-0.04582192606976	4.23785551039733
H	0.36722164303017	-1.66476572059863	-1.81408529816255
Si	-1.29387251493575	-1.71502461377402	0.04345953545361
H	-2.43995302479799	-2.58106897920549	2.08527085018685
Si	-0.82775797905502	0.44191771599790	0.85176079794519
H	-2.51683537275651	0.11166859441883	5.00548919825576
H	0.77162700396309	1.17747029307723	-2.25834370039580
H	0.87178362668607	3.44566928549192	-0.15021795365679
Si	-2.18990580118067	0.94334755887658	2.70422387412579

H	-1.12041332138535	3.09594917850647	3.36004365878316
C	-0.27911755435050	1.42924310382108	-2.42218185804992
C	-0.19424826183948	3.63047344122934	-0.30484237532436
C	-2.13308000587225	2.77729509026228	3.10343969587776
Si	-1.07227166653767	2.05768095353553	-0.83856410691591
C	-2.83385101747675	-1.68301673269598	-1.03551406877106
H	-0.78480652807889	0.53698877087670	-2.79870260746032
H	-0.60350715412031	4.02204835177641	0.62896247059926
H	-3.07076692372729	-2.69100210490179	-1.38932646614901
H	-2.78327730122876	2.99589616185112	3.95600560566090
H	-4.03166248367891	-0.58734355016633	1.99933717254056
H	-0.29456796037568	4.40457060539071	-1.07150670401832
H	-0.32377203332356	2.19552782186831	-3.20186890323617
C	-3.93821869725937	0.48701874322092	2.17428305535838
H	-2.68794585420885	-1.04675745698885	-1.91170230846911
H	-3.70053677413368	-1.30629150472346	-0.48762056653052
H	-2.47501837394140	3.37965275059007	2.25859060948056
H	-4.65030643211610	0.75909732469745	2.95950781536627
C	-2.89053398903189	2.42067681853635	-1.14624485099209
H	-4.23350529743577	1.00349091732709	1.25836407598000
H	-3.43709563566714	1.51538699059636	-1.42054192737930
H	-3.36531566478462	2.84593665100239	-0.25883429220875
H	-3.00131381377910	3.14152200640776	-1.96180968793733

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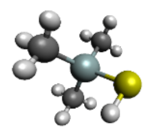
H= -807.63087449 Eh



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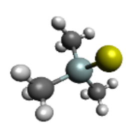
S	3.00380431065943	-0.05095337423937	-0.13088627962310
Si	0.84912406590392	-0.01617043224118	-0.04830921864569
H	3.14523021704940	1.28028654162588	-0.02246823252862
C	0.34290926768795	-1.80797598342223	-0.18635972103132
C	0.16552674318241	0.98133495997650	-1.47299660188984
C	0.28458395752793	0.71800017528391	1.57477954124854
H	0.49012262117018	0.56685538734433	-2.42960141811516
H	0.50110690558509	2.02014317516394	-1.42395609585883
H	-0.92844485186673	0.98163630737493	-1.45086590521620
H	0.68750938677239	-2.24496331568746	-1.12617700198075
H	-0.74710834644561	-1.89113096156819	-0.15451837861477
H	0.75097227239822	-2.39994131622204	0.63577288463571
H	0.68822622818036	0.15322284762543	2.41761943066360
H	-0.80728874627758	0.70835513029092	1.64361629994292
H	0.61676596847263	1.75447085869464	1.67270069701352

$Me_3SiS^{\bullet}$
E= -806.99374916 Eh
H= -807.03705311 Eh



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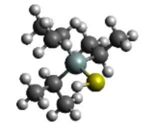
S	2.99199578251031	-0.04678863873788	-0.12735998159497
Si	0.85166535008725	-0.00939119233510	-0.04804257049154
C	0.35316879294058	-1.81179499286769	-0.18750420434966
C	0.16235001058198	0.98092290000587	-1.47551407504078
C	0.28323719655807	0.71768023369609	1.57735700235083
H	0.47316540625468	0.55402419683163	-2.43107273539918
H	0.50956483770249	2.01601270329187	-1.43870657919659
H	-0.93123820626807	0.99179585778485	-1.43980107233364
H	0.69403615732998	-2.24855765244734	-1.12786007597372
H	-0.73881856292393	-1.87821823134672	-0.15536280583311
H	0.75598519404162	-2.40308487417618	0.63659727505050
H	0.67182688493088	0.13945854152135	2.41792989297797
H	-0.80937881223767	0.72277337260561	1.63399547280018
H	0.62988996849181	1.74792777617360	1.68618445703370

***i*Pr_3SiSH**
E= -1043.18144924 Eh
H= -1043.12030454 Eh



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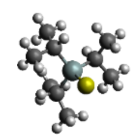
S	2.93651963738553	0.00750309846613	0.41296420014587
Si	0.84698344410901	0.07717002871758	-0.14172956897762
H	3.06992791353126	1.33345932593543	0.57518726364394
C	0.44588797686043	-1.74291326741676	-0.47331210657351
C	0.60219649635978	1.14278713053394	-1.69376053260786
C	-0.17493915685072	0.71599679193705	1.31731770468296
H	0.86907423605893	0.47281064404641	-2.52178539499823
C	1.51629259110264	2.36096012738190	-1.78389746251259
C	-0.86052416471159	1.55100538174326	-1.87129078061808
H	0.76065498211520	-2.25954515567923	0.44335197368111
C	1.24605444639343	-2.32430761068023	-1.63542087668085
C	-1.04841293987198	-1.99526293950122	-0.66307091941322
C	-0.09201223048672	-0.21730602276208	2.52079452553523
H	-1.21345217530494	0.72402839407921	0.95824912119242
C	0.19732936088274	2.14087945853409	1.71629451713992
H	2.32136613060495	-2.18131720548635	-1.50927088867624
H	0.96123226386269	-1.86026657991877	-2.58413998806913
H	1.06028060782749	-3.39864302198370	-1.73375610309074
H	-1.25471522656703	-3.06905895106377	-0.71454013580875
H	-1.40898447676006	-1.55617502350109	-1.59738575553600
H	-1.65041123667352	-1.58411478708041	0.15090607822773
H	-1.00257141449129	2.06751349102335	-2.82608119761657
H	-1.17941368897127	2.23845164228437	-1.08301010939101
H	-1.54117241340644	0.69708016730619	-1.85581979740262
H	1.34704472257562	2.89823707653566	-2.72282256147460
H	2.57016841810730	2.07970354412002	-1.74771795635940
H	1.32979159879710	3.06929037031591	-0.97184707893000
H	0.07385390246680	2.85039818405965	0.89540703833790
H	1.23710902875044	2.19557735331296	2.05200645543479
H	-0.42702706353746	2.48681239061223	2.54646877176121
H	-0.44618751271468	-1.22466368422507	2.29047880511946
H	-0.69879801339906	0.16475584046204	3.34822122956609
H	0.93845395595541	-0.30198619210868	2.87676153026839

***i*$Pr_3SiS^{\bullet}$**
E= -1042.54456035 Eh
H= -1042.48406019 Eh



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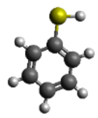
S	2.92210832308561	0.08792337519865	0.39322519006501
Si	0.84290578413642	0.06077621686232	-0.12969796022668
C	0.42061995373019	-1.75988395463724	-0.47986530276290
C	0.68779691490126	1.13883072409141	-1.68801158210053
C	-0.19931700515651	0.69345672968582	1.31554955417188
H	1.04316680600152	0.48630443642893	-2.49526373962085
C	1.57050391634752	2.38413015733944	-1.67965029621756
C	-0.76815062268890	1.50212021994930	-1.97170989459132
H	0.81422846630063	-2.30497937624037	0.38811045942050
C	1.12461278613992	-2.29119659873488	-1.72317251064431
C	-1.08409780090719	-2.01441604749733	-0.54702680207066
C	-0.02461665257848	-0.20171179904203	2.53954450336439
H	-1.24572832651284	0.63009106242154	0.98701671662122
C	0.10605356889258	2.14593538970165	1.66670489503324
H	2.20105872592016	-2.11107028660166	-1.69004341569802
H	0.73541622107426	-1.82013345800768	-2.63041890385846
H	0.96464843401911	-3.36918016308134	-1.82653108589630
H	-1.28642189917151	-3.08664395977579	-0.63635308713768
H	-1.53224165815989	-1.53044808451788	-1.41889648465299
H	-1.61114401711821	-1.65414645505219	0.33895429593830
H	-0.84668201562805	2.05388019370946	-2.91438318238469

H	-1.18032339304586	2.14315290001449	-1.18786738973520
H	-1.41276674415447	0.62424588055554	-2.05085357592665
H	1.46532354260164	2.93229924122362	-2.62174143680574
H	2.62684132457318	2.13251638195993	-1.55822056418105
H	1.29982419772168	3.06924617587875	-0.87327440046046
H	-0.14295118361292	2.82960167610784	0.85263659331188
H	1.16638346104098	2.27722940322829	1.90150324782569
H	-0.46639182401964	2.45994361860374	2.54569449778837
H	-0.29808106349042	-1.24076806801435	2.34056718637697
H	-0.64562296938912	0.15056059518887	3.36940829319741
H	1.01485474914731	-0.19130612694682	2.88090618185720

PhSH

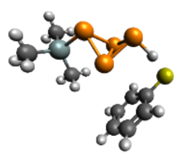


E= -630.05716043 Eh
H= -630.01940342 Eh

0 1

S	2.56588250164266	-0.00946555604700	-0.11531930938568
C	0.17508042134928	-1.27092288114327	-0.15668742065460
C	0.80871856464140	-0.03518442552593	-0.04892352087953
C	0.04039119315924	1.11495110460617	0.10670572771601
C	-1.34142289841786	1.02563387628877	0.15134462021337
C	-1.97317514667809	-0.20405840264503	0.04449013724095
C	-1.20646877463352	-1.34978033180712	-0.10946709187243
H	0.76649386493813	-2.17155291388536	-0.27803180026055
H	0.52050374549226	2.08297155505007	0.19343981903349
H	-1.92739879715992	1.92967816926956	0.27123642032981
H	-3.05373084267719	-0.26900252667760	0.08065475155316
H	-1.68596022184374	-2.31807426782027	-0.19480973655502
H	2.70721239018735	1.31921560033702	-0.00434759647898

TS((Me$_3$Si)P$_4^{\bullet}$→(Me$_3$Si)P$_4$H) with PhSH

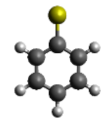


E= -2404.00991199 Eh
im. freq. = 613.81 *i*

0 2

S	2.14872124853627	0.46173831623764	2.91558115400222
C	3.06119641408370	0.54270015751460	0.34276553496687
C	2.02029893497958	0.85439035930127	1.22629481720517
C	0.88189071102449	1.50156559961553	0.73021229843234
C	0.79639414754645	1.83977503871454	-0.60779111286871
C	1.83836450621916	1.53099698233466	-1.47387461890103
C	2.96621012188961	0.87685674398997	-0.99684143425646
H	3.94220059724210	0.04573102856969	0.72958479509927
H	0.07634578242925	1.73718020701509	1.41497378404292
H	-0.08583576692118	2.34795905906020	-0.97917055544858
H	1.76854258681977	1.79808820606375	-2.52192509922021
H	3.78039853504470	0.63590451793218	-1.67028550616176
H	2.66178074590515	2.01679752898120	3.42065345227524
H	6.17845647667509	7.42310815782314	-0.16260237000479
P	5.28264286919392	4.96936211539747	2.07507437810249
P	3.42126902182637	3.39850213771627	3.57162891628660
H	8.49371483348101	5.75936957909196	1.13490996977730
C	5.93490256242087	6.55933434335756	-0.78553357646588
H	4.86595615315137	6.59369192338781	-1.00797713203645
C	8.22015188937469	4.92777266064592	0.48150386033508
Si	6.39354360810251	4.95813811475053	0.06989869851327
P	3.49324070554366	3.82440166660633	1.41671304269601
P	5.14075266401901	2.77357605555609	2.35333288779409
H	6.48117816026239	6.65750583180569	-1.72817901514177
H	8.49117549681744	3.99815986481692	0.98726273170538
H	8.81863693472835	5.00353531375850	-0.43108594316444
C	5.94805553985787	3.49042752907379	-1.00340738315224
H	4.88380514595385	3.46960107569824	-1.24734050124800
H	6.19853852608478	2.54456157593446	-0.51843090550467
H	6.51141084770601	3.54966830924790	-1.94003516765930

PhS$^{\bullet}$

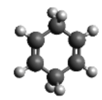


E= -629.43446638 Eh
H= -629.39752933 Eh

0 2

C	0.00000023103084	-0.00000015803615	-2.22512584858054
C	-0.00000000132722	1.20696485466739	-1.53175678442517
C	-0.00000060032364	1.21145705282857	-0.15242840981621
C	-0.00000035533568	-0.00000007195274	0.56906425574294
C	-0.00000000915220	-1.21145705331380	-0.15242818003967
C	-0.00000043482932	-1.20696499407865	-1.53175688634728
H	0.00000072791710	0.00000063806544	-3.30893987047651
H	0.00000020762139	2.14428389445272	-2.07556498285729
H	-0.00000043226030	2.14151539188980	0.40260306927496
H	0.00000003197047	-2.14151504275576	0.40260422281231
H	-0.00000034636263	-2.14428399952163	-2.07556511298903
S	0.00000098105120	-0.00000051224520	2.27610452770149

1,4-CHD

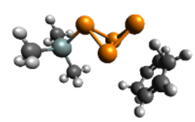


E= -233.13043463 Eh
H= -233.09575335 Eh

0 1

C	0.25914522071808	-1.34441116077819	-0.14734431717976
C	0.84127882912225	0.02690785806039	-0.04182267763781
C	0.10996900796243	1.12663617075972	0.08487002883856
C	-1.38266752527305	1.12448127732812	0.13552804067298
C	-1.96480488102972	-0.24682765513613	0.02988207292192
C	-1.23349413353694	-1.34655556660946	-0.09680874390628
H	0.60414879856170	2.09121925932012	0.15669699122489
H	1.92417765260425	0.10621841947398	-0.07165021541718
H	0.60195439029541	-1.82498025546379	-1.07474662892349
H	0.65995219640370	-1.98220942952743	0.65338412177901
H	-1.72767560420367	-2.31112931905112	-0.16873059251744
H	-3.04770804906985	-0.32613017658517	0.05961199467164
H	-1.72539863432608	1.60492438967556	1.06302765226774
H	-1.78354726822851	1.76238618853341	-0.66507772679477

TS((Me$_3$Si)P$_4^{\bullet}$→(Me$_3$Si)P$_4$H) with 1,4-CHD



E= -2007.07520011Eh
im. freq. = 1491.20 *i*

0 2

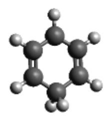
H	6.45069229120128	7.85696029527981	0.26187859345653
P	5.75833375129288	4.81261537934821	1.71899407196054
P	3.94975174504601	2.84092306284788	2.77635086898715
H	8.88806151021088	6.03383466597736	0.99373090561541
C	6.23420991305293	7.19281159804176	-0.57803898469380
H	5.15815693416604	7.22474066986941	-0.76423376750398
C	8.63973100609805	5.40763174949084	0.13365633985571
Si	6.79939732411705	5.44206989826567	-0.21975116877177
P	3.92777498593360	3.90914131917086	0.84617908237588
P	5.60548008358464	2.63163169883529	1.33447052382302
H	6.74310882575228	7.58884228236348	-1.46183024100763
H	8.97709086235727	4.39089520030628	0.34816998420248
H	9.20378196521689	5.77761461108120	-0.72767965827694
C	6.40468701560457	4.32781658863508	-1.67354441035270
H	5.33883226542857	4.33640940605838	-1.91123819010467
H	6.69916476763484	3.29413527173304	-1.47895636122828
H	6.95216479468822	4.67510378183780	-2.55532193976559
H	3.15294292839448	1.53189533135945	2.14358430428919
C	2.56688739076324	0.44722518449823	1.42127093429498

C	3.69675105759989	-0.40225889159735	1.09867218818043
H	4.10648965113135	-1.03253234468048	1.88091667794827
C	1.91147397089717	1.09386889520231	0.30194459570971
H	0.96748127224316	1.59841166168024	0.47866766576194
C	4.26552978943289	-0.39090831186980	-0.11446774989384
H	4.51250102304725	1.22449434634250	-1.47944792264305
C	2.46232101658443	1.12178686735097	-0.91959639433361
H	1.93164786385303	0.12843964233096	2.24506852146676
C	3.75962149179326	0.45729696318210	-1.23136669312147
H	5.12964414942818	-1.01670269738227	-0.31129380103555
H	1.95980415248927	1.64490725565637	-1.72641022998079
H	3.66973420095495	-0.13872138121647	-2.15052774521434

1,4-CHD$^{\bullet}$

E= -232.52005407 Eh

H= -232.48524300 Eh



0 2

C	0.26948888905695	-1.36181394827597	-0.10152732807081
C	0.85738733115205	0.00655860256977	-0.06571913299054
C	0.08468850676011	1.12295235580218	-0.05713081963625
C	-1.32376223918753	1.04390231197007	-0.08008572548266
C	-1.94649216867039	-0.22153476614782	-0.11110917671395
C	-1.22009952573342	-1.36860901687294	-0.12086599572583
H	0.55832250072825	2.09876130392976	-0.03163554246819
H	1.93843809006007	0.09172732495963	-0.04697142237086
H	0.65928175189093	-1.91579662566891	-0.97336761129940
H	0.63855566764027	-1.95378671444347	0.75381894888813
H	-1.72075799483254	-2.33031824855731	-0.14420161043242
H	-3.02990206378874	-0.27650383843774	-0.12713575320029
H	-1.92107874507603	1.94643125917276	-0.07234883049692