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Free Radical Chemistry of Phosphasilenes

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A. Experimental Procedures

1. Materials and Methods

General

All manipulations were carried out under a protective atmosphere of argon, using Schlenk techniques or a glove box. All solvents used were purified by a PureSolvMD5 solvent purification system by Innovative Technology. Deuterated benzene (C_6D_6) was refluxed over potassium, then distilled and stored under argon. UV/vis spectra were recorded on a PerkinElmer Lamda 750 UV/vis spectrometer with quartz cells with a path length of 0.1 cm. NMR spectra were recorded on a Bruker Avance III 300 MHz and/or a Bruker Avance III HD 400 MHz spectrometer. Chemical shifts are reported in ppm. Elemental analyses were carried out with an elementar vario Micro Cube. Phosphasilenes **1**[1] and **4**[2] were synthesized according to literature procedures.

X-Ray Structure Determination

Crystals of **2** and **3** suitable for single-crystal x-ray analysis were obtained by recrystallization from *n*-hexane. The data were collected at -130°C on a BrukerAXS X8 Apex CCD diffractometer operating with graphite-monochromatized Mo Kα radiation. Frames of 0.5° oscillation were exposed; deriving 88964/52437 reflections in the θ range of 2 to 27° with a completeness of ~99%. Structure solution and full least-squares refinement with anisotropic thermal parameters of all non-hydrogen atoms were performed using SHELX. [3]

Crystallographic data for the structures have been deposited with the Cambridge Crystallographic Data Centre, CCDC, 12 Union Road, Cambridge CB21EZ, UK. Copies of the data can be obtained free of charge from www.ccdc.cam.ac.uk/data_request/cif by quoting the depository numbers, CCDC: 1989735, 1989736.

Synthesis of Si=P-Tip Phosphasilene 2

A suspension of 1.5 g (1.91 mmol, 1.0 eq.) of phosphasilene **4** and 815 mg (2.87 mmol, 1.5 eq.) of TipLi·Et_2O in 20 mL of toluene was stirred for three days at 50°C. After removal of toluene in vacuo, the solid residue was taken up in 20 mL of *n*-hexane and lithium salts were removed by filtration. Crystallization from *n*-hexane yielded 611 mg (0.647 mmol, 33%) of Si=P-Tip phosphasilene **2** as yellow-red crystals.
Overlapping of resonances due to presence of an *E*/*Z*-mixture in solution (ca 2:1) neglects individual assignment and integration in the according ^{1}H and ^{13}C NMR spectra.

^{1}H-NMR (400 MHz, C_6D_6, 300 K): 0.09 (d), 0.22 (d), 0.27 (d), 0.36-0.43 (m), 0.54 (d), 0.83 (d), 0.87-0.91 (m), 0.96 (d), 1.02-1.07 (m), 1.13 (d), 1.18-1.22 (m), 1.24 (d, residual 1,3,5-triisopropylbenzene), 1.27-1.32 (m), 1.44-1.46 (m), 1.51-1.54 (m), 1.63-1.68 (m), 1.82 (d), 2.38-2.44 (m), 2.48 (d), 2.51-2.88 (m, residual 1,3,5-triisopropylbenzene), 2.95 (sept), 3.16-3.32 (m), 3.50 (d), 3.62 (tr), 3.78 (sept), 3.91 (tr), 4.16 (sept), 5.79 (sept), 6.72 (s), 6.88 (s), 6.93 (s), 6.95 (s), 6.99 (s, residual 1,3,5-triisopropylbenzene), 7.03 (br), 7.12 (s), 7.21 (s), 7.26 (s), 7.26 (s), 7.28 (s).

^{13}C{^{1}H} NMR (75.47 MHz, C_6D_6, 300 K): δ = 14.4, 22.4, 23.1, 23.2, 23.3, 23.6, 23.7, 23.8, 24.0, 24.5, 24.7, 24.9, 25.2, 25.5, 25.7, 26.2, 26.4, 27.5, 27.7, 27.8, 28.0, 28.2, 29.5, 30.6, 32.0, 34.1, 34.6, 34.7, 34.8, 35.0, 36.1, 36.6, 37.0, 37.7, 37.9, 42.2, 42.7, 43.1 (*i*Pr-*C*H, *i*Pr-*C*H_3 and -N(*C*H_3)$_2$), 121.4, 121.7, 122.1, 122.2, 122.4, 122.5, 122.8, 123.3, 134.7, 135.7, 136.2, 136.4, 137.9, 138.8, 148.1, 148.2, 149.1, 149.7, 150.0, 150.5, 150.8, 151.5, 151.6, 153.1, 153.3, 154.1, 154.5, 154.8, 155.2, 155.5, 156.0, 156.5, 156.6 (Tip-*C*) ppm.

^{31}P{^{1}H}-NMR (121.5 MHz, C_6D_6, 300 K): δ = 217.3 ($^1J_{P\text{-}Si}$ = 190.7 Hz, $^2J_{P\text{-}Si}$ = 29.5 Hz, *Z*-**2**), 231.9 ($^1J_{P\text{-}Si}$ = 193.6 Hz, $^2J_{P\text{-}Si}$ = 49.4 Hz, *E*-**2**) ppm.

^{29}Si{^{1}H}-NMR (59.62 MHz, C_6D_6, 300 K): δ = −8.4 (d, $^{2}J_{Si-P}$ = 29.8 Hz, *Z*-**2**), −5.5 (d, $^{2}J_{Si-P}$ = 49.4 Hz, *E*-**2**), 181.5 (d, $^{1}J_{Si-P}$ = 193.0 Hz, *E*-**2**), 186.8 (d, $^{1}J_{Si-P}$ = 191.0 Hz, *Z*-**2**) ppm.

UV/vis (*n*-hexane): $\lambda_{max}(\varepsilon)$ = 382 nm (7770 $M^{-1}cm^{-1}$).

Elemental analysis: Calculated for $C_{62}H_{98}NPSi_2$: C: 78.83, H: 10.46, N: 1.48. Found: C: 77.82, H: 10.69, N: 2.39.

m.p.: 165°C.

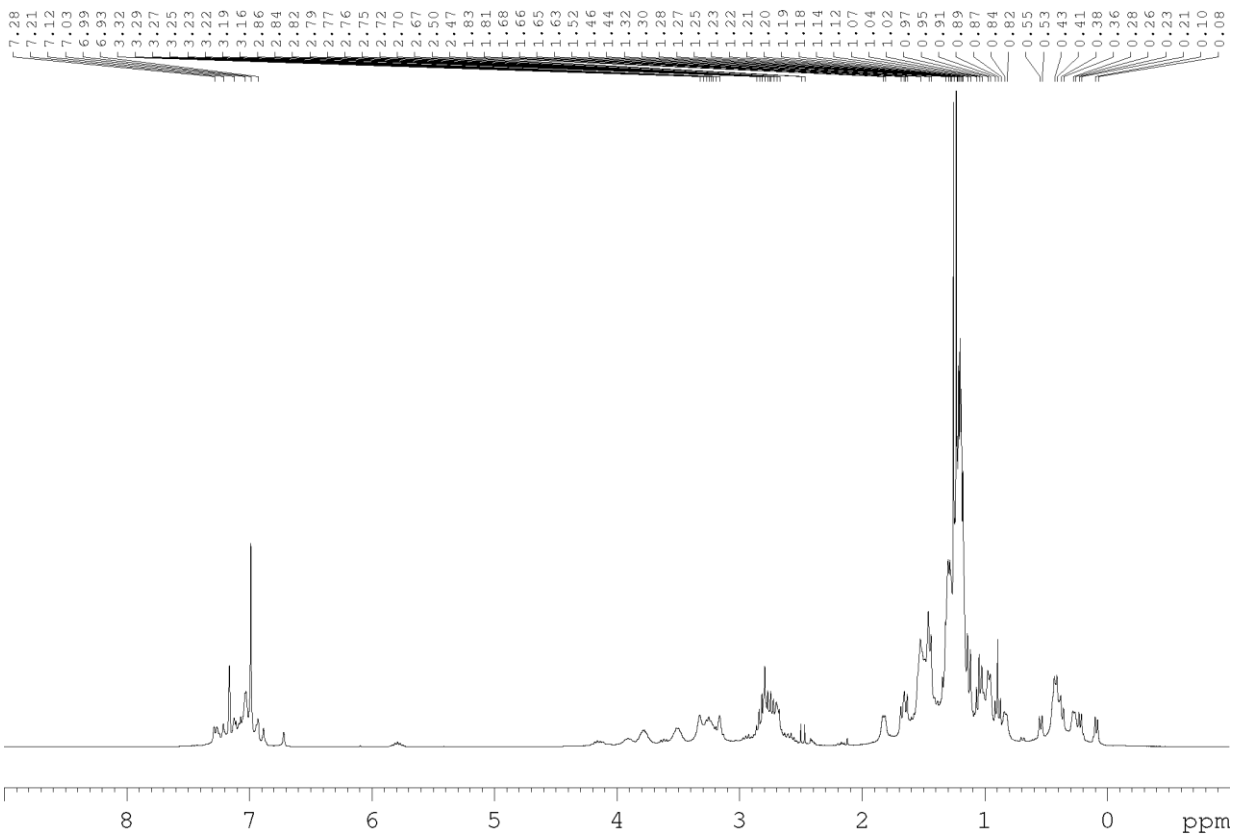

Figure S1: ^{1}H NMR spectrum of Si=P-Tip phosphasilene **2**.

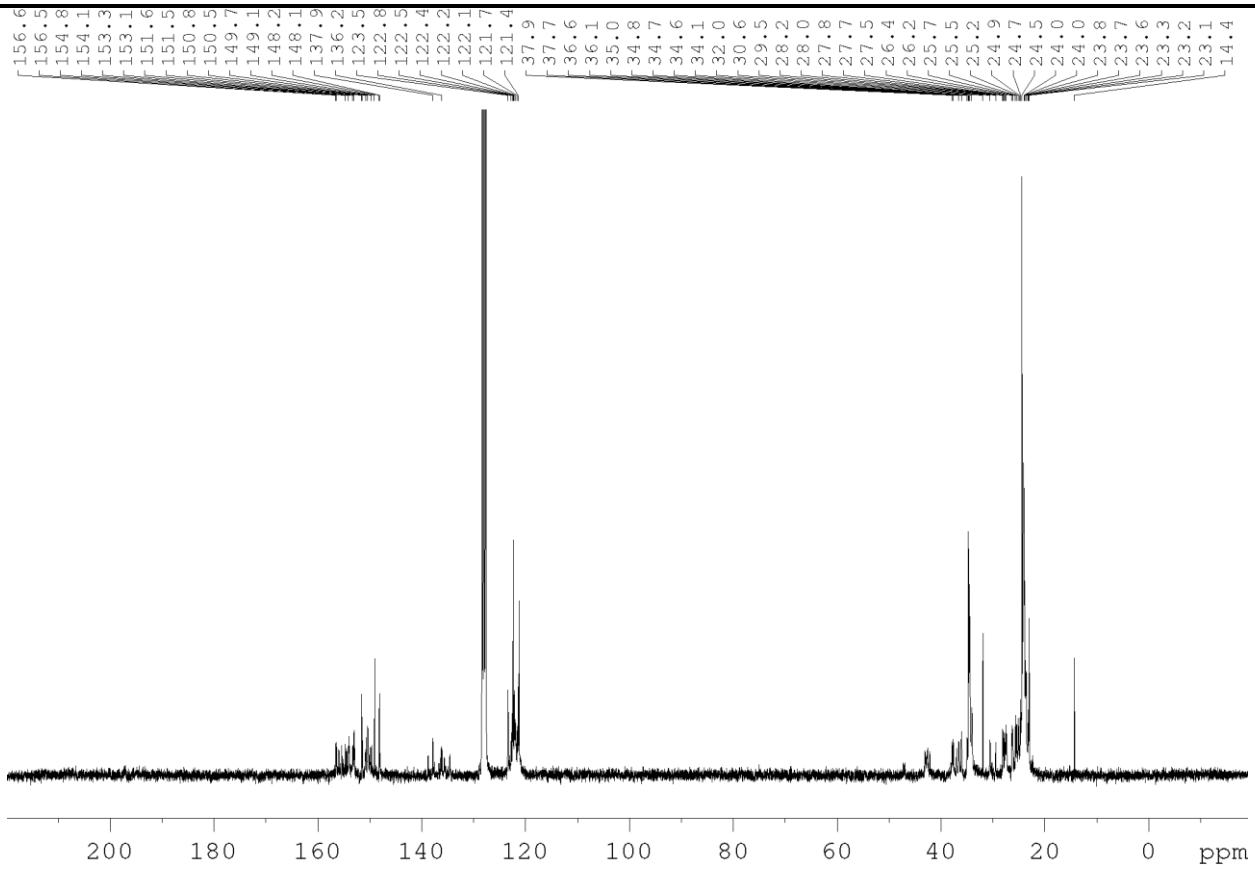

Figure S2: ^{13}C NMR spectrum of Si=P-Tip phosphasilene **2**.

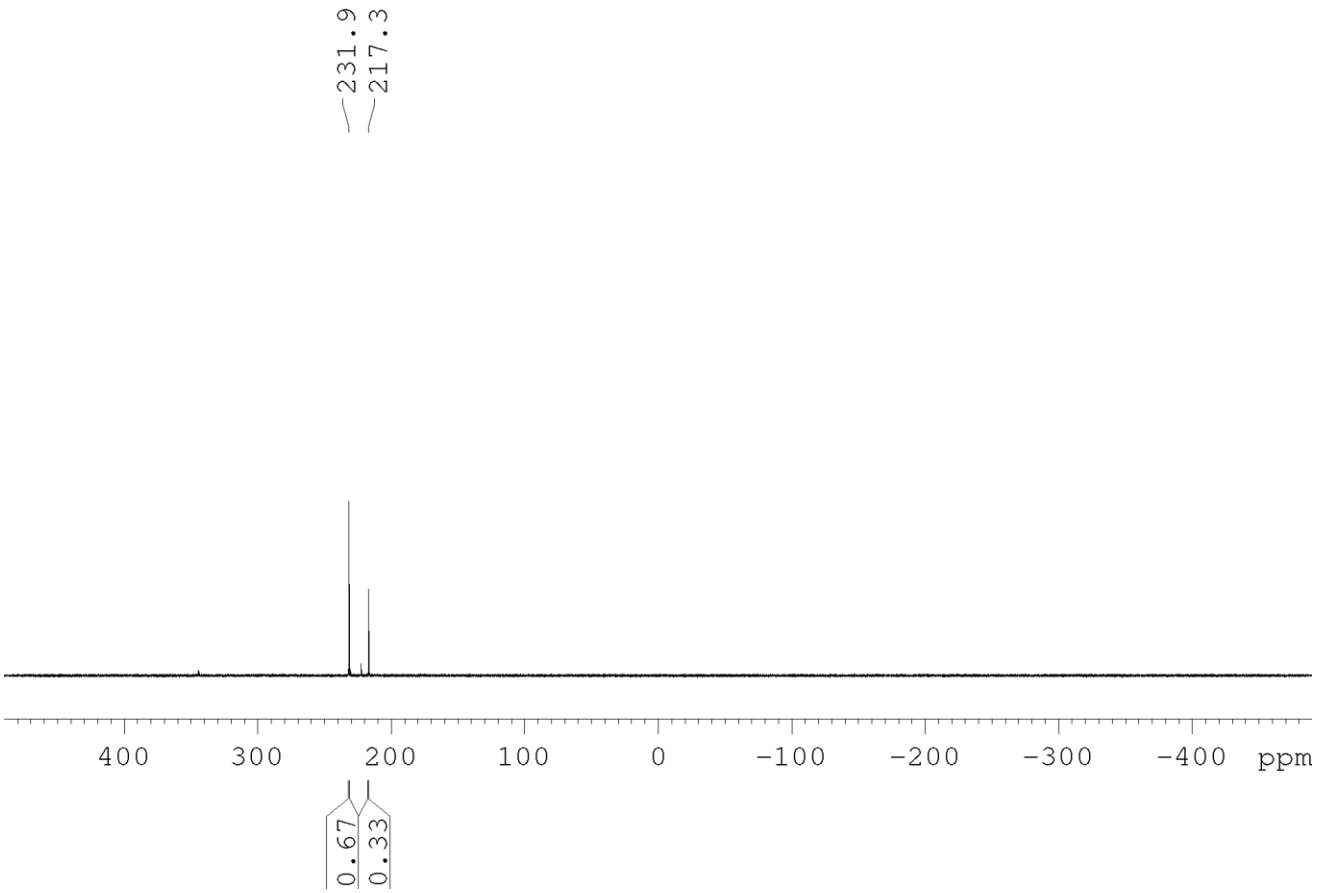

Figure S3: ^{31}P NMR spectrum of Si=P-Tip phosphasilene **2**.

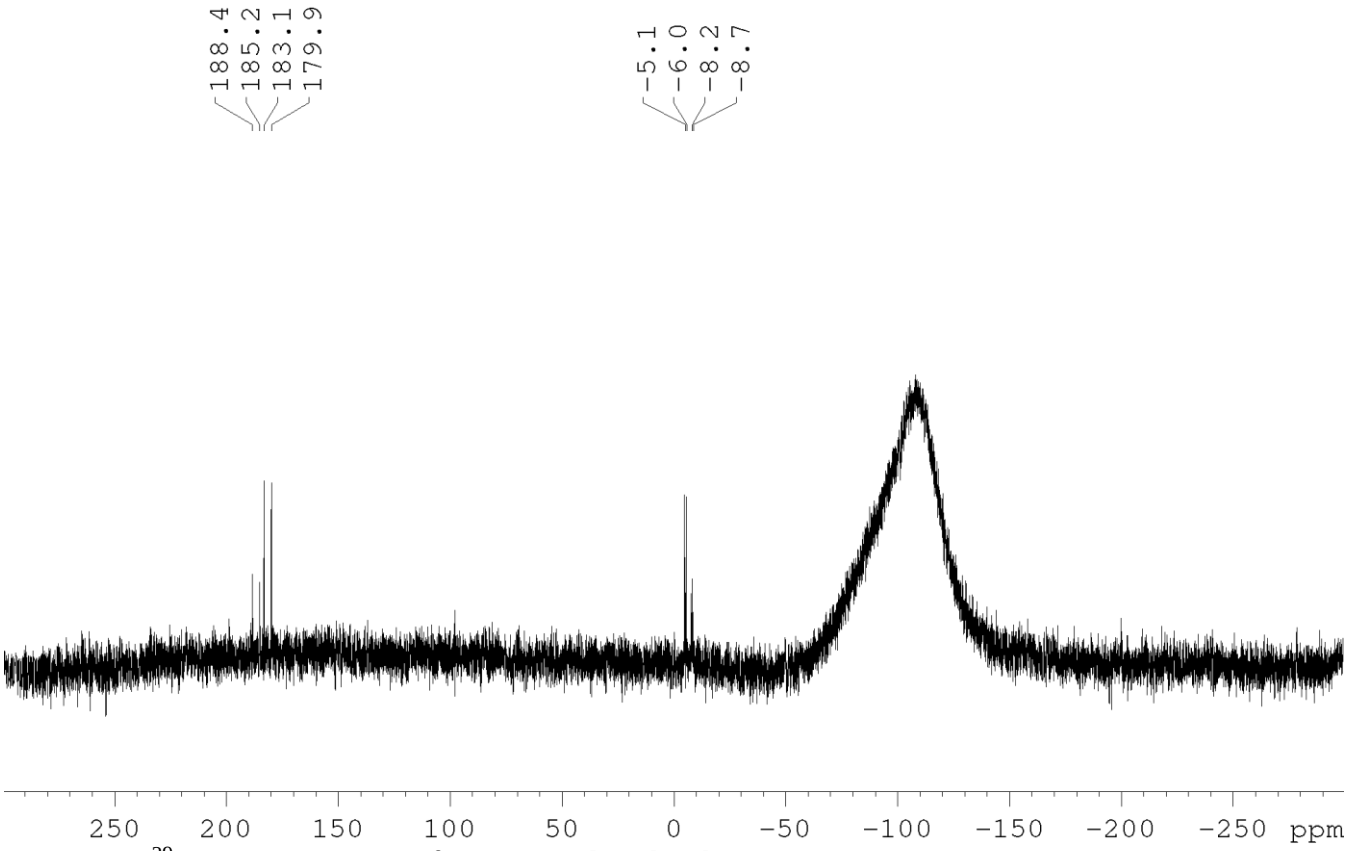

Figure S4: ^{29}Si NMR spectrum of Si=P-Tip phosphasilene **2**.

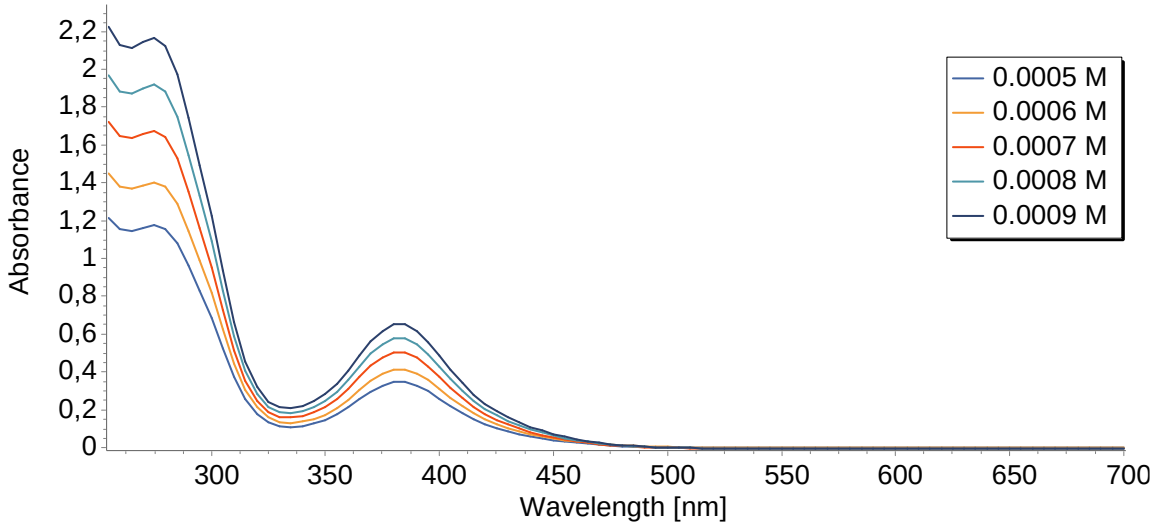

Figure S5: UV/vis spectra of **2** in *n*-hexane at different concentrations (5×10^{-4} – 9×10^{-4} M).

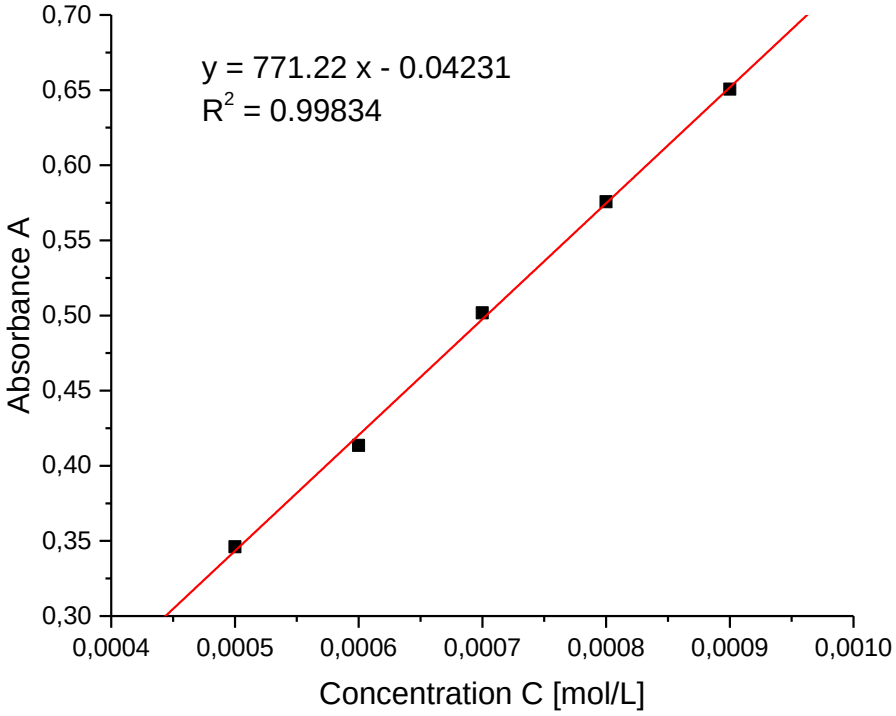

Figure S6: Determination of extinction coefficient ε (7770 $M^{-1}cm^{-1}$) by linear regression of absorbance (λ = 382 nm) of **2** against concentration.

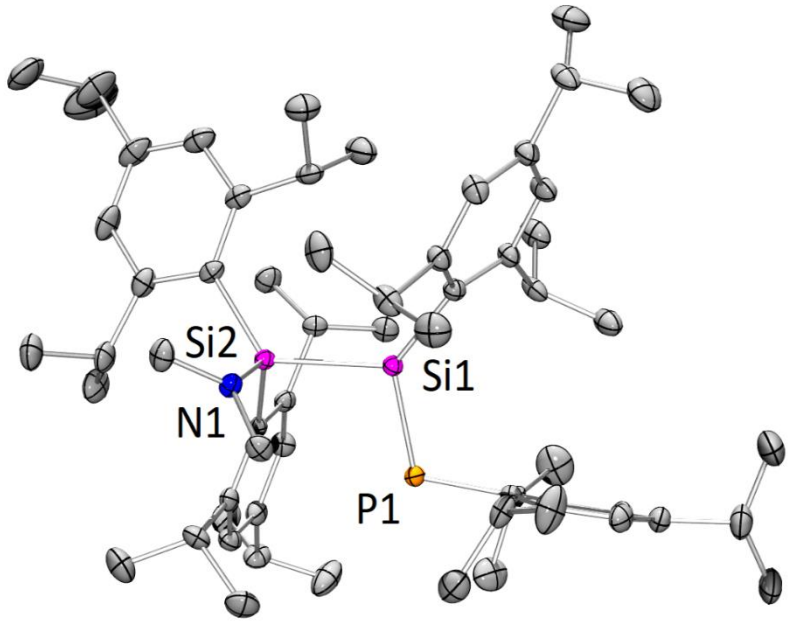

Figure S7: Molecular structure of *E*-**2** in the solid state (thermal ellipsoids at 50%, H atoms omitted for clarity). Selected bond lengths [Å] and angles [°]: Si1=P1 2.0939(8), Si1-Si2 2.4123(8), Si2-N1 1.7316(18), P1-C1 1.847(2), C1-P1-Si1 108.49(7).

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Table S1: Crystal data and structure refinement for *E*-**2** (CCDC-1989736)

Identification code	sh3951	
Empirical formula	C62 H98 N P Si2	
Formula weight	944.56	
Temperature	142(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 10.6736(4) Å	α= 90°.
	b = 38.2291(15) Å	β= 94.5421(18)°.
	c = 14.4974(6) Å	γ = 90°.
Volume	5897.0(4) $Å^3$	
Z	4	
Density (calculated)	1.064 Mg/m^3	
Absorption coefficient	0.124 mm^{-1}	
F(000)	2080	
Crystal size	0.498 x 0.147 x 0.066 mm^3	
Theta range for data collection	1.065 to 27.176°.	
Index ranges	-11<=h<=13, -49<=k<=46, -18<=l<=18	
Reflections collected	52437	
Independent reflections	13098 [R(int) = 0.0685]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	13098 / 0 / 621	
Goodness-of-fit on F^2	1.016	
Final R indices [I>2sigma(I)]	R1 = 0.0554, wR2 = 0.1118	
R indices (all data)	R1 = 0.1040, wR2 = 0.1294	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.979 and -0.448 $e.Å^{-3}$	

Synthesis of Si=P-Dur Phosphasilene 3

A suspension of 1.5 g (1.91 mmol, 1.0 eq.) of phosphasilene **4** and 525 mg (2.87 mmol, 1.5 eq.) of duryl lithium in 20 mL of toluene was stirred for three days at 50°C. After removal of toluene in vacuo, the solid residue was taken up in 20 mL of *n*-hexane and lithium salts were removed by filtration. Crystallization from *n*-hexane yielded 698 mg (0.798 mmol, 40%) of Si=P-Dur phosphasilene **3** as yellow-brown crystals.

Overlapping of resonances due to presence of an *E*/*Z*-mixture in solution (ca 4:1) neglects individual assignment and integration in the according ^{1}H and ^{13}C NMR spectra.

^{1}H-NMR (300 MHz, C_6D_6, 300 K): δ = 0.11 (d), 0.24 (d), 0.33-0.38 (m), 0.44 (d), 0.59 (d), 0.65 (d), 0.81 (d), 0.85-0.91 (m), 0.95 (d) 1.01 (tr), 1.12 (d), 1.17-1.34 (m), 1.39-1.46 (m), 1.54 (br), 1.61 (d), 1.67-1.73 (m), 1.88 (d), 1.92 (s), 2.03 (s), 2.08 (s), 2.34 (s), 2.47 (s), 2.62-2.93 (m), 3.11-3.60 (m), 3.92 (tr), 4.18 (sept), 5.68 (sept), 6.62, 6.69, 6.73, 6.82, 6.85, 6.87, 6.97, 7.04, 7.11, 7.16, 7.21, 7.30 (each s).
^{13}C{^{1}H} NMR (75.47 MHz, C_6D_6, 300 K): δ = 14.2, 19.1, 20.6, 20.7, 21.5, 21.6, 22.9, 23.0, 23.1, 23.5, 23.7, 23.9, 24.0, 24.2, 24.3, 24.5, 24.8, 24.9, 25.4, 25.7, 27.2, 27.4, 27.5, 27.9, 28.0, 28.3, 29.3, 30.5, 31.8, 34.0, 34.2, 34.4, 34.5, 34.9, 35.7, 36.5, 36.7 38.5 (*i*Pr-*C*H, *i*Pr-*C*H_3 and Dur-*C*H_3), 42.6 (-N(*C*H_3)$_2$), 121.6, 121.8, 121.9, 122.0, 122.3, 122.5, 123.2, 130.6, 133.0, 133.1, 135.2, 135.3, 135.5, 135.7, 135.8, 136.2, 137.2, 142.1, 142.9, 149.6, 150.0, 150.4, 150.6, 151.3, 151.4, 153.1, 153.4, 154.2, 154.5, 154.7, 155.0, 156.0, 156.3, 156.5 (Ar-*C*).

^{31}P{^{1}H}-NMR (121.5 MHz, C_6D_6, 300 K): δ = 227.3 ($^{1}J_{P\text{-}Si}$ = 185.3 Hz, $^{2}J_{P\text{-}Si}$ = 29.4 Hz, *Z*-**3**), 242.3 ($^{1}J_{P\text{-}Si}$ = 189.6 Hz, $^{2}J_{P\text{-}Si}$ = 46.9 Hz, *E*-**3**) ppm.

^{29}Si{^{1}H}-NMR (59.62 MHz, C_6D_6, 300 K): δ = −9.6 (d, $^{2}J_{Si\text{-}P}$ = 29.2 Hz, *Z*-**3**), −6.5 (d, $^{2}J_{Si\text{-}P}$ = 46.3 Hz, *E*-**3**), 186.5 (d, $^{1}J_{Si\text{-}P}$ = 185.5 Hz, *Z*-**3**), 187.7 (d, $^{1}J_{Si\text{-}P}$ = 190.0 Hz, *E*-**3**) ppm.

UV/vis (*n*-hexane): $\lambda_{max}(\varepsilon)$ = 373 nm (9170 $M^{-1}cm^{-1}$).

Elemental analysis: Calculated for $C_{57}H_{88}NPSi_2$: C: 78.29, H: 10.14, N: 1.60. Found: C: 77.87, H: 10.19, N: 2.28.

m.p.: 183°C.

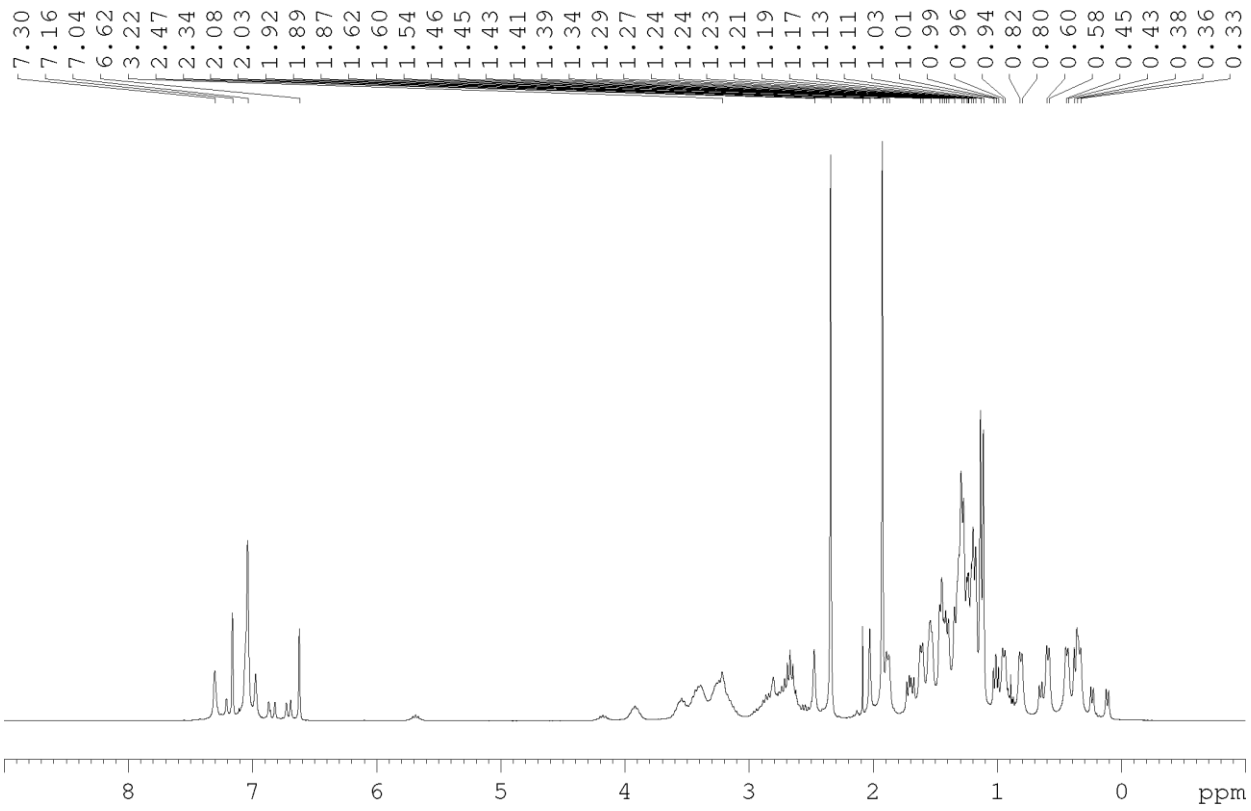


Figure S8: ^{1}H NMR spectrum of Si=P-Dur phosphasilene **3**.

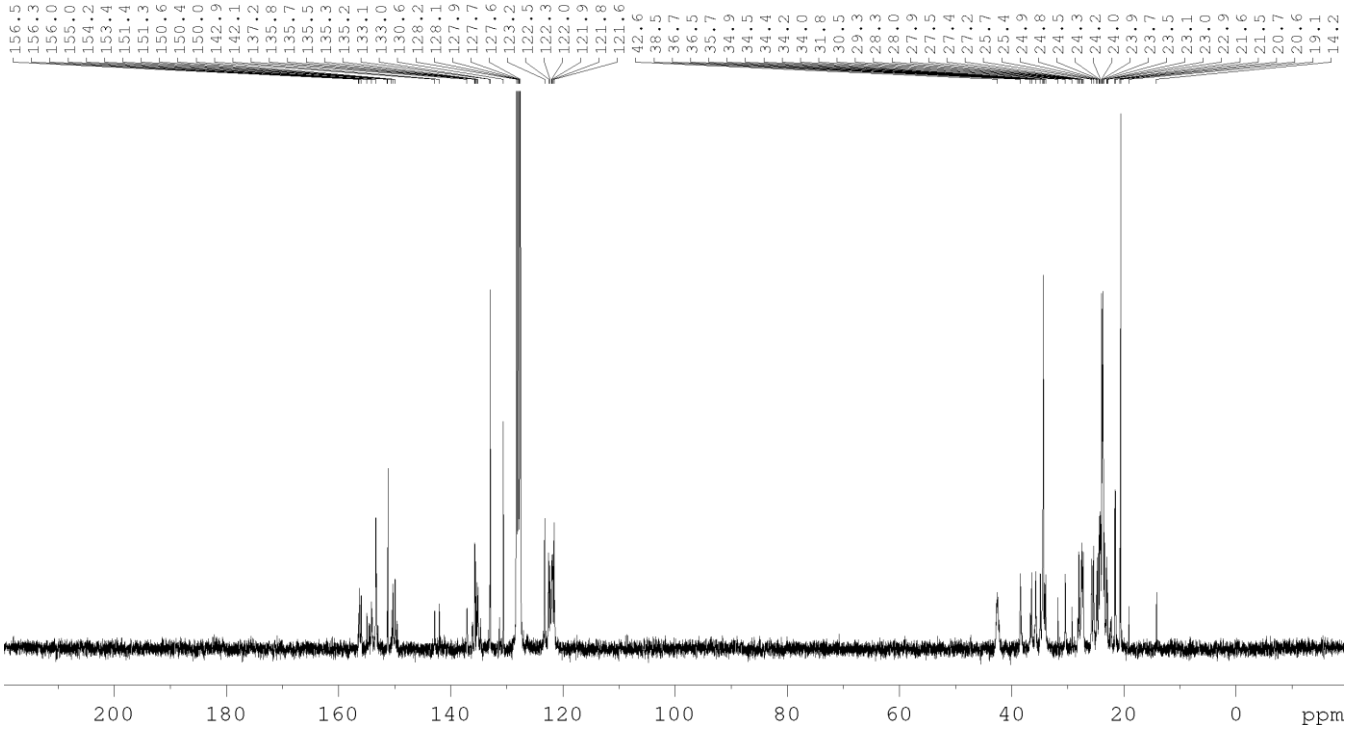


Figure S9: ^{13}C NMR spectrum of Si=P-Dur phosphasilene **3**.

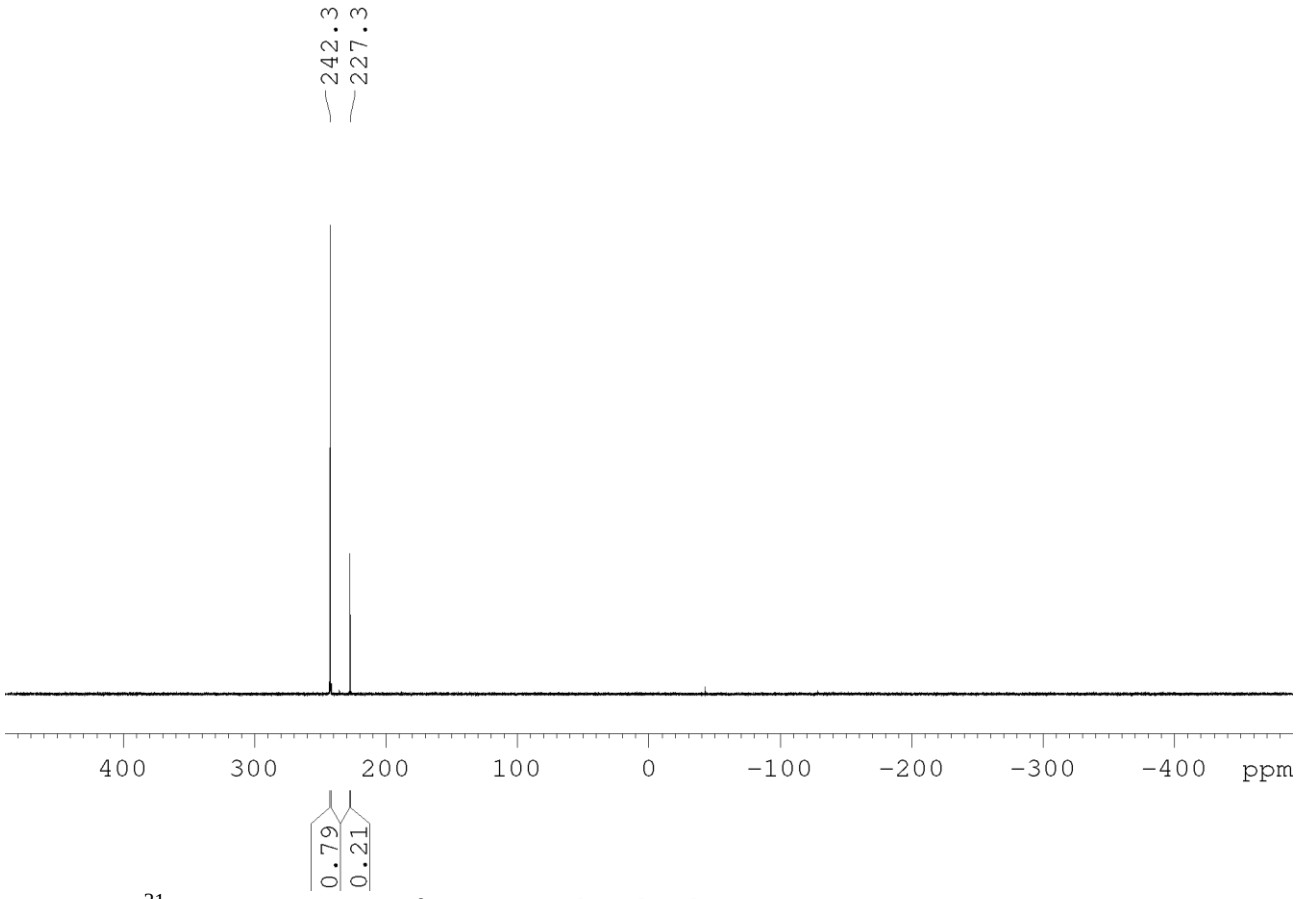


Figure S10: ^{31}P NMR spectrum of Si=P-Dur phosphasilene **3**.

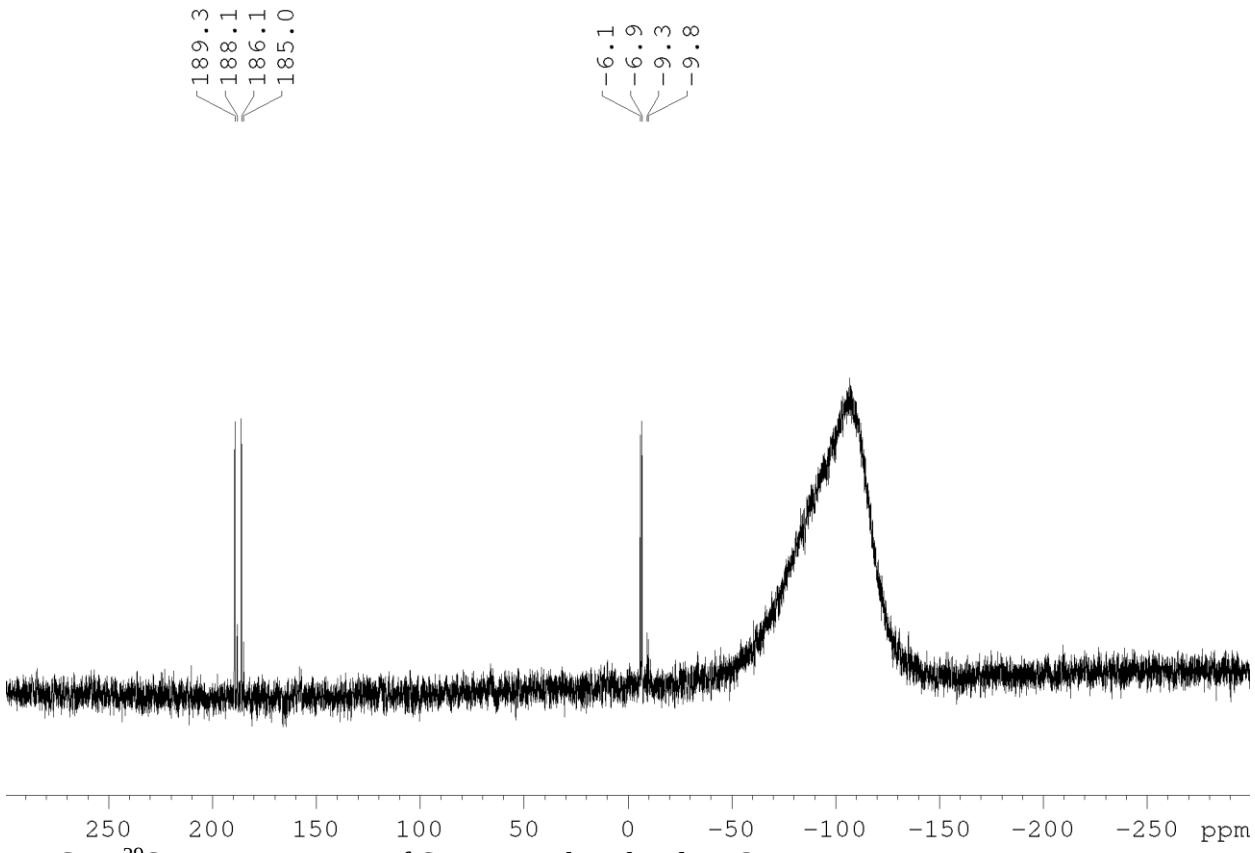


Figure S11: ^{29}Si NMR spectrum of Si=P-Dur phosphasilene **3**.

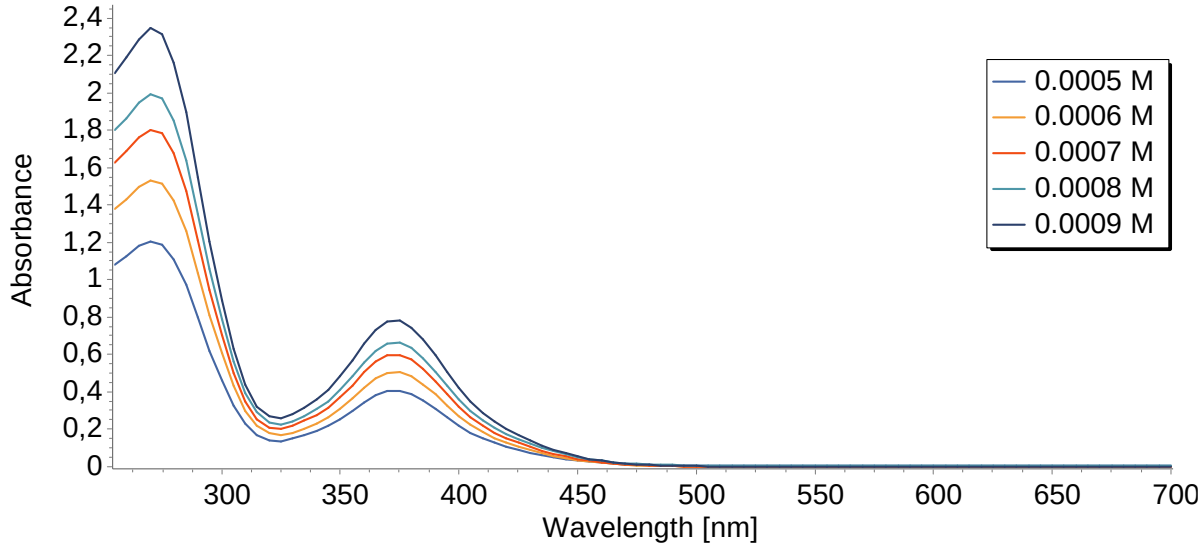


Figure S12: UV/vis spectra of **3** in *n*-hexane at different concentrations (5×10^{-4} – 9×10^{-4} M).

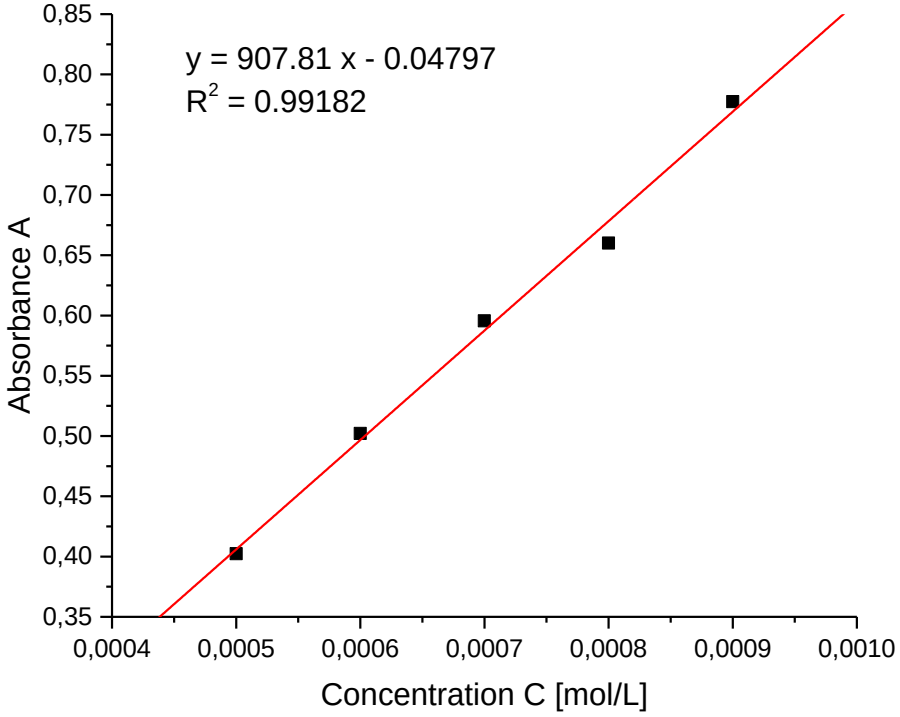


Figure S13: Determination of extinction coefficient ε (9170 $M^{-1}cm^{-1}$) by linear regression of absorbance (λ = 373 nm) of **3** against concentration.

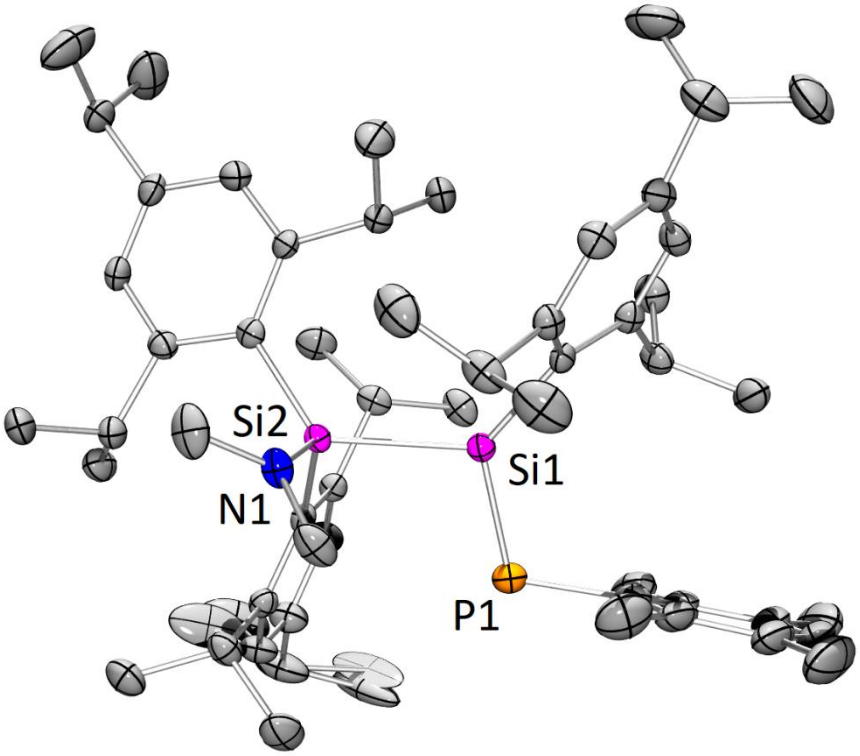


Figure S14: Molecular structure of *E*-**3** in the solid state (thermal ellipsoids at 50%, H atoms omitted for clarity). Selected bond lengths [Å] and angles [°]: Si1=P1 2.0903(10), Si1-Si2 2.4210(10), Si2-N1 1.731(2), P1-C1 1.853(3), C1-P1-Si1 108.02(9).

Table S2: Crystal data and structure refinement for *E*-**3** (CCDC-1989735).

Identification code	sh3948	
Empirical formula	C57 H88 N P Si2	
Formula weight	874.43	
Temperature	142(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.6545(10) Å	α= 78.981(3)°.
	b = 19.8563(14) Å	β= 89.555(3)°.
	c = 26.305(2) Å	γ = 85.188(3)°.
Volume	5443.1(8) $Å^3$	
Z	4	
Density (calculated)	1.067 Mg/m^3	
Absorption coefficient	0.129 mm^{-1}	
F(000)	1920	
Crystal size	0.369 x 0.181 x 0.179 mm^3	
Theta range for data collection	1.185 to 27.193°.	
Index ranges	-13<=h<=13, -25<=k<=25, -33<=l<=33	
Reflections collected	88964	
Independent reflections	23910 [R(int) = 0.0648]	
Completeness to theta = 25.242°	99.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7455 and 0.6562	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	23910 / 42 / 1168	
Goodness-of-fit on F^2	1.009	
Final R indices [I>2sigma(I)]	R1 = 0.0668, wR2 = 0.1536	
R indices (all data)	R1 = 0.1203, wR2 = 0.1786	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.024 and -0.392 $e.Å^{-3}$	

2. Samples for Muon Spin Spectroscopy

Each of the phosphasilenes **1**-**4** was dissolved in dry and oxygen-free tetrahydrofuran (THF) and sealed under inert atmosphere in a stainless-steel cell equipped with a thin stainless-steel window for muon spin spectroscopy experiments. The concentrations were close to saturation, ca. 0.5 M. Earlier experiments employed a sample of **4** dissolved in hexane (0.4 M) and sealed in a similar sample cell.

3. Muon Spin Rotation Spectroscopy (μSR)

Transverse-field muon spin rotation (μSR) experiments were carried out at TRIUMF in Vancouver, Canada, at the M15 and M20 beam lines. Beams of about 4.1 MeV positive muons were used, this being sufficient for the muons to penetrate the steel foil window of the sample cell and stop in the sample itself. The HELIOS μSR spectrometer was installed at the end of each beam line in two separate beam periods. The spectrometer incorporates a superconducting solenoid magnet whose axis is aligned along the direction of the incoming beam. Incoming muons trigger a plastic scintillator detector and enter the sample cell, which was mounted on the cold tip of a cryostat. Additional detectors are arranged in phase quadrature about the sample to register passage of decay positrons. The muon spin polarization of the beam was adjusted to be transverse to the beam direction so that the spins of stopped muons precess in a plane perpendicular to the applied magnetic field.

At TRIUMF the beam is quasi-continuous (i.e. not pulsed as in some other accelerators), and therefore μSR functions in single-particle counting mode. Accordingly, the muon beam rate was limited to about 7×10^4 s^{-1} to avoid "pile-up" (more than one muon or positron detected in the 7 μs data gate). As each individual muon decays, its positron is emitted in a direction influenced by the instantaneous muon spin orientation (the asymmetric probability distribution has a maximum along the spin direction). The elapsed time between muon arrival and detection of the decay positron is recorded in a separate histogram for each positron detector. Such a histogram comprises a lifetime decay curve (τ_μ = 2.197 μs) with additional oscillations which correspond to the spin precession frequencies of the muon. These frequencies are conveniently displayed in Fourier transform spectra, but quantitative analysis was accomplished in time space, using Wimda,[4] a multi-parameter curve-fitting program for μSR histograms.

A substantial fraction of muons become incorporated in diamagnetic molecules during thermalization or shortly thereafter (picoseconds). These precess at the muon Larmor frequency ν_D. The remainder form muonium which, in the presence of suitable reactants, is converted to a muoniated free radical. At sufficiently high field (typically a few kG) a muoniated radical is characterized by two spin precession frequencies, ν_{R1} and ν_{R2} , one above and one below ν_D. The difference in these frequencies gives the muon hyperfine constant A_μ:

$$A_\mu = \nu_{R2} - \nu_{R1} \qquad \text{(S1)}$$

Sometimes the upper frequency can not be determined due to low signal intensity, which might be due to loss of spin coherence during the radical formation reaction, or simply to limited time resolution of the spectrometer. In such cases it is still possible to determine A_μ from the single radical frequency, the muon Larmor frequency ν_D and electron Larmor frequency ν_e:

$$A_\mu = 2\frac{(\nu_D - \nu_{R1})(\nu_e + \nu_{R1})}{\nu_e - \nu_D + 2\nu_{R1}} \qquad \text{(S2)}$$

B. Additional μSR Spectra and Results

1. Phosphasilene 1 in THF at 53.5°C

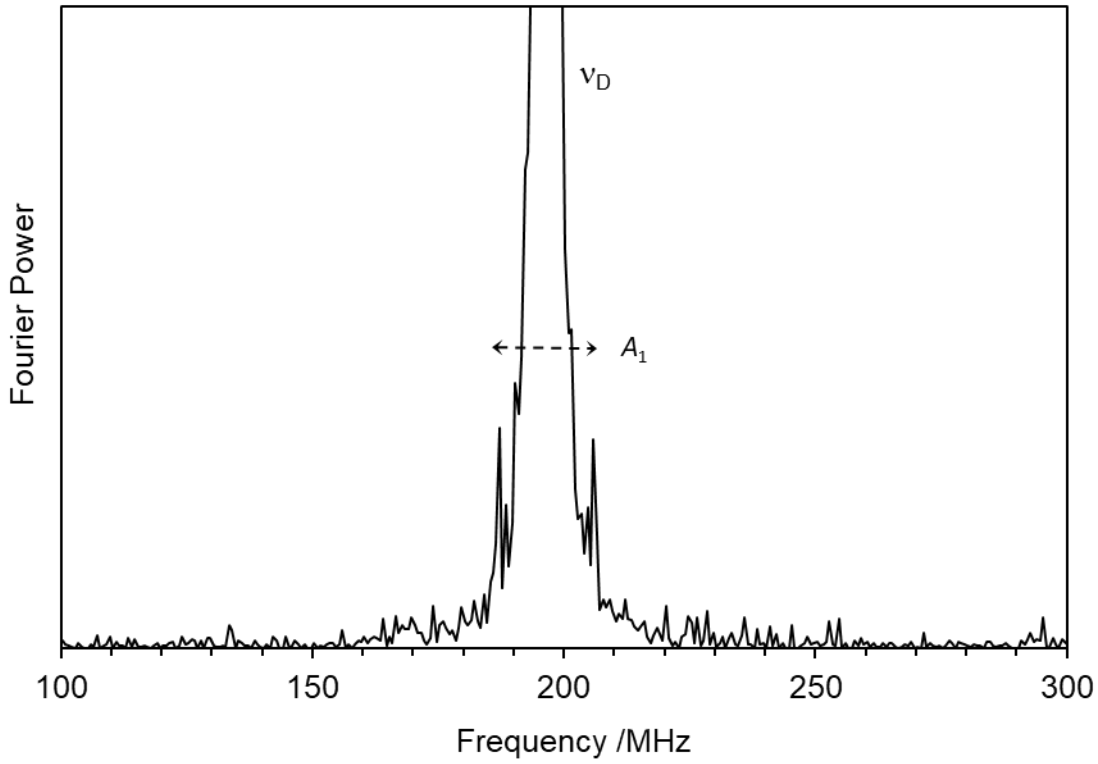


Figure S15: Transverse-field μSR spectrum at 14.48 kG obtained from a 0.5 M solution of **1** in tetrahydrofuran at 53.5°C. This Fourier transform corresponds to a 2.5 μs time window delayed by 75 ns. The truncated signal labelled ν_D is due to muons in diamagnetic molecules, whose spins precess at the muon Larmor frequency (196.25 MHz at this magnetic field). A_1 denotes the separation of the pair of radical precession frequencies and thus comprises the muon hyperfine constant.

Precession Frequency /MHz	A_μ /MHz	Label
196.2349 ± 0.0005		ν_D
186.81 ± 0.04	18.99 ± 0.07	A_1
205.80 ± 0.05		

2. Phosphasilene 2 in THF at 53.7°C with Fourier transform delay of 38 ns

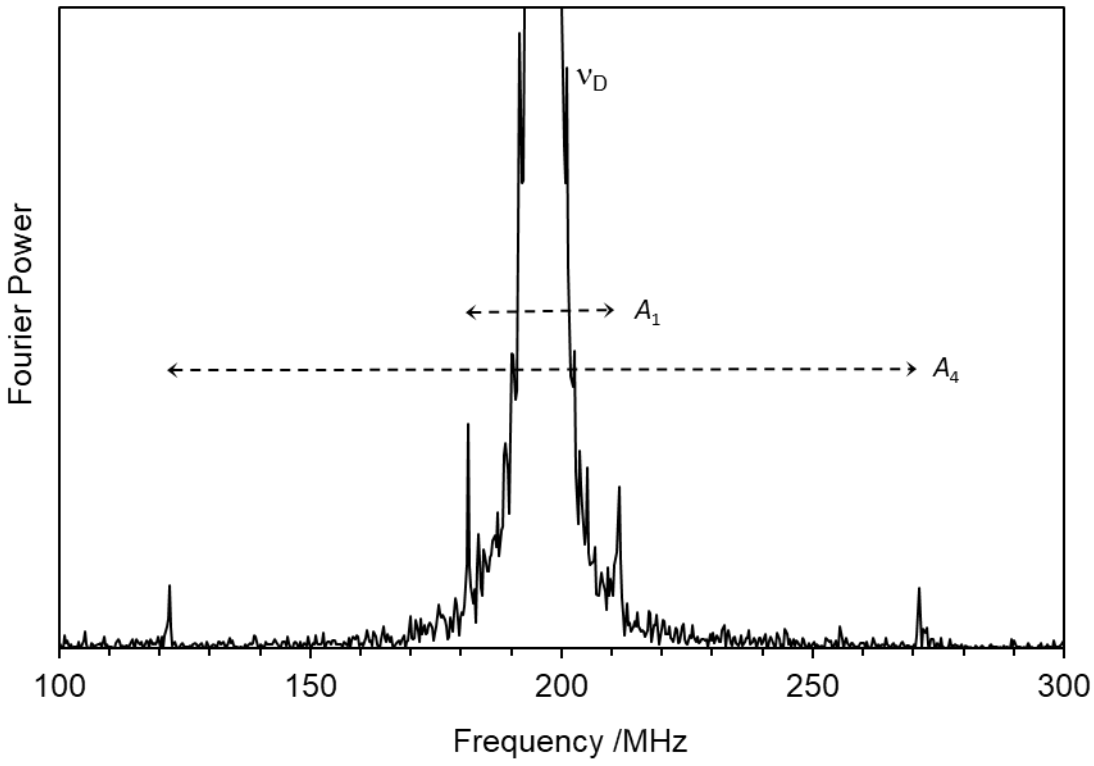


Figure S16: Transverse-field μSR spectrum at 14.48 kG obtained from a 0.5 M solution of **2** in tetrahydrofuran at 53.7°C. This Fourier transform corresponds to a 2.5 μs time window delayed by 38 ns. The truncated signal labelled ν_D is due to muons in diamagnetic molecules, whose spins precess at the muon Larmor frequency (196.25 MHz at this magnetic field). A_1 and A_4 denote the separation of the pairs of radical precession frequencies and thus comprise the muon hyperfine constants.

Precession Frequency /MHz	A_μ /MHz	Label
196.2514 ± 0.0003		ν_D
181.18 ± 0.02	30.09 ± 0.05	A_1
211.27 ± 0.04		
121.88 ± 0.04	149.01 ± 0.08[a]	A_4

[a] Calculated from a single radical frequency and ν_D.

3. Phosphasilene 2 in THF at 53.7°C with Fourier transform delay of 53 ns

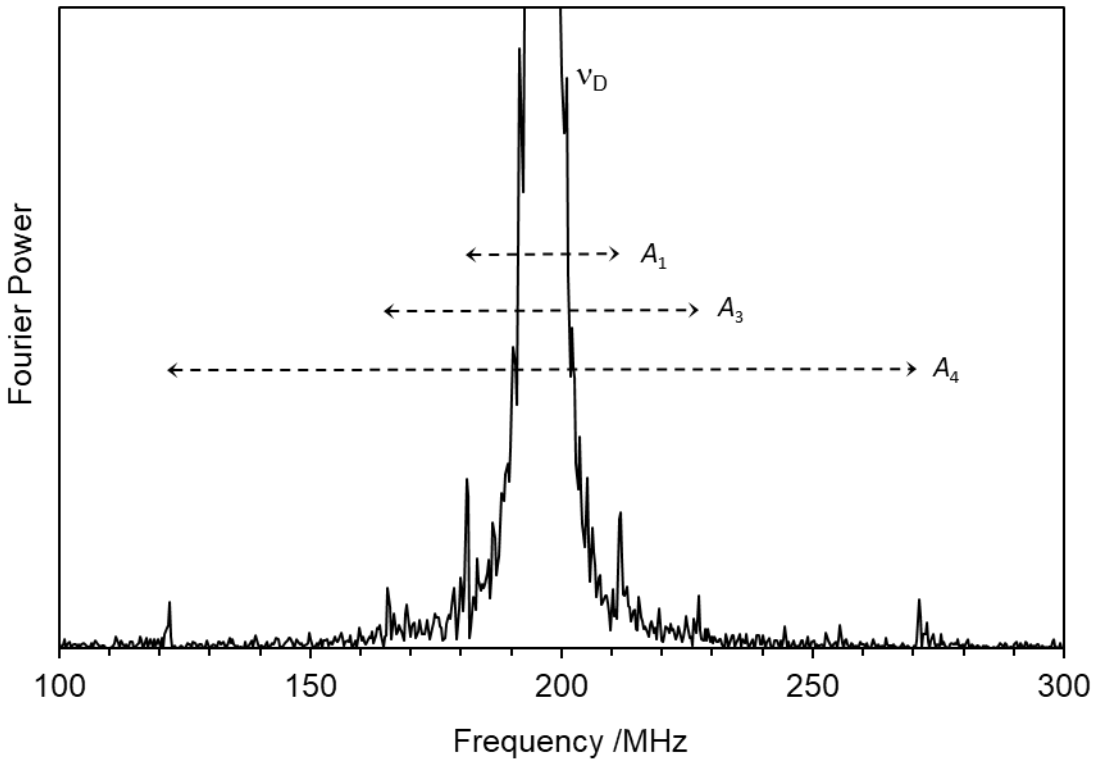


Figure S17: Transverse-field μSR spectrum at 14.48 kG obtained from a 0.5 M solution of **2** in tetrahydrofuran at 53.7°C. This Fourier transform corresponds to a 2.5 μs time window delayed by 53 ns. The truncated signal labelled ν_D is due to muons in diamagnetic molecules, whose spins precess at the muon Larmor frequency (196.25 MHz at this magnetic field). A_1, A_3 and A_4 denote the separation of the pairs of radical precession frequencies and thus comprise the muon hyperfine constants.

Precession Frequency /MHz	A_μ /MHz	Label
196.2514 ± 0.0003		ν_D
181.18 ± 0.02	30.09 ± 0.05	A_1
211.27 ± 0.04		
165.44 ± 0.03	61.66 ± 0.07[a]	A_3
121.88 ± 0.04	149.01 ± 0.08[a]	A_4

[a] Calculated from a single radical frequency and ν_D.

4. Phosphasilene 3 in THF at 54.6°C

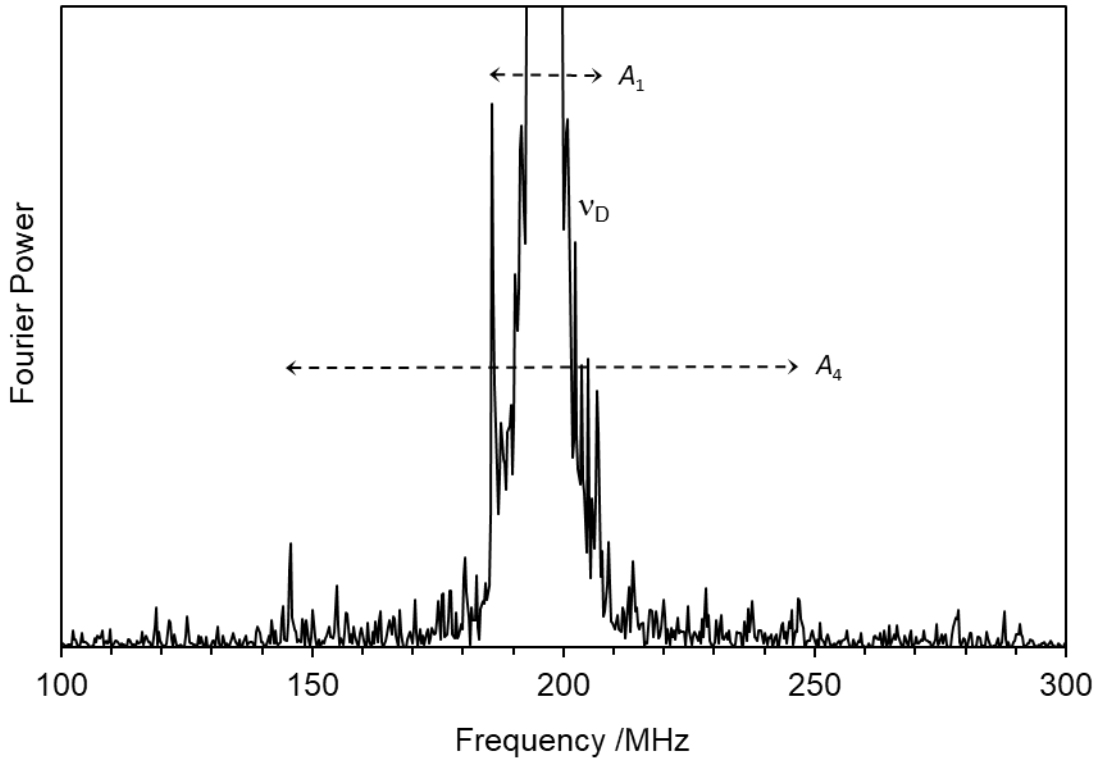


Figure S18: Transverse-field μSR spectrum at 14.48 kG obtained from a 0.5 M solution of **3** in tetrahydrofuran at 54.6°C. This Fourier transform corresponds to a 2.5 μs time window delayed by 50 ns. The truncated signal labelled ν_D is due to muons in diamagnetic molecules, whose spins precess at the muon Larmor frequency (196.25 MHz at this magnetic field). A_1 and A_4 denote the separation of the pairs of radical precession frequencies and thus comprise the muon hyperfine constants.

Precession Frequency /MHz	A_μ /MHz	Label
196.2349 ± 0.0005		ν_D
185.54 ± 0.03	21.35 ± 0.05	A_1
206.89 ± 0.04		
145.51 ± 0.05	101.89 ± 0.07	A_4
247.40 ± 0.05		

5. Phosphasilene 4 in THF at 25.3°C at 25.3°C with Fourier transform delay of 30 ns

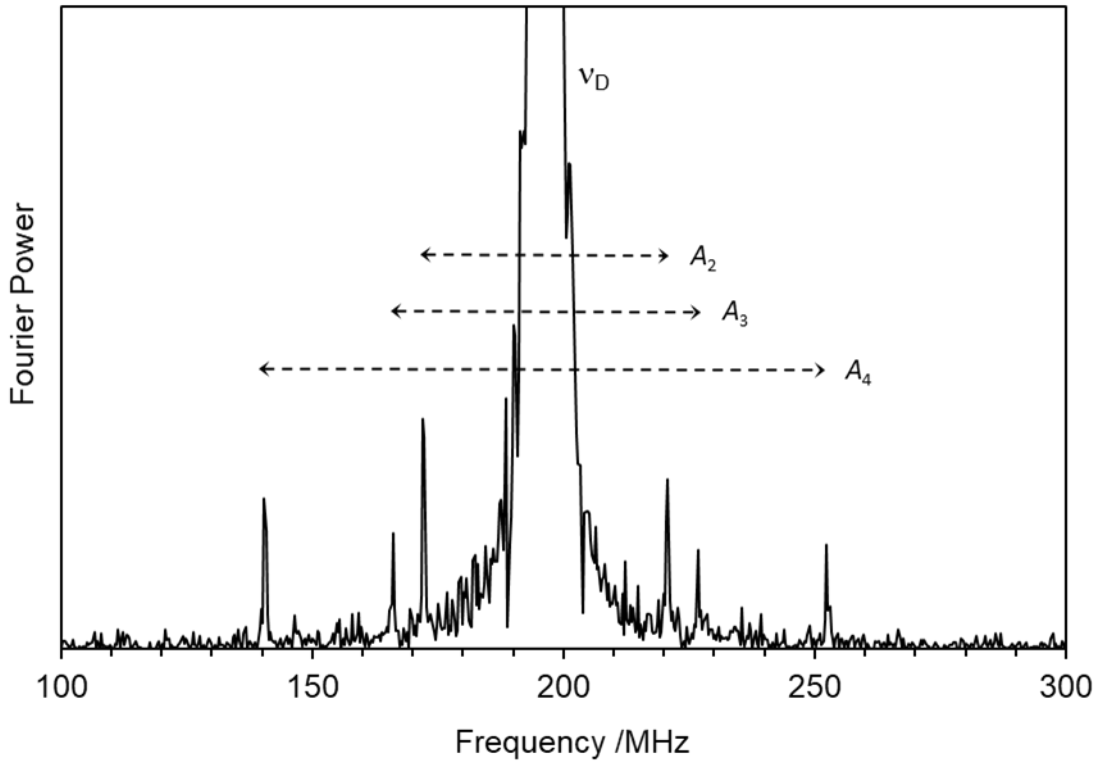


Figure S19: Transverse-field μSR spectrum at 14.48 kG obtained from a 0.5 M solution of **4** in tetrahydrofuran at 25.3°C. This Fourier transform corresponds to a 3 μs time window delayed by 30 ns. The truncated signal labelled ν_D is due to muons in diamagnetic molecules, whose spins precess at the muon Larmor frequency (196.25 MHz at this magnetic field). A_1, A_2, A_3 and A_4 denote the separation of the pairs of radical precession frequencies and thus comprise the muon hyperfine constants.

Precession Frequency /MHz	A_μ /MHz	Label
196.2509 ± 0.0004		ν_D
172.02 ± 0.03	48.49 ± 0.05[a]	A_2
166.05 ± 0.03	60.44 ± 0.06[a]	A_3
140.39 ± 0.04	111.87 ± 0.08[a]	A_4

[a] Calculated from a single radical frequency and ν_D.

6. Phosphasilene 4 in THF at 25.3°C with Fourier transform delay of 86 ns

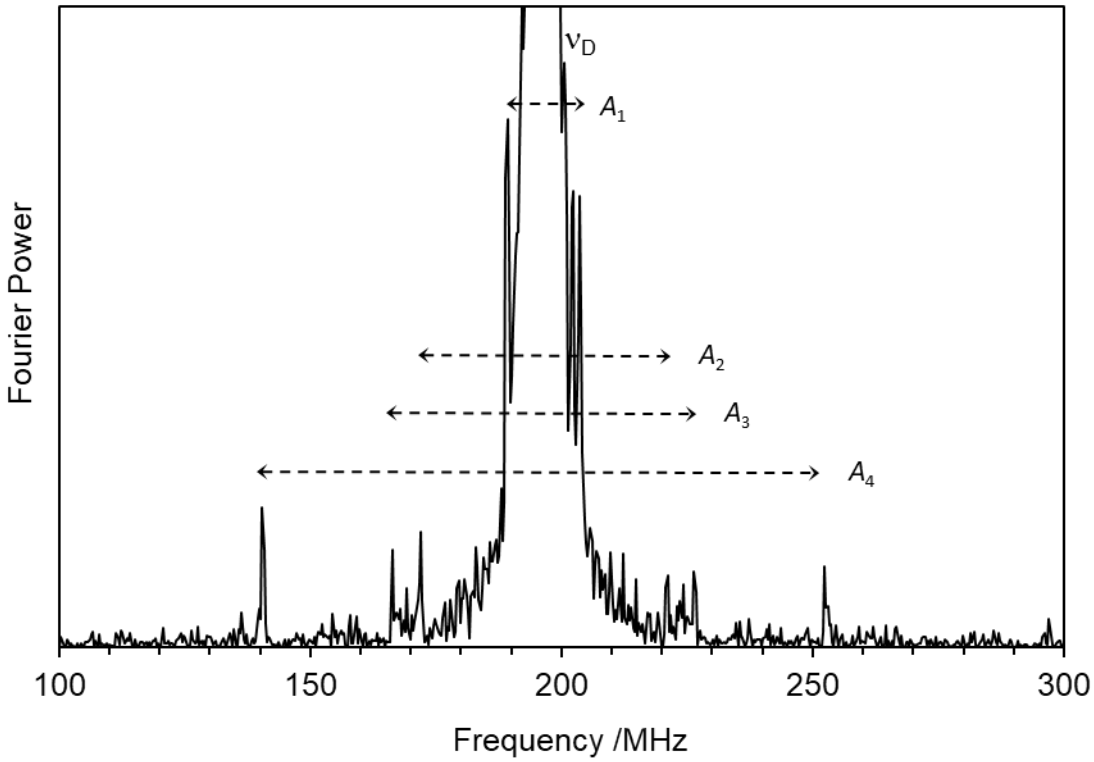


Figure S20: Transverse-field μSR spectrum at 14.48 kG obtained from a 0.5 M solution of **4** in tetrahydrofuran at 25.3°C. This Fourier transform corresponds to a 3 μs time window delayed by 86 ns. The truncated signal labelled ν_D is due to muons in diamagnetic molecules, whose spins precess at the muon Larmor frequency (196.25 MHz at this magnetic field). A_1, A_3 and A_4 denote the separation of the pairs of radical precession frequencies and thus comprise the muon hyperfine constants.

Precession Frequency /MHz	A_μ /MHz	Label
196.2509 ± 0.0004		ν_D
188.77 ± 0.03	14.96 ± 0.06[a]	A_1
172.02 ± 0.03	48.49 ± 0.05[a]	A_2
166.05 ± 0.03	60.44 ± 0.06[a]	A_3
140.39 ± 0.04	111.87 ± 0.08[a]	A_4

[a] Calculated from a single radical frequency and ν_D.

7. Phosphasilene 4 in hexane at 50.6°C

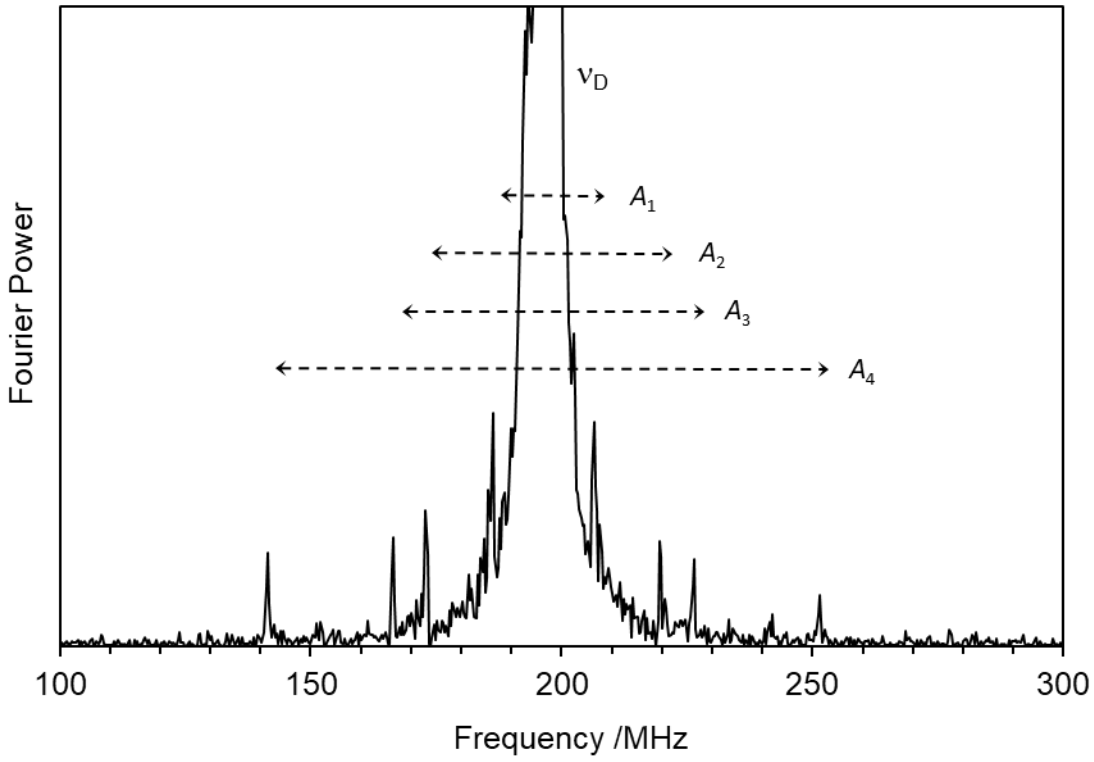


Figure S21: Transverse-field μSR spectrum at 14.48 kG obtained from a 0.4 M solution of **4** in hexane at 50.6°C. This Fourier transform corresponds to a 3 μs time window delayed by 85 ns. The truncated signal labelled ν_D is due to muons in diamagnetic molecules, whose spins precess at the muon Larmor frequency (196.15 MHz at this magnetic field). A_1, A_2, A_3 and A_4 denote the separation of the pairs of radical precession frequencies and thus comprise the muon hyperfine constants.

Precession Frequency /MHz	A_μ /MHz	Label
196.1549 ± 0.0009		ν_D
186.29 ± 0.10	19.87 ± 0.12	A_1
206.15 ± 0.07		
172.49 ± 0.03	46.25± 0.06[a]	A_2
166.08 ± 0.04	60.19± 0.08[a]	A_3
141.20 ± 0.05	110.06± 0.09[a]	A_4

[a] Calculated from a single radical frequency and ν_D.

C. DFT Calculations

1. Computational Details

Geometry optimizations of the parent phosphasilenes were carried out without symmetry restraints using Gaussian 09, Revision D.01,[5] at the density functional level of theory (DFT) using the hybrid three-parameter functional of Becke[6] and the correlation functional of Lee, Yang, and Parr [7] (B3LYP). The 6-31G(d) basis set was used for all atoms. Similarly, the unrestricted functional (UB3LYP) was used to optimize the geometries of the free radicals formed by adding H to either end of the Si=P bond. The polarizable continuum model (PCM) was employed to account for possible solvent effects (THF for **1**-**3**, and hexane for **4**).[8]

Relaxed potential energy surface (PES) scans were performed for rotation about the Si-P bond of each radical. Dihedral angles were incremented in steps of 10°. It was assumed that each PES applies to the analogous muoniated radical, i.e. no account was taken of zero-point energy.

Isotropic hyperfine coupling constants were calculated using UB3LYP/cc-pVDZ. [9] at each radical geometry corresponding to a local minimum on a PES. Muon hyperfine coupling constants were scaled from the proton hyperfine constants by the ratio of the muon/proton magnetic moment (3.1833). No attempt was made to account for mass-dependent isotope effects.

For ease of comparison across different phosphasilenes and sites of Mu addition, the energies of the radicals are displayed as reaction energies: $\Delta E = E$(radical)-E(parent)-E(H).

2. PES Scans of rotation about the Si-P bond of each radical

1 Si=P-Mes

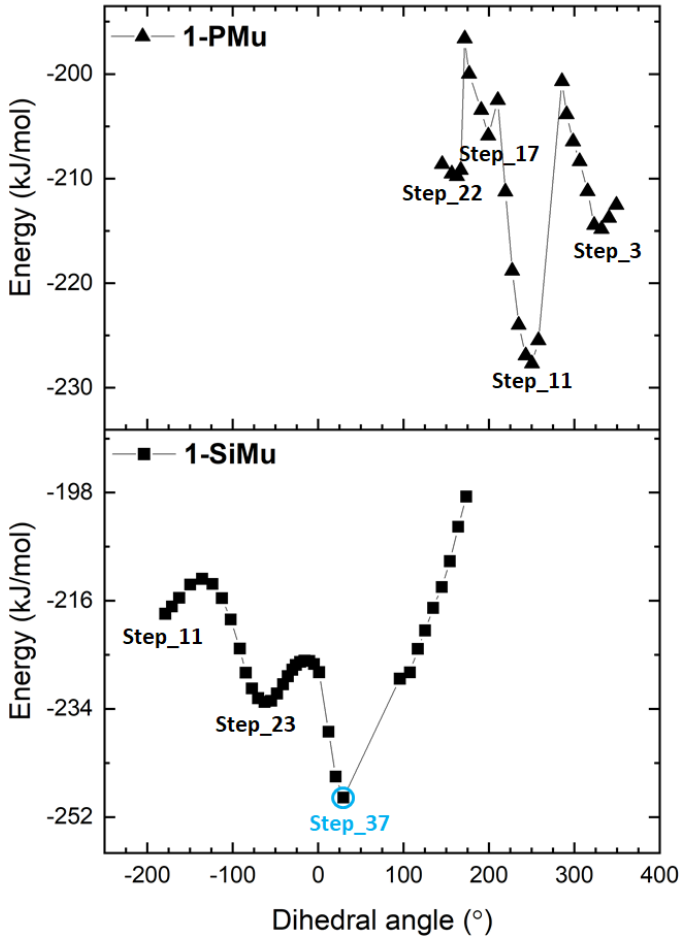


Figure S22: Potential energy surface scans for rotation about the Si-P bonds of radicals **1-PMu** and **1-SiMu**. The blue label denotes a radical conformation detected by muon spin spectroscopy.

The PES scan over the dihedral angle Mu^{62}-Si^{2}-P^{3}-C^{4} of **1-SiMu** (Mu addition to the Si atom in **1**) shows three minima at -179° (**Step 11**), -63° (**Step 23**), and 30° (**Step 37**), with calculated muon hfcs of 5 MHz, 139 MHz, and 22 MHz, respectively. The barriers from the local minima at -63°, -179° to the global minimum at 30° (**Step 37**) are ca. 7 kJ/mol, so interconversion from these local minima to the global minimum is unlikely. The barrier from the global minimum at 30° to the local minimum at -63° is ca. 23 kJ/mol, ensuring stability for this rotamer.

The PES scan over the dihedral angle Mu^{24}-P^{3}-Si^{2}-Si^{1} of **1-PMu** (Mu addition to the P atom in **1**) shows four minima at 332° (i.e. -28° at **Step 3**), 251° (i.e. -109° at **Step 11**), 199° (i.e. -161° at **Step 17**) and 163° (**Step 22**), with calculated hfcs of 19 MHz, 80 MHz, -4 MHz and 63 MHz, respectively. The barrier from the local minimum at 163° to the global minimum at 251° is ca. 13 kJ/mol, sufficient to prevent interconversion. There is only a low barrier from the local minimum at 199° to the global minimum (ca. 3.4 kJ/mol) and the predicted hfc is too low for the signals to be detected. The remaining rotamer, at 332°, has a sufficient barrier to prevent conversion to the global minimum at 251°. However, even if formed it would be unlikely to be detected, because its predicted hfc is close to that found for **step 37** of **1-SiMu**, the lowest energy product for **1**.

The conclusion is that the single radical signal detected from phosphasilene **1** is the radical formed by Mu addition to the Si atom, resulting in a rotamer with the dihedral angle Mu^{62}-Si^{2}-P^{3}-C^{4} of 30° (**step 37**).

Summary of findings for **1**:

Rotamer dihedral angle		**A_μ /MHz**		**Energy/kJ mol^{-1}**	
		calc.	**exp.**	**Reaction**	**Relative**
1-SiMu: Mu^{62}-Si^{2}-P^{3}-C^{4} [b]	**Step_11** (-179°)	5	–[a]	-218.2	30.6
	Step_23 (-63°)	139	–	-232.8	16.0
	Step_37 (30°)	22	20	-248.8	0.0
1-PMu: Mu^{24}-P^{3}-Si^{2}-Si^{1}	**Step_3** (-28°/332°)	19	–	-214.8	34.0
	Step_11 (-109°/251°)	80	–	-227.7	21.1
	Step_17 (-161°/199°)	-4	–	-205.9	42.9
	Step_22 (163°)	63	–	-209.8	39.0

[a] Too close to the diamagnetic peak to be detected; [b] The superscript digit denotes the atom number in the calculation.

2 Si=P-Tip

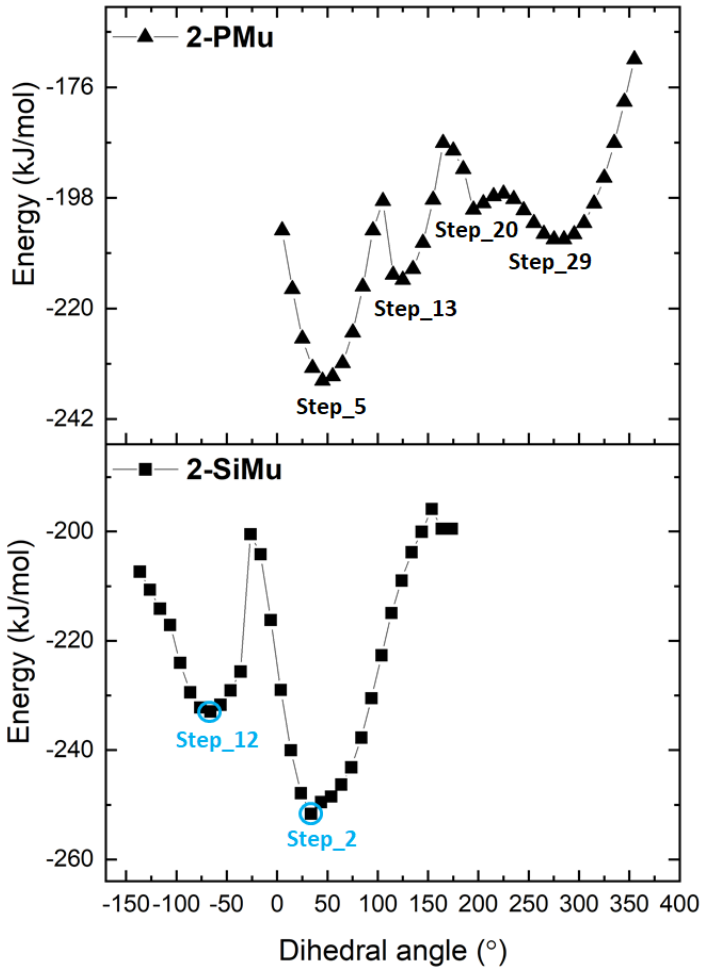


Figure S23: Potential energy surface scans for rotation about the Si-P bonds of radicals **2-PMu** and **2-SiMu**. The blue labels denote radical conformations detected by muon spin spectroscopy.

The PES scan over the dihedral angle Mu^{56}-Si^{2}-P^{3}-C^{4} of **2-SiMu** (Mu addition to Si atom in **2**) shows two minima at 34° (**Step 2**) and -66° (**Step 12**), with calculated hfcs of 31 MHz and 141 MHz, respectively. The barrier between these two minima is sufficiently high (ca. 33 kJ/mol in one direction and ca 51 kJ/mol in the reverse direction) that both rotamers may be stable. Furthermore, the predicted hfcs are consistent with the experimental values (30 MHz and 149 MHz).

The PES scan over the dihedral angle Mu^{165}-P^{3}-Si^{2}-Si^{1} of **2-PMu** (Mu addition to the P atom in **2**) shows four minima at 45° (**Step 5**), 125° (**Step 13**), 195° (**Step 20**), and 285° (i.e. -75° at **Step 29**), with calculated hfcs of 17 MHz, 155 MHz, 25 MHz and 154 MHz, respectively. The low barrier between the local minima at 195° and 285° (ca. 3.1 kJ/mol) suggests that the former would not be stable. In contrast, the barriers between the other minima are sufficiently high that interconversion is unlikely. Although no signal was identified with hfc 17 MHz (the lowest energy rotamer of **2-PMu**, there is a possibility that a weak signal was obscured by the intense diamagnetic peak (Figure S16). Also, the possible existence of the other rotamers of **2-PMu** cannot be completely excluded, since the predicted hfc values lie close to those calculated for the lower energy radical **2-SiMu**.

In view of the above considerations we assign the two clear radical signals detected from phosphasilene **2** (Figure S16) to two rotamers of **2-SiMu**, one with the dihedral angle Mu^{56}-Si^{2}-P^{3}-C^{4} of -66° (**step 12**) and the other 34° (**step 2)**.

Summary of findings for **2**:

Rotamer dihedral angle		A_μ /MHz		Energy/kJ mol^{-1}	
		calc.	exp.	Reaction	Relative
2-SiMu: **Mu^{56}-Si^{2}-P^{3}-C^{4}** [a]	**Step_2** (34°)	31	30	-251.6	0.0
	Step_12 (-66°)	141	149	-232.9	18.7
2-PMu: **Mu^{165}-P^{3}-Si^{2}-Si^{1}**	**Step_5** (45°)	17	–	-234.4	17.3
	Step_13 (125°)	155	–	-214.3	37.3
	Step_20 (-165°/195°)	25	–	-200.3	51.3
	Step_29 (-75°/285°)	154	–	-206.2	45.4

[a] The superscript digit denotes the atom number in the calculation.

An additional signal displayed in Figure S17 has an hfc of 62 MHz but this matches none of the predictions. If the three lowest energy rotamers are considered, then an alternative assignment includes the **2-PMu** radical, as shown below. Further investigation of the Mu/H isotope effect will be necessary before this possibility can be evaluated.

Possible alternative assignments for **2**:

Rotamer dihedral angle		A_μ /MHz		Energy/kJ/mol	
		calc.	exp.	Reaction	Relative
2-SiMu: **Mu^{56}-Si^{2}-P^{3}-C^{4}** [a]	**Step_2** (34°)	31	62	-251.6	0.0
	Step_12 (-66°)	141	149	-232.9	18.7
2-PMu: **Mu^{165}-P^{3}-Si^{2}-Si^{1}**	**Step_5** (45°)	17	30	-234.4	17.3
	Step_13 (125°)	155	–	-214.3	37.3
	Step_20 (-165°/195°)	25	–	-200.3	51.3
	Step_29 (-75°/285°)	154	–	-206.2	45.4

3 Si=P-Dur

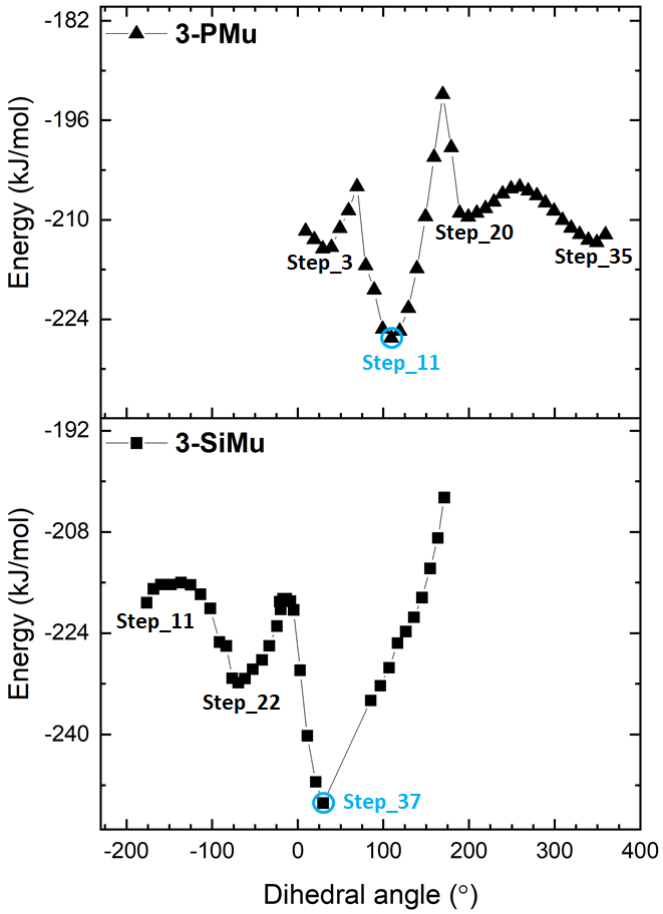


Figure S24: Potential energy surface scans for rotation about the Si-P bonds of radicals **3-PMu** and **3-SiMu**. The blue labels denote radical conformations detected by muon spin spectroscopy.

The PES scan over the dihedral angle Mu^{65}-Si^{2}-P^{3}-C^{4} of **3-SiMu** (Mu addition to the Si atom in **3**) shows three minima at -176° (**Step 11**), -70° (**Step 22**), and 30° (**Step 37**), with calculated hfcs of -6 MHz, 158 MHz, and 21 MHz, respectively. There is only a low barrier between **Step 11** and **Step 22**.so the former is unlikely to be stable. However, the barrier between **Step 22** and **Step 37** is sufficiently high that both rotamers are possible.

The PES scan over the dihedral angle Mu^{27}-P^{3}-Si^{2}-Si^{1} of **3-PMu** (Mu addition to the P atom in **3**) shows four minima at 29° (**Step 3**), 109° (**Step 11**), 200° (**Step 20**), and 11° (**Step 35**), with calculated hfcs of 26 MHz, 81 MHz, 70 MHz, and 4 MHz, respectively. However, the barrier between **Step 3** and **Step 35** is negligible (ca. 1.6 kJ/mol), so stable conformations are unlikely. The rotamer at **Step 20** is higher in energy, with a low barrier (ca. 4 kJ/mol) to **Step 35**, so this one is also unlikely. In contrast, the global minimum at **Step 11** has high barriers to conversion and this rotamer can be considered stable.

Two radicals were detected experimentally. One has a muon hfc of 21 MHz, which agrees well with the prediction for **3-SiMu Step 37** (dihedral angle Mu^{65}-Si^{2}-P^{3}-C^{4} of 30°). The second radical has a muon hfc of 102 MHz, which is consistent with the prediction for **3-PMu Step 11** (dihedral angle Mu^{27}-P^{3}-Si^{2}-Si^{1} of 109°).

Summary of findings for **3**:

Rotamer dihedral angle (°)		A_μ /MHz		Energy/kJ mol^{-1}	
		calc.	exp.	Reaction	Relative
3-SiMu: **Mu^{65}-Si^{2}-P^{3}-C^{4}** [b]	**Step_11** (-176°)	-6	–[a]	-219.2	31.6
	Step_22 (-70°)	158	–	-231.8	19 0
	Step_37 (30°)	21	21	-250.8	0.0
3-PMu: **Mu^{27}-P^{3}-Si^{2}-Si^{1}**	**Step_3** (29°)	26	–	-214.1	36.7
	Step_11 (109°)	81	100	-226.6	24.2
	Step_20 (200°)	70	–	-209.6	41.2
	Step_35 (11°)	4	–[a]	-213.2	37.6

[a] Too close to the diamagnetic peak to be detected; [b] The superscript digit denotes the atom number in the calculation.

4 Si=P-NMe$_2$

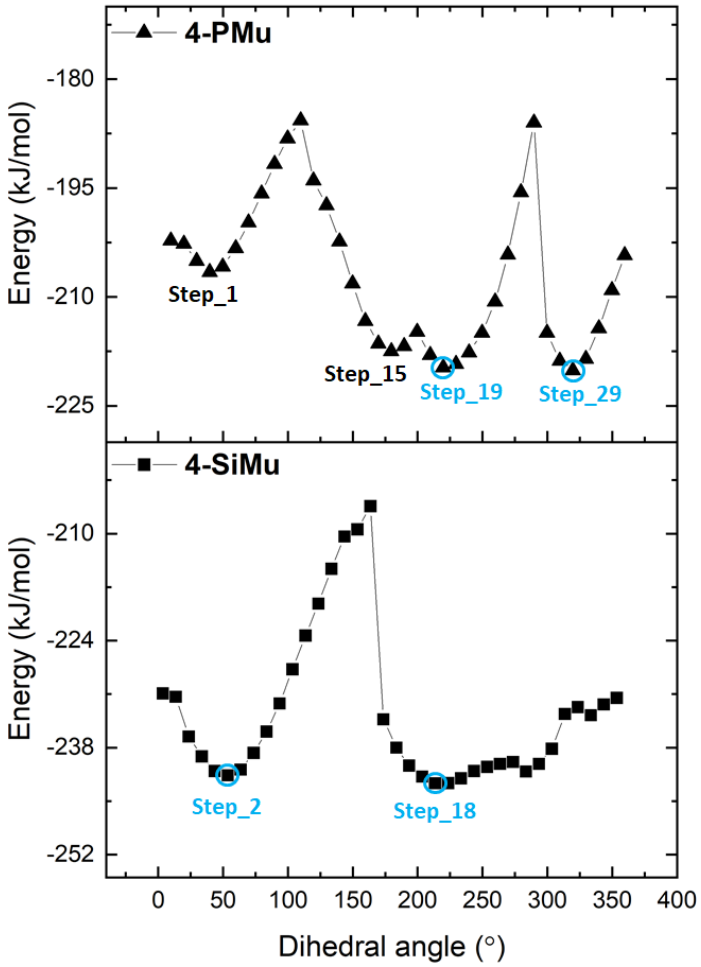


Figure S25: Potential energy surface scans for rotation about the Si-P bonds of radicals **4-PMu** and **4-SiMu**. The blue labels denote radical conformations detected by muon spin spectroscopy.

The PES scan over the dihedral angle Mu^3-Si^2-P^{42}-N^{43} of **4-SiMu** (Mu addition to the Si atom in **4**) has two minima at 53° (**Step 2**) and 213° (i.e. -147° at **Step 18**), with calculated hfcs of 90 MHz and 43 MHz, respectively. They are approximately equiergic (±1 kJ/mol), but the barrier between them is sufficiently high (ca. 11 kJ/mol) that interconversion is unlikely. Thus both rotamers should be stable.

The PES scan over the dihedral angle Mu^{51}-P^{41}-Si^2-Si^1 of **4-PMu** (Mu addition to the P atom in **4**) shows four minima at 40° (**Step 1**), 180° (**Step 15**), 220° (i.e. -140° at **Step 19**), and 320° (i.e. -40° at **Step 29**), with calculated hfcs of 115 MHz, 5 MHz, 57 MHz, and 19 MHz, respectively. The lowest energy rotamers, at **Step 19** and 320° **Step 29**, are essentially equiergic (±0.3 kJ/mol) but separated by a large barrier (ca. 34 kJ/mol) so interconversion is unlikely. There is also a local minimum at **Step 1**, which is well-separated from **Step 19** but not from **Step 29** (a barrier of only ca. 5 kJ/mol).

Four radicals were detected experimentally. The three smallest hfcs have good matches with predictions for **4-PMu Step 29**, **4-SiMu Step 18** and **4-PMu Step 19**. The largest measured hfc (110 MHz) is temptingly close to the prediction for **Step 1** of **4-PMu**. However, the stability of that rotamer is questionable, in contrast to **Step 2** of **4-SiMu**. The difference in hfcs (90 MHz predicted, 110 observed) might be due to the neglect of vibrational averaging in the calculations.

On balance we assign the four detected radicals to two rotamers of **4-SiMu** (dihedral angles Mu^3-Si^2-P^{42}-N^{43} 53° and 213°) and two rotamers of **4-PMu** (dihedral angles Mu^{51}-P^{41}-Si^2-Si^1 220° and 320°).

Summary of findings for **4**:

Rotamer dihedral angle (°)		A_μ /MHz		Energy/kJ mol^{-1}	
		calc.	**exp.**	**Reaction**	**Relative**
4-SiMu:	**Step_2** (53°)	90	110[a]	-241.6	1.0
Mu^3-Si^2-P^{42}-N^{43} [b]	**Step_18** (-147°/213°)	43	46	-242.7	0.0
	Step_1 (40°)	115	110[a]	-206.6	36.1
4-PMu:	**Step_15** (180°)	5	–[c]	-217.5	25.2
Mu^{51}-P^{41}-Si^2-Si^1	**Step_19** (-140°/220°)	57	60	-219.7	22.9
	Step_29 (-40°/320°)	19	20	-220.1	22.6

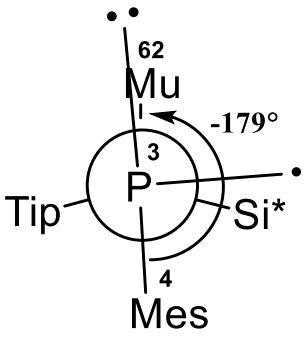
[a] Alternative assignments; [b] The superscript digit denotes the atom number in the calculation;
[c] Too close to the diamagnetic peak to be detected.

3. XYZ Coordinates of radical geometry at local minima on each PES

Mu-Si-P-Mes – Dihedral angle 62(Mu)-2(Si)-3(P)-4(C)

Rotamer: Step-11

Atom #	Symbol	x	y	z
1	Si	0.907	0.391	-0.727
2	Si	-1.135	-0.309	0.546
3	P	-0.982	-2.442	1.478
4	C/Mes	-1.245	-3.833	0.293
5	C	-2.481	-4.103	-0.350
6	C	-2.590	-5.214	-1.195
7	C	-1.530	-6.100	-1.402
8	C	-0.351	-5.878	-0.685
9	C	-0.193	-4.783	0.172
10	C	1.081	-4.677	0.981
11	H	1.639	-3.757	0.781
12	H	1.744	-5.521	0.765
13	H	0.864	-4.688	2.057
14	H	0.472	-6.584	-0.785
15	C	-1.657	-7.263	-2.357
16	H	-1.017	-8.099	-2.057
17	H	-1.358	-6.974	-3.374
18	H	-2.689	-7.624	-2.414
19	H	-3.542	-5.402	-1.688
20	C	-3.729	-3.306	-0.053
21	H	-3.554	-2.229	-0.032
22	H	-4.126	-3.583	0.933
23	H	-4.513	-3.510	-0.789
24	C	-2.988	0.237	0.273
25	C	-3.578	0.544	-0.985
26	C	-4.883	1.053	-1.044
27	C	-5.655	1.279	0.094
28	C	-5.092	0.928	1.322
29	C	-3.804	0.394	1.441
30	C	-3.403	-0.039	2.86
31	C	-4.352	-1.130	3.401
32	H	-4.395	-1.990	2.726
33	H	-5.373	-0.754	3.534
34	H	-3.998	-1.483	4.377
35	C	-3.327	1.143	3.845
36	H	-3.021	0.789	4.837
37	H	-2.603	1.893	3.514
38	H	-4.299	1.639	3.956
39	H	-2.411	-0.490	2.830
40	H	-5.684	1.057	2.224
41	C	-7.056	1.863	-0.011
42	C	-7.165	3.219	0.712
43	H	-6.997	3.109	1.791



step 11

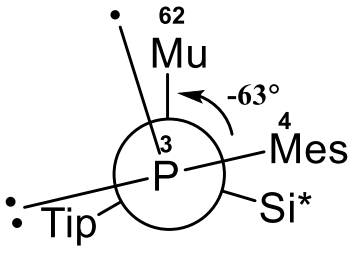
44	H	-8.162	3.651	0.572
45	H	-6.426	3.932	0.330
46	C	-8.130	0.881	0.496
47	H	-9.133	1.300	0.351
48	H	-8.006	0.672	1.565
49	H	-8.078	-0.074	-0.04
50	H	-7.252	2.042	-1.077
51	H	-5.317	1.280	-2.014
52	C	-2.886	0.280	-2.321
53	C	-3.026	1.427	-3.341
54	H	-2.744	2.392	-2.914
55	H	-2.379	1.235	-4.205
56	H	-4.050	1.514	-3.722
57	C	-3.418	-1.024	-2.955
58	H	-3.181	-1.903	-2.350
59	H	-4.508	-0.978	-3.071
60	H	-2.986	-1.175	-3.952
61	H	-1.818	0.160	-2.125
62	H/Mu	-0.838	0.377	1.826
63	N	0.616	-0.045	-2.404
64	C	0.949	0.781	-3.557
65	H	1.786	0.360	-4.139
66	H	1.219	1.791	-3.248
67	H	0.085	0.852	-4.234
68	C	0.085	-1.339	-2.813
69	H	0.829	-1.938	-3.359
70	H	-0.771	-1.210	-3.486
71	H	-0.243	-1.927	-1.950
72	C	2.331	-0.576	0.230
73	C	3.156	-1.601	-0.341
74	C	4.086	-2.283	0.456
75	C	4.292	-1.991	1.804
76	C	3.534	-0.956	2.342
77	C	2.573	-0.252	1.602
78	C	1.882	0.885	2.364
79	C	1.223	0.409	3.675
80	H	0.618	1.216	4.107
81	H	1.973	0.129	4.423
82	H	0.572	-0.456	3.514
83	C	2.855	2.044	2.663
84	H	3.275	2.461	1.744
85	H	2.332	2.849	3.193
86	H	3.685	1.711	3.298
87	H	1.090	1.299	1.739
88	H	3.700	-0.682	3.381
89	C	5.310	-2.744	2.648
90	H	5.271	-2.316	3.658
91	C	4.961	-4.240	2.767
92	H	3.956	-4.380	3.181

93	H	4.994	-4.735	1.789
94	H	5.675	-4.751	3.423
95	C	6.746	-2.554	2.122
96	H	7.466	-3.056	2.780
97	H	6.862	-2.977	1.117
98	H	7.013	-1.493	2.072
99	H	4.684	-3.066	-0.004
100	C	3.160	-2.013	-1.822
101	C	2.646	-3.451	-2.034
102	H	1.628	-3.587	-1.659
103	H	2.648	-3.702	-3.102
104	H	3.289	-4.178	-1.524
105	C	4.556	-1.884	-2.471
106	H	5.270	-2.603	-2.055
107	H	4.979	-0.884	-2.342
108	H	4.482	-2.083	-3.547
109	H	2.504	-1.333	-2.360
110	C	1.422	2.283	-0.718
111	C	2.764	2.646	-1.061
112	C	3.203	3.967	-0.900
113	C	2.384	4.986	-0.421
114	C	1.062	4.646	-0.144
115	C	0.566	3.344	-0.298
116	C	-0.929	3.191	-0.029
117	C	-1.763	4.085	-0.970
118	H	-1.476	3.943	-2.017
119	H	-1.634	5.148	-0.733
120	H	-2.829	3.850	-0.869
121	C	-1.300	3.490	1.436
122	H	-0.745	2.852	2.131
123	H	-2.369	3.320	1.597
124	H	-1.084	4.533	1.693
125	H	-1.219	2.160	-0.243
126	H	0.382	5.422	0.197
127	C	2.912	6.401	-0.233
128	C	2.172	7.416	-1.124
129	H	2.613	8.414	-1.017
130	H	2.227	7.131	-2.181
131	H	1.113	7.489	-0.850
132	C	2.871	6.831	1.246
133	H	1.841	6.865	1.621
134	H	3.434	6.135	1.877
135	H	3.304	7.831	1.368
136	H	3.965	6.395	-0.545
137	H	4.229	4.213	-1.162
138	C	3.804	1.691	-1.657
139	C	4.280	2.161	-3.049
140	H	3.442	2.334	-3.731
141	H	4.932	1.403	-3.499

142	H	4.856	3.092	-2.986
143	C	5.020	1.505	-0.726
144	H	5.757	0.835	-1.184
145	H	5.520	2.461	-0.537
146	H	4.726	1.077	0.236
147	H	3.339	0.714	-1.795

Rotamer: Step-23

Atom #	Symbol	x	y	z
1	Si	0.250	0.792	-0.815
2	Si	-0.638	-1.309	0.222
3	P	0.182	-3.407	-0.348
4	C/Mes	2.007	-3.647	-0.292
5	C	2.576	-4.368	-1.382
6	C	3.927	-4.723	-1.345
7	C	4.750	-4.410	-0.259
8	C	4.172	-3.734	0.819
9	C	2.828	-3.347	0.828
10	C	2.298	-2.648	2.056
11	H	2.099	-1.589	1.861
12	H	3.025	-2.701	2.872
13	H	1.362	-3.095	2.408
14	H	4.785	-3.504	1.688
15	C	6.213	-4.782	-0.255
16	H	6.593	-4.902	0.764
17	H	6.819	-4.004	-0.739
18	H	6.391	-5.715	-0.801
19	H	4.348	-5.266	-2.189
20	C	1.767	-4.770	-2.598
21	H	1.379	-3.901	-3.142
22	H	0.899	-5.382	-2.325
23	H	2.383	-5.349	-3.293
24	C	-2.514	-1.806	0.229
25	C	-3.203	-2.045	-0.991
26	C	-4.547	-2.444	-0.979
27	C	-5.256	-2.638	0.202
28	C	-4.570	-2.430	1.402
29	C	-3.231	-2.023	1.450
30	C	-2.588	-1.902	2.838
31	C	-1.913	-3.231	3.234
32	H	-1.177	-3.550	2.488
33	H	-2.660	-4.029	3.325
34	H	-1.401	-3.134	4.200
35	C	-3.545	-1.454	3.959
36	H	-2.965	-1.232	4.862
37	H	-4.101	-0.551	3.685
38	H	-4.269	-2.231	4.228
39	H	-1.808	-1.140	2.783



step 23

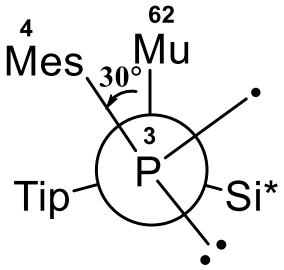
40	H	-5.099	-2.593	2.336
41	C	-6.717	-3.065	0.179
42	C	-7.636	-1.994	0.797
43	H	-7.410	-1.841	1.859
44	H	-8.687	-2.296	0.720
45	H	-7.519	-1.031	0.288
46	C	-6.929	-4.431	0.860
47	H	-7.977	-4.743	0.778
48	H	-6.676	-4.390	1.926
49	H	-6.306	-5.205	0.397
50	H	-7.003	-3.175	-0.875
51	H	-5.054	-2.619	-1.926
52	C	-2.534	-1.936	-2.361
53	C	-3.233	-0.937	-3.301
54	H	-3.259	0.068	-2.873
55	H	-2.700	-0.884	-4.258
56	H	-4.264	-1.238	-3.518
57	C	-2.430	-3.315	-3.045
58	H	-1.917	-4.039	-2.406
59	H	-3.425	-3.711	-3.282
60	H	-1.873	-3.232	-3.987
61	H	-1.517	-1.563	-2.209
62	H/Mu	-0.238	-1.137	1.634
63	N	0.294	0.467	-2.545
64	C	-0.128	1.395	-3.589
65	H	0.722	1.717	-4.212
66	H	-0.598	2.280	-3.163
67	H	-0.857	0.911	-4.255
68	C	0.771	-0.777	-3.135
69	H	1.645	-0.610	-3.784
70	H	-0.007	-1.240	-3.760
71	H	1.067	-1.495	-2.368
72	C	1.936	0.932	0.192
73	C	3.244	0.737	-0.352
74	C	4.372	0.791	0.479
75	C	4.295	1.073	1.841
76	C	3.026	1.307	2.364
77	C	1.859	1.235	1.589
78	C	0.560	1.557	2.341
79	C	0.393	0.746	3.643
80	H	-0.612	0.903	4.054
81	H	1.106	1.064	4.412
82	H	0.530	-0.327	3.481
83	C	0.452	3.061	2.666
84	H	0.497	3.674	1.764
85	H	-0.496	3.272	3.176
86	H	1.266	3.371	3.332
87	H	-0.289	1.305	1.699
88	H	2.943	1.555	3.419

89	C	5.534	1.146	2.722
90	H	5.191	1.359	3.744
91	C	6.294	-0.193	2.761
92	H	5.644	-1.008	3.097
93	H	6.681	-0.460	1.770
94	H	7.148	-0.132	3.447
95	C	6.469	2.297	2.300
96	H	7.324	2.370	2.983
97	H	6.862	2.138	1.289
98	H	5.942	3.257	2.308
99	H	5.349	0.620	0.035
100	C	3.542	0.490	-1.836
101	C	4.084	-0.930	-2.082
102	H	3.410	-1.699	-1.698
103	H	4.228	-1.106	-3.156
104	H	5.055	-1.069	-1.591
105	C	4.526	1.520	-2.432
106	H	5.526	1.431	-1.994
107	H	4.186	2.548	-2.282
108	H	4.627	1.352	-3.512
109	H	2.609	0.599	-2.386
110	C	-0.602	2.553	-0.666
111	C	0.173	3.720	-0.960
112	C	-0.369	4.997	-0.757
113	C	-1.662	5.208	-0.285
114	C	-2.431	4.072	-0.045
115	C	-1.943	2.772	-0.235
116	C	-2.952	1.657	0.021
117	C	-4.196	1.797	-0.881
118	H	-3.918	1.933	-1.932
119	H	-4.809	2.658	-0.589
120	H	-4.821	0.901	-0.805
121	C	-3.388	1.589	1.497
122	H	-2.536	1.428	2.166
123	H	-4.094	0.766	1.645
124	H	-3.882	2.518	1.806
125	H	-2.485	0.703	-0.229
126	H	-3.455	4.195	0.297
127	C	-2.202	6.614	-0.067
128	C	-3.406	6.915	-0.980
129	H	-3.737	7.952	-0.850
130	H	-3.149	6.769	-2.036
131	H	-4.255	6.262	-0.748
132	C	-2.553	6.868	1.411
133	H	-3.361	6.207	1.747
134	H	-1.687	6.694	2.059
135	H	-2.885	7.903	1.555
136	H	-1.399	7.313	-0.340
137	H	0.244	5.866	-0.982

138	C	1.596	3.711	-1.531
139	C	1.683	4.461	-2.879
140	H	0.945	4.097	-3.599
141	H	2.679	4.327	-3.318
142	H	1.525	5.538	-2.754
143	C	2.616	4.305	-0.539
144	H	3.623	4.299	-0.972
145	H	2.369	5.345	-0.298
146	H	2.646	3.735	0.394
147	H	1.887	2.678	-1.726

Rotamer: Step-37

Atom #	Symbol	x	y	z
1	Si	1.251	-0.315	0.954
2	Si	-1.102	0.192	0.331
3	P	-1.898	1.961	1.635
4	C/Mes	-2.854	2.991	0.426
5	C	-4.269	2.906	0.392
6	C	-4.988	3.758	-0.452
7	C	-4.359	4.707	-1.263
8	C	-2.965	4.791	-1.203
9	C	-2.203	3.962	-0.373
10	C	-0.705	4.150	-0.328
11	H	-0.372	4.464	0.669
12	H	-0.388	4.918	-1.040
13	H	-0.162	3.229	-0.566
14	H	-2.451	5.528	-1.817
15	C	-5.162	5.634	-2.145
16	H	-4.563	6.010	-2.981
17	H	-5.521	6.506	-1.583
18	H	-6.045	5.131	-2.556
19	H	-6.073	3.674	-0.476
20	C	-5.027	1.910	1.242
21	H	-4.803	2.038	2.308
22	H	-4.773	0.875	0.983
23	H	-6.107	2.031	1.112
24	C	-2.563	-1.071	0.208
25	C	-3.054	-1.712	1.378
26	C	-4.197	-2.521	1.314
27	C	-4.894	-2.729	0.127
28	C	-4.399	-2.112	-1.025
29	C	-3.256	-1.304	-1.024
30	C	-2.837	-0.691	-2.368
31	C	-3.535	0.663	-2.607
32	H	-3.306	1.387	-1.821
33	H	-4.624	0.533	-2.637
34	H	-3.221	1.091	-3.567
35	C	-3.078	-1.607	-3.584



step 37

36	H	-2.582	-1.179	-4.463
37	H	-2.679	-2.614	-3.428
38	H	-4.141	-1.699	-3.832
39	H	-1.761	-0.505	-2.332
40	H	-4.921	-2.271	-1.963
41	C	-6.139	-3.605	0.093
42	C	-5.937	-4.855	-0.786
43	H	-5.768	-4.581	-1.834
44	H	-6.824	-5.498	-0.748
45	H	-5.075	-5.441	-0.449
46	C	-7.386	-2.816	-0.350
47	H	-8.278	-3.452	-0.309
48	H	-7.283	-2.452	-1.379
49	H	-7.556	-1.948	0.297
50	H	-6.317	-3.952	1.120
51	H	-4.556	-3.000	2.221
52	C	-2.392	-1.560	2.746
53	C	-1.923	-2.908	3.325
54	H	-1.245	-3.425	2.641
55	H	-1.395	-2.749	4.273
56	H	-2.769	-3.574	3.529
57	C	-3.305	-0.842	3.759
58	H	-3.616	0.140	3.394
59	H	-4.207	-1.431	3.964
60	H	-2.779	-0.698	4.711
61	H	-1.495	-0.947	2.615
62	H/Mu	-0.971	0.821	-1.000
63	N	1.267	-0.611	2.694
64	C	1.993	-1.697	3.346
65	H	2.765	-1.310	4.030
66	H	2.473	-2.349	2.617
67	H	1.303	-2.310	3.947
68	C	0.552	0.169	3.697
69	H	1.245	0.624	4.423
70	H	-0.135	-0.469	4.273
71	H	-0.028	0.977	3.249
72	C	2.056	1.321	0.209
73	C	2.595	2.398	0.980
74	C	3.115	3.535	0.349
75	C	3.170	3.670	-1.038
76	C	2.665	2.613	-1.791
77	C	2.106	1.463	-1.215
78	C	1.619	0.409	-2.222
79	C	0.656	0.991	-3.280
80	H	0.217	0.178	-3.871
81	H	1.179	1.652	-3.980
82	H	-0.160	1.562	-2.827
83	C	2.794	-0.282	-2.944
84	H	3.473	-0.768	-2.241

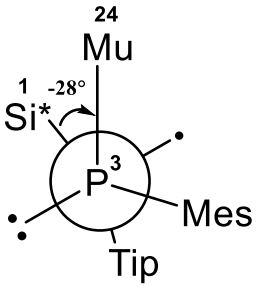
85	H	2.417	-1.044	-3.637
86	H	3.370	0.445	-3.530
87	H	1.072	-0.371	-1.685
88	H	2.710	2.688	-2.874
89	C	3.770	4.899	-1.706
90	H	3.664	4.760	-2.791
91	C	3.016	6.189	-1.330
92	H	1.952	6.114	-1.581
93	H	3.094	6.397	-0.256
94	H	3.433	7.049	-1.867
95	C	5.275	5.033	-1.402
96	H	5.702	5.889	-1.939
97	H	5.45	5.188	-0.331
98	H	5.822	4.133	-1.705
99	H	3.504	4.338	0.969
100	C	2.669	2.408	2.510
101	C	1.700	3.443	3.117
102	H	0.668	3.273	2.790
103	H	1.720	3.394	4.213
104	H	1.979	4.462	2.824
105	C	4.096	2.655	3.044
106	H	4.459	3.661	2.805
107	H	4.813	1.936	2.635
108	H	4.106	2.556	4.137
109	H	2.378	1.422	2.864
110	C	2.311	-1.790	0.232
111	C	3.740	-1.712	0.287
112	C	4.520	-2.699	-0.331
113	C	3.973	-3.794	-0.996
114	C	2.584	-3.902	-0.988
115	C	1.756	-2.947	-0.382
116	C	0.265	-3.274	-0.381
117	C	-0.019	-4.558	0.426
118	H	0.399	-4.496	1.436
119	H	0.416	-5.439	-0.059
120	H	-1.099	-4.724	0.511
121	C	-0.312	-3.406	-1.802
122	H	-0.153	-2.494	-2.387
123	H	-1.389	-3.597	-1.754
124	H	0.151	-4.236	-2.347
125	H	-0.270	-2.461	0.115
126	H	2.121	-4.766	-1.458
127	C	4.860	-4.830	-1.671
128	C	4.700	-6.225	-1.038
129	H	5.393	-6.939	-1.501
130	H	4.906	-6.199	0.038
131	H	3.683	-6.611	-1.176
132	C	4.619	-4.883	-3.192
133	H	3.596	-5.204	-3.421

134	H	4.773	-3.900	-3.651
135	H	5.307	-5.592	-3.666
136	H	5.901	-4.514	-1.513
137	H	5.603	-2.613	-0.285
138	C	4.530	-0.632	1.037
139	C	5.414	-1.241	2.148
140	H	4.836	-1.872	2.830
141	H	5.878	-0.442	2.738
142	H	6.223	-1.852	1.731
143	C	5.396	0.226	0.095
144	H	5.923	1.002	0.663
145	H	6.155	-0.384	-0.410
146	H	4.791	0.720	-0.669
147	H	3.823	0.037	1.529

Si-P(Mu)-Mes: Dihedral angle 24(Mu)-3(P)-2(Si)-1(Si)

Rotamer: Step-3

Atom #	Symbol	*x*	*y*	*z*
1	Si	-0.042	-0.092	-0.099
2	Si	0.074	-0.549	2.3
3	P	1.866	0.292	3.481
4	C	2.561	-1.135	4.463
5	C	2.155	-1.259	5.816
6	C	2.709	-2.263	6.618
7	C	3.671	-3.154	6.136
8	C	4.067	-3.016	4.804
9	C	3.536	-2.032	3.961
10	C	4.044	-1.978	2.539
11	H	3.222	-2.023	1.817
12	H	4.716	-2.816	2.337
13	H	4.598	-1.053	2.335
14	H	4.813	-3.699	4.402
15	C	4.282	-4.205	7.031
16	H	4.674	-5.047	6.45
17	H	5.117	-3.794	7.613
18	H	3.551	-4.596	7.748
19	H	2.38	-2.345	7.652
20	C	1.135	-0.332	6.44
21	H	0.15	-0.434	5.972
22	H	1.433	0.718	6.335
23	H	1.02	-0.546	7.507
24	H/Mu	2.773	0.295	2.394
25	C	-1.372	-0.927	3.512
26	C	-1.697	-2.285	3.786
27	C	-2.745	-2.586	4.667
28	C	-3.494	-1.597	5.305
29	C	-3.155	-0.266	5.047
30	C	-2.117	0.09	4.178



step 3

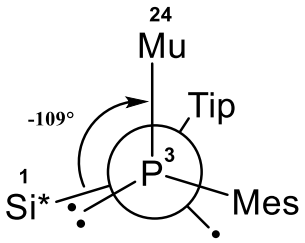
31	C	-1.825	1.581	4.006
32	C	-1.55	2.284	5.351
33	H	-0.757	1.783	5.914
34	H	-2.445	2.313	5.983
35	H	-1.239	3.32	5.177
36	C	-2.942	2.322	3.247
37	H	-2.724	3.395	3.199
38	H	-3.047	1.957	2.22
39	H	-3.909	2.204	3.751
40	H	-0.912	1.667	3.409
41	H	-3.716	0.525	5.539
42	C	-4.624	-1.964	6.257
43	C	-5.981	-1.415	5.781
44	H	-5.987	-0.319	5.769
45	H	-6.785	-1.745	6.449
46	H	-6.216	-1.763	4.768
47	C	-4.322	-1.513	7.699
48	H	-5.12	-1.837	8.379
49	H	-4.25	-0.421	7.767
50	H	-3.377	-1.935	8.058
51	H	-4.695	-3.06	6.264
52	H	-2.981	-3.628	4.871
53	C	-0.923	-3.462	3.192
54	C	-1.814	-4.415	2.375
55	H	-2.326	-3.886	1.565
56	H	-1.207	-5.212	1.929
57	H	-2.577	-4.892	3.001
58	C	-0.148	-4.235	4.276
59	H	0.532	-3.576	4.827
60	H	-0.83	-4.699	4.999
61	H	0.447	-5.035	3.82
62	H	-0.178	-3.045	2.501
63	N	0.128	-1.718	-0.768
64	C	-0.328	-2.077	-2.108
65	H	0.501	-2.119	-2.836
66	H	-1.067	-1.363	-2.473
67	H	-0.795	-3.073	-2.093
68	C	0.95	-2.785	-0.213
69	H	1.834	-2.997	-0.836
70	H	0.37	-3.718	-0.141
71	H	1.298	-2.527	0.789
72	C	1.429	1.193	-0.339
73	C	2.635	0.899	-1.055
74	C	3.666	1.845	-1.133
75	C	3.57	3.115	-0.57
76	C	2.384	3.417	0.093
77	C	1.33	2.502	0.234
78	C	0.113	3.043	1.002
79	C	0.509	3.662	2.359

80	H	-0.389	3.959	2.912
81	H	1.113	4.566	2.226
82	H	1.081	2.967	2.981
83	C	-0.673	4.097	0.194
84	H	-1.069	3.688	-0.737
85	H	-1.52	4.465	0.787
86	H	-0.038	4.958	-0.049
87	H	-0.575	2.215	1.204
88	H	2.277	4.411	0.518
89	C	4.697	4.133	-0.67
90	H	4.345	5.052	-0.181
91	C	5.955	3.664	0.084
92	H	5.731	3.453	1.136
93	H	6.367	2.75	-0.36
94	H	6.736	4.434	0.049
95	C	5.03	4.488	-2.132
96	H	5.8	5.267	-2.172
97	H	5.411	3.616	-2.677
98	H	4.144	4.855	-2.662
99	H	4.572	1.579	-1.671
100	C	2.906	-0.402	-1.823
101	C	4.106	-1.179	-1.248
102	H	3.971	-1.397	-0.185
103	H	4.234	-2.132	-1.777
104	H	5.04	-0.615	-1.355
105	C	3.127	-0.153	-3.331
106	H	4.038	0.426	-3.518
107	H	2.291	0.389	-3.782
108	H	3.231	-1.11	-3.857
109	H	2.029	-1.037	-1.731
110	C	-1.647	0.61	-0.947
111	C	-1.571	1.468	-2.086
112	C	-2.704	2.187	-2.499
113	C	-3.944	2.057	-1.879
114	C	-4.053	1.087	-0.879
115	C	-2.956	0.342	-0.432
116	C	-3.26	-0.875	0.448
117	C	-3.599	-2.075	-0.466
118	H	-2.779	-2.316	-1.146
119	H	-4.487	-1.854	-1.07
120	H	-3.818	-2.965	0.136
121	C	-4.405	-0.696	1.459
122	H	-4.292	0.205	2.064
123	H	-4.426	-1.553	2.139
124	H	-5.381	-0.653	0.962
125	H	-2.361	-1.136	1.014
126	H	-5.03	0.884	-0.453
127	C	-5.138	2.887	-2.33
128	C	-6.258	2.013	-2.926

129	H	-7.075	2.639	-3.301
130	H	-5.885	1.404	-3.757
131	H	-6.677	1.334	-2.174
132	C	-5.677	3.773	-1.191
133	H	-6.063	3.166	-0.363
134	H	-4.892	4.425	-0.791
135	H	-6.496	4.407	-1.551
136	H	-4.783	3.555	-3.127
137	H	-2.618	2.855	-3.353
138	C	-0.362	1.533	-3.029
139	C	-0.737	0.922	-4.399
140	H	-1.165	-0.08	-4.298
141	H	0.153	0.848	-5.035
142	H	-1.469	1.544	-4.925
143	C	0.225	2.941	-3.241
144	H	1.046	2.896	-3.966
145	H	-0.526	3.633	-3.639
146	H	0.62	3.359	-2.313
147	H	0.431	0.912	-2.61

Rotamer: Step-11

Atom #	Symbol	*x*	*y*	*z*
1	Si	1.297	-0.267	0.966
2	Si	-1.066	0.112	0.333
3	P	-1.689	2.077	1.416
4	C	-2.979	2.942	0.393
5	C	-2.518	3.860	-0.584
6	C	-3.440	4.618	-1.313
7	C	-4.816	4.519	-1.097
8	C	-5.255	3.628	-0.116
9	C	-4.373	2.833	0.628
10	C	-4.970	1.891	1.651
11	H	-4.661	0.855	1.478
12	H	-6.063	1.925	1.607
13	H	-4.676	2.152	2.676
14	H	-6.323	3.539	0.077
15	C	-5.796	5.332	-1.910
16	H	-6.099	4.796	-2.820
17	H	-6.708	5.546	-1.343
18	H	-5.359	6.285	-2.228
19	H	-3.068	5.315	-2.062
20	C	-1.044	4.063	-0.850
21	H	-0.545	3.143	-1.175
22	H	-0.516	4.400	0.050
23	H	-0.891	4.815	-1.631
24	H/Mu	-2.553	1.462	2.354
25	C	-2.514	-1.171	0.251



Step-11

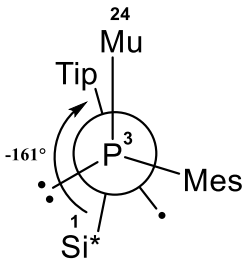
26	C	-2.898	-1.966	1.366
27	C	-3.942	-2.892	1.238
28	C	-4.647	-3.064	0.047
29	C	-4.290	-2.255	-1.035
30	C	-3.253	-1.317	-0.962
31	C	-3.016	-0.442	-2.195
32	C	-4.168	0.564	-2.389
33	H	-4.316	1.184	-1.501
34	H	-5.110	0.043	-2.601
35	H	-3.955	1.228	-3.236
36	C	-2.798	-1.240	-3.494
37	H	-2.556	-0.556	-4.315
38	H	-1.982	-1.961	-3.400
39	H	-3.700	-1.790	-3.786
40	H	-2.102	0.141	-2.012
41	H	-4.842	-2.350	-1.966
42	C	-5.771	-4.086	-0.054
43	C	-5.467	-5.172	-1.104
44	H	-5.397	-4.743	-2.111
45	H	-6.261	-5.928	-1.117
46	H	-4.519	-5.677	-0.888
47	C	-7.131	-3.417	-0.330
48	H	-7.933	-4.165	-0.337
49	H	-7.137	-2.913	-1.304
50	H	-7.368	-2.670	0.436
51	H	-5.842	-4.584	0.923
52	H	-4.223	-3.494	2.100
53	C	-2.254	-1.812	2.742
54	C	-1.708	-3.130	3.320
55	H	-0.981	-3.595	2.651
56	H	-1.215	-2.944	4.282
57	H	-2.511	-3.854	3.502
58	C	-3.232	-1.171	3.749
59	H	-3.626	-0.218	3.384
60	H	-4.085	-1.834	3.938
61	H	-2.731	-0.989	4.708
62	H	-1.400	-1.135	2.625
63	N	1.341	-0.525	2.711
64	C	2.030	-1.634	3.365
65	H	2.774	-1.265	4.089
66	H	2.541	-2.266	2.640
67	H	1.317	-2.262	3.921
68	C	0.588	0.244	3.695
69	H	1.253	0.664	4.465
70	H	-0.147	-0.387	4.217
71	H	0.056	1.078	3.233
72	C	2.024	1.399	0.221
73	C	2.541	2.496	0.979
74	C	2.998	3.652	0.331

75	C	3.009	3.788	-1.056
76	C	2.532	2.709	-1.795
77	C	2.037	1.538	-1.203
78	C	1.583	0.456	-2.196
79	C	0.519	0.967	-3.187
80	H	0.160	0.140	-3.811
81	H	0.921	1.733	-3.859
82	H	-0.343	1.396	-2.667
83	C	2.773	-0.139	-2.977
84	H	3.518	-0.572	-2.306
85	H	2.423	-0.929	-3.652
86	H	3.265	0.627	-3.588
87	H	1.125	-0.366	-1.642
88	H	2.547	2.782	-2.880
89	C	3.539	5.040	-1.742
90	H	3.423	4.888	-2.824
91	C	2.730	6.295	-1.363
92	H	1.669	6.169	-1.602
93	H	2.809	6.512	-0.291
94	H	3.102	7.170	-1.908
95	C	5.040	5.249	-1.465
96	H	5.416	6.121	-2.013
97	H	5.227	5.419	-0.398
98	H	5.625	4.374	-1.771
99	H	3.375	4.470	0.939
100	C	2.669	2.516	2.507
101	C	1.720	3.551	3.144
102	H	0.683	3.392	2.832
103	H	1.765	3.490	4.239
104	H	2.003	4.572	2.859
105	C	4.113	2.778	2.984
106	H	4.459	3.783	2.717
107	H	4.820	2.059	2.559
108	H	4.164	2.695	4.077
109	H	2.397	1.531	2.878
110	C	2.397	-1.706	0.240
111	C	3.821	-1.573	0.267
112	C	4.627	-2.516	-0.386
113	C	4.109	-3.618	-1.061
114	C	2.726	-3.788	-1.016
115	C	1.875	-2.881	-0.370
116	C	0.402	-3.274	-0.327
117	C	0.203	-4.607	0.423
118	H	0.662	-4.580	1.417
119	H	0.649	-5.445	-0.125
120	H	-0.866	-4.820	0.543
121	C	-0.222	-3.359	-1.730
122	H	-0.094	-2.42	-2.278
123	H	-1.294	-3.569	-1.660

124	H	0.241	-4.156	-2.324
125	H	-0.144	-2.509	0.233
126	H	2.289	-4.663	-1.489
127	C	5.022	-4.599	-1.782
128	C	4.940	-6.014	-1.179
129	H	5.651	-6.685	-1.675
130	H	5.173	-6.003	-0.108
131	H	3.938	-6.442	-1.300
132	C	4.741	-4.629	-3.297
133	H	3.729	-4.995	-3.506
134	H	4.833	-3.629	-3.736
135	H	5.449	-5.293	-3.806
136	H	6.051	-4.242	-1.645
137	H	5.707	-2.388	-0.360
138	C	4.580	-0.485	1.036
139	C	5.477	-1.094	2.136
140	H	4.910	-1.744	2.809
141	H	5.928	-0.295	2.737
142	H	6.294	-1.685	1.708
143	C	5.424	0.412	0.109
144	H	5.938	1.186	0.692
145	H	6.193	-0.170	-0.412
146	H	4.804	0.911	-0.641
147	H	3.854	0.152	1.542

Rotamer: Step-17

Atom #	Symbol	*x*	*y*	*z*
1	Si	-0.141	-0.281	-0.071
2	Si	-0.216	-0.906	2.309
3	P	1.728	-1.909	3.111
4	C	2.841	-0.736	4.029
5	C	4.089	-0.421	3.436
6	C	5.005	0.371	4.137
7	C	4.737	0.864	5.415
8	C	3.514	0.523	5.999
9	C	2.566	-0.267	5.339
10	C	1.294	-0.611	6.077
11	H	0.407	-0.434	5.465
12	H	1.205	-0.015	6.99
13	H	1.269	-1.669	6.371
14	H	3.289	0.878	7.003
15	C	5.728	1.746	6.137
16	H	5.545	2.807	5.92
17	H	5.659	1.622	7.223
18	H	6.756	1.527	5.832
19	H	5.962	0.598	3.671
20	C	4.475	-0.918	2.062



step 17

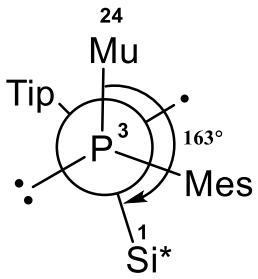
21	H	3.882	-0.43	1.282
22	H	4.318	-1.999	1.956
23	H	5.528	-0.703	1.855
24	H/Mu	1.061	-2.467	4.229
25	C	-1.692	-1.747	3.228
26	C	-2.027	-3.118	3.063
27	C	-3.11	-3.661	3.768
28	C	-3.886	-2.906	4.646
29	C	-3.533	-1.565	4.827
30	C	-2.457	-0.975	4.154
31	C	-2.143	0.491	4.471
32	C	-2.189	0.809	5.979
33	H	-1.623	0.082	6.568
34	H	-3.216	0.824	6.361
35	H	-1.763	1.803	6.162
36	C	-3.05	1.475	3.707
37	H	-2.801	2.509	3.976
38	H	-2.94	1.374	2.623
39	H	-4.105	1.311	3.959
40	H	-1.115	0.677	4.132
41	H	-4.111	-0.961	5.52
42	C	-5.054	-3.533	5.395
43	C	-6.389	-2.836	5.071
44	H	-6.384	-1.791	5.404
45	H	-7.219	-3.342	5.576
46	H	-6.589	-2.843	3.994
47	C	-4.805	-3.565	6.915
48	H	-5.63	-4.071	7.43
49	H	-4.725	-2.552	7.326
50	H	-3.877	-4.097	7.154
51	H	-5.134	-4.574	5.053
52	H	-3.352	-4.714	3.635
53	C	-1.224	-4.064	2.173
54	C	-2.077	-4.728	1.076
55	H	-2.551	-3.981	0.433
56	H	-1.451	-5.37	0.446
57	H	-2.866	-5.356	1.504
58	C	-0.493	-5.14	3.002
59	H	0.149	-4.692	3.767
60	H	-1.206	-5.802	3.508
61	H	0.136	-5.76	2.352
62	H	-0.458	-3.467	1.665
63	N	-0.032	-1.759	-1.022
64	C	-0.543	-1.89	-2.381
65	H	0.266	-1.879	-3.132
66	H	-1.235	-1.08	-2.616
67	H	-1.078	-2.844	-2.497
68	C	0.791	-2.909	-0.665
69	H	1.617	-3.055	-1.378

70	H	0.191	-3.832	-0.674
71	H	1.228	-2.793	0.329
72	C	1.422	0.913	-0.063
73	C	2.591	0.709	-0.869
74	C	3.685	1.577	-0.764
75	C	3.697	2.682	0.086
76	C	2.551	2.902	0.841
77	C	1.428	2.062	0.792
78	C	0.258	2.51	1.681
79	C	0.68	2.632	3.16
80	H	-0.191	2.858	3.785
81	H	1.402	3.443	3.304
82	H	1.139	1.709	3.527
83	C	-0.364	3.842	1.213
84	H	-0.769	3.765	0.202
85	H	-1.184	4.127	1.884
86	H	0.373	4.653	1.227
87	H	-0.535	1.759	1.63
88	H	2.526	3.771	1.494
89	C	4.893	3.619	0.179
90	H	4.626	4.412	0.891
91	C	6.139	2.903	0.732
92	H	5.934	2.455	1.711
93	H	6.47	2.103	0.059
94	H	6.971	3.608	0.846
95	C	5.2	4.298	-1.17
96	H	6.026	5.011	-1.062
97	H	5.492	3.563	-1.929
98	H	4.327	4.842	-1.548
99	H	4.557	1.385	-1.383
100	C	2.75	-0.395	-1.926
101	C	3.865	-1.398	-1.567
102	H	3.679	-1.887	-0.607
103	H	3.935	-2.179	-2.335
104	H	4.843	-0.906	-1.509
105	C	3.014	0.181	-3.335
106	H	3.989	0.677	-3.398
107	H	2.252	0.909	-3.628
108	H	3.01	-0.628	-4.075
109	H	1.816	-0.948	-1.98
110	C	-1.68	0.693	-0.764
111	C	-1.517	1.798	-1.654
112	C	-2.576	2.694	-1.864
113	C	-3.832	2.52	-1.288
114	C	-4.041	1.338	-0.573
115	C	-3.017	0.413	-0.335
116	C	-3.442	-0.958	0.198
117	C	-3.905	-1.832	-0.992
118	H	-3.122	-1.957	-1.742

119	H	-4.773	-1.375	-1.482
120	H	-4.205	-2.827	-0.642
121	C	-4.569	-0.942	1.246
122	H	-4.374	-0.242	2.059
123	H	-4.674	-1.94	1.683
124	H	-5.534	-0.683	0.795
125	H	-2.574	-1.448	0.65
126	H	-5.04	1.115	-0.212
127	C	-4.944	3.536	-1.506
128	C	-6.098	2.954	-2.344
129	H	-6.859	3.72	-2.537
130	H	-5.738	2.58	-3.309
131	H	-6.588	2.122	-1.824
132	C	-5.464	4.11	-0.175
133	H	-5.928	3.33	0.441
134	H	-4.652	4.559	0.408
135	H	-6.22	4.883	-0.358
136	H	-4.511	4.369	-2.078
137	H	-2.423	3.543	-2.525
138	C	-0.304	1.975	-2.575
139	C	-0.725	1.678	-4.034
140	H	-1.203	0.697	-4.125
141	H	0.151	1.692	-4.693
142	H	-1.433	2.429	-4.404
143	C	0.378	3.352	-2.501
144	H	1.214	3.395	-3.21
145	H	-0.313	4.162	-2.764
146	H	0.775	3.551	-1.503
147	H	0.443	1.229	-2.305

Rotamer: Step-22

Atom #	Symbol	*x*	*y*	*z*
1	Si	-0.189	0.915	0.879
2	Si	0.634	-1.243	-0.068
3	P	-0.307	-3.255	0.640
4	C	-2.116	-3.554	0.315
5	C	-2.898	-3.996	1.413
6	C	-4.244	-4.328	1.211
7	C	-4.850	-4.247	-0.043
8	C	-4.060	-3.840	-1.121
9	C	-2.712	-3.498	-0.969
10	C	-1.934	-3.105	-2.200
11	H	-1.439	-2.139	-2.066
12	H	-2.592	-3.036	-3.072
13	H	-1.147	-3.834	-2.432
14	H	-4.502	-3.792	-2.115



step 22

15	C	-6.312	-4.576	-0.230
16	H	-6.928	-3.667	-0.206
17	H	-6.494	-5.062	-1.195
18	H	-6.679	-5.239	0.561
19	H	-4.832	-4.666	2.062
20	C	-2.335	-4.168	2.811
21	H	-1.931	-3.235	3.219
22	H	-1.518	-4.898	2.831
23	H	-3.116	-4.516	3.494
24	H/Mu	0.221	-3.942	-0.485
25	C	2.471	-1.886	-0.039
26	C	3.255	-1.980	1.145
27	C	4.588	-2.406	1.068
28	C	5.191	-2.771	-0.136
29	C	4.399	-2.732	-1.287
30	C	3.064	-2.313	-1.265
31	C	2.284	-2.417	-2.579
32	C	2.061	-3.893	-2.969
33	H	1.576	-4.457	-2.165
34	H	3.013	-4.388	-3.193
35	H	1.429	-3.963	-3.863
36	C	2.937	-1.662	-3.752
37	H	2.302	-1.732	-4.643
38	H	3.083	-0.604	-3.521
39	H	3.913	-2.088	-4.012
40	H	1.295	-1.968	-2.414
41	H	4.831	-3.049	-2.233
42	C	6.646	-3.217	-0.180
43	C	7.507	-2.270	-1.038
44	H	7.185	-2.280	-2.086
45	H	8.560	-2.576	-1.009
46	H	7.442	-1.238	-0.676
47	C	6.787	-4.675	-0.658
48	H	7.837	-4.990	-0.622
49	H	6.440	-4.791	-1.691
50	H	6.205	-5.357	-0.029
51	H	7.029	-3.169	0.848
52	H	5.177	-2.471	1.981
53	C	2.679	-1.720	2.536
54	C	3.510	-0.747	3.391
55	H	3.638	0.219	2.897
56	H	3.010	-0.574	4.352
57	H	4.506	-1.147	3.613
58	C	2.484	-3.048	3.297
59	H	1.854	-3.741	2.733
60	H	3.449	-3.535	3.484
61	H	2.008	-2.866	4.269
62	H	1.693	-1.265	2.401
63	N	-0.184	0.759	2.633

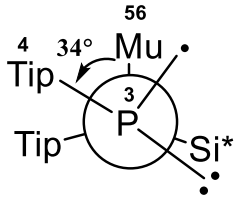
64	C	0.378	1.730	3.565
65	H	-0.389	2.105	4.262
66	H	0.807	2.581	3.036
67	H	1.173	1.269	4.171
68	C	-0.638	-0.430	3.341
69	H	-1.439	-0.192	4.057
70	H	0.181	-0.890	3.915
71	H	-1.025	-1.179	2.648
72	C	-1.905	0.967	-0.071
73	C	-3.196	0.843	0.531
74	C	-4.348	0.810	-0.266
75	C	-4.312	0.924	-1.654
76	C	-3.059	1.094	-2.237
77	C	-1.870	1.118	-1.495
78	C	-0.598	1.390	-2.313
79	C	-0.420	0.437	-3.510
80	H	0.547	0.620	-3.992
81	H	-1.194	0.586	-4.271
82	H	-0.450	-0.611	-3.200
83	C	-0.555	2.849	-2.812
84	H	-0.601	3.560	-1.984
85	H	0.374	3.033	-3.366
86	H	-1.394	3.055	-3.487
87	H	0.274	1.248	-1.669
88	H	-3.007	1.221	-3.316
89	C	-5.576	0.891	-2.501
90	H	-5.262	0.965	-3.552
91	C	-6.342	-0.436	-2.342
92	H	-5.699	-1.294	-2.564
93	H	-6.719	-0.558	-1.319
94	H	-7.204	-0.467	-3.020
95	C	-6.492	2.095	-2.209
96	H	-7.369	2.082	-2.867
97	H	-6.852	2.078	-1.173
98	H	-5.963	3.042	-2.364
99	H	-5.311	0.699	0.225
100	C	-3.449	0.756	2.041
101	C	-4.009	-0.622	2.442
102	H	-3.376	-1.436	2.084
103	H	-4.095	-0.702	3.533
104	H	-5.008	-0.778	2.018
105	C	-4.396	1.860	2.558
106	H	-5.408	1.755	2.151
107	H	-4.037	2.861	2.302
108	H	-4.476	1.799	3.650
109	H	-2.498	0.900	2.551
110	C	0.679	2.634	0.536
111	C	-0.078	3.836	0.711
112	C	0.469	5.073	0.345

113	C	1.750	5.210	-0.183
114	C	2.509	4.046	-0.293
115	C	2.016	2.785	0.069
116	C	3.016	1.638	-0.040
117	C	4.268	1.894	0.823
118	H	4.001	2.151	1.854
119	H	4.871	2.718	0.423
120	H	4.901	1.000	0.844
121	C	3.430	1.368	-1.497
122	H	2.562	1.140	-2.124
123	H	4.117	0.517	-1.549
124	H	3.936	2.238	-1.931
125	H	2.545	0.730	0.346
126	H	3.527	4.116	-0.665
127	C	2.294	6.573	-0.586
128	C	3.501	6.987	0.278
129	H	3.839	7.995	0.008
130	H	3.244	6.987	1.343
131	H	4.346	6.303	0.136
132	C	2.645	6.630	-2.085
133	H	3.455	5.933	-2.332
134	H	1.780	6.371	-2.705
135	H	2.976	7.637	-2.364
136	H	1.495	7.304	-0.407
137	H	-0.129	5.971	0.482
138	C	-1.476	3.908	1.337
139	C	-1.480	4.770	2.619
140	H	-0.727	4.432	3.337
141	H	-2.461	4.715	3.105
142	H	-1.282	5.824	2.397
143	C	-2.531	4.437	0.345
144	H	-3.518	4.480	0.820
145	H	-2.285	5.451	0.010
146	H	-2.608	3.794	-0.536
147	H	-1.777	2.903	1.634

Mu-Si-P-Tip: Dihedral angle: 56(Mu)-2(Si)-3(P)-4(C)

Rotamer: Step-2

Atom #	Symbol	x	y	z
1	Si	1.759	-0.082	0.948
2	Si	-0.631	-0.428	0.322
3	P	-2.011	0.868	1.695
4	C/Tip	-3.417	1.431	0.605
5	C	-3.304	2.601	-0.192
6	C	-4.430	3.074	-0.875
7	C	-5.673	2.438	-0.803
8	C	-5.768	1.298	-0.004



Step-2

9	C	-4.675	0.781	0.702
10	C	-4.891	-0.441	1.592
11	H	-3.904	-0.858	1.822
12	H	-6.728	0.794	0.071
13	C	-6.885	2.965	-1.558
14	H	-7.719	2.282	-1.345
15	H	-4.333	3.971	-1.480
16	C	-2.008	3.404	-0.273
17	H	-1.183	2.742	0.017
18	C	-1.503	-2.148	0.138
19	C	-1.662	-2.997	1.268
20	C	-2.387	-4.192	1.158
21	C	-2.973	-4.600	-0.037
22	C	-2.804	-3.770	-1.150
23	C	-2.085	-2.570	-1.102
24	C	-1.992	-1.762	-2.405
25	C	-3.160	-0.764	-2.530
26	H	-3.200	-0.073	-1.685
27	H	-4.118	-1.298	-2.574
28	H	-3.063	-0.175	-3.451
29	C	-1.922	-2.620	-3.684
30	H	-1.674	-1.978	-4.537
31	H	-1.159	-3.402	-3.617
32	H	-2.879	-3.101	-3.916
33	H	-1.067	-1.183	-2.374
34	H	-3.245	-4.076	-2.093
35	C	-3.754	-5.904	-0.123
36	C	-3.098	-6.902	-1.096
37	H	-3.103	-6.518	-2.123
38	H	-3.640	-7.855	-1.094
39	H	-2.057	-7.101	-0.818
40	C	-5.231	-5.667	-0.491
41	H	-5.783	-6.615	-0.494
42	H	-5.327	-5.223	-1.489
43	H	-5.715	-4.993	0.223
44	H	-3.733	-6.358	0.877
45	H	-2.497	-4.826	2.035
46	C	-1.063	-2.681	2.638
47	C	-0.082	-3.771	3.112
48	H	0.721	-3.933	2.390
49	H	0.372	-3.482	4.068
50	H	-0.591	-4.729	3.269
51	C	-2.137	-2.450	3.719
52	H	-2.799	-1.619	3.463
53	H	-2.753	-3.345	3.863
54	H	-1.663	-2.216	4.680
55	H	-0.483	-1.759	2.544
56	H/Mu	-0.771	0.244	-0.989
57	N	1.880	-0.419	2.677

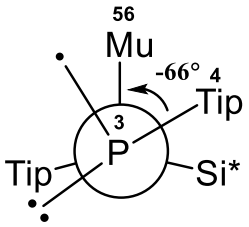
58	C	2.937	-1.213	3.297
59	H	3.530	-0.610	4.003
60	H	3.611	-1.631	2.551
61	H	2.501	-2.047	3.867
62	C	0.943	0.029	3.700
63	H	1.438	0.669	4.447
64	H	0.522	-0.827	4.248
65	H	0.116	0.600	3.277
66	C	1.958	1.760	0.277
67	C	2.113	2.924	1.093
68	C	2.264	4.188	0.508
69	C	2.307	4.382	-0.871
70	C	2.162	3.249	-1.668
71	C	1.979	1.962	-1.140
72	C	1.866	0.844	-2.190
73	C	0.761	1.109	-3.232
74	H	0.648	0.237	-3.886
75	H	1.005	1.964	-3.872
76	H	-0.205	1.310	-2.761
77	C	3.204	0.611	-2.922
78	H	4.009	0.365	-2.227
79	H	3.105	-0.216	-3.636
80	H	3.499	1.504	-3.487
81	H	1.610	-0.092	-1.687
82	H	2.205	3.371	-2.748
83	C	2.553	5.752	-1.489
84	H	2.438	5.641	-2.576
85	C	1.535	6.808	-1.021
86	H	0.508	6.500	-1.244
87	H	1.607	6.985	0.059
88	H	1.718	7.765	-1.525
89	C	3.995	6.228	-1.224
90	H	4.184	7.187	-1.722
91	H	4.173	6.366	-0.151
92	H	4.726	5.502	-1.595
93	H	2.376	5.050	1.161
94	C	2.149	2.900	2.624
95	C	0.864	3.500	3.228
96	H	-0.033	2.988	2.864
97	H	0.878	3.424	4.322
98	H	0.768	4.562	2.968
99	C	3.384	3.610	3.217
100	H	3.366	4.691	3.042
101	H	4.317	3.219	2.799
102	H	3.412	3.458	4.303
103	H	2.218	1.861	2.936
104	C	3.274	-1.058	0.184
105	C	4.586	-0.493	0.288
106	C	5.667	-1.102	-0.363

107	C	5.543	-2.271	-1.110
108	C	4.280	-2.857	-1.151
109	C	3.165	-2.294	-0.515
110	C	1.884	-3.120	-0.587
111	C	2.071	-4.499	0.080
112	H	2.476	-4.404	1.093
113	H	2.761	-5.130	-0.493
114	H	1.112	-5.025	0.140
115	C	1.381	-3.303	-2.030
116	H	1.199	-2.341	-2.522
117	H	0.444	-3.869	-2.032
118	H	2.107	-3.855	-2.637
119	H	1.103	-2.600	-0.027
120	H	4.153	-3.794	-1.687
121	C	6.743	-2.884	-1.818
122	C	7.086	-4.280	-1.264
123	H	7.984	-4.677	-1.751
124	H	7.271	-4.244	-0.185
125	H	6.269	-4.990	-1.440
126	C	6.542	-2.930	-3.345
127	H	5.706	-3.585	-3.616
128	H	6.331	-1.933	-3.747
129	H	7.442	-3.315	-3.840
130	H	7.603	-2.231	-1.618
131	H	6.651	-0.647	-0.279
132	C	4.947	0.740	1.125
133	C	5.993	0.407	2.213
134	H	5.682	-0.436	2.836
135	H	6.142	1.275	2.867
136	H	6.966	0.157	1.774
137	C	5.460	1.905	0.255
138	H	5.686	2.778	0.879
139	H	6.382	1.627	-0.268
140	H	4.720	2.204	-0.491
141	H	4.053	1.084	1.646
142	C	-7.300	4.366	-1.069
143	H	-8.207	4.702	-1.587
144	H	-7.502	4.367	0.008
145	H	-6.513	5.105	-1.263
146	C	-6.660	2.958	-3.082
147	H	-5.848	3.637	-3.367
148	H	-6.399	1.956	-3.439
149	H	-7.566	3.283	-3.607
150	C	-5.691	-1.567	0.913
151	H	-6.733	-1.280	0.730
152	H	-5.242	-1.854	-0.044
153	H	-5.705	-2.453	1.559
154	C	-5.546	-0.032	2.926
155	H	-4.947	0.721	3.450

156	H	-6.543	0.390	2.756
157	H	-5.655	-0.901	3.588
158	C	-2.034	4.575	0.731
159	H	-2.838	5.279	0.481
160	H	-2.203	4.221	1.754
161	H	-1.084	5.120	0.712
162	C	-1.695	3.917	-1.690
163	H	-0.677	4.319	-1.723
164	H	-1.767	3.115	-2.433
165	H	-2.377	4.720	-1.995

Rotamer: Step-12

Atom #	Symbol	*x*	*y*	*z*
1	Si	0.670	-0.947	-0.818
2	Si	0.289	1.266	0.315
3	P	-1.535	2.686	-0.048
4	C/Tip	-3.232	1.931	-0.057
5	C	-4.040	2.125	-1.216
6	C	-5.380	1.731	-1.189
7	C	-5.970	1.158	-0.057
8	C	-5.174	1.007	1.078
9	C	-3.827	1.388	1.111
10	C	-3.083	1.304	2.440
11	H	-2.019	1.458	2.236
12	H	-5.625	0.590	1.976
13	C	-7.434	0.739	-0.044
14	H	-7.635	0.305	0.945
15	H	-5.987	1.881	-2.078
16	C	-3.510	2.817	-2.474
17	H	-2.414	2.802	-2.427
18	C	1.605	2.689	0.343
19	C	1.973	3.338	-0.867
20	C	2.900	4.390	-0.852
21	C	3.478	4.856	0.326
22	C	3.088	4.240	1.519
23	C	2.176	3.179	1.561
24	C	1.783	2.649	2.945
25	C	0.547	3.407	3.475
26	H	-0.295	3.348	2.778
27	H	0.783	4.468	3.622
28	H	0.223	2.995	4.439
29	C	2.905	2.690	3.998
30	H	2.585	2.143	4.892
31	H	3.827	2.227	3.632
32	H	3.142	3.712	4.318
33	H	1.503	1.599	2.838
34	H	3.509	4.602	2.451
35	C	4.482	6.000	0.308



Step-12

36	C	5.862	5.560	0.835
37	H	5.809	5.263	1.889
38	H	6.583	6.383	0.756
39	H	6.251	4.709	0.265
40	C	3.965	7.230	1.078
41	H	4.680	8.058	1.002
42	H	3.828	7.005	2.142
43	H	3.003	7.571	0.680
44	H	4.611	6.298	-0.741
45	H	3.172	4.868	-1.790
46	C	1.367	2.979	-2.224
47	C	2.414	2.506	-3.249
48	H	2.943	1.616	-2.900
49	H	1.928	2.260	-4.201
50	H	3.159	3.284	-3.450
51	C	0.555	4.153	-2.808
52	H	-0.201	4.506	-2.100
53	H	1.207	4.998	-3.059
54	H	0.046	3.843	-3.729
55	H	0.674	2.145	-2.074
56	H/Mu	0.069	0.830	1.714
57	N	0.323	-0.639	-2.516
58	C	1.112	-1.122	-3.643
59	H	0.536	-1.825	-4.267
60	H	2.017	-1.624	-3.305
61	H	1.409	-0.281	-4.287
62	C	-0.802	0.155	-2.989
63	H	-1.464	-0.434	-3.644
64	H	-0.458	1.018	-3.578
65	H	-1.410	0.524	-2.160
66	C	-0.547	-2.073	0.246
67	C	-1.762	-2.660	-0.231
68	C	-2.542	-3.462	0.612
69	C	-2.177	-3.761	1.923
70	C	-0.987	-3.203	2.384
71	C	-0.181	-2.369	1.596
72	C	1.099	-1.872	2.284
73	C	0.818	-1.169	3.628
74	H	1.739	-0.713	4.013
75	H	0.467	-1.877	4.387
76	H	0.063	-0.383	3.530
77	C	2.108	-3.017	2.510
78	H	2.378	-3.509	1.573
79	H	3.025	-2.629	2.969
80	H	1.691	-3.772	3.186
81	H	1.587	-1.139	1.635
82	H	-0.673	-3.430	3.400
83	C	-3.015	-4.673	2.808
84	H	-2.523	-4.710	3.790

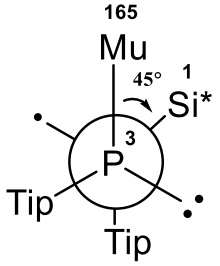
85	C	-4.439	-4.128	3.025
86	H	-4.418	-3.121	3.456
87	H	-4.995	-4.076	2.081
88	H	-5.000	-4.779	3.706
89	C	-3.056	-6.112	2.257
90	H	-3.613	-6.769	2.935
91	H	-3.549	-6.146	1.278
92	H	-2.046	-6.520	2.139
93	H	-3.463	-3.882	0.217
94	C	-2.305	-2.490	-1.654
95	C	-3.571	-1.612	-1.663
96	H	-3.396	-0.641	-1.193
97	H	-3.914	-1.440	-2.691
98	H	-4.388	-2.100	-1.119
99	C	-2.602	-3.828	-2.363
100	H	-3.421	-4.377	-1.884
101	H	-1.728	-4.485	-2.384
102	H	-2.903	-3.636	-3.400
103	H	-1.54	-1.993	-2.246
104	C	2.368	-1.934	-0.836
105	C	2.351	-3.322	-1.191
106	C	3.521	-4.089	-1.096
107	C	4.741	-3.567	-0.677
108	C	4.769	-2.206	-0.383
109	C	3.633	-1.389	-0.469
110	C	3.876	0.088	-0.177
111	C	4.917	0.692	-1.143
112	H	4.677	0.466	-2.187
113	H	5.922	0.302	-0.944
114	H	4.953	1.781	-1.027
115	C	4.318	0.333	1.278
116	H	3.576	-0.031	1.996
117	H	4.460	1.404	1.453
118	H	5.266	-0.173	1.494
119	H	2.942	0.631	-0.336
120	H	5.710	-1.753	-0.084
121	C	5.981	-4.444	-0.573
122	C	7.080	-3.999	-1.557
123	H	7.940	-4.678	-1.505
124	H	6.711	-3.994	-2.588
125	H	7.438	-2.989	-1.323
126	C	6.522	-4.501	0.868
127	H	6.854	-3.512	1.207
128	H	5.755	-4.854	1.566
129	H	7.380	-5.181	0.930
130	H	5.680	-5.462	-0.853
131	H	3.477	-5.142	-1.365
132	C	1.130	-4.083	-1.720
133	C	1.388	-4.685	-3.120

134	H	1.739	-3.931	-3.831
135	H	0.463	-5.119	-3.518
136	H	2.135	-5.485	-3.084
137	C	0.683	-5.196	-0.751
138	H	-0.207	-5.706	-1.135
139	H	1.469	-5.950	-0.631
140	H	0.443	-4.793	0.237
141	H	0.300	-3.384	-1.827
142	C	-8.374	1.948	-0.217
143	H	-9.422	1.633	-0.149
144	H	-8.194	2.704	0.556
145	H	-8.232	2.426	-1.193
146	C	-7.736	-0.346	-1.094
147	H	-7.573	0.027	-2.112
148	H	-7.097	-1.225	-0.953
149	H	-8.781	-0.669	-1.022
150	C	-3.214	-0.064	3.130
151	H	-4.245	-0.265	3.446
152	H	-2.896	-0.877	2.470
153	H	-2.587	-0.092	4.029
154	C	-3.534	2.439	3.383
155	H	-3.394	3.422	2.918
156	H	-4.595	2.337	3.639
157	H	-2.957	2.418	4.315
158	C	-3.939	4.298	-2.496
159	H	-5.031	4.387	-2.540
160	H	-3.595	4.823	-1.598
161	H	-3.522	4.809	-3.372
162	C	-3.909	2.116	-3.785
163	H	-3.397	2.59	-4.631
164	H	-3.638	1.055	-3.773
165	H	-4.985	2.186	-3.979

Si-P(Mu)-Tip: Dihedral angle 165(Mu)-3(P)-2(Si)-1(Si)

Rotamer: Step-5

Atom #	Symbol	*x*	*y*	*z*
1	Si	1.829	-0.125	0.967
2	Si	-0.523	-0.464	0.233
3	P	-1.814	1.062	1.396
4	N	1.929	-0.458	2.697
5	C	-3.290	1.624	0.395
6	C	-3.251	2.703	-0.529
7	C	-4.450	3.145	-1.104
8	C	-5.686	2.566	-0.819
9	C	-5.704	1.498	0.080
10	C	-4.542	1.014	0.688



Step-5

11	C	-1.970	3.458	-0.881
12	C	-4.686	-0.132	1.692
13	C	-1.527	-2.118	0.157
14	C	-1.669	-2.998	1.266
15	C	-2.458	-4.150	1.145
16	C	-3.120	-4.485	-0.036
17	C	-2.981	-3.616	-1.120
18	C	-2.209	-2.448	-1.053
19	C	-1.015	-2.734	2.622
20	C	-0.197	-3.931	3.145
21	C	-2.052	-2.319	3.685
22	C	-3.962	-5.751	-0.125
23	C	-3.395	-6.744	-1.158
24	C	-5.442	-5.439	-0.418
25	C	-2.188	-1.559	-2.301
26	C	-3.541	-0.851	-2.513
27	C	-1.794	-2.308	-3.589
28	C	2.045	1.722	0.321
29	C	2.235	2.877	1.141
30	C	2.396	4.142	0.561
31	C	2.412	4.346	-0.818
32	C	2.228	3.221	-1.619
33	C	2.040	1.933	-1.095
34	C	2.310	2.845	2.673
35	C	1.083	3.517	3.322
36	C	3.600	3.486	3.227
37	C	2.692	5.709	-1.438
38	H	2.513	5.614	-2.518
39	C	1.764	6.819	-0.912
40	H	0.711	6.577	-1.091
41	H	1.896	6.978	0.164
42	H	1.983	7.768	-1.415
43	C	4.172	6.103	-1.251
44	H	4.386	7.053	-1.754
45	H	4.415	6.222	-0.188
46	H	4.840	5.339	-1.664
47	C	1.884	0.824	-2.146
48	C	0.699	1.081	-3.097
49	C	3.175	0.618	-2.964
50	C	3.321	-1.124	0.197
51	C	4.638	-0.565	0.240
52	C	5.686	-1.182	-0.456
53	C	5.523	-2.357	-1.187
54	C	4.261	-2.945	-1.154
55	C	3.180	-2.374	-0.468
56	C	5.040	0.658	1.072
57	C	6.091	0.289	2.143
58	C	5.563	1.818	0.203
59	C	6.685	-2.977	-1.950

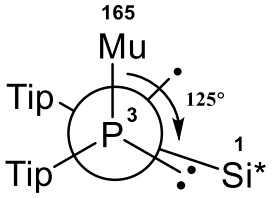
60	C	7.071	-4.358	-1.385
61	C	6.397	-3.061	-3.461
62	C	1.901	-3.207	-0.445
63	C	2.139	-4.570	0.237
64	C	1.313	-3.413	-1.850
65	C	2.962	-1.280	3.320
66	C	0.972	-0.011	3.702
67	H	-1.124	2.783	-0.725
68	H	-3.696	-0.567	1.853
69	H	-2.562	-4.810	2.003
70	H	-3.494	-3.848	-2.05
71	H	-0.315	-1.903	2.491
72	H	0.549	-4.262	2.419
73	H	0.326	-3.652	4.068
74	H	-0.838	-4.788	3.383
75	H	-2.575	-1.400	3.405
76	H	-2.800	-3.108	3.828
77	H	-1.562	-2.145	4.651
78	H	-3.917	-6.237	0.858
79	H	-3.423	-6.324	-2.170
80	H	-3.982	-7.670	-1.164
81	H	-2.355	-7.001	-0.930
82	H	-6.037	-6.360	-0.415
83	H	-5.564	-4.968	-1.401
84	H	-5.861	-4.760	0.333
85	H	-1.434	-0.778	-2.134
86	H	-3.833	-0.263	-1.640
87	H	-4.335	-1.581	-2.712
88	H	-3.485	-0.176	-3.376
89	H	-1.702	-1.596	-4.418
90	H	-0.842	-2.833	-3.485
91	H	-2.555	-3.044	-3.877
92	H	2.539	4.996	1.218
93	H	2.246	3.349	-2.699
94	H	2.329	1.803	2.981
95	H	0.146	3.050	3.006
96	H	1.142	3.450	4.415
97	H	1.031	4.580	3.056
98	H	3.637	4.566	3.044
99	H	4.498	3.043	2.786
100	H	3.65	3.339	4.313
101	H	1.677	-0.121	-1.639
102	H	0.566	0.226	-3.771
103	H	0.864	1.967	-3.721
104	H	-0.233	1.227	-2.543
105	H	4.024	0.378	-2.319
106	H	3.043	-0.208	-3.674
107	H	3.427	1.515	-3.541
108	H	6.676	-0.732	-0.418

109	H	4.108	-3.891	-1.667
110	H	4.161	1.017	1.609
111	H	5.753	-0.537	2.777
112	H	6.287	1.153	2.790
113	H	7.043	-0.005	1.689
114	H	5.821	2.679	0.830
115	H	6.469	1.526	-0.342
116	H	4.815	2.142	-0.525
117	H	7.550	-2.314	-1.815
118	H	7.946	-4.757	-1.912
119	H	7.314	-4.297	-0.318
120	H	6.254	-5.079	-1.503
121	H	5.551	-3.727	-3.668
122	H	6.157	-2.075	-3.874
123	H	7.269	-3.453	-3.997
124	H	1.152	-2.679	0.153
125	H	2.561	-4.448	1.241
126	H	2.831	-5.193	-0.341
127	H	1.194	-5.119	0.325
128	H	1.105	-2.455	-2.336
129	H	0.377	-3.977	-1.793
130	H	2.004	-3.971	-2.493
131	H	3.562	-0.696	4.037
132	H	3.633	-1.705	2.575
133	H	2.504	-2.111	3.880
134	H	1.446	0.643	4.450
135	H	0.553	-0.868	4.249
136	H	0.140	0.541	3.259
137	H	-4.422	3.976	-1.804
138	H	-6.653	1.027	0.321
139	C	-6.961	3.090	-1.467
140	H	-6.670	3.918	-2.127
141	C	-7.644	2.021	-2.341
142	H	-6.960	1.642	-3.108
143	H	-7.979	1.169	-1.739
144	H	-8.523	2.440	-2.845
145	C	-7.942	3.657	-0.423
146	H	-7.472	4.448	0.173
147	H	-8.826	4.080	-0.915
148	H	-8.285	2.877	0.267
149	C	-5.183	0.399	3.052
150	H	-4.511	1.169	3.447
151	H	-6.182	0.840	2.956
152	H	-5.242	-0.413	3.787
153	C	-5.582	-1.280	1.194
154	H	-6.631	-0.977	1.099
155	H	-5.246	-1.656	0.223
156	H	-5.548	-2.111	1.909
157	C	-1.786	4.668	0.060

158	H	-2.589	5.399	-0.093
159	H	-1.806	4.369	1.114
160	H	-0.828	5.164	-0.130
161	C	-1.892	3.913	-2.350
162	H	-2.095	3.086	-3.039
163	H	-2.595	4.723	-2.575
164	H	-0.885	4.290	-2.561
165	H/Mu	-0.947	2.157	1.194

Rotamer: Step-13

Atom #	Symbol	*x*	*y*	*z*
1	Si	1.621	-0.418	-0.909
2	Si	-0.468	0.236	0.155
3	P	-1.656	-1.577	0.945
4	N	1.251	-0.663	-2.615
5	C	-3.470	-1.453	0.474
6	C	-4.424	-0.683	1.195
7	C	-5.784	-0.812	0.878
8	C	-6.250	-1.650	-0.134
9	C	-5.300	-2.383	-0.846
10	C	-3.931	-2.306	-0.568
11	C	-4.062	0.255	2.347
12	C	-3.001	-3.207	-1.382
13	C	-1.333	1.954	0.166
14	C	-2.170	2.383	-0.900
15	C	-2.737	3.665	-0.866
16	C	-2.524	4.551	0.191
17	C	-1.731	4.107	1.253
18	C	-1.143	2.838	1.269
19	C	-2.515	1.495	-2.095
20	C	-1.945	2.043	-3.416
21	C	-4.033	1.260	-2.222
22	C	-3.152	5.938	0.187
23	C	-2.085	7.050	0.190
24	C	-4.144	6.123	1.351
25	C	-0.331	2.451	2.506
26	C	-1.148	2.572	3.807
27	C	0.983	3.244	2.634
28	C	2.099	-1.973	0.202
29	C	2.198	-3.308	-0.305
30	C	2.542	-4.369	0.543
31	C	2.821	-4.194	1.896
32	C	2.735	-2.896	2.389
33	C	2.379	-1.796	1.594
34	C	1.971	-3.707	-1.768
35	C	0.757	-4.645	-1.919
36	C	3.219	-4.356	-2.404



Step-13

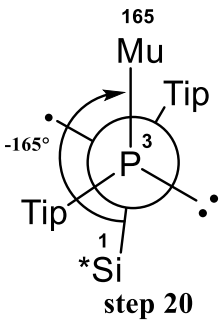
37	C	3.211	-5.357	2.799
38	H	3.373	-4.944	3.804
39	C	2.085	-6.403	2.906
40	H	1.154	-5.947	3.262
41	H	1.880	-6.870	1.935
42	H	2.365	-7.199	3.607
43	C	4.531	-6.012	2.349
44	H	4.823	-6.808	3.045
45	H	4.434	-6.458	1.352
46	H	5.344	-5.278	2.311
47	C	2.334	-0.458	2.349
48	C	1.373	-0.527	3.555
49	C	3.723	0.004	2.835
50	C	3.114	0.830	-0.897
51	C	4.460	0.383	-0.721
52	C	5.470	1.306	-0.407
53	C	5.236	2.675	-0.318
54	C	3.960	3.123	-0.669
55	C	2.918	2.245	-0.993
56	C	4.934	-1.041	-1.039
57	C	5.820	-1.021	-2.307
58	C	5.691	-1.746	0.101
59	C	6.347	3.640	0.071
60	C	6.727	4.579	-1.090
61	C	5.985	4.445	1.334
62	C	1.672	2.863	-1.633
63	C	1.917	3.007	-3.153
64	C	1.251	4.233	-1.075
65	C	2.256	-0.613	-3.671
66	C	-0.005	-1.196	-3.123
67	H	-3.006	0.514	2.248
68	H	-1.970	-2.911	-1.170
69	H	-3.371	3.984	-1.690
70	H	-1.566	4.770	2.099
71	H	-2.052	0.516	-1.919
72	H	-0.855	2.128	-3.376
73	H	-2.204	1.379	-4.249
74	H	-2.353	3.035	-3.643
75	H	-4.452	0.848	-1.299
76	H	-4.563	2.191	-2.455
77	H	-4.238	0.552	-3.034
78	H	-3.721	6.031	-0.748
79	H	-1.487	7.025	1.109
80	H	-2.558	8.037	0.128
81	H	-1.400	6.945	-0.659
82	H	-4.627	7.105	1.291
83	H	-3.637	6.059	2.321
84	H	-4.926	5.355	1.330
85	H	-0.063	1.394	2.391

86	H	-2.082	2.005	3.751
87	H	-1.401	3.614	4.031
88	H	-0.567	2.186	4.653
89	H	1.515	2.953	3.549
90	H	1.652	3.062	1.788
91	H	0.793	4.322	2.692
92	H	2.601	-5.368	0.121
93	H	2.958	-2.733	3.440
94	H	1.759	-2.806	-2.334
95	H	-0.145	-4.198	-1.490
96	H	0.565	-4.857	-2.978
97	H	0.923	-5.604	-1.414
98	H	3.475	-5.308	-1.926
99	H	4.096	-3.703	-2.334
100	H	3.035	-4.560	-3.466
101	H	1.959	0.319	1.676
102	H	1.301	0.452	4.041
103	H	1.730	-1.235	4.311
104	H	0.367	-0.839	3.259
105	H	4.412	0.159	2.002
106	H	3.631	0.953	3.377
107	H	4.170	-0.727	3.519
108	H	6.483	0.942	-0.252
109	H	3.777	4.191	-0.719
110	H	4.060	-1.649	-1.272
111	H	5.323	-0.522	-3.146
112	H	6.061	-2.046	-2.616
113	H	6.765	-0.499	-2.123
114	H	6.020	-2.739	-0.229
115	H	6.587	-1.187	0.397
116	H	5.061	-1.878	0.983
117	H	7.232	3.035	0.307
118	H	7.567	5.223	-0.805
119	H	7.020	4.010	-1.980
120	H	5.889	5.229	-1.368
121	H	5.113	5.086	1.160
122	H	5.750	3.781	2.173
123	H	6.820	5.090	1.632
124	H	0.827	2.180	-1.502
125	H	2.126	2.045	-3.626
126	H	2.771	3.669	-3.339
127	H	1.040	3.446	-3.643
128	H	1.183	4.237	0.014
129	H	0.266	4.501	-1.470
130	H	1.948	5.024	-1.377
131	H	2.563	-1.619	-4.006
132	H	3.146	-0.078	-3.336
133	H	1.854	-0.089	-4.550
134	H	0.107	-2.211	-3.536

135	H	-0.396	-0.557	-3.928
136	H	-0.754	-1.242	-2.330
137	H	-6.511	-0.235	1.442
138	H	-5.632	-3.049	-1.638
139	C	-7.738	-1.755	-0.440
140	H	-8.257	-1.074	0.249
141	C	-8.064	-1.297	-1.874
142	H	-7.717	-0.273	-2.052
143	H	-7.587	-1.947	-2.617
144	H	-9.146	-1.326	-2.051
145	C	-8.278	-3.174	-0.178
146	H	-8.085	-3.487	0.853
147	H	-9.361	-3.211	-0.350
148	H	-7.810	-3.908	-0.845
149	C	-3.147	-4.677	-0.941
150	H	-2.932	-4.792	0.127
151	H	-4.166	-5.040	-1.121
152	H	-2.457	-5.319	-1.500
153	C	-3.205	-3.068	-2.902
154	H	-4.184	-3.440	-3.222
155	H	-3.123	-2.024	-3.224
156	H	-2.445	-3.650	-3.436
157	C	-4.252	-0.449	3.707
158	H	-5.304	-0.719	3.860
159	H	-3.660	-1.369	3.771
160	H	-3.949	0.208	4.531
161	C	-4.837	1.587	2.321
162	H	-4.742	2.084	1.351
163	H	-5.903	1.454	2.535
164	H	-4.436	2.262	3.086
165	H/Mu	-1.786	-1.137	2.286

Rotamer: Step-20

Atom #	Symbol	*x*	*y*	*z*
1	Si	-0.414	0.061	0.679
2	Si	-0.545	0.616	3.078
3	P	1.32	1.119	4.363
4	N	-0.997	-1.604	0.726
5	C	2.532	-0.29	4.611
6	C	2.206	-1.528	5.226
7	C	3.233	-2.445	5.496
8	C	4.567	-2.193	5.186
9	C	4.873	-0.966	4.593
10	C	3.895	-0.008	4.304
11	C	0.796	-1.893	5.689
12	C	4.354	1.343	3.743
13	C	-2.083	1.327	4.023
14	C	-3.19	0.459	4.255



step 20

15	C	-4.358	0.95	4.855
16	C	-4.481	2.271	5.28
17	C	-3.37	3.101	5.113
18	C	-2.186	2.67	4.503
19	C	-3.147	-1.04	3.963
20	C	-4.245	-1.518	2.998
21	C	-3.195	-1.851	5.273
22	C	-5.768	2.77	5.924
23	C	-6.419	3.899	5.103
24	C	-5.548	3.208	7.385
25	C	-1.035	3.68	4.471
26	C	-0.469	3.901	5.891
27	C	-1.408	5.047	3.864
28	C	1.468	0.436	0.271
29	C	2.471	-0.543	0.005
30	C	3.76	-0.153	-0.388
31	C	4.127	1.18	-0.553
32	C	3.156	2.138	-0.259
33	C	1.857	1.807	0.146
34	C	2.24	-2.054	0.115
35	C	2.906	-2.625	1.382
36	C	2.706	-2.846	-1.124
37	C	5.492	1.625	-1.073
38	H	5.8	2.487	-0.463
39	C	6.596	0.564	-0.963
40	H	6.701	0.186	0.059
41	H	6.401	-0.291	-1.622
42	H	7.558	0.994	-1.264
43	C	5.375	2.118	-2.531
44	H	6.34	2.498	-2.889
45	H	5.067	1.299	-3.192
46	H	4.637	2.921	-2.627
47	C	0.924	2.999	0.398
48	C	1.479	3.954	1.474
49	C	0.629	3.785	-0.896
50	C	-1.411	0.856	-0.811
51	C	-0.961	0.636	-2.152
52	C	-1.556	1.33	-3.216
53	C	-2.614	2.219	-3.045
54	C	-3.11	2.359	-1.752
55	C	-2.551	1.692	-0.652
56	C	0.104	-0.386	-2.566
57	C	-0.485	-1.465	-3.502
58	C	1.323	0.275	-3.237
59	C	-3.214	2.965	-4.228
60	C	-4.674	2.549	-4.488
61	C	-3.098	4.492	-4.061
62	C	-3.283	1.883	0.671
63	C	-4.721	1.329	0.595

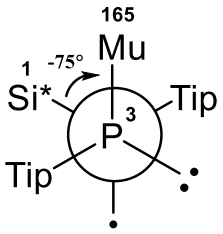
64	C	-3.305	3.356	1.113
65	C	-1.927	-2.195	-0.231
66	C	-0.625	-2.588	1.734
67	H	0.088	-1.281	5.122
68	H	3.544	1.747	3.127
69	H	-5.194	0.273	5.013
70	H	-3.424	4.125	5.474
71	H	-2.182	-1.251	3.488
72	H	-4.174	-1.015	2.031
73	H	-4.154	-2.598	2.827
74	H	-5.248	-1.334	3.402
75	H	-2.405	-1.539	5.965
76	H	-4.155	-1.723	5.786
77	H	-3.068	-2.921	5.067
78	H	-6.47	1.925	5.936
79	H	-5.775	4.786	5.065
80	H	-7.374	4.199	5.55
81	H	-6.61	3.58	4.072
82	H	-6.498	3.505	7.844
83	H	-4.865	4.064	7.446
84	H	-5.121	2.394	7.982
85	H	-0.233	3.264	3.853
86	H	-0.188	2.959	6.371
87	H	-1.212	4.393	6.531
88	H	0.42	4.541	5.854
89	H	-0.521	5.691	3.832
90	H	-1.794	4.952	2.847
91	H	-2.164	5.567	4.463
92	H	4.493	-0.928	-0.586
93	H	3.419	3.189	-0.364
94	H	1.167	-2.215	0.195
95	H	2.557	-2.12	2.288
96	H	2.69	-3.696	1.482
97	H	3.996	-2.507	1.337
98	H	3.796	-2.84	-1.237
99	H	2.271	-2.452	-2.048
100	H	2.398	-3.895	-1.028
101	H	-0.035	2.626	0.772
102	H	0.752	4.747	1.684
103	H	2.404	4.438	1.143
104	H	1.691	3.428	2.41
105	H	0.197	3.142	-1.667
106	H	-0.079	4.598	-0.692
107	H	1.544	4.236	-1.299
108	H	-1.185	1.157	-4.223
109	H	-3.971	3.002	-1.586
110	H	0.456	-0.903	-1.673
111	H	-1.367	-1.946	-3.068
112	H	0.263	-2.244	-3.695

113	H	-0.776	-1.043	-4.47
114	H	2.077	-0.481	-3.487
115	H	1.036	0.774	-4.17
116	H	1.789	1.015	-2.582
117	H	-2.63	2.686	-5.116
118	H	-5.068	3.058	-5.376
119	H	-4.755	1.468	-4.651
120	H	-5.319	2.809	-3.64
121	H	-3.676	4.842	-3.197
122	H	-2.056	4.797	-3.913
123	H	-3.482	5.007	-4.949
124	H	-2.758	1.314	1.444
125	H	-4.732	0.288	0.255
126	H	-5.334	1.912	-0.102
127	H	-5.198	1.375	1.58
128	H	-2.291	3.766	1.158
129	H	-3.758	3.455	2.104
130	H	-3.882	3.973	0.414
131	H	-1.45	-3.001	-0.814
132	H	-2.309	-1.448	-0.925
133	H	-2.784	-2.638	0.298
134	H	-0.111	-3.454	1.287
135	H	-1.515	-2.975	2.251
136	H	0.041	-2.155	2.483
137	H	2.985	-3.389	5.974
138	H	5.908	-0.744	4.356
139	C	5.648	-3.22	5.497
140	H	5.151	-4.078	5.971
141	C	6.335	-3.735	4.218
142	H	5.604	-4.159	3.519
143	H	6.865	-2.927	3.699
144	H	7.067	-4.513	4.461
145	C	6.686	-2.678	6.499
146	H	6.206	-2.348	7.427
147	H	7.418	-3.454	6.751
148	H	7.233	-1.824	6.082
149	C	4.612	2.344	4.888
150	H	3.716	2.497	5.497
151	H	5.413	1.981	5.545
152	H	4.919	3.317	4.485
153	C	5.594	1.258	2.838
154	H	6.507	1.035	3.403
155	H	5.473	0.496	2.063
156	H	5.752	2.222	2.342
157	C	0.617	-1.557	7.184
158	H	1.301	-2.154	7.799
159	H	0.821	-0.5	7.389
160	H	-0.407	-1.775	7.511
161	C	0.421	-3.364	5.428

162	H	0.611	-3.651	4.388
163	H	0.977	-4.055	6.072
164	H	-0.643	-3.518	5.635
165	H/Mu	0.579	0.943	5.559

Rotamer: Step-29

Atom #	Symbol	*x*	*y*	*z*
1	Si	0.646	1.010	0.853
2	Si	0.439	-1.245	-0.228
3	P	-1.324	-2.762	-0.070
4	N	0.419	0.731	2.575
5	C	-3.063	-2.146	0.187
6	C	-3.797	-2.351	1.391
7	C	-5.166	-2.047	1.404
8	C	-5.844	-1.543	0.296
9	C	-5.109	-1.352	-0.876
10	C	-3.747	-1.650	-0.958
11	C	-3.193	-2.955	2.662
12	C	-3.060	-1.512	-2.319
13	C	1.807	-2.626	-0.234
14	C	2.382	-3.157	0.953
15	C	3.406	-4.111	0.868
16	C	3.876	-4.597	-0.352
17	C	3.262	-4.120	-1.514
18	C	2.242	-3.162	-1.484
19	C	1.867	-2.805	2.348
20	C	2.949	-2.252	3.293
21	C	1.181	-4.024	3.000
22	C	4.996	-5.627	-0.404
23	C	6.243	-5.078	-1.125
24	C	4.532	-6.952	-1.038
25	C	1.574	-2.805	-2.815
26	C	0.684	-3.967	-3.300
27	C	2.559	-2.397	-3.925
28	C	-0.739	1.990	-0.135
29	C	-1.953	2.511	0.414
30	C	-2.841	3.235	-0.393
31	C	-2.592	3.513	-1.736
32	C	-1.406	3.014	-2.269
33	C	-0.492	2.262	-1.517
34	C	-2.390	2.344	1.873
35	C	-3.589	1.383	1.983
36	C	-2.733	3.676	2.572
37	C	-3.546	4.346	-2.581
38	H	-3.147	4.352	-3.605
39	C	-4.961	3.742	-2.640



Step-29

40	H	-4.937	2.712	-3.013
41	H	-5.433	3.730	-1.651
42	H	-5.601	4.332	-3.307
43	C	-3.593	5.809	-2.096
44	H	-4.238	6.412	-2.747
45	H	-3.992	5.873	-1.076
46	H	-2.594	6.258	-2.093
47	C	0.761	1.813	-2.279
48	C	0.415	0.968	-3.521
49	C	1.648	3.008	-2.682
50	C	2.255	2.127	0.726
51	C	2.145	3.520	1.037
52	C	3.234	4.378	0.826
53	C	4.46	3.943	0.333
54	C	4.585	2.577	0.089
55	C	3.533	1.673	0.288
56	C	0.908	4.192	1.644
57	C	1.220	4.840	3.011
58	C	0.301	5.242	0.693
59	C	5.607	4.915	0.100
60	C	6.818	4.603	0.999
61	C	6.020	4.964	-1.384
62	C	3.883	0.210	0.037
63	C	5.040	-0.258	0.945
64	C	4.238	-0.063	-1.435
65	C	1.280	1.240	3.636
66	C	-0.603	-0.155	3.114
67	H	-2.130	-2.699	2.690
68	H	-1.976	-1.480	-2.156
69	H	3.840	-4.504	1.785
70	H	3.578	-4.516	-2.475
71	H	1.113	-2.019	2.230
72	H	3.384	-1.327	2.908
73	H	2.516	-2.040	4.278
74	H	3.762	-2.972	3.441
75	H	0.413	-4.455	2.349
76	H	1.910	-4.812	3.219
77	H	0.707	-3.736	3.947
78	H	5.285	-5.842	0.634
79	H	6.028	-4.854	-2.176
80	H	7.057	-5.813	-1.099
81	H	6.601	-4.157	-0.652
82	H	5.338	-7.695	-1.010
83	H	4.243	-6.812	-2.086
84	H	3.669	-7.365	-0.504
85	H	0.918	-1.943	-2.632
86	H	-0.058	-4.242	-2.544
87	H	1.288	-4.855	-3.523
88	H	0.152	-3.685	-4.218

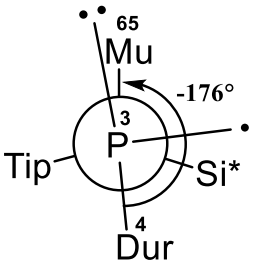
89	H	2.006	-2.084	-4.818
90	H	3.201	-1.567	-3.616
91	H	3.207	-3.230	-4.222
92	H	-3.757	3.609	0.056
93	H	-1.182	3.221	-3.312
94	H	-1.556	1.915	2.424
95	H	-3.384	0.417	1.514
96	H	-3.845	1.206	3.036
97	H	-4.475	1.806	1.493
98	H	-3.620	4.153	2.140
99	H	-1.909	4.393	2.517
100	H	-2.948	3.493	3.632
101	H	1.361	1.174	-1.626
102	H	1.332	0.582	-3.982
103	H	-0.111	1.558	-4.279
104	H	-0.219	0.116	-3.257
105	H	1.954	3.591	-1.809
106	H	2.552	2.655	-3.191
107	H	1.118	3.677	-3.371
108	H	3.120	5.434	1.062
109	H	5.538	2.192	-0.262
110	H	0.150	3.429	1.825
111	H	1.673	4.128	3.707
112	H	0.297	5.217	3.466
113	H	1.905	5.690	2.909
114	H	-0.595	5.691	1.137
115	H	1.012	6.053	0.498
116	H	0.018	4.798	-0.265
117	H	5.243	5.915	0.374
118	H	7.607	5.350	0.855
119	H	6.537	4.604	2.058
120	H	7.244	3.619	0.766
121	H	6.411	3.996	-1.720
122	H	5.170	5.223	-2.024
123	H	6.806	5.713	-1.540
124	H	3.014	-0.404	0.285
125	H	4.857	-0.007	1.994
126	H	5.989	0.209	0.655
127	H	5.165	-1.343	0.867
128	H	3.421	0.225	-2.105
129	H	4.441	-1.128	-1.585
130	H	5.130	0.497	-1.739
131	H	0.719	1.885	4.331
132	H	2.110	1.815	3.226
133	H	1.698	0.410	4.226
134	H	-1.255	0.369	3.829
135	H	-0.152	-1.002	3.653
136	H	-1.237	-0.555	2.319
137	H	-5.73	-2.209	2.318

138	H	-5.615	-0.974	-1.760
139	C	-7.333	-1.230	0.366
140	H	-7.664	-1.468	1.386
141	C	-7.618	0.264	0.124
142	H	-7.071	0.892	0.837
143	H	-7.321	0.568	-0.886
144	H	-8.689	0.475	0.235
145	C	-8.150	-2.109	-0.600
146	H	-7.981	-3.174	-0.407
147	H	-9.223	-1.908	-0.489
148	H	-7.880	-1.911	-1.644
149	C	-3.360	-2.745	-3.196
150	H	-3.054	-3.673	-2.701
151	H	-4.434	-2.813	-3.409
152	H	-2.829	-2.677	-4.153
153	C	-3.423	-0.218	-3.066
154	H	-4.471	-0.209	-3.388
155	H	-3.247	0.666	-2.446
156	H	-2.808	-0.126	-3.970
157	C	-3.297	-4.495	2.634
158	H	-4.348	-4.808	2.618
159	H	-2.810	-4.919	1.749
160	H	-2.826	-4.932	3.523
161	C	-3.793	-2.410	3.971
162	H	-3.795	-1.315	3.989
163	H	-4.820	-2.754	4.135
164	H	-3.197	-2.763	4.821
165	H/Mu	-1.039	-3.208	1.238

Mu-Si-P-Dur: Dihedral angle: 65(Mu)-2(Si)-3(P)-4(C)

Rotamer: Step-11

Atom #	Symbol	*x*	*y*	*z*
1	Si	0.972	0.410	-0.734
2	Si	-1.117	-0.128	0.549
3	P	-1.215	-2.257	1.498
4	C/Dur	-1.552	-3.639	0.305
5	C	-2.824	-3.840	-0.284
6	C	-3.039	-4.974	-1.094
7	C	-1.999	-5.886	-1.274
8	C	-0.760	-5.749	-0.640
9	C	-0.533	-4.623	0.173
10	C	0.760	-4.495	0.952
11	H	1.510	-5.216	0.621
12	H	0.585	-4.673	2.023
13	H	1.206	-3.501	0.864



Step-11

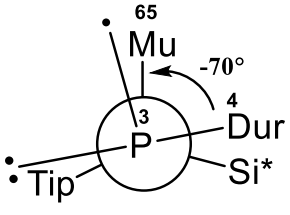
14	C	0.282	-6.831	-0.834
15	H	0.544	-7.324	0.110
16	H	-0.09	-7.603	-1.515
17	H	1.214	-6.438	-1.258
18	H	-2.171	-6.757	-1.903
19	C	-4.379	-5.233	-1.747
20	H	-4.360	-6.169	-2.314
21	H	-5.186	-5.309	-1.006
22	H	-4.663	-4.431	-2.440
23	C	-3.997	-2.938	0.025
24	H	-4.626	-2.760	-0.852
25	H	-3.687	-1.966	0.409
26	H	-4.642	-3.401	0.786
27	C	-2.927	0.555	0.290
28	C	-3.504	0.871	-0.970
29	C	-4.778	1.453	-1.035
30	C	-5.530	1.745	0.100
31	C	-4.980	1.391	1.333
32	C	-3.723	0.787	1.460
33	C	-3.340	0.369	2.889
34	C	-4.334	-0.667	3.455
35	H	-4.407	-1.546	2.806
36	H	-5.340	-0.249	3.569
37	H	-3.999	-1.006	4.443
38	C	-3.212	1.568	3.848
39	H	-2.927	1.221	4.848
40	H	-2.451	2.275	3.505
41	H	-4.159	2.113	3.944
42	H	-2.368	-0.123	2.870
43	H	-5.557	1.577	2.235
44	C	-6.896	2.407	-0.012
45	C	-6.905	3.803	0.640
46	H	-6.712	3.740	1.718
47	H	-7.880	4.287	0.502
48	H	-6.138	4.451	0.200
49	C	-8.018	1.523	0.565
50	H	-8.996	1.994	0.409
51	H	-7.891	1.369	1.643
52	H	-8.034	0.538	0.084
53	H	-7.101	2.542	-1.082
54	H	-5.202	1.686	-2.009
55	C	-2.833	0.545	-2.302
56	C	-2.896	1.686	-3.335
57	H	-2.538	2.632	-2.922
58	H	-2.273	1.436	-4.202
59	H	-3.914	1.845	-3.709
60	C	-3.448	-0.731	-2.918
61	H	-3.257	-1.613	-2.301
62	H	-4.533	-0.620	-3.028

63	H	-3.033	-0.920	-3.915
64	H	-1.775	0.357	-2.103
65	H/Mu	-0.756	0.539	1.824
66	N	0.641	0.023	-2.416
67	C	1.066	0.825	-3.557
68	H	1.882	0.343	-4.121
69	H	1.404	1.811	-3.237
70	H	0.226	0.963	-4.254
71	C	0.008	-1.217	-2.849
72	H	0.707	-1.875	-3.384
73	H	-0.817	-1.006	-3.539
74	H	-0.392	-1.781	-2.000
75	C	2.322	-0.673	0.207
76	C	3.073	-1.742	-0.383
77	C	3.967	-2.490	0.395
78	C	4.203	-2.229	1.744
79	C	3.515	-1.157	2.303
80	C	2.597	-0.381	1.580
81	C	1.994	0.793	2.363
82	C	1.297	0.343	3.663
83	H	0.763	1.188	4.115
84	H	2.020	-0.019	4.404
85	H	0.576	-0.459	3.482
86	C	3.055	1.866	2.682
87	H	3.516	2.256	1.771
88	H	2.592	2.707	3.215
89	H	3.849	1.463	3.322
90	H	1.239	1.281	1.746
91	H	3.706	-0.908	3.344
92	C	5.183	-3.053	2.567
93	H	5.186	-2.631	3.581
94	C	4.742	-4.525	2.682
95	H	3.738	-4.605	3.111
96	H	4.729	-5.013	1.700
97	H	5.433	-5.084	3.324
98	C	6.620	-2.950	2.021
99	H	7.315	-3.507	2.661
100	H	6.693	-3.366	1.010
101	H	6.955	-1.907	1.980
102	H	4.509	-3.303	-0.081
103	C	3.025	-2.143	-1.866
104	C	2.397	-3.535	-2.073
105	H	1.381	-3.593	-1.674
106	H	2.357	-3.782	-3.141
107	H	2.995	-4.310	-1.578
108	C	4.416	-2.116	-2.538
109	H	5.080	-2.891	-2.140
110	H	4.916	-1.153	-2.410
111	H	4.308	-2.300	-3.614

112	H	2.414	-1.412	-2.390
113	C	1.637	2.254	-0.707
114	C	3.006	2.515	-1.032
115	C	3.546	3.795	-0.844
116	C	2.802	4.868	-0.361
117	C	1.452	4.632	-0.114
118	C	0.858	3.376	-0.293
119	C	-0.649	3.334	-0.063
120	C	-1.388	4.277	-1.035
121	H	-1.093	4.092	-2.073
122	H	-1.176	5.328	-0.811
123	H	-2.472	4.131	-0.952
124	C	-1.037	3.670	1.388
125	H	-0.536	3.010	2.103
126	H	-2.118	3.561	1.525
127	H	-0.771	4.703	1.641
128	H	-1.003	2.323	-0.279
129	H	0.828	5.457	0.220
130	C	3.438	6.235	-0.145
131	C	2.820	7.307	-1.063
132	H	3.333	8.267	-0.931
133	H	2.900	7.020	-2.118
134	H	1.758	7.461	-0.837
135	C	3.371	6.669	1.331
136	H	2.333	6.799	1.661
137	H	3.839	5.925	1.985
138	H	3.889	7.624	1.475
139	H	4.499	6.142	-0.414
140	H	4.592	3.963	-1.089
141	C	3.972	1.494	-1.643
142	C	4.483	1.953	-3.027
143	H	3.660	2.200	-3.705
144	H	5.077	1.157	-3.492
145	H	5.125	2.837	-2.946
146	C	5.168	1.198	-0.716
147	H	5.843	0.469	-1.178
148	H	5.750	2.107	-0.524
149	H	4.839	0.794	0.244
150	H	3.434	0.557	-1.801

Rotamer: Step-22

Atom #	Symbol	*x*	*y*	*z*
1	Si	0.972	0.410	-0.734
2	Si	-1.117	-0.128	0.549
3	P	-1.215	-2.257	1.498
4	C/Dur	-1.552	-3.639	0.305
5	C	-2.824	-3.840	-0.284
6	C	-3.039	-4.974	-1.094



Step-22

7	C	-1.999	-5.886	-1.274
8	C	-0.760	-5.749	-0.640
9	C	-0.533	-4.623	0.173
10	C	0.760	-4.495	0.952
11	H	1.510	-5.216	0.621
12	H	0.585	-4.673	2.023
13	H	1.206	-3.501	0.864
14	C	0.282	-6.831	-0.834
15	H	0.544	-7.324	0.110
16	H	-0.090	-7.603	-1.515
17	H	1.214	-6.438	-1.258
18	H	-2.171	-6.757	-1.903
19	C	-4.379	-5.233	-1.747
20	H	-4.360	-6.169	-2.314
21	H	-5.186	-5.309	-1.006
22	H	-4.663	-4.431	-2.440
23	C	-3.997	-2.938	0.025
24	H	-4.626	-2.760	-0.852
25	H	-3.687	-1.966	0.409
26	H	-4.642	-3.401	0.786
27	C	-2.927	0.555	0.290
28	C	-3.504	0.871	-0.970
29	C	-4.778	1.453	-1.035
30	C	-5.530	1.745	0.100
31	C	-4.980	1.391	1.333
32	C	-3.723	0.787	1.460
33	C	-3.340	0.369	2.889
34	C	-4.334	-0.667	3.455
35	H	-4.407	-1.546	2.806
36	H	-5.340	-0.249	3.569
37	H	-3.999	-1.006	4.443
38	C	-3.212	1.568	3.848
39	H	-2.927	1.221	4.848
40	H	-2.451	2.275	3.505
41	H	-4.159	2.113	3.944
42	H	-2.368	-0.123	2.870
43	H	-5.557	1.577	2.235
44	C	-6.896	2.407	-0.012
45	C	-6.905	3.803	0.640
46	H	-6.712	3.740	1.718
47	H	-7.880	4.287	0.502
48	H	-6.138	4.451	0.200
49	C	-8.018	1.523	0.565
50	H	-8.996	1.994	0.409
51	H	-7.891	1.369	1.643
52	H	-8.034	0.538	0.084
53	H	-7.101	2.542	-1.082
54	H	-5.202	1.686	-2.009
55	C	-2.833	0.545	-2.302

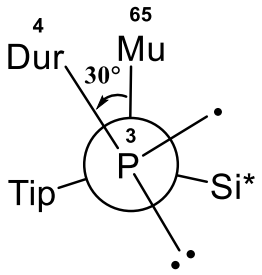
56	C	-2.896	1.686	-3.335
57	H	-2.538	2.632	-2.922
58	H	-2.273	1.436	-4.202
59	H	-3.914	1.845	-3.709
60	C	-3.448	-0.731	-2.918
61	H	-3.257	-1.613	-2.301
62	H	-4.533	-0.620	-3.028
63	H	-3.033	-0.920	-3.915
64	H	-1.775	0.357	-2.103
65	H/Mu	-0.756	0.539	1.824
66	N	0.641	0.023	-2.416
67	C	1.066	0.825	-3.557
68	H	1.882	0.343	-4.121
69	H	1.404	1.811	-3.237
70	H	0.226	0.963	-4.254
71	C	0.008	-1.217	-2.849
72	H	0.707	-1.875	-3.384
73	H	-0.817	-1.006	-3.539
74	H	-0.392	-1.781	-2.000
75	C	2.322	-0.673	0.207
76	C	3.073	-1.742	-0.383
77	C	3.967	-2.490	0.3950
78	C	4.203	-2.229	1.744
79	C	3.515	-1.157	2.303
80	C	2.597	-0.381	1.580
81	C	1.994	0.793	2.363
82	C	1.297	0.343	3.663
83	H	0.763	1.188	4.115
84	H	2.02	-0.019	4.404
85	H	0.576	-0.459	3.482
86	C	3.055	1.866	2.682
87	H	3.516	2.256	1.771
88	H	2.592	2.707	3.215
89	H	3.849	1.463	3.322
90	H	1.239	1.281	1.746
91	H	3.706	-0.908	3.344
92	C	5.183	-3.053	2.567
93	H	5.186	-2.631	3.581
94	C	4.742	-4.525	2.682
95	H	3.738	-4.605	3.111
96	H	4.729	-5.013	1.700
97	H	5.433	-5.084	3.324
98	C	6.620	-2.950	2.021
99	H	7.315	-3.507	2.661
100	H	6.693	-3.366	1.010
101	H	6.955	-1.907	1.980
102	H	4.509	-3.303	-0.081
103	C	3.025	-2.143	-1.866
104	C	2.397	-3.535	-2.073

105	H	1.381	-3.593	-1.674
106	H	2.357	-3.782	-3.141
107	H	2.995	-4.310	-1.578
108	C	4.416	-2.116	-2.538
109	H	5.080	-2.891	-2.140
110	H	4.916	-1.153	-2.410
111	H	4.308	-2.300	-3.614
112	H	2.414	-1.412	-2.390
113	C	1.637	2.254	-0.707
114	C	3.006	2.515	-1.032
115	C	3.546	3.795	-0.844
116	C	2.802	4.868	-0.361
117	C	1.452	4.632	-0.114
118	C	0.858	3.376	-0.293
119	C	-0.649	3.334	-0.063
120	C	-1.388	4.277	-1.035
121	H	-1.093	4.092	-2.073
122	H	-1.176	5.328	-0.811
123	H	-2.472	4.131	-0.952
124	C	-1.037	3.670	1.388
125	H	-0.536	3.010	2.103
126	H	-2.118	3.561	1.525
127	H	-0.771	4.703	1.641
128	H	-1.003	2.323	-0.279
129	H	0.828	5.457	0.220
130	C	3.438	6.235	-0.145
131	C	2.820	7.307	-1.063
132	H	3.333	8.267	-0.931
133	H	2.900	7.020	-2.118
134	H	1.758	7.461	-0.837
135	C	3.371	6.669	1.331
136	H	2.333	6.799	1.661
137	H	3.839	5.925	1.985
138	H	3.889	7.624	1.475
139	H	4.499	6.142	-0.414
140	H	4.592	3.963	-1.089
141	C	3.972	1.494	-1.643
142	C	4.483	1.953	-3.027
143	H	3.660	2.200	-3.705
144	H	5.077	1.157	-3.492
145	H	5.125	2.837	-2.946
146	C	5.168	1.198	-0.716
147	H	5.843	0.469	-1.178
148	H	5.750	2.107	-0.524
149	H	4.839	0.794	0.244
150	H	3.434	0.557	-1.801

Rotamer: Step-37

SUPPORTING INFORMATION

Atom #	Symbol	*x*	*y*	*z*
1	Si	1.313	-0.335	0.978
2	Si	-1.052	0.104	0.345
3	P	-1.913	1.838	1.651
4	C/Dur	-2.893	2.844	0.430
5	C	-4.307	2.710	0.427
6	C	-5.077	3.521	-0.427
7	C	-4.426	4.452	-1.243
8	C	-3.041	4.615	-1.237
9	C	-2.258	3.806	-0.390
10	C	-0.763	4.023	-0.370
11	H	-0.517	5.040	-0.036
12	H	-0.323	3.905	-1.368
13	H	-0.243	3.329	0.293
14	C	-2.405	5.656	-2.130
15	H	-1.691	5.209	-2.834
16	H	-3.163	6.184	-2.716
17	H	-1.847	6.405	-1.553
18	H	-5.024	5.079	-1.901
19	C	-6.587	3.419	-0.497
20	H	-6.984	4.126	-1.232
21	H	-6.920	2.416	-0.791
22	H	-7.063	3.644	0.465
23	C	-4.979	1.690	1.323
24	H	-4.658	1.804	2.366
25	H	-4.730	0.664	1.023
26	H	-6.066	1.781	1.305
27	C	-2.463	-1.211	0.195
28	C	-2.932	-1.888	1.354
29	C	-4.034	-2.751	1.271
30	C	-4.712	-2.977	0.077
31	C	-4.240	-2.321	-1.064
32	C	-3.137	-1.459	-1.044
33	C	-2.741	-0.806	-2.375
34	C	-3.500	0.518	-2.594
35	H	-3.310	1.236	-1.792
36	H	-4.581	0.337	-2.634
37	H	-3.200	0.979	-3.543
38	C	-2.932	-1.711	-3.608
39	H	-2.456	-1.242	-4.478
40	H	-2.483	-2.699	-3.468
41	H	-3.989	-1.852	-3.861
42	H	-1.675	-0.571	-2.329
43	H	-4.750	-2.491	-2.007
44	C	-5.918	-3.905	0.024
45	C	-5.675	-5.114	-0.899
46	H	-5.534	-4.800	-1.940
47	H	-6.532	-5.797	-0.871
48	H	-4.784	-5.673	-0.593



Step-37

49	C	-7.201	-3.152	-0.380
50	H	-8.066	-3.825	-0.354
51	H	-7.122	-2.749	-1.396
52	H	-7.398	-2.315	0.299
53	H	-6.071	-4.292	1.040
54	H	-4.377	-3.258	2.171
55	C	-2.290	-1.718	2.729
56	C	-1.733	-3.043	3.285
57	H	-1.004	-3.489	2.605
58	H	-1.240	-2.871	4.249
59	H	-2.532	-3.775	3.451
60	C	-3.256	-1.087	3.751
61	H	-3.637	-0.123	3.402
62	H	-4.114	-1.743	3.941
63	H	-2.745	-0.923	4.707
64	H	-1.438	-1.041	2.619
65	H/Mu	-0.934	0.752	-0.978
66	N	1.324	-0.638	2.717
67	C	2.098	-1.688	3.373
68	H	2.866	-1.266	4.042
69	H	2.590	-2.333	2.647
70	H	1.437	-2.316	3.991
71	C	0.578	0.116	3.717
72	H	1.251	0.599	4.443
73	H	-0.085	-0.546	4.292
74	H	-0.031	0.900	3.265
75	C	2.072	1.328	0.243
76	C	2.575	2.417	1.022
77	C	3.066	3.572	0.398
78	C	3.126	3.713	-0.987
79	C	2.655	2.646	-1.747
80	C	2.125	1.478	-1.180
81	C	1.674	0.417	-2.197
82	C	0.701	0.979	-3.255
83	H	0.296	0.160	-3.861
84	H	1.205	1.668	-3.941
85	H	-0.138	1.513	-2.799
86	C	2.874	-0.235	-2.916
87	H	3.559	-0.711	-2.211
88	H	2.523	-1.000	-3.619
89	H	3.435	0.512	-3.489
90	H	1.147	-0.382	-1.669
91	H	2.706	2.728	-2.830
92	C	3.690	4.963	-1.648
93	H	3.617	4.814	-2.734
94	C	2.870	6.220	-1.299
95	H	1.818	6.096	-1.577
96	H	2.910	6.435	-0.225
97	H	3.263	7.095	-1.829

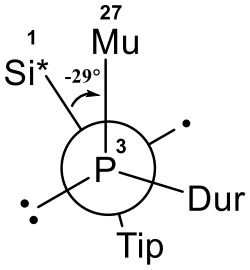
98	C	5.179	5.166	-1.309
99	H	5.581	6.037	-1.842
100	H	5.323	5.336	-0.236
101	H	5.773	4.289	-1.592
102	H	3.429	4.383	1.023
103	C	2.640	2.424	2.553
104	C	1.641	3.430	3.158
105	H	0.614	3.228	2.835
106	H	1.666	3.386	4.254
107	H	1.887	4.456	2.860
108	C	4.057	2.708	3.094
109	H	4.390	3.727	2.868
110	H	4.797	2.016	2.679
111	H	4.067	2.597	4.185
112	H	2.375	1.429	2.901
113	C	2.420	-1.773	0.254
114	C	3.846	-1.651	0.309
115	C	4.657	-2.602	-0.325
116	C	4.143	-3.703	-1.006
117	C	2.759	-3.860	-0.992
118	C	1.901	-2.943	-0.370
119	C	0.423	-3.323	-0.367
120	C	0.190	-4.640	0.401
121	H	0.613	-4.596	1.411
122	H	0.652	-5.490	-0.114
123	H	-0.883	-4.846	0.487
124	C	-0.160	-3.432	-1.787
125	H	-0.031	-2.502	-2.350
126	H	-1.231	-3.654	-1.740
127	H	0.324	-4.234	-2.356
128	H	-0.138	-2.546	0.159
129	H	2.325	-4.734	-1.472
130	C	5.062	-4.699	-1.701
131	C	4.982	-6.098	-1.060
132	H	5.691	-6.782	-1.542
133	H	5.218	-6.059	0.009
134	H	3.979	-6.528	-1.167
135	C	4.788	-4.770	-3.215
136	H	3.778	-5.143	-3.420
137	H	4.883	-3.783	-3.682
138	H	5.500	-5.448	-3.702
139	H	6.090	-4.335	-1.568
140	H	5.736	-2.482	-0.280
141	C	4.602	-0.562	1.081
142	C	5.498	-1.167	2.184
143	H	4.939	-1.834	2.846
144	H	5.931	-0.366	2.796
145	H	6.330	-1.740	1.758
146	C	5.450	0.335	0.158

147	H	5.963	1.106	0.744
148	H	6.218	-0.248	-0.363
149	H	4.833	0.835	-0.593
150	H	3.874	0.078	1.582

Si-P(Mu)-Dur: Dihedral angle: 27(Mu)-3(P)-2(Si)-1(Si)

Rotamer: Step-3

Atom #	Symbol	*x*	*y*	*z*
1	Si	-1.317	-0.071	0.928
2	Si	0.988	-0.284	0.153
3	P	1.512	-2.095	-1.168
4	C	3.077	-2.829	-0.449
5	C	4.302	-2.445	-1.053
6	C	5.510	-3.009	-0.594
7	C	5.468	-3.962	0.422
8	C	4.273	-4.376	1.015
9	C	3.061	-3.795	0.591
10	C	1.769	-4.225	1.249
11	H	1.148	-3.363	1.505
12	H	1.948	-4.786	2.168
13	H	1.167	-4.867	0.591
14	C	4.329	-5.435	2.097
15	H	3.719	-6.312	1.850
16	H	5.358	-5.779	2.242
17	H	3.971	-5.059	3.064
18	H	6.401	-4.405	0.763
19	C	6.846	-2.610	-1.182
20	H	7.665	-3.096	-0.643
21	H	6.933	-2.894	-2.239
22	H	7.009	-1.527	-1.132
23	C	4.363	-1.433	-2.176
24	H	4.553	-0.420	-1.796
25	H	3.426	-1.397	-2.736
26	H	5.164	-1.668	-2.883
27	H/Mu	0.542	-2.972	-0.631
28	C	2.312	1.095	-0.068
29	C	3.227	1.340	0.995
30	C	4.193	2.347	0.863
31	C	4.305	3.132	-0.284
32	C	3.418	2.870	-1.332
33	C	2.438	1.874	-1.255
34	C	1.552	1.664	-2.483
35	C	2.370	1.461	-3.774
36	H	3.125	0.679	-3.657
37	H	2.883	2.381	-4.078
38	H	1.706	1.173	-4.598



Step-3

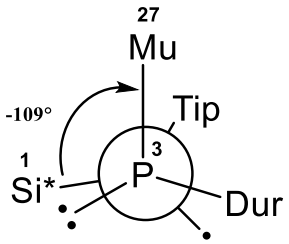
39	C	0.538	2.807	-2.685
40	H	-0.035	2.651	-3.607
41	H	-0.173	2.872	-1.856
42	H	1.048	3.774	-2.774
43	H	0.980	0.745	-2.318
44	H	3.491	3.460	-2.242
45	C	5.370	4.215	-0.389
46	C	4.754	5.612	-0.594
47	H	4.214	5.674	-1.546
48	H	5.537	6.379	-0.604
49	H	4.048	5.855	0.208
50	C	6.397	3.899	-1.493
51	H	7.187	4.660	-1.514
52	H	5.925	3.880	-2.482
53	H	6.869	2.923	-1.328
54	H	5.909	4.230	0.568
55	H	4.888	2.521	1.682
56	C	3.244	0.522	2.286
57	C	3.012	1.383	3.541
58	H	2.064	1.926	3.482
59	H	2.986	0.750	4.436
60	H	3.813	2.118	3.680
61	C	4.541	-0.300	2.421
62	H	4.686	-0.958	1.558
63	H	5.420	0.350	2.504
64	H	4.503	-0.924	3.322
65	H	2.415	-0.195	2.229
66	N	-1.132	-0.286	2.672
67	C	-2.122	0.183	3.637
68	H	-2.773	-0.632	3.999
69	H	-2.754	0.958	3.203
70	H	-1.618	0.608	4.517
71	C	-0.164	-1.157	3.325
72	H	-0.639	-2.041	3.782
73	H	0.357	-0.614	4.129
74	H	0.586	-1.507	2.613
75	C	-2.213	-1.477	-0.118
76	C	-2.749	-2.676	0.456
77	C	-3.326	-3.660	-0.359
78	C	-3.449	-3.520	-1.739
79	C	-2.960	-2.342	-2.294
80	C	-2.343	-1.335	-1.537
81	C	-1.874	-0.119	-2.353
82	C	-1.007	-0.530	-3.562
83	H	-0.620	0.362	-4.066
84	H	-1.591	-1.085	-4.303
85	H	-0.158	-1.155	-3.268
86	C	-3.050	0.741	-2.862
87	H	-3.643	1.150	-2.043

88	H	-2.668	1.582	-3.453
89	H	-3.712	0.153	-3.509
90	H	-1.261	0.522	-1.709
91	H	-3.066	-2.201	-3.367
92	C	-4.087	-4.595	-2.609
93	H	-4.090	-4.214	-3.639
94	C	-3.261	-5.896	-2.600
95	H	-2.230	-5.712	-2.923
96	H	-3.225	-6.337	-1.597
97	H	-3.704	-6.638	-3.276
98	C	-5.550	-4.867	-2.214
99	H	-6.002	-5.598	-2.895
100	H	-5.621	-5.273	-1.197
101	H	-6.149	-3.950	-2.252
102	H	-3.707	-4.562	0.112
103	C	-2.791	-2.987	1.958
104	C	-1.958	-4.233	2.317
105	H	-0.920	-4.130	1.989
106	H	-1.958	-4.394	3.402
107	H	-2.365	-5.138	1.850
108	C	-4.235	-3.162	2.477
109	H	-4.722	-4.040	2.038
110	H	-4.858	-2.290	2.251
111	H	-4.228	-3.298	3.565
112	H	-2.363	-2.142	2.489
113	C	-2.324	1.587	0.761
114	C	-3.738	1.582	0.563
115	C	-4.395	2.758	0.167
116	C	-3.733	3.973	0.012
117	C	-2.384	4.009	0.375
118	C	-1.683	2.867	0.779
119	C	-0.308	3.088	1.416
120	C	-0.499	3.379	2.923
121	H	-1.001	2.556	3.436
122	H	-1.100	4.286	3.062
123	H	0.471	3.544	3.407
124	C	0.535	4.222	0.807
125	H	0.613	4.149	-0.279
126	H	1.550	4.180	1.217
127	H	0.127	5.209	1.055
128	H	0.275	2.167	1.331
129	H	-1.867	4.964	0.370
130	C	-4.473	5.215	-0.461
131	C	-4.515	6.312	0.621
132	H	-5.109	7.167	0.278
133	H	-4.962	5.936	1.548
134	H	-3.509	6.678	0.857
135	C	-3.884	5.761	-1.776
136	H	-2.849	6.095	-1.640

137	H	-3.889	4.995	-2.560
138	H	-4.468	6.618	-2.133
139	H	-5.510	4.915	-0.664
140	H	-5.468	2.727	-0.005
141	C	-4.650	0.403	0.929
142	C	-5.541	0.786	2.133
143	H	-4.954	1.168	2.974
144	H	-6.102	-0.090	2.481
145	H	-6.270	1.558	1.859
146	C	-5.538	-0.115	-0.218
147	H	-6.190	-0.917	0.148
148	H	-6.184	0.677	-0.614
149	H	-4.944	-0.516	-1.041
150	H	-4.021	-0.429	1.251

Rotamer: Step-11

Atom #	Symbol	*x*	*y*	*z*
1	Si	1.363	-0.283	0.978
2	Si	-1.008	-0.026	0.324
3	P	-1.725	1.917	1.379
4	C	-3.046	2.745	0.349
5	C	-2.610	3.692	-0.610
6	C	-3.559	4.462	-1.311
7	C	-4.913	4.287	-1.029
8	C	-5.369	3.361	-0.088
9	C	-4.433	2.562	0.602
10	C	-4.938	1.529	1.588
11	H	-4.46	0.557	1.431
12	H	-6.014	1.378	1.494
13	H	-4.746	1.822	2.629
14	C	-6.862	3.248	0.149
15	H	-7.128	3.410	1.200
16	H	-7.399	3.994	-0.446
17	H	-7.254	2.262	-0.133
18	H	-5.642	4.894	-1.562
19	C	-3.135	5.480	-2.345
20	H	-4.006	5.985	-2.774
21	H	-2.408	6.249	-1.917
22	H	-2.577	5.018	-3.169
23	C	-1.147	3.930	-0.917
24	H	-0.474	3.284	-0.351
25	H	-0.863	4.968	-0.698
26	H	-0.936	3.767	-1.980
27	H/Mu	-2.563	1.285	2.326
28	C	-2.397	-1.370	0.218
29	C	-2.752	-2.196	1.321
30	C	-3.766	-3.151	1.180
31	C	-4.468	-3.327	-0.013



Step-11

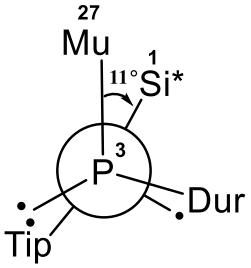
32	C	-4.137	-2.492	-1.083
33	C	-3.129	-1.524	-0.997
34	C	-2.912	-0.631	-2.222
35	C	-4.091	0.342	-2.418
36	H	-4.255	0.962	-1.533
37	H	-5.019	-0.206	-2.628
38	H	-3.897	1.008	-3.268
39	C	-2.663	-1.414	-3.524
40	H	-2.430	-0.718	-4.338
41	H	-1.830	-2.115	-3.428
42	H	-3.548	-1.985	-3.829
43	H	-2.017	-0.024	-2.028
44	H	-4.684	-2.592	-2.017
45	C	-5.560	-4.382	-0.128
46	C	-5.219	-5.447	-1.187
47	H	-5.159	-5.006	-2.189
48	H	-5.990	-6.226	-1.211
49	H	-4.257	-5.926	-0.972
50	C	-6.939	-3.753	-0.402
51	H	-7.718	-4.525	-0.418
52	H	-6.958	-3.240	-1.371
53	H	-7.201	-3.020	0.370
54	H	-5.618	-4.891	0.844
55	H	-4.027	-3.775	2.032
56	C	-2.108	-2.045	2.698
57	C	-1.543	-3.361	3.263
58	H	-0.819	-3.816	2.584
59	H	-1.042	-3.176	4.220
60	H	-2.336	-4.095	3.449
61	C	-3.095	-1.430	3.712
62	H	-3.494	-0.473	3.363
63	H	-3.943	-2.103	3.885
64	H	-2.600	-1.262	4.676
65	H	-1.264	-1.355	2.587
66	N	1.399	-0.561	2.721
67	C	2.125	-1.648	3.370
68	H	2.845	-1.259	4.107
69	H	2.669	-2.251	2.643
70	H	1.431	-2.311	3.911
71	C	0.596	0.161	3.700
72	H	1.230	0.601	4.486
73	H	-0.118	-0.508	4.204
74	H	0.034	0.977	3.240
75	C	2.021	1.427	0.269
76	C	2.491	2.531	1.049
77	C	2.916	3.710	0.424
78	C	2.938	3.868	-0.961
79	C	2.503	2.786	-1.721
80	C	2.043	1.590	-1.152

81	C	1.630	0.512	-2.167
82	C	0.549	1.008	-3.148
83	H	0.211	0.181	-3.784
84	H	0.931	1.794	-3.810
85	H	-0.320	1.408	-2.618
86	C	2.841	-0.027	-2.954
87	H	3.599	-0.446	-2.287
88	H	2.521	-0.817	-3.645
89	H	3.309	0.765	-3.550
90	H	1.199	-0.336	-1.631
91	H	2.525	2.877	-2.805
92	C	3.437	5.146	-1.621
93	H	3.327	5.012	-2.706
94	C	2.597	6.373	-1.221
95	H	1.539	6.226	-1.464
96	H	2.669	6.572	-0.145
97	H	2.948	7.268	-1.749
98	C	4.932	5.385	-1.336
99	H	5.288	6.277	-1.866
100	H	5.112	5.538	-0.265
101	H	5.539	4.532	-1.659
102	H	3.256	4.532	1.048
103	C	2.593	2.534	2.579
104	C	1.583	3.513	3.212
105	H	0.561	3.308	2.879
106	H	1.612	3.440	4.307
107	H	1.821	4.550	2.943
108	C	4.014	2.857	3.087
109	H	4.315	3.882	2.846
110	H	4.763	2.182	2.662
111	H	4.050	2.754	4.179
112	H	2.362	1.532	2.931
113	C	2.540	-1.658	0.248
114	C	3.956	-1.460	0.296
115	C	4.814	-2.356	-0.355
116	C	4.357	-3.474	-1.049
117	C	2.983	-3.707	-1.028
118	C	2.082	-2.848	-0.384
119	C	0.627	-3.309	-0.370
120	C	0.479	-4.664	0.353
121	H	0.921	-4.634	1.355
122	H	0.971	-5.470	-0.202
123	H	-0.580	-4.927	0.451
124	C	0.028	-3.396	-1.783
125	H	0.115	-2.441	-2.310
126	H	-1.033	-3.662	-1.733
127	H	0.538	-4.157	-2.386
128	H	0.038	-2.581	0.196
129	H	2.593	-4.595	-1.518

130	C	5.325	-4.405	-1.766
131	C	5.296	-5.830	-1.181
132	H	6.046	-6.462	-1.671
133	H	5.508	-5.821	-0.106
134	H	4.317	-6.301	-1.327
135	C	5.073	-4.427	-3.286
136	H	4.082	-4.833	-3.519
137	H	5.131	-3.419	-3.711
138	H	5.818	-5.054	-3.790
139	H	6.335	-4.004	-1.605
140	H	5.886	-2.180	-0.312
141	C	4.652	-0.345	1.084
142	C	5.565	-0.920	2.189
143	H	5.022	-1.603	2.850
144	H	5.971	-0.107	2.803
145	H	6.415	-1.468	1.766
146	C	5.461	0.601	0.174
147	H	5.928	1.395	0.768
148	H	6.263	0.063	-0.343
149	H	4.825	1.073	-0.580
150	H	3.891	0.251	1.588

Rotamer: Step-20

Atom #	Symbol	x	y	z
1	Si	-0.110	0.962	0.880
2	Si	0.645	-1.216	-0.084
3	P	-0.368	-3.209	0.571
4	C	-2.198	-3.434	0.264
5	C	-2.997	-3.794	1.381
6	C	-4.357	-4.117	1.185
7	C	-4.881	-4.099	-0.106
8	C	-4.110	-3.769	-1.222
9	C	-2.758	-3.418	-1.041
10	C	-1.933	-3.073	-2.259
11	H	-1.139	-2.364	-2.018
12	H	-2.547	-2.628	-3.046
13	H	-1.454	-3.965	-2.689
14	C	-4.747	-3.813	-2.594
15	H	-4.205	-4.478	-3.278
16	H	-5.779	-4.173	-2.528
17	H	-4.773	-2.824	-3.070
18	H	-5.926	-4.363	-0.251
19	C	-5.249	-4.497	2.345
20	H	-6.265	-4.714	2.000
21	H	-4.879	-5.385	2.873
22	H	-5.314	-3.694	3.091
23	C	-2.467	-3.877	2.799
24	H	-1.408	-3.633	2.867



Step-20

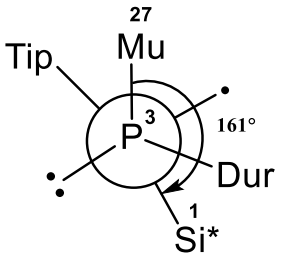
25	H	-2.598	-4.889	3.204
26	H	-3.015	-3.200	3.466
27	H/Mu	0.111	-3.885	-0.580
28	C	2.457	-1.931	-0.049
29	C	3.224	-2.071	1.142
30	C	4.532	-2.570	1.076
31	C	5.126	-2.960	-0.124
32	C	4.352	-2.869	-1.283
33	C	3.040	-2.379	-1.272
34	C	2.270	-2.431	-2.596
35	C	1.981	-3.890	-3.007
36	H	1.463	-4.440	-2.215
37	H	2.911	-4.427	-3.231
38	H	1.354	-3.918	-3.907
39	C	2.970	-1.694	-3.753
40	H	2.341	-1.723	-4.650
41	H	3.164	-0.646	-3.508
42	H	3.928	-2.161	-4.010
43	H	1.303	-1.936	-2.434
44	H	4.777	-3.201	-2.227
45	C	6.556	-3.483	-0.154
46	C	7.481	-2.563	-0.974
47	H	7.176	-2.528	-2.026
48	H	8.515	-2.925	-0.937
49	H	7.465	-1.538	-0.585
50	C	6.629	-4.935	-0.665
51	H	7.660	-5.306	-0.621
52	H	6.293	-5.009	-1.706
53	H	6.002	-5.600	-0.061
54	H	6.922	-3.480	0.881
55	H	5.104	-2.672	1.995
56	C	2.650	-1.780	2.527
57	C	3.533	-0.866	3.396
58	H	3.732	0.090	2.906
59	H	3.033	-0.662	4.350
60	H	4.497	-1.332	3.630
61	C	2.364	-3.095	3.282
62	H	1.698	-3.746	2.708
63	H	3.295	-3.642	3.478
64	H	1.890	-2.887	4.250
65	H	1.698	-1.260	2.383
66	N	-0.131	0.771	2.630
67	C	0.460	1.700	3.587
68	H	-0.298	2.095	4.282
69	H	0.931	2.541	3.079
70	H	1.228	1.195	4.193
71	C	-0.642	-0.412	3.309
72	H	-1.439	-0.154	4.024
73	H	0.150	-0.919	3.879

74	H	-1.057	-1.129	2.599
75	C	-1.816	1.128	-0.079
76	C	-3.116	1.090	0.515
77	C	-4.263	1.190	-0.283
78	C	-4.211	1.359	-1.666
79	C	-2.946	1.425	-2.242
80	C	-1.764	1.315	-1.497
81	C	-0.470	1.474	-2.307
82	C	-0.381	0.496	-3.494
83	H	0.603	0.574	-3.972
84	H	-1.133	0.715	-4.259
85	H	-0.521	-0.540	-3.172
86	C	-0.292	2.920	-2.814
87	H	-0.291	3.638	-1.990
88	H	0.658	3.019	-3.353
89	H	-1.098	3.194	-3.505
90	H	0.383	1.258	-1.658
91	H	-2.876	1.581	-3.316
92	C	-5.469	1.503	-2.511
93	H	-5.147	1.567	-3.559
94	C	-6.399	0.281	-2.388
95	H	-5.876	-0.644	-2.651
96	H	-6.780	0.170	-1.366
97	H	-7.263	0.387	-3.056
98	C	-6.226	2.804	-2.180
99	H	-7.097	2.923	-2.836
100	H	-6.585	2.799	-1.144
101	H	-5.581	3.680	-2.307
102	H	-5.235	1.146	0.202
103	C	-3.384	0.956	2.020
104	C	-4.028	-0.403	2.351
105	H	-3.439	-1.234	1.955
106	H	-4.126	-0.530	3.436
107	H	-5.031	-0.478	1.915
108	C	-4.264	2.090	2.587
109	H	-5.281	2.063	2.180
110	H	-3.847	3.079	2.375
111	H	-4.346	1.985	3.676
112	H	-2.429	1.017	2.538
113	C	0.842	2.645	0.568
114	C	0.141	3.878	0.761
115	C	0.744	5.094	0.410
116	C	2.029	5.180	-0.118
117	C	2.734	3.985	-0.244
118	C	2.185	2.743	0.102
119	C	3.134	1.556	-0.023
120	C	4.396	1.746	0.844
121	H	4.138	2.005	1.876
122	H	5.036	2.546	0.453

123	H	4.988	0.824	0.856
124	C	3.541	1.290	-1.483
125	H	2.666	1.109	-2.116
126	H	4.191	0.412	-1.545
127	H	4.084	2.144	-1.904
128	H	2.625	0.663	0.348
129	H	3.754	4.015	-0.615
130	C	2.634	6.522	-0.506
131	C	3.868	6.865	0.349
132	H	4.249	7.860	0.091
133	H	3.625	6.858	1.417
134	H	4.679	6.145	0.184
135	C	2.970	6.583	-2.009
136	H	3.736	5.846	-2.275
137	H	2.084	6.383	-2.622
138	H	3.353	7.575	-2.276
139	H	1.872	7.288	-0.307
140	H	0.187	6.016	0.560
141	C	-1.251	4.006	1.387
142	C	-1.218	4.854	2.678
143	H	-0.481	4.477	3.393
144	H	-2.202	4.837	3.164
145	H	-0.975	5.901	2.468
146	C	-2.278	4.594	0.398
147	H	-3.266	4.667	0.867
148	H	-1.990	5.604	0.084
149	H	-2.373	3.972	-0.496
150	H	-1.598	3.013	1.673

Rotamer: Step-35

Atom #	Symbol	*x*	*y*	*z*
1	Si	0.600	0.781	-0.847
2	Si	-0.932	-0.906	0.085
3	P	-0.017	-2.604	1.344
4	C	0.472	-4.094	0.320
5	C	-0.522	-4.800	-0.396
6	C	-0.166	-5.943	-1.138
7	C	1.160	-6.374	-1.114
8	C	2.142	-5.741	-0.349
9	C	1.800	-4.593	0.395
10	C	2.839	-3.947	1.289
11	H	3.144	-2.958	0.928
12	H	3.741	-4.558	1.358
13	H	2.462	-3.812	2.310
14	C	3.544	-6.318	-0.349
15	H	3.840	-6.685	0.642
16	H	3.608	-7.162	-1.042



Step-35

17	H	4.296	-5.580	-0.654
18	H	1.435	-7.252	-1.695
19	C	-1.179	-6.715	-1.957
20	H	-0.688	-7.515	-2.519
21	H	-1.949	-7.181	-1.328
22	H	-1.702	-6.075	-2.678
23	C	-1.962	-4.347	-0.364
24	H	-2.244	-3.969	0.624
25	H	-2.650	-5.161	-0.608
26	H	-2.150	-3.536	-1.076
27	H/Mu	1.253	-1.994	1.420
28	C	-2.856	-0.824	0.209
29	C	-3.643	-0.802	-0.980
30	C	-5.031	-0.620	-0.900
31	C	-5.703	-0.506	0.315
32	C	-4.937	-0.600	1.480
33	C	-3.545	-0.749	1.461
34	C	-2.854	-0.898	2.819
35	C	-3.125	-2.297	3.411
36	H	-2.810	-3.093	2.731
37	H	-4.194	-2.430	3.618
38	H	-2.580	-2.426	4.354
39	C	-3.246	0.176	3.852
40	H	-2.645	0.047	4.761
41	H	-3.077	1.187	3.475
42	H	-4.298	0.097	4.148
43	H	-1.775	-0.810	2.659
44	H	-5.441	-0.554	2.441
45	C	-7.212	-0.316	0.361
46	C	-7.603	1.011	1.040
47	H	-7.295	1.026	2.093
48	H	-8.690	1.153	1.009
49	H	-7.133	1.865	0.541
50	C	-7.920	-1.509	1.033
51	H	-9.008	-1.376	1.005
52	H	-7.623	-1.608	2.084
53	H	-7.677	-2.449	0.526
54	H	-7.563	-0.269	-0.678
55	H	-5.611	-0.587	-1.820
56	C	-3.058	-1.025	-2.375
57	C	-3.102	0.236	-3.255
58	H	-2.496	1.040	-2.829
59	H	-2.715	0.016	-4.257
60	H	-4.128	0.605	-3.369
61	C	-3.743	-2.196	-3.113
62	H	-3.779	-3.102	-2.500
63	H	-4.772	-1.945	-3.396
64	H	-3.197	-2.428	-4.035
65	H	-2.005	-1.297	-2.242

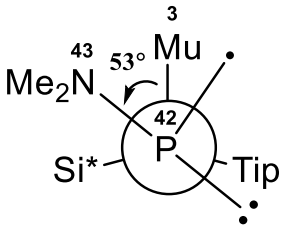
66	N	0.502	0.443	-2.575
67	C	0.516	1.455	-3.626
68	H	1.442	1.411	-4.222
69	H	0.423	2.457	-3.208
70	H	-0.326	1.296	-4.315
71	C	0.462	-0.891	-3.159
72	H	1.351	-1.093	-3.777
73	H	-0.414	-1.001	-3.814
74	H	0.41	-1.663	-2.387
75	C	2.238	0.350	0.140
76	C	3.402	-0.263	-0.420
77	C	4.521	-0.522	0.383
78	C	4.575	-0.185	1.736
79	C	3.446	0.423	2.278
80	C	2.292	0.691	1.528
81	C	1.160	1.386	2.298
82	C	0.728	0.600	3.553
83	H	-0.145	1.078	4.012
84	H	1.522	0.577	4.308
85	H	0.464	-0.435	3.319
86	C	1.538	2.827	2.695
87	H	1.798	3.430	1.821
88	H	0.697	3.312	3.206
89	H	2.393	2.834	3.381
90	H	0.280	1.453	1.651
91	H	3.468	0.707	3.327
92	C	5.814	-0.442	2.583
93	H	5.583	-0.104	3.602
94	C	6.163	-1.940	2.663
95	H	5.322	-2.524	3.053
96	H	6.423	-2.342	1.676
97	H	7.024	-2.099	3.324
98	C	7.021	0.377	2.086
99	H	7.886	0.226	2.743
100	H	7.314	0.077	1.073
101	H	6.791	1.448	2.065
102	H	5.387	-0.995	-0.072
103	C	3.538	-0.664	-1.893
104	C	3.502	-2.196	-2.069
105	H	2.593	-2.635	-1.648
106	H	3.547	-2.462	-3.133
107	H	4.360	-2.666	-1.574
108	C	4.806	-0.097	-2.565
109	H	5.722	-0.538	-2.157
110	H	4.879	0.989	-2.450
111	H	4.788	-0.322	-3.638
112	H	2.690	-0.244	-2.430
113	C	0.414	2.728	-0.723
114	C	1.556	3.555	-0.979

115	C	1.487	4.938	-0.758
116	C	0.333	5.580	-0.318
117	C	-0.797	4.785	-0.144
118	C	-0.785	3.398	-0.347
119	C	-2.132	2.703	-0.172
120	C	-3.180	3.242	-1.168
121	H	-2.815	3.205	-2.199
122	H	-3.443	4.283	-0.945
123	H	-4.098	2.646	-1.110
124	C	-2.661	2.829	1.267
125	H	-1.939	2.437	1.990
126	H	-3.596	2.271	1.381
127	H	-2.859	3.875	1.528
128	H	-2.006	1.638	-0.382
129	H	-1.729	5.256	0.155
130	C	0.310	7.083	-0.077
131	C	-0.628	7.805	-1.064
132	H	-0.589	8.890	-0.901
133	H	-0.345	7.598	-2.103
134	H	-1.668	7.485	-0.930
135	C	-0.055	7.425	1.379
136	H	-1.073	7.098	1.623
137	H	0.630	6.940	2.084
138	H	-0.005	8.508	1.544
139	H	1.327	7.454	-0.259
140	H	2.372	5.541	-0.947
141	C	2.889	3.060	-1.552
142	C	3.225	3.748	-2.895
143	H	2.408	3.659	-3.617
144	H	4.118	3.291	-3.337
145	H	3.436	4.815	-2.759
146	C	4.057	3.253	-0.566
147	H	4.989	2.867	-0.996
148	H	4.213	4.316	-0.345
149	H	3.877	2.731	0.377
150	H	2.803	1.993	-1.760

Mu-Si-P-NMe$_2$: Dihedral angle: 3(Mu)-2(Si)-42(P)-43(N)

Rotamer: Step-2

Atom #	Symbol	*x*	*y*	*z*
1	Si	0.988	-0.307	0.933
2	Si	-1.289	-1.386	0.715
3	H/Mu	-1.009	-2.677	0.049
4	C	-2.823	-0.67	-0.225
5	C	-3.419	-1.392	-1.31
6	C	-4.649	-0.973	-1.827
7	C	-5.334	0.143	-1.341



Step-2

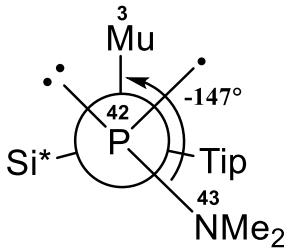
8	C	-4.735	0.856	-0.309
9	C	-3.506	0.48	0.253
10	C	-2.974	1.381	1.367
11	H	-1.988	1.006	1.671
12	C	-2.773	2.826	0.869
13	H	-2.338	3.446	1.66
14	H	-2.103	2.86	0.006
15	H	-3.728	3.28	0.581
16	C	-3.882	1.37	2.614
17	H	-4.011	0.359	3.01
18	H	-3.449	1.995	3.405
19	H	-4.874	1.774	2.381
20	H	-5.245	1.735	0.078
21	C	-6.678	0.57	-1.916
22	H	-6.985	1.476	-1.375
23	C	-6.576	0.936	-3.408
24	H	-5.827	1.719	-3.575
25	H	-6.291	0.067	-4.013
26	H	-7.54	1.3	-3.783
27	C	-7.764	-0.497	-1.682
28	H	-7.867	-0.729	-0.616
29	H	-8.735	-0.148	-2.052
30	H	-7.523	-1.43	-2.205
31	H	-5.091	-1.538	-2.642
32	C	-2.802	-2.645	-1.942
33	H	-1.725	-2.612	-1.772
34	C	-2.988	-2.741	-3.468
35	H	-2.369	-3.556	-3.861
36	H	-4.023	-2.961	-3.753
37	H	-2.69	-1.815	-3.972
38	C	-3.34	-3.922	-1.264
39	H	-4.422	-4.012	-1.418
40	H	-2.862	-4.816	-1.685
41	H	-3.158	-3.911	-0.184
42	P	-2.43	-2.073	2.597
43	N	-1.471	-3.254	3.411
44	C	-0.258	-3.886	2.917
45	H	0.328	-4.268	3.762
46	H	-0.475	-4.733	2.247
47	H	0.355	-3.159	2.382
48	C	-2.135	-4.006	4.472
49	H	-2.466	-4.997	4.124
50	H	-1.449	-4.152	5.317
51	H	-3.011	-3.457	4.827
52	C	0.771	1.552	0.35
53	C	0.495	1.782	-1.033
54	C	0.359	3.09	-1.52
55	C	0.459	4.213	-0.704
56	C	0.719	3.989	0.647

57	C	0.89	2.707	1.185
58	C	1.221	2.662	2.683
59	H	1.509	1.642	2.93
60	C	0.003	3.039	3.549
61	H	-0.317	4.069	3.348
62	H	-0.852	2.384	3.359
63	H	0.25	2.971	4.615
64	C	2.416	3.56	3.069
65	H	3.301	3.347	2.462
66	H	2.185	4.625	2.957
67	H	2.68	3.395	4.121
68	H	0.805	4.845	1.311
69	C	0.299	5.616	-1.273
70	H	0.107	5.507	-2.35
71	C	-0.91	6.35	-0.662
72	H	-0.776	6.507	0.415
73	H	-1.039	7.335	-1.127
74	H	-1.834	5.78	-0.804
75	C	1.585	6.449	-1.117
76	H	1.468	7.432	-1.589
77	H	1.827	6.614	-0.061
78	H	2.441	5.948	-1.582
79	H	0.168	3.239	-2.58
80	C	0.37	0.674	-2.088
81	H	0.357	-0.298	-1.583
82	C	1.574	0.665	-3.052
83	H	2.521	0.537	-2.523
84	H	1.475	-0.154	-3.776
85	H	1.623	1.603	-3.617
86	C	-0.934	0.779	-2.904
87	H	-1.814	0.838	-2.26
88	H	-0.927	1.659	-3.557
89	H	-1.042	-0.1	-3.549
90	C	2.561	-0.988	-0.042
91	C	3.714	-0.147	-0.193
92	C	4.755	-0.52	-1.051
93	C	4.757	-1.718	-1.765
94	C	3.695	-2.583	-1.529
95	C	2.631	-2.262	-0.674
96	C	1.645	-3.395	-0.409
97	H	0.869	-3.017	0.253
98	C	0.952	-3.905	-1.684
99	H	0.476	-3.087	-2.235
100	H	1.662	-4.392	-2.363
101	H	0.179	-4.641	-1.433
102	C	2.333	-4.558	0.337
103	H	2.8	-4.212	1.267
104	H	1.602	-5.335	0.59
105	H	3.115	-5.022	-0.274

106	H	3.702	-3.557	-2.013
107	C	5.887	-2.091	-2.715
108	H	5.636	-3.071	-3.143
109	C	7.231	-2.241	-1.976
110	H	7.159	-2.977	-1.168
111	H	8.016	-2.569	-2.668
112	H	7.551	-1.29	-1.535
113	C	6.006	-1.092	-3.881
114	H	5.063	-1.014	-4.433
115	H	6.266	-0.09	-3.522
116	H	6.788	-1.409	-4.582
117	H	5.606	0.149	-1.151
118	C	3.969	1.136	0.607
119	H	3.122	1.306	1.27
120	C	5.214	0.985	1.511
121	H	5.32	1.865	2.157
122	H	5.145	0.101	2.153
123	H	6.133	0.898	0.921
124	C	4.12	2.38	-0.29
125	H	4.284	3.275	0.322
126	H	4.979	2.281	-0.963
127	H	3.228	2.546	-0.898
128	N	1.368	-0.643	2.623
129	C	2.642	-1.156	3.111
130	H	3.172	-0.411	3.728
131	H	2.478	-2.043	3.744
132	H	3.292	-1.446	2.286
133	C	0.462	-0.395	3.738
134	H	0.245	-1.322	4.286
135	H	0.895	0.32	4.455
136	H	-0.491	0.014	3.396

Rotamer: Step-18

Atom #	Symbol	*x*	*y*	*z*
1	Si	1.012	-0.302	0.930
2	Si	-1.196	-1.329	0.355
3	H/Mu	-0.767	-2.075	-0.856
4	C	-2.844	-0.508	-0.251
5	C	-3.656	-1.266	-1.156
6	C	-4.822	-0.700	-1.680
7	C	-5.272	0.572	-1.320
8	C	-4.509	1.275	-0.393
9	C	-3.313	0.773	0.142
10	C	-2.606	1.655	1.169
11	H	-1.610	1.235	1.348
12	C	-2.403	3.097	0.669
13	H	-1.797	3.663	1.382



Step-18

14	H	-1.889	3.115	-0.296
15	H	-3.358	3.624	0.559
16	C	-3.366	1.662	2.513
17	H	-3.437	0.659	2.946
18	H	-2.862	2.309	3.240
19	H	-4.386	2.041	2.383
20	H	-4.857	2.256	-0.077
21	C	-6.548	1.165	-1.899
22	H	-6.678	2.156	-1.443
23	C	-6.442	1.369	-3.422
24	H	-5.581	1.998	-3.678
25	H	-6.323	0.412	-3.944
26	H	-7.346	1.852	-3.811
27	C	-7.790	0.327	-1.540
28	H	-7.888	0.209	-0.455
29	H	-8.701	0.807	-1.915
30	H	-7.736	-0.675	-1.982
31	H	-5.408	-1.281	-2.387
32	C	-3.347	-2.703	-1.600
33	H	-2.553	-3.104	-0.969
34	C	-2.843	-2.749	-3.055
35	H	-2.613	-3.779	-3.351
36	H	-3.598	-2.360	-3.749
37	H	-1.936	-2.149	-3.177
38	C	-4.548	-3.651	-1.407
39	H	-5.383	-3.413	-2.076
40	H	-4.244	-4.683	-1.62
41	H	-4.922	-3.615	-0.378
42	P	-1.517	-3.106	1.822
43	N	-2.814	-2.768	2.908
44	C	-4.080	-2.120	2.596
45	H	-4.848	-2.863	2.325
46	H	-4.447	-1.569	3.473
47	H	-3.967	-1.426	1.766
48	C	-2.919	-3.661	4.061
49	H	-3.223	-3.089	4.948
50	H	-3.668	-4.452	3.895
51	H	-1.954	-4.130	4.263
52	C	1.012	1.555	0.315
53	C	0.820	1.797	-1.079
54	C	0.825	3.108	-1.577
55	C	0.996	4.223	-0.761
56	C	1.180	3.986	0.601
57	C	1.206	2.699	1.153
58	C	1.482	2.634	2.663
59	H	1.610	1.588	2.936
60	C	0.307	3.192	3.489
61	H	0.123	4.249	3.258
62	H	-0.619	2.643	3.296

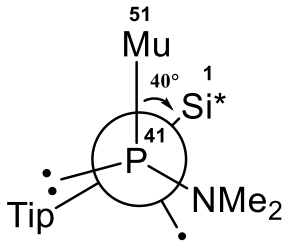
63	H	0.523	3.121	4.562
64	C	2.780	3.369	3.065
65	H	3.642	3.022	2.488
66	H	2.699	4.452	2.921
67	H	2.992	3.196	4.127
68	H	1.323	4.837	1.264
69	C	0.995	5.630	-1.342
70	H	0.839	5.531	-2.425
71	C	-0.163	6.482	-0.786
72	H	-0.061	6.633	0.296
73	H	-0.177	7.470	-1.260
74	H	-1.130	6.001	-0.967
75	C	2.347	6.338	-1.134
76	H	2.345	7.324	-1.614
77	H	2.558	6.487	-0.068
78	H	3.170	5.752	-1.558
79	H	0.693	3.266	-2.645
80	C	0.628	0.693	-2.128
81	H	0.572	-0.275	-1.621
82	C	1.818	0.607	-3.105
83	H	2.756	0.410	-2.581
84	H	1.655	-0.204	-3.825
85	H	1.931	1.538	-3.674
86	C	-0.685	0.865	-2.919
87	H	-1.553	0.931	-2.258
88	H	-0.663	1.768	-3.539
89	H	-0.834	0.012	-3.591
90	C	2.562	-1.172	0.103
91	C	3.773	-0.444	-0.135
92	C	4.769	-0.978	-0.962
93	C	4.667	-2.241	-1.546
94	C	3.558	-3.004	-1.196
95	C	2.535	-2.518	-0.370
96	C	1.513	-3.549	0.097
97	H	0.717	-3.022	0.626
98	C	0.868	-4.366	-1.036
99	H	0.463	-3.721	-1.823
100	H	1.586	-5.052	-1.500
101	H	0.047	-4.974	-0.638
102	C	2.151	-4.493	1.138
103	H	2.574	-3.931	1.977
104	H	1.397	-5.181	1.537
105	H	2.956	-5.088	0.690
106	H	3.496	-4.026	-1.561
107	C	5.748	-2.793	-2.464
108	H	5.409	-3.783	-2.801
109	C	7.083	-2.991	-1.722
110	H	6.96	-3.646	-0.852
111	H	7.832	-3.441	-2.386

112	H	7.486	-2.035	-1.366
113	C	5.937	-1.919	-3.718
114	H	4.996	-1.805	-4.268
115	H	6.292	-0.915	-3.453
116	H	6.676	-2.366	-4.393
117	H	5.668	-0.392	-1.135
118	C	4.148	0.858	0.581
119	H	3.307	1.162	1.204
120	C	5.342	0.617	1.533
121	H	5.549	1.521	2.119
122	H	5.145	-0.201	2.233
123	H	6.252	0.367	0.977
124	C	4.463	2.025	-0.372
125	H	4.703	2.929	0.200
126	H	5.328	1.801	-1.007
127	H	3.613	2.253	-1.021
128	N	1.152	-0.606	2.653
129	C	2.365	-1.054	3.321
130	H	2.778	-0.279	3.991
131	H	2.156	-1.942	3.937
132	H	3.133	-1.321	2.594
133	C	0.068	-0.405	3.601
134	H	-0.138	-1.330	4.158
135	H	0.306	0.383	4.334
136	H	-0.855	-0.113	3.094

Si-P(Mu)-NMe$_2$: Dihedral angle: 51(Mu)-41(P)-2(Si)-1(Si)

Rotamer: Step-1

Atom #	Symbol	*x*	*y*	*z*
1	Si	0.977	-0.241	1.051
2	Si	-1.186	-1.287	1.070
3	C	-2.710	-0.644	0.119
4	C	-3.336	-1.466	-0.857
5	C	-4.459	-0.997	-1.544
6	C	-5.000	0.267	-1.305
7	C	-4.402	1.053	-0.320
8	C	-3.280	0.625	0.398
9	C	-2.753	1.513	1.520
10	H	-1.706	1.240	1.690
11	C	-2.771	3.011	1.182
12	H	-2.237	3.577	1.951
13	H	-2.278	3.200	0.225
14	H	-3.792	3.406	1.135
15	C	-3.526	1.231	2.823
16	H	-3.466	0.173	3.102
17	H	-3.125	1.829	3.652



Step-1

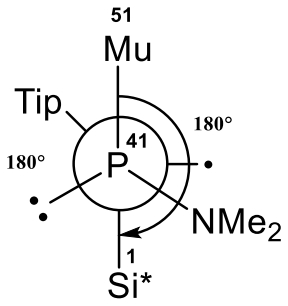
18	H	-4.586	1.485	2.704
19	H	-4.831	2.029	-0.107
20	C	-6.197	0.774	-2.093
21	H	-6.452	1.768	-1.701
22	C	-5.849	0.936	-3.585
23	H	-4.987	1.599	-3.718
24	H	-5.598	-0.032	-4.035
25	H	-6.697	1.355	-4.139
26	C	-7.430	-0.130	-1.908
27	H	-7.692	-0.227	-0.849
28	H	-8.294	0.282	-2.442
29	H	-7.244	-1.136	-2.301
30	H	-4.923	-1.635	-2.291
31	C	-2.857	-2.881	-1.163
32	H	-1.885	-3.013	-0.668
33	C	-2.644	-3.139	-2.664
34	H	-2.203	-4.130	-2.820
35	H	-3.590	-3.109	-3.217
36	H	-1.975	-2.396	-3.107
37	C	-3.823	-3.922	-0.567
38	H	-4.811	-3.848	-1.039
39	H	-3.446	-4.939	-0.730
40	H	-3.953	-3.769	0.509
41	P	-2.028	-2.68	2.713
42	N	-1.018	-4.092	2.887
43	C	0.377	-3.921	3.280
44	H	0.842	-4.905	3.415
45	H	0.973	-3.352	2.551
46	H	0.425	-3.392	4.237
47	C	-1.222	-5.093	1.844
48	H	-0.790	-4.807	0.870
49	H	-0.762	-6.041	2.150
50	H	-2.293	-5.262	1.698
51	H/Mu	-1.543	-2.022	3.876
52	C	0.65	1.566	0.419
53	C	0.245	1.733	-0.938
54	C	0.054	3.021	-1.458
55	C	0.211	4.171	-0.691
56	C	0.583	4.003	0.641
57	C	0.819	2.746	1.203
58	C	1.263	2.741	2.668
59	H	1.606	1.738	2.909
60	C	0.091	3.085	3.607
61	H	-0.278	4.099	3.411
62	H	-0.746	2.395	3.474
63	H	0.407	3.038	4.656
64	C	2.452	3.681	2.952
65	H	3.297	3.472	2.290
66	H	2.184	4.736	2.830

67	H	2.790	3.548	3.986
68	H	0.703	4.884	1.265
69	C	-0.023	5.552	-1.280
70	H	-0.282	5.419	-2.339
71	C	-1.208	6.258	-0.595
72	H	-1.003	6.425	0.469
73	H	-1.400	7.234	-1.058
74	H	-2.121	5.656	-0.668
75	C	1.249	6.416	-1.215
76	H	1.083	7.388	-1.695
77	H	1.547	6.602	-0.176
78	H	2.087	5.921	-1.718
79	H	-0.229	3.132	-2.502
80	C	0.036	0.579	-1.927
81	H	0.000	-0.365	-1.371
82	C	1.200	0.478	-2.934
83	H	2.162	0.354	-2.437
84	H	1.048	-0.377	-3.603
85	H	1.247	1.384	-3.550
86	C	-1.294	0.697	-2.699
87	H	-2.139	0.881	-2.034
88	H	-1.255	1.507	-3.437
89	H	-1.490	-0.229	-3.250
90	C	2.431	-0.903	-0.049
91	C	3.551	-0.046	-0.285
92	C	4.508	-0.385	-1.246
93	C	4.436	-1.560	-1.994
94	C	3.401	-2.437	-1.692
95	C	2.423	-2.149	-0.729
96	C	1.441	-3.275	-0.427
97	H	0.715	-2.914	0.308
98	C	0.644	-3.707	-1.668
99	H	0.126	-2.854	-2.115
100	H	1.292	-4.146	-2.434
101	H	-0.107	-4.46	-1.402
102	C	2.177	-4.472	0.206
103	H	2.729	-4.166	1.100
104	H	1.466	-5.254	0.494
105	H	2.894	-4.912	-0.496
106	H	3.360	-3.387	-2.218
107	C	5.451	-1.875	-3.079
108	H	5.195	-2.859	-3.494
109	C	6.882	-1.963	-2.517
110	H	6.947	-2.710	-1.718
111	H	7.591	-2.241	-3.306
112	H	7.204	-1.001	-2.102
113	C	5.369	-0.848	-4.224
114	H	4.357	-0.803	-4.640
115	H	5.629	0.156	-3.869

116	H	6.064	-1.110	-5.031
117	H	5.336	0.296	-1.421
118	C	3.826	1.243	0.491
119	H	3.053	1.359	1.250
120	C	5.168	1.168	1.249
121	H	5.289	2.052	1.886
122	H	5.222	0.280	1.886
123	H	6.020	1.139	0.561
124	C	3.794	2.483	-0.421
125	H	3.951	3.398	0.162
126	H	4.589	2.431	-1.174
127	H	2.838	2.575	-0.940
128	N	1.505	-0.519	2.704
129	C	2.844	-0.949	3.082
130	H	3.397	-0.150	3.604
131	H	2.788	-1.812	3.764
132	H	3.419	-1.249	2.207
133	C	0.687	-0.264	3.881
134	H	0.592	-1.169	4.496
135	H	1.125	0.519	4.520
136	H	-0.316	0.064	3.600

Rotamer: Step-15

Atom #	Symbol	*x*	*y*	*z*
1	Si	1.033	-0.248	0.974
2	Si	-1.200	-1.151	0.709
3	C	-2.744	-0.520	-0.237
4	C	-3.397	-1.383	-1.166
5	C	-4.571	-0.963	-1.799
6	C	-5.149	0.284	-1.548
7	C	-4.509	1.118	-0.632
8	C	-3.327	0.751	0.023
9	C	-2.746	1.725	1.046
10	H	-1.710	1.421	1.238
11	C	-2.690	3.177	0.539
12	H	-2.164	3.806	1.265
13	H	-2.156	3.244	-0.413
14	H	-3.691	3.605	0.404
15	C	-3.511	1.638	2.383
16	H	-3.448	0.631	2.811
17	H	-3.095	2.345	3.112
18	H	-4.570	1.887	2.245
19	H	-4.955	2.086	-0.418
20	C	-6.434	0.723	-2.237
21	H	-6.669	1.730	-1.869
22	C	-6.264	0.819	-3.765
23	H	-5.442	1.494	-4.030
24	H	-6.046	-0.161	-4.205



Step-15

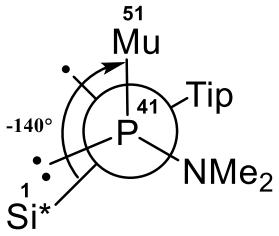
25	H	-7.181	1.197	-4.233
26	C	-7.621	-0.189	-1.871
27	H	-7.767	-0.233	-0.786
28	H	-8.547	0.181	-2.325
29	H	-7.461	-1.214	-2.228
30	H	-5.05	-1.632	-2.509
31	C	-2.882	-2.781	-1.51
32	H	-1.965	-2.949	-0.929
33	C	-2.504	-2.917	-2.997
34	H	-2.104	-3.917	-3.200
35	H	-3.374	-2.768	-3.647
36	H	-1.744	-2.183	-3.284
37	C	-3.885	-3.880	-1.110
38	H	-4.809	-3.810	-1.697
39	H	-3.455	-4.874	-1.289
40	H	-4.156	-3.813	-0.052
41	P	-1.626	-2.700	2.349
42	N	-2.963	-2.071	3.300
43	C	-4.303	-2.133	2.724
44	H	-4.684	-3.169	2.650
45	H	-5.002	-1.565	3.352
46	H	-4.308	-1.691	1.727
47	C	-2.951	-2.510	4.697
48	H	-3.622	-1.868	5.284
49	H	-3.285	-3.555	4.829
50	H	-1.944	-2.420	5.112
51	H/Mu	-2.332	-3.650	1.538
52	C	0.977	1.567	0.251
53	C	0.757	1.726	-1.152
54	C	0.732	3.008	-1.721
55	C	0.889	4.170	-0.971
56	C	1.091	4.014	0.400
57	C	1.154	2.760	1.020
58	C	1.438	2.788	2.528
59	H	1.616	1.765	2.855
60	C	0.235	3.339	3.320
61	H	0.026	4.380	3.044
62	H	-0.672	2.757	3.135
63	H	0.439	3.316	4.398
64	C	2.705	3.593	2.888
65	H	3.579	3.249	2.328
66	H	2.584	4.664	2.691
67	H	2.924	3.482	3.957
68	H	1.221	4.902	1.013
69	C	0.854	5.542	-1.630
70	H	0.668	5.380	-2.701
71	C	-0.296	6.413	-1.089
72	H	-0.164	6.630	-0.022
73	H	-0.336	7.371	-1.620

74	H	-1.263	5.913	-1.211
75	C	2.204	6.272	-1.502
76	H	2.175	7.234	-2.028
77	H	2.450	6.473	-0.453
78	H	3.019	5.676	-1.927
79	H	0.587	3.104	-2.794
80	C	0.572	0.565	-2.139
81	H	0.462	-0.369	-1.576
82	C	1.798	0.394	-3.059
83	H	2.712	0.214	-2.489
84	H	1.647	-0.457	-3.735
85	H	1.950	1.287	-3.677
86	C	-0.699	0.723	-2.998
87	H	-1.594	0.849	-2.384
88	H	-0.624	1.583	-3.672
89	H	-0.839	-0.165	-3.625
90	C	2.533	-1.166	0.126
91	C	3.773	-0.472	-0.057
92	C	4.794	-1.039	-0.828
93	C	4.685	-2.301	-1.412
94	C	3.525	-3.019	-1.141
95	C	2.469	-2.498	-0.377
96	C	1.347	-3.482	-0.052
97	H	0.545	-2.931	0.448
98	C	0.725	-4.136	-1.298
99	H	0.373	-3.382	-2.01
100	H	1.439	-4.782	-1.822
101	H	-0.129	-4.760	-1.012
102	C	1.837	-4.554	0.943
103	H	2.239	-4.096	1.853
104	H	1.009	-5.212	1.234
105	H	2.625	-5.176	0.502
106	H	3.444	-4.033	-1.523
107	C	5.797	-2.893	-2.266
108	H	5.462	-3.890	-2.585
109	C	7.101	-3.080	-1.466
110	H	6.936	-3.702	-0.579
111	H	7.867	-3.562	-2.085
112	H	7.503	-2.117	-1.129
113	C	6.044	-2.059	-3.537
114	H	5.127	-1.953	-4.126
115	H	6.400	-1.052	-3.288
116	H	6.804	-2.534	-4.169
117	H	5.715	-0.478	-0.960
118	C	4.129	0.852	0.629
119	H	3.279	1.166	1.235
120	C	5.317	0.668	1.599
121	H	5.496	1.596	2.157
122	H	5.130	-0.131	2.323

123	H	6.242	0.424	1.064
124	C	4.431	1.985	-0.369
125	H	4.670	2.912	0.166
126	H	5.293	1.739	-1.000
127	H	3.577	2.184	-1.021
128	N	1.285	-0.478	2.698
129	C	2.459	-1.105	3.293
130	H	2.996	-0.407	3.957
131	H	2.164	-1.975	3.900
132	H	3.152	-1.448	2.525
133	C	0.305	-0.147	3.723
134	H	0.023	-1.044	4.293
135	H	0.701	0.589	4.440
136	H	-0.606	0.269	0.000

Rotamer: Step-19

Atom #	Symbol	*x*	*y*	*z*
1	Si	1.033	-0.248	0.974
2	Si	-1.200	-1.151	0.709
3	C	-2.744	-0.520	-0.237
4	C	-3.397	-1.383	-1.166
5	C	-4.571	-0.963	-1.799
6	C	-5.149	0.284	-1.548
7	C	-4.509	1.118	-0.632
8	C	-3.327	0.751	0.023
9	C	-2.746	1.725	1.046
10	H	-1.710	1.421	1.238
11	C	-2.690	3.177	0.539
12	H	-2.164	3.806	1.265
13	H	-2.156	3.244	-0.413
14	H	-3.691	3.605	0.404
15	C	-3.511	1.638	2.383
16	H	-3.448	0.631	2.811
17	H	-3.095	2.345	3.112
18	H	-4.570	1.887	2.245
19	H	-4.955	2.086	-0.418
20	C	-6.434	0.723	-2.237
21	H	-6.669	1.730	-1.869
22	C	-6.264	0.819	-3.765
23	H	-5.442	1.494	-4.030
24	H	-6.046	-0.161	-4.205
25	H	-7.181	1.197	-4.233
26	C	-7.621	-0.189	-1.871
27	H	-7.767	-0.233	-0.786
28	H	-8.547	0.181	-2.325
29	H	-7.461	-1.214	-2.228
30	H	-5.050	-1.632	-2.509
31	C	-2.882	-2.781	-1.510



Step-19

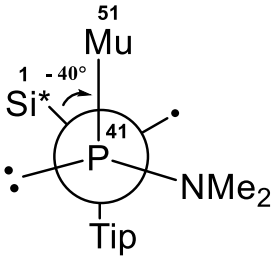
32	H	-1.965	-2.949	-0.929
33	C	-2.504	-2.917	-2.997
34	H	-2.104	-3.917	-3.200
35	H	-3.374	-2.768	-3.647
36	H	-1.744	-2.183	-3.284
37	C	-3.885	-3.880	-1.110
38	H	-4.809	-3.810	-1.697
39	H	-3.455	-4.874	-1.289
40	H	-4.156	-3.813	-0.052
41	P	-1.626	-2.700	2.349
42	N	-2.963	-2.071	3.300
43	C	-4.303	-2.133	2.724
44	H	-4.684	-3.169	2.650
45	H	-5.002	-1.565	3.352
46	H	-4.308	-1.691	1.727
47	C	-2.951	-2.510	4.697
48	H	-3.622	-1.868	5.284
49	H	-3.285	-3.555	4.829
50	H	-1.944	-2.420	5.112
51	H/Mu	-2.332	-3.650	1.538
52	C	0.977	1.567	0.251
53	C	0.757	1.726	-1.152
54	C	0.732	3.008	-1.721
55	C	0.889	4.170	-0.971
56	C	1.091	4.014	0.400
57	C	1.154	2.760	1.020
58	C	1.438	2.788	2.528
59	H	1.616	1.765	2.855
60	C	0.235	3.339	3.320
61	H	0.026	4.380	3.044
62	H	-0.672	2.757	3.135
63	H	0.439	3.316	4.398
64	C	2.705	3.593	2.888
65	H	3.579	3.249	2.328
66	H	2.584	4.664	2.691
67	H	2.924	3.482	3.957
68	H	1.221	4.902	1.013
69	C	0.854	5.542	-1.630
70	H	0.668	5.380	-2.701
71	C	-0.296	6.413	-1.089
72	H	-0.164	6.630	-0.022
73	H	-0.336	7.371	-1.620
74	H	-1.263	5.913	-1.211
75	C	2.204	6.272	-1.502
76	H	2.175	7.234	-2.028
77	H	2.450	6.473	-0.453
78	H	3.019	5.676	-1.927
79	H	0.587	3.104	-2.794
80	C	0.572	0.565	-2.139

81	H	0.462	-0.369	-1.576
82	C	1.798	0.394	-3.059
83	H	2.712	0.214	-2.489
84	H	1.647	-0.457	-3.735
85	H	1.950	1.287	-3.677
86	C	-0.699	0.723	-2.998
87	H	-1.594	0.849	-2.384
88	H	-0.624	1.583	-3.672
89	H	-0.839	-0.165	-3.625
90	C	2.533	-1.166	0.126
91	C	3.773	-0.472	-0.057
92	C	4.794	-1.039	-0.828
93	C	4.685	-2.301	-1.412
94	C	3.525	-3.019	-1.141
95	C	2.469	-2.498	-0.377
96	C	1.347	-3.482	-0.052
97	H	0.545	-2.931	0.448
98	C	0.725	-4.136	-1.298
99	H	0.373	-3.382	-2.010
100	H	1.439	-4.782	-1.822
101	H	-0.129	-4.760	-1.012
102	C	1.837	-4.554	0.943
103	H	2.239	-4.096	1.853
104	H	1.009	-5.212	1.234
105	H	2.625	-5.176	0.502
106	H	3.444	-4.033	-1.523
107	C	5.797	-2.893	-2.266
108	H	5.462	-3.890	-2.585
109	C	7.101	-3.080	-1.466
110	H	6.936	-3.702	-0.579
111	H	7.867	-3.562	-2.085
112	H	7.503	-2.117	-1.129
113	C	6.044	-2.059	-3.537
114	H	5.127	-1.953	-4.126
115	H	6.400	-1.052	-3.288
116	H	6.804	-2.534	-4.169
117	H	5.715	-0.478	-0.960
118	C	4.129	0.852	0.629
119	H	3.279	1.166	1.235
120	C	5.317	0.668	1.599
121	H	5.496	1.596	2.157
122	H	5.130	-0.131	2.323
123	H	6.242	0.424	1.064
124	C	4.431	1.985	-0.369
125	H	4.670	2.912	0.166
126	H	5.293	1.739	-1.000
127	H	3.577	2.184	-1.021
128	N	1.285	-0.478	2.698
129	C	2.459	-1.105	3.293

130	H	2.996	-0.407	3.957
131	H	2.164	-1.975	3.900
132	H	3.152	-1.448	2.525
133	C	0.305	-0.147	3.723
134	H	0.023	-1.044	4.293
135	H	0.701	0.589	4.440
136	H	-0.606	0.269	3.286

Rotamer: Step-29

Atom #	Symbol	*x*	*y*	*z*
1	Si	1.029	-0.253	1.022
2	Si	-1.247	-1.143	0.791
3	C	-2.772	-0.350	-0.076
4	C	-3.448	-1.094	-1.087
5	C	-4.566	-0.547	-1.726
6	C	-5.072	0.712	-1.396
7	C	-4.424	1.419	-0.384
8	C	-3.294	0.922	0.279
9	C	-2.713	1.768	1.409
10	H	-1.731	1.347	1.663
11	C	-2.484	3.236	1.006
12	H	-1.984	3.776	1.817
13	H	-1.856	3.311	0.113
14	H	-3.430	3.753	0.807
15	C	-3.598	1.680	2.669
16	H	-3.708	0.644	3.006
17	H	-3.162	2.263	3.490
18	H	-4.599	2.081	2.468
19	H	-4.821	2.390	-0.099
20	C	-6.292	1.294	-2.096
21	H	-6.479	2.280	-1.650
22	C	-6.042	1.509	-3.601
23	H	-5.166	2.146	-3.770
24	H	-5.867	0.557	-4.116
25	H	-6.909	1.988	-4.072
26	C	-7.551	0.438	-1.864
27	H	-7.755	0.315	-0.794
28	H	-8.427	0.906	-2.328
29	H	-7.439	-0.563	-2.299
30	H	-5.063	-1.129	-2.498
31	C	-3.046	-2.513	-1.491
32	H	-2.145	-2.773	-0.918
33	C	-2.685	-2.639	-2.982
34	H	-2.384	-3.668	-3.215
35	H	-3.535	-2.391	-3.628
36	H	-1.857	-1.976	-3.253
37	C	-4.139	-3.529	-1.109
38	H	-5.065	-3.348	-1.669



Step-29

39	H	-3.809	-4.550	-1.337
40	H	-4.366	-3.468	-0.041
41	P	-2.005	-2.065	2.758
42	N	-2.986	-3.434	2.302
43	C	-2.327	-4.633	1.802
44	H	-1.745	-5.157	2.582
45	H	-3.075	-5.334	1.410
46	H	-1.647	-4.372	0.987
47	C	-4.065	-3.741	3.244
48	H	-4.815	-4.368	2.744
49	H	-3.718	-4.281	4.142
50	H	-4.552	-2.818	3.567
51	H/Mu	-0.784	-2.706	3.148
52	C	1.007	1.588	0.348
53	C	0.711	1.793	-1.035
54	C	0.709	3.088	-1.573
55	C	0.958	4.225	-0.809
56	C	1.232	4.026	0.543
57	C	1.281	2.755	1.130
58	C	1.662	2.742	2.617
59	H	1.825	1.707	2.912
60	C	0.537	3.323	3.498
61	H	0.348	4.374	3.251
62	H	-0.403	2.778	3.370
63	H	0.813	3.275	4.559
64	C	2.978	3.494	2.910
65	H	3.801	3.137	2.283
66	H	2.882	4.574	2.748
67	H	3.265	3.347	3.959
68	H	1.432	4.892	1.168
69	C	0.941	5.612	-1.435
70	H	0.685	5.483	-2.495
71	C	-0.136	6.517	-0.807
72	H	0.068	6.702	0.254
73	H	-0.166	7.489	-1.314
74	H	-1.129	6.061	-0.882
75	C	2.327	6.283	-1.375
76	H	2.308	7.254	-1.884
77	H	2.642	6.455	-0.339
78	H	3.090	5.660	-1.856
79	H	0.508	3.217	-2.633
80	C	0.418	0.669	-2.039
81	H	0.266	-0.268	-1.491
82	C	1.599	0.443	-3.006
83	H	2.520	0.193	-2.474
84	H	1.371	-0.379	-3.695
85	H	1.785	1.341	-3.607
86	C	-0.866	0.931	-2.852
87	H	-1.724	1.131	-2.208

88	H	-0.743	1.780	-3.534
89	H	-1.101	0.058	-3.471
90	C	2.460	-1.199	0.084
91	C	3.708	-0.535	-0.150
92	C	4.670	-1.110	-0.989
93	C	4.495	-2.355	-1.593
94	C	3.333	-3.048	-1.271
95	C	2.335	-2.518	-0.440
96	C	1.215	-3.487	-0.065
97	H	0.45	-2.933	0.489
98	C	0.515	-4.107	-1.287
99	H	0.139	-3.335	-1.966
100	H	1.186	-4.757	-1.859
101	H	-0.336	-4.723	-0.970
102	C	1.744	-4.584	0.881
103	H	2.206	-4.149	1.774
104	H	0.926	-5.238	1.206
105	H	2.497	-5.209	0.386
106	H	3.205	-4.052	-1.669
107	C	5.54	-2.953	-2.524
108	H	5.166	-3.938	-2.837
109	C	6.888	-3.176	-1.813
110	H	6.770	-3.809	-0.927
111	H	7.603	-3.661	-2.487
112	H	7.329	-2.226	-1.489
113	C	5.720	-2.102	-3.795
114	H	4.770	-1.975	-4.326
115	H	6.103	-1.103	-3.552
116	H	6.434	-2.576	-4.480
117	H	5.597	-0.569	-1.159
118	C	4.141	0.758	0.548
119	H	3.335	1.081	1.206
120	C	5.371	0.511	1.450
121	H	5.608	1.416	2.022
122	H	5.194	-0.302	2.162
123	H	6.259	0.251	0.862
124	C	4.428	1.908	-0.436
125	H	4.726	2.812	0.108
126	H	5.246	1.651	-1.119
127	H	3.547	2.151	-1.035
128	N	1.373	-0.518	2.730
129	C	2.542	-1.221	3.245
130	H	3.163	-0.562	3.875
131	H	2.236	-2.075	3.871
132	H	3.162	-1.601	2.434
133	C	0.497	-0.115	3.820
134	H	0.172	-0.984	4.410
135	H	1.004	0.574	4.514
136	H	-0.396	0.392	3.448

4. NBO analysis of the P-centred radicals

The natural bond orbitals (NBO) calculations were performed using the NBO 7.0 program as implemented in the Gaussian 09 package.[10]

Table S3: NBO analysis of the P-centred radicals at the local minima on each PES

Rotamers	Occupancy	Atom	Atom #	Composition (%)			s/p	hfc of calc. A_μ (MHz)	Mu-SOMO angle (°) *
				s	p	d			
1-SiMu_step_11	0.93506	P	3	4.02	95.92	0.06	0.04	5	89
1-SiMu_step_23	0.91918	P	3	8.15	91.78	0.07	0.09	139	27
1-SiMu_step_37	0.94445	P	3	1.88	98.07	0.05	0.02	**22**	**60**
2-SiMu_step_2	0.94106	P	3	1.05	98.89	0.06	0.01	**31**	**56**
2-SiMu_step_12	0.93278	P	3	8.23	91.70	0.06	0.09	**141**	**24**
3-SiMu_step_11	0.93833	P	3	3.92	96.02	0.06	0.04	-6	86
3-SiMu_step_22	0.93073	P	3	9.42	90.51	0.06	0.10	158	20
3-SiMu_step_37	0.94199	P	3	2.11	97.83	0.06	0.02	**21**	**60**
4-SiMu_step_2	0.93280	P	42	2.99	96.93	0.08	0.03	**90**	**37**
4-SiMu_step_18	0.94388	P	42	0.00	99.93	0.07	0.00	**43**	**57**

*Mu-SOMO dihedral angle designates the Mu-Si-bond–P-centred-p_z dihedral angle. The rotamers in bold indicates the assigned P-centred radicals.

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