Supporting Information

An Ylide-Like Phosphasilene and Striking Formation of a 4π-Electron, Resonance-Stabilized 2,4-Disila-1,3-diphosphacyclobutadiene.

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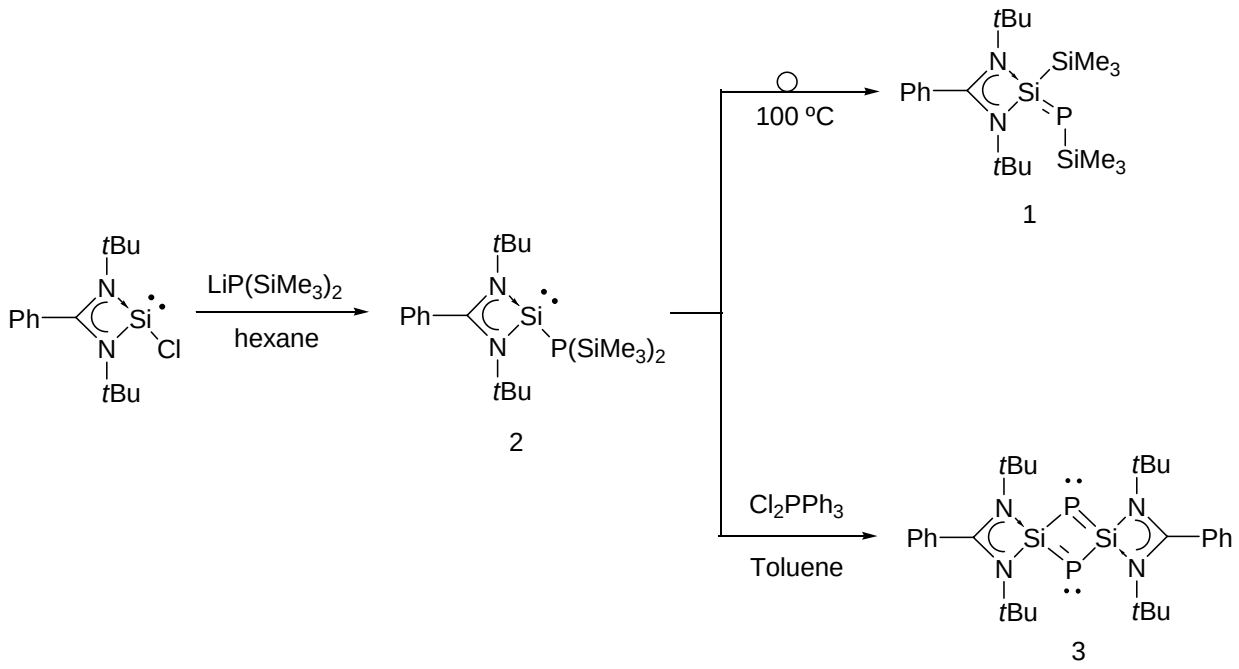
Experimental Section

General Procedures.

All experiments and manipulations were carried out under dry oxygen-free nitrogen using standard Schlenk techniques or in an MBraun inert atmosphere dry box containing an atmosphere of purified nitrogen. All solvents were dried by standard methods and freshly distilled prior to use. Triphenylphosphine dichloride Cl_2PPh_3 (Aldrich) was used as received. The starting material, silylene chloride [LSiCl][1] and lithium bis(trimethylsilyl)phosphate (dme)LiP$(SiMe_3)_2$[2] were prepared according to the literature. The ^1H, ^{13}C, ^{31}P, and ^{29}Si, NMR spectra were recorded on Brucker ARX200 and AV 400 Spectrometers.

Single-Crystal X-ray Structure Determinations: Crystals were each mounted on a glass capillary in perfluorinated oil and measured in a cold N_2 flow. The data of Compounds **1**, **2** and **3** were collected on an Oxford Diffraction Xcalibur S Sapphire at 150 K (Mo-Kαradiation, λ = 0.71073 Å). The structures were solved by direct methods and refined on F^2 with the SHELX-97 software package.[3] The positions of the H atoms were calculated and considered isotropically according to a riding model.

Scheme S1



Preparation of 1 [LSi(SiMe$_3$)=P(SiMe$_3$)] (L = PhC(N*t*Bu)$_2$): When a mixture of bis(trimethylsilyl)phosphino silylene **2** (70 mg, 0.16 mmol) and toluene (0.5 mL) in a sealed NMR tube

was kept at 100 ºC for 5 days in the dark, the initial yellow solution turned gradually pale yellow. The quantitative formation of phosphasilene **1** was confirmed by NMR spectroscopy. The solvent was removed, and the remaining solid was crystallized from hexane at –30 ºC suitable for single crystal measurement (61 mg, 0.14 mmol, 87%). M.p. 230-231 °C. ^{1}H NMR (400.13 MHz, C_6D_6, 298K): δ = 0.44 (s, 9 H, SiSi*Me*$_3$), 0.71 (d, $^{3}J_{P\text{-}H}$ = 3.4 Hz, 9 H, PSi*Me*$_3$), 1.14 (s, 18 H, *t*Bu), 7.23- 7.26 (m, 5 H, Ph). ^{13}C NMR (100.61 MHz, C_6D_6, 298K): δ = –0.1 (d, $^{3}J_{C\text{-}P}$ = 3.3 Hz, SiSi*Me*$_3$), 7.1 (d, $^{3}J_{C\text{-}P}$ = 10.3 Hz, PSi*Me*$_3$), 31.7 (d, $^{4}J_{C\text{-}P}$ = 0.6 Hz, C*Me*$_3$), 54.7 (*C*Me$_3$), 128.3, 129.0, 129.9, 131.5 (Ph), 169.5 (N*C*N). ^{29}Si NMR (79.49 MHz, C_6D_6, 298K): δ = –17.5 (d, $^{2}J_{Si\text{-}P}$ = 36.3 Hz, SiSi*Me*$_3$), 3.0 (d, $^{1}J_{Si\text{-}P}$ = 70.5 Hz, PSi*Me*$_3$), 40.5 (d, $^{1}J_{Si\text{-}P}$ = 191.4 Hz, *Si*=P). ^{31}P NMR (81.012 MHz, C_6D_6, 298K) δ = –252.9. UV-vis (hexane) λ_{max} (ε) = 333 (3500). HRMS calcd for $C_{21}H_{41}N_2PSi_3$, 436.2315, Found 436.2411.

Preparation of 2 [LSiP(SiMe$_3$)$_2$]: Toluene (20 mL) was added to a mixture of chloro silylene [LSiCl] (302 mg, 1.02 mmol) and lithium bis(trimethylsilyl)phosphate (285 mg, 1.03 mmol) at ambient temperature. The solution turned to a yellow color and was stirred for 3 h. The solvent was removed and the residue was extracted with hexane (30 mL). The filtrate was concentrated and stored at –30 ºC for 24 h yielding **2** as yellow crystals (371 mg, 0.85 mmol, 83%). M.p. 149-150 °C. ^{1}H NMR (400.13 MHz, C_6D_6, 298K): δ = 0.58 (d, $^{3}J_{P\text{-}H}$ = 4.4 Hz, 18 H, Si*Me*$_3$), 1.24 (s, 18 H, *t*Bu), 6.81-6.99 (m, 2 H, Ph), 7.34-7.41 (m, 3 H, Ph). ^{13}C NMR (100.61 MHz, C_6D_6, 298K): δ = 4.4 (d, $^{3}J_{C\text{-}P}$ = 10.0 Hz, Si*Me*$_3$), 31.5 (d, $^{4}J_{C\text{-}P}$ = 1.6 Hz, C*Me*$_3$), 54.0 (*C*Me$_3$), 128.9, 129.2, 129.3, 134.4, (Ph), 157.2 (d, $^{3}J_{C\text{-}P}$ = 9.5 Hz, N*C*N). ^{29}Si NMR (79.49 MHz, C_6D_6, 298K): δ = 3.1 (d, $^{1}J_{Si\text{-}P}$ = 22.9 Hz, SiSi*Me*$_3$), 44,0 (d, $^{1}J_{Si\text{-}P}$ = 194.3 Hz, Si=P). ^{31}P NMR (81.012 MHz, C_6D_6, 298K) δ = –211.0. HRMS calcd for $C_{21}H_{41}N_2PSi_3$, 436.2315, Found 436.2524.

Preparation of 3 [L$_2$Si$_2$P$_2$]: Toluene (20 mL) was added to a mixture of **2** (309 mg, 0.71 mmol) and triphenylphosphine dichloride (237 mg, 0.71 mmol) at room temperature. The solution was stirred for 24 h. The solvent was removed and the residue was extracted with THF (30 mL). The filtrate was concentrated to yield yellow crystals of **3** (148 mg, 0.25 mmol, 72%). M.p. > 174 °C (decomp.). ^{1}H NMR (400.13 MHz, THF-D_8, 298K): δ = 1.35 (s, 18 H, *t*Bu), 7.05-7.33 (m, 10 H, Ph). ^{13}C NMR (100.61 MHz, THF-D_8, 298K): δ = 33.1 (C*Me*$_3$), 53.4 (*C*Me$_3$), 125.6, 127.6, 129.4, 135.9 (Ph), 171.0 (N*C*N). ^{29}Si NMR (79.49 MHz, THF-D_8, 298K): δ = 26.7 (t, $^{1}J_{Si\text{-}P}$ = 99.8 Hz). ^{31}P NMR (81.012 MHz, THF-D_8, 298K) δ = –164.9. HRMS calcd for $C_{30}H_{46}N_4P_2Si_2$, 580.2736, Found 580.2361.

Crystallographic data for compound 1:

Empirical formula	C21 H41 N2 P Si3

Formula weight	436.80	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 14.020(2) Å	α= 90°.
	b = 11.5941(12) Å	β= 108.598(19)°.
	c = 17.583(3) Å	γ = 90°.
Volume	2708.8(7) $Å^3$	
Z	4	
Density (calculated)	1.071 Mg/m^3	
Absorption coefficient	0.243 mm^{-1}	
F(000)	952	
Crystal size	0.48 x 0.26 x 0.09 mm^3	
Theta range for data collection	3.41 to 25.00°.	
Index ranges	-12<=h<=16, -13<=k<=12, -20<=l<=19	
Reflections collected	10268	
Independent reflections	4753 [R(int) = 0.0637]	
Completeness to theta = 25.00°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9785 and 0.8922	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4753 / 0 / 256	
Goodness-of-fit on F^2	1.446	
Final R indices [I>2sigma(I)]	R1 = 0.1033, wR2 = 0.2631	
R indices (all data)	R1 = 0.1526, wR2 = 0.2751	
Largest diff. peak and hole	1.184 and -0.456 $e.Å^{-3}$	

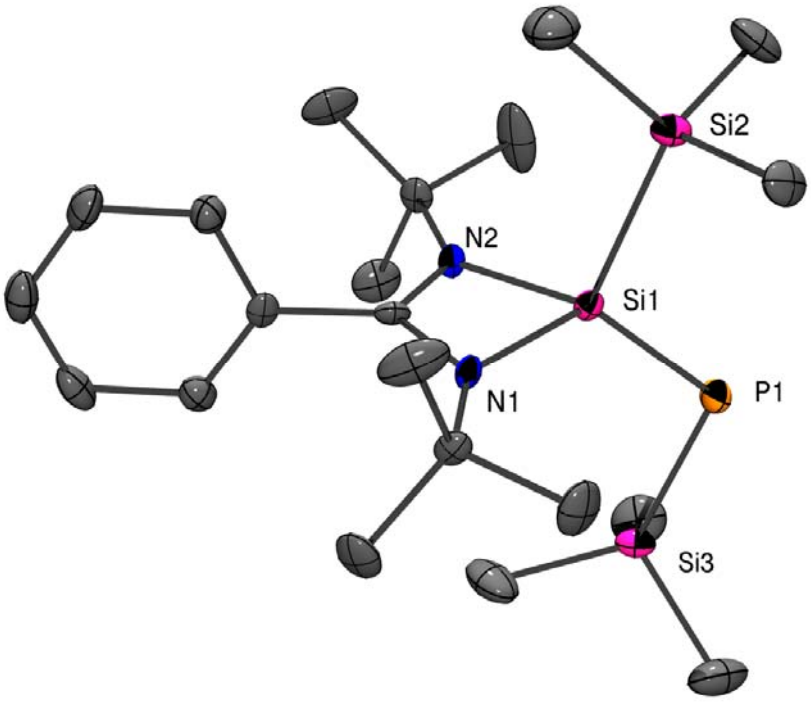


Figure 1. Molecular structure of compound **1.** Thermal ellipsoids are drawn at 30% probability level. Hydrogen atoms are omitted for clarity.

Table 1. Selected bond lengths and angles of compound **1**

Interatomic distances (Å)		Angles(°)	
Si(1)-N(2)	1.849(5)	N(2)-Si(1)-N(1)	70.8(2)
Si(1)-N(1)	1.862(5)	N(2)-Si(1)-P(1)	126.6(2)
Si(1)-P(1)	2.095(3)	N(1)-Si(1)-P(1)	127.5(2)
Si(1)-C(1)	2.299(7)	N(2)-Si(1)-C(1)	35.2(2)
Si(1)-Si(2)	2.366(3)	N(1)-Si(1)-C(1)	35.7(2)
Si(2)-C(18)	1.838(8)	P(1)-Si(1)-C(1)	139.82(19)
Si(2)-C(16)	1.849(9)	N(2)-Si(1)-Si(2)	108.6(2)
Si(2)-C(17)	1.879(7)	N(1)-Si(1)-Si(2)	108.35(19)
Si(3)-C(20)	1.855(8)	P(1)-Si(1)-Si(2)	109.50(10)
Si(3)-C(19)	1.859(9)	C(1)-Si(1)-Si(2)	110.67(18)
Si(3)-C(21)	1.865(8)	C(18)-Si(2)-C(16)	110.4(4)
Si(3)-P(1)	2.201(3)	C(18)-Si(2)-C(17)	105.6(4)

N(1)-C(1)	1.341(8)	C(16)-Si(2)-C(17)	109.6(4)
N(1)-C(8)	1.475(7)	C(18)-Si(2)-Si(1)	111.3(3)
N(2)-C(1)	1.325(8)	C(16)-Si(2)-Si(1)	110.6(3)
N(2)-C(12)	1.504(7)	C(17)-Si(2)-Si(1)	109.3(3)
C(1)-C(2)	1.501(9)	C(20)-Si(3)-C(19)	107.1(4)
C(2)-C(7)	1.368(9)	C(20)-Si(3)-C(21)	106.3(4)
C(2)-C(3)	1.387(10)	C(19)-Si(3)-C(21)	105.7(4)
C(3)-C(4)	1.373(9)	C(20)-Si(3)-P(1)	111.1(3)
C(4)-C(5)	1.368(11)	C(19)-Si(3)-P(1)	118.4(3)
C(5)-C(6)	1.359(11)	C(21)-Si(3)-P(1)	107.6(3)
C(6)-C(7)	1.416(10)	Si(1)-P(1)-Si(3)	106.61(11)
C(8)-C(11)	1.507(10)	C(1)-N(1)-C(8)	131.8(5)
C(8)-C(9)	1.511(9)	C(1)-N(1)-Si(1)	90.2(4)
C(8)-C(10)	1.534(9)	C(8)-N(1)-Si(1)	137.3(4)
C(12)-C(14)	1.499(10)	C(1)-N(2)-C(12)	131.8(5)
C(12)-C(15)	1.508(9)	C(1)-N(2)-Si(1)	91.3(4)
C(12)-C(13)	1.523(10)	C(12)-N(2)-Si(1)	136.9(4)
		N(2)-C(1)-N(1)	107.4(5)
		N(2)-C(1)-C(2)	126.6(5)
		N(1)-C(1)-C(2)	126.0(5)
		N(2)-C(1)-Si(1)	53.5(3)
		N(1)-C(1)-Si(1)	54.1(3)
		C(2)-C(1)-Si(1)	175.9(5)

Crystallographic data for compound 2:

Empirical formula	C21 H41 N2 P Si3	
Formula weight	436.80	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 19.3556(7) Å	α= 90°.
	b = 14.2399(4) Å	β= 90°.
	c = 19.9777(6) Å	γ = 90°.
Volume	5506.3(3) $Å^3$	
Z	8	
Density (calculated)	1.054 Mg/m^3	
Absorption coefficient	0.239 mm^{-1}	
F(000)	1904	
Crystal size	0.39 x 0.36 x 0.16 mm^3	
Theta range for data collection	3.51 to 25.00°.	
Index ranges	-13<=h<=23, -16<=k<=16, -23<=l<=22	
Reflections collected	19912	
Independent reflections	4836 [R(int) = 0.0961]	
Completeness to theta = 25.00°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9627 and 0.9125	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4836 / 18 / 287	
Goodness-of-fit on F^2	0.906	
Final R indices [I>2sigma(I)]	R1 = 0.0571, wR2 = 0.0889	
R indices (all data)	R1 = 0.1270, wR2 = 0.1032	
Largest diff. peak and hole	0.316 and -0.214 $e.Å^{-3}$	

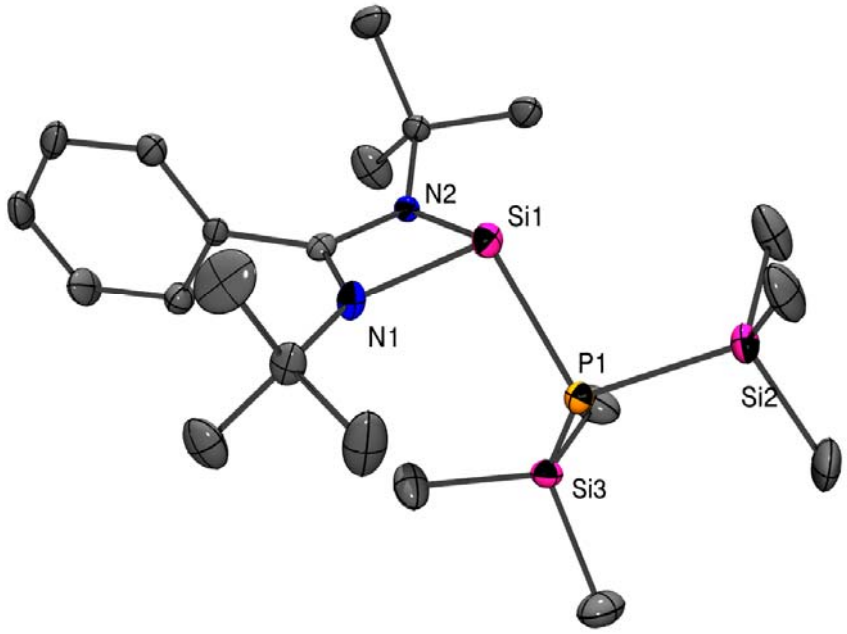


Figure 2. Molecular structure of compound **2.** Thermal ellipsoids are drawn at 30% probability level. Hydrogen atoms are omitted for clarity. The *t*Bu group on the N1 atom was disordered over two positions with occupancy factors of 0.71 : 0.29. The structure with higher occupancy is shown.

Table 2. Selected bond lengths and angles of compound **2**

Interatomic distances (Å)		Angles(°)	
P(1)-Si(2)	2.2264(13)	Si(2)-P(1)-Si(3)	108.59(5)
P(1)-Si(3)	2.2321(12)	Si(2)-P(1)-Si(1)	103.90(5)
P(1)-Si(1)	2.2838(12)	Si(3)-P(1)-Si(1)	118.22(5)
Si(1)-N(1)	1.877(3)	N(1)-Si(1)-N(2)	69.10(11)
Si(1)-N(2)	1.882(2)	N(1)-Si(1)-P(1)	99.98(9)
Si(2)-C(21)	1.847(4)	N(2)-Si(1)-P(1)	108.54(8)
Si(2)-C(20)	1.851(4)	C(21)-Si(2)-C(20)	106.90(18)
Si(2)-C(19)	1.866(4)	C(21)-Si(2)-C(19)	110.4(2)
Si(3)-C(16)	1.860(4)	C(20)-Si(2)-C(19)	108.1(2)
Si(3)-C(17)	1.862(3)	C(21)-Si(2)-P(1)	106.96(13)

Si(3)-C(18)	1.864(3)	C(20)-Si(2)-P(1)	116.12(12)
N(1)-C(9)	1.334(4)	C(19)-Si(2)-P(1)	108.30(14)
N(1)-C(5)	1.472(4)	C(16)-Si(3)-C(17)	106.74(18)
N(2)-C(9)	1.343(4)	C(16)-Si(3)-C(18)	109.11(18)
N(2)-C(1)	1.476(4)	C(17)-Si(3)-C(18)	107.73(17)
C(1)-C(4)	1.519(4)	C(16)-Si(3)-P(1)	115.90(12)
C(1)-C(3)	1.519(4)	C(17)-Si(3)-P(1)	108.89(13)
C(1)-C(2)	1.526(4)	C(18)-Si(3)-P(1)	108.20(12)
C(5)-C(7)	1.519(13)	C(9)-N(1)-C(5)	130.9(3)
C(5)-C(8)	1.523(8)	C(9)-N(1)-Si(1)	92.0(2)
C(5)-C(6)	1.571(7)	C(5)-N(1)-Si(1)	135.8(2)
		C(9)-N(2)-C(1)	128.6(2)
		C(9)-N(2)-Si(1)	91.53(19)
		C(1)-N(2)-Si(1)	132.4(2)

Crystallographic data for compound 3· $(toluene)_2$:

Empirical formula	C44 H60 N4 P2 Si2	
Formula weight	763.08	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 23.841(3) Å	α= 90°.
	b = 10.1993(12) Å	β= 108.346(12)°.
	c = 19.369(2) Å	γ = 90°.
Volume	4470.3(9) $Å^3$	
Z	4	
Density (calculated)	1.134 Mg/m^3	
Absorption coefficient	0.184 mm^{-1}	
F(000)	1640	
Crystal size	0.76 x 0.57 x 0.55 mm^3	
Theta range for data collection	3.53 to 25.00°.	
Index ranges	-28<=h<=28, -12<=k<=12, -20<=l<=23	
Reflections collected	16197	
Independent reflections	3927 [R(int) = 0.0447]	
Completeness to theta = 25.00°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9053 and 0.8725	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3927 / 0 / 251	
Goodness-of-fit on F^2	1.034	
Final R indices [I>2sigma(I)]	R1 = 0.0618, wR2 = 0.1393	
R indices (all data)	R1 = 0.0843, wR2 = 0.1489	
Largest diff. peak and hole	0.721 and -0.649 $e.Å^{-3}$	

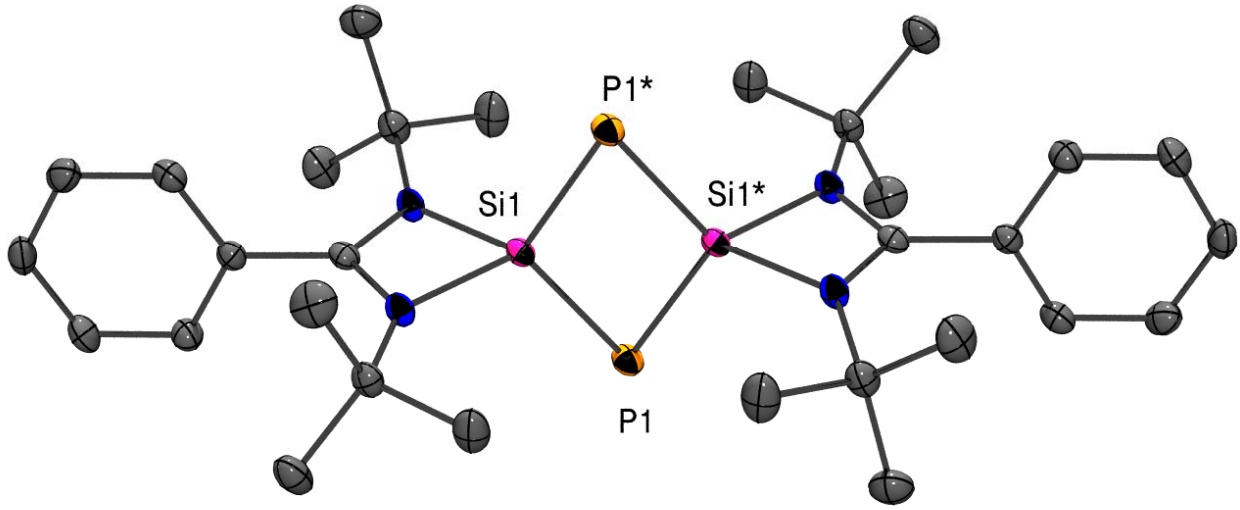


Figure 3. Molecular structure of **3**. Thermal ellipsoids are drawn at 30% probability level. Hydrogen atoms and solvents molecules are omitted for clarity.

Table 3. Selected bond legths and angles of compound **3**

Interatomic distances (Å)		Angles(°)	
P(1)-Si(1)	2.1701(12)	Si(1)-P(1)-Si(1)#1	72.34(4)
P(1)-Si(1)#1	2.1717(11)	N(2)-Si(1)-N(1)	70.78(11)
Si(1)-N(2)	1.856(2)	N(2)-Si(1)-P(1)	118.83(9)
Si(1)-N(1)	1.858(3)	N(1)-Si(1)-P(1)	120.41(9)
Si(1)-P(1)#1	2.1717(11)	N(2)-Si(1)-P(1)#1	118.48(9)
Si(1)-C(1)	2.315(3)	N(1)-Si(1)-P(1)#1	117.32(9)
Si(1)-Si(1)#1	2.5626(16)	P(1)-Si(1)-P(1)#1	107.66(4)

N(1)-C(1)	1.345(4)	N(2)-Si(1)-C(1)	35.31(10)
N(1)-C(8)	1.491(4)	N(1)-Si(1)-C(1)	35.50(10)
C(1)-N(2)	1.339(4)	P(1)-Si(1)-C(1)	128.47(8)
C(1)-C(2)	1.486(4)	P(1)#1-Si(1)-C(1)	123.87(8)
N(2)-C(12)	1.487(4)	N(2)-Si(1)-Si(1)#1	144.34(9)
C(2)-C(7)	1.384(4)	N(1)-Si(1)-Si(1)#1	144.84(9)
C(2)-C(3)	1.395(4)	P(1)-Si(1)-Si(1)#1	53.86(4)
C(3)-C(4)	1.385(4)	P(1)#1-Si(1)-Si(1)#1	53.80(4)
C(4)-C(5)	1.375(5)	C(1)-Si(1)-Si(1)#1	177.64(9)
C(5)-C(6)	1.382(5)	C(1)-N(1)-C(8)	130.9(3)
C(6)-C(7)	1.387(5)	C(1)-N(1)-Si(1)	91.15(18)
C(8)-C(10)	1.521(5)	C(8)-N(1)-Si(1)	136.73(19)
C(8)-C(9)	1.525(4)	N(2)-C(1)-N(1)	106.5(3)
C(8)-C(11)	1.530(4)	N(2)-C(1)-C(2)	126.9(3)
C(12)-C(15)	1.520(4)	N(1)-C(1)-C(2)	126.6(3)
C(12)-C(14)	1.523(5)	N(2)-C(1)-Si(1)	53.26(14)
C(12)-C(13)	1.528(4)	N(1)-C(1)-Si(1)	53.35(15)
		C(2)-C(1)-Si(1)	178.8(2)
		C(1)-N(2)-C(12)	131.1(3)
		C(1)-N(2)-Si(1)	91.43(18)
		C(12)-N(2)-Si(1)	137.0(2)
		N(1)-C(8)-C(10)	109.5(3)
		N(1)-C(8)-C(9)	106.1(3)
		N(1)-C(8)-C(11)	111.4(3)
		N(2)-C(12)-C(15)	105.6(2)
		N(2)-C(12)-C(14)	109.7(3)
		N(2)-C(12)-C(13)	112.3(2)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1/2,-y+1/2,-z+1 #2 -x+1,y,-z+3/2 #3 -x+1,-y+1,-z+1

Computational Methods

DFT calculations of the compounds **1-3** and **6** were performed at the B3LYP level using 6-31G(d) basis set with the GAUSSIAN-03 program package.[4] The structure obtained by X-ray analysis was used as input for the calculations of **1-3**. Compound **6** is by 46.2 kcal mol^{-1} less stable than its isomer **1**. Optimized structures of **1-3** and **6** are shown in Figure 4-7. Cartesian coordinates of optimized structures are shown in Table 4-7. The NBO approach was used to calculate the orbital populations, Wiberg Bond Indices (WBI), and Natural Population Analysis (NPA). The GIAO calculations was performed at B3LYP level using 6-311(d) basis sets for H, C, N, and P atoms and 6-311+G(3d) basis set for the Si atom, respectively.

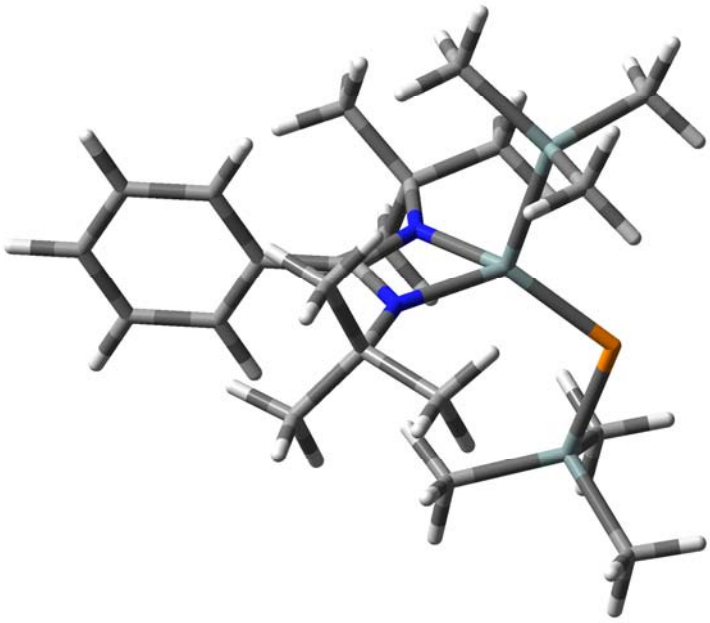


Figure 4. Optimized structure of compound **1**.

Table 4. Cartesian coordinates (x, y, z) for the optimized structure of **1**.

Si	-1.03369529	0.73778813	0.02910002	C	2.56938446	-0.63527358	-0.00850226
Si	-1.00252718	3.10403072	0.23571219	C	0.59627506	-1.80991186	2.73178481
Si	-2.97421736	-2.23794161	-0.21259353	H	-0.3383055	-2.24441083	2.36450132
P	-3.02610058	0.0140224	-0.08836522	H	0.68295069	-2.03751001	3.80046414
N	0.43700934	0.22530971	-1.06871712	H	1.43291602	-2.29361692	2.21921797
N	0.38453194	0.03405826	1.0823847	C	-1.57002888	3.91795566	-1.38712106
C	0.79627231	0.33287427	-2.50589141	H	-1.67744815	5.00188242	-1.25006211
C	1.15941305	-0.14125715	0.00070506	H	-2.54201358	3.52051739	-1.69995626
C	0.60913054	-0.28350522	2.51559167	H	-0.86238511	3.75862601	-2.20878506

C	5.21579902	-1.55861133	-0.02722927
H	6.24147261	-1.9164939	-0.0346764
C	4.95262258	-0.1893238	0.04575438
H	5.77174911	0.52235957	0.09775573
C	4.15689234	-2.46623038	-0.09095671
H	4.35446951	-3.53274149	-0.15095612
C	3.63624171	0.27223023	0.05585186
H	3.43381161	1.33664071	0.12906542
C	2.83868593	-2.00906167	-0.08243206
H	2.01667401	-2.71514283	-0.15157308
C	1.92787434	0.3138967	3.04495024
H	2.80761743	-0.16948165	2.61484722
H	1.97291905	0.18059399	4.13177446
H	1.98196316	1.38752642	2.83407303
C	0.73625342	3.75307983	0.67107703
H	0.73475782	4.84948845	0.7202199
H	1.48280736	3.45847858	-0.07597049
H	1.07175526	3.3798773	1.64561303
C	1.47026161	-0.95040186	-3.03136565
H	2.46994582	-1.09712293	-2.6177396
H	1.56798477	-0.88271066	-4.12063663
H	0.86396867	-1.83162654	-2.79957858
C	-0.51691969	0.5405192	-3.28217679
H	-1.19879221	-0.30275306	-3.14399667
H	-0.29472178	0.64102941	-4.35004392
H	-1.04091832	1.44404613	-2.95813677
C	1.72163006	1.54402878	-2.74302352
H	1.25280128	2.46816813	-2.38989237
H	1.92685589	1.65595168	-3.81396209
H	2.68048666	1.42199761	-2.23040482
C	-2.21586455	3.62697767	1.59867519
H	-1.89655296	3.28844328	2.59059183
H	-3.20931924	3.20563093	1.41126012
H	-2.30713143	4.72047138	1.63217374
C	-0.5594459	0.34265621	3.29776915
H	-0.54268244	1.43508497	3.22187036
H	-0.47443198	0.07811686	4.35710005
H	-1.52546703	-0.01089189	2.92571908
C	-4.32109329	-2.75545731	-1.45292903
H	-4.42727996	-3.8477682	-1.49228985
H	-4.08946042	-2.40022342	-2.46366359
H	-5.29381734	-2.33399021	-1.17315725
C	-1.34794059	-3.05829914	-0.78020225
H	-0.52511406	-2.85263876	-0.08627537
H	-1.0512993	-2.7041153	-1.77332845
H	-1.47360898	-4.1477937	-0.83585719
C	-3.44531326	-3.01726183	1.46165365
H	-4.40476555	-2.61911398	1.81192878
H	-2.70289866	-2.80437474	2.24001804
H	-3.54339732	-4.10834394	1.37959387

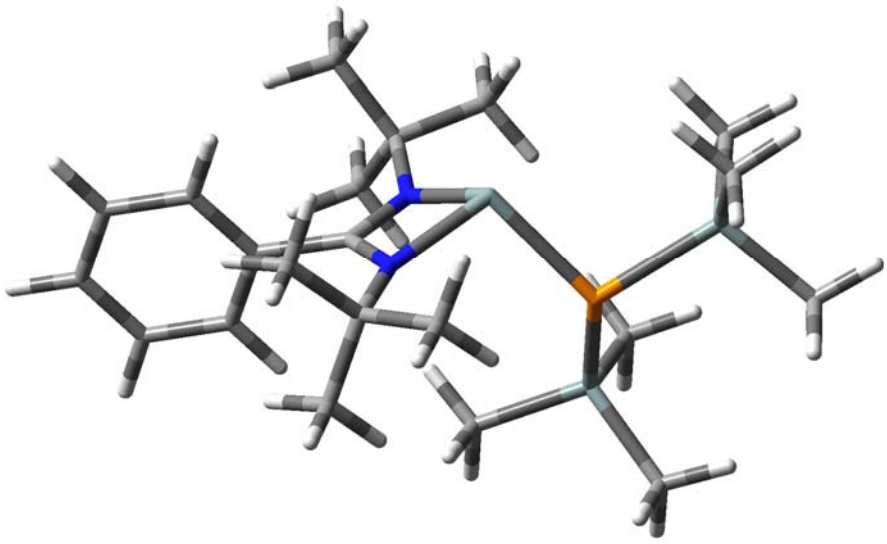


Figure 5. Optimized structure of compound **2**.

Table 5. Cartesian coordinates (x, y, z) for the optimized structure of **2**.

Si	0.38513755	0.44719484	-1.38538268
N	-0.8506894	-0.87040755	-0.71768208
N	1.09081749	1.25653209	-0.4742225
C	1.06963476	-2.29630647	-1.06024785
C	1.54247542	2.64779967	-0.23554447
C	3.16351163	-0.12069567	0.03002236
C	3.48258287	-0.40378616	1.36617318
C	4.80980169	-0.60185195	1.749862
C	5.83296111	-0.52211961	0.80381603
C	5.52399695	-0.24023619	-0.52815211
C	4.19798495	-0.0385683	-0.91345052
P	2.09625575	0.7377159	0.1543678
Si	3.97090163	0.20621893	-1.00366919
C	4.10903882	1.44641346	-2.43169343
C	5.48146317	0.4038723	0.1314437
Si	2.10063949	-0.38063051	2.12727588
C	2.66284783	-2.19684668	2.05153764
C	3.2645704	0.52839572	3.32308544
C	0.35307869	-0.33306458	2.86725816
C	1.57193913	-3.09352634	0.15920684
C	0.29970914	-2.85592325	-1.4843893
C	2.04827086	-2.45474223	-2.24301842
C	-1.962783	2.83973971	1.23448246
C	-2.6992039	3.03815928	-1.17936011
C	0.34258445	3.56504186	-0.53288265
C	1.73321068	0.08565388	-0.36380868
C	4.01101284	-1.54733584	-1.73453591
H	2.68799722	-0.46513218	2.10381088
H	5.04202259	-0.81879088	2.78883514
H	6.86583403	-0.67793068	1.10269358
H	6.31496147	-0.1756549	-1.27024085
H	3.96317094	0.18324359	-1.95015436
H	3.2341654	1.39195108	-3.08928215
H	5.0007234	1.24089348	-3.03844234
H	4.18225678	2.47374591	-2.05794607
H	6.40531409	0.28075913	-0.44874681
H	5.49585382	-0.34332655	0.93331243
H	5.50677662	1.39608177	0.59532762
H	2.00153013	-2.8072759	1.42681806
H	2.66291809	-2.63173973	3.06020348
H	3.67943469	-2.29292922	1.65296182
H	3.2526372	0.04775187	4.31057048
H	2.95698591	1.57220587	3.45115829
H	4.30011486	0.53082506	2.9658751
H	0.01829198	0.69420286	2.95082271
H	-0.3492895	-0.89931471	2.24717629
H	0.35372909	-0.77334536	3.87278567
H	2.56300259	-2.7672299	0.48370596
H	0.87936758	-2.98925213	1.00122438
H	-1.6372201	-4.15739097	-0.09674937
H	0.67360114	-2.34236149	-2.37678498
H	0.21223435	-3.92215913	-1.71859074
H	1.03907178	-2.73745115	-0.68730975
H	-1.7181255	-1.85023574	-3.09491966
H	2.08506123	-3.5028668	-2.56270667
H	3.06382746	-2.15406306	-1.97293269
H	1.14090475	2.57008654	1.90559021
H	2.21814338	3.89058357	1.41345767
H	2.83632701	2.2346788	1.49177924
H	2.42244632	2.84903578	-2.222404
H	2.91829287	4.10719449	-1.07468629
H	3.61588634	2.4874885	-0.95515717
H	0.50770102	3.3308585	0.11324953
H	0.01692205	3.45988452	-1.57392676
H	0.63052938	4.60960293	-0.37212299
H	3.91077241	-2.31430568	-0.95862228
H	3.20027224	-1.69367025	-2.45691727
H	4.96006511	-1.72265951	-2.25886237

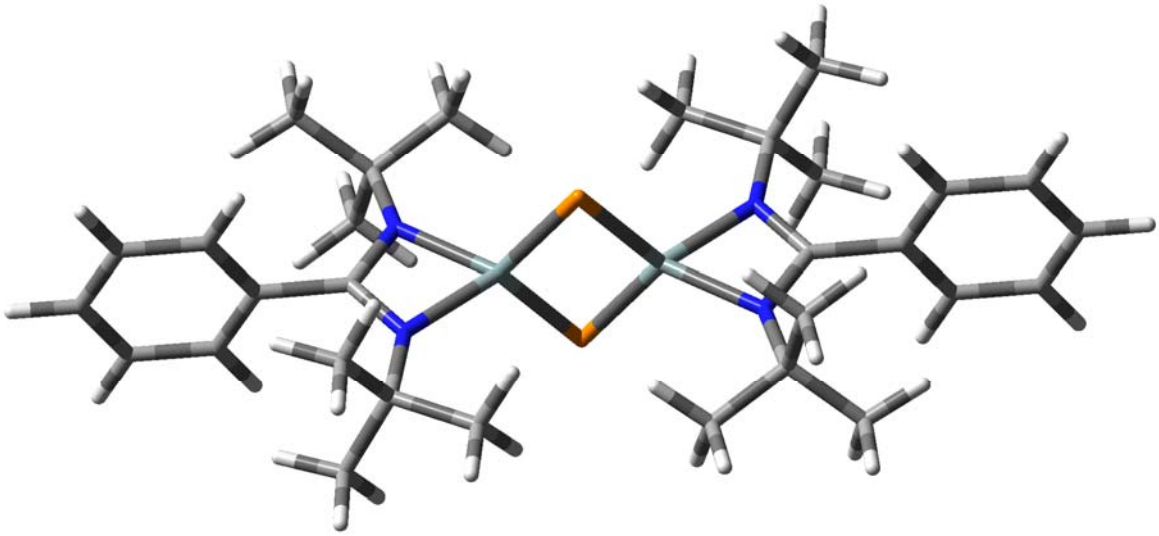


Figure 6. Optimized structure of compound **3**.

Table 6. Cartesian coordinates (x, y, z) for the optimized structure of **3**.

P	-0.04949504	0.162273	-1.77138217	C	3.16810376	2.53641361	0.02048358
Si	1.29488425	0.00558011	-0.03832924	C	3.90756383	2.9376519	-1.27130384
N	2.8553013	-1.06486224	-0.15654872	C	3.99015781	2.92635466	1.26492282
C	3.64785176	0.01140655	-0.05011275	C	1.82112235	3.27549518	0.06742135
N	2.85297545	1.08721034	0.02650551	P	0.0495641	-0.16148182	1.76863169
C	5.14189026	0.00526899	-0.0217157	Si	-1.29479595	-0.00490401	0.03560624
C	5.87209197	0.02647899	-1.21811668	N	-2.85533592	1.06514532	0.15461485
C	7.26646111	0.00804681	-1.18995086	C	-3.64777848	-0.01136382	0.04970141
C	7.94358229	-0.03628307	0.03049114	N	-2.85273306	-1.08696171	-0.02787527
C	7.22106061	-0.05940376	1.22441922	C	-5.14186666	-0.0056791	0.02358763
C	5.82568815	-0.03682011	1.20089214	C	-5.87028948	-0.02661037	1.22108207
C	3.14881585	-2.51305101	-0.03130461	C	-7.26470895	-0.00868005	1.19497399
C	1.87009563	-3.2501393	-0.46193255	C	-7.94366521	0.03488588	-0.02447429
C	3.46412468	-2.85849749	1.4384065	C	-7.22293009	0.05774973	-1.21948211
C	4.30172934	-2.95904887	-0.95043434	C	-5.82751603	0.03566737	-1.19801035

C	-3.1494007	2.51327974	0.03025596
C	-1.86939217	3.25052302	0.45679314
C	-3.46938494	2.85878396	-1.43842989
C	-4.2994556	2.9590483	0.95308001
C	-3.16754701	-2.53623324	-0.02150829
C	-3.90588866	-2.93767237	1.27085852
C	-3.99048243	-2.92636419	-1.26530814
C	-1.82045444	-3.27502311	-0.06948865
H	5.3463368	0.04958669	-2.16795033
H	7.82280256	0.0251901	-2.12292975
H	9.02970209	-0.05283811	0.05056529
H	7.74143415	-0.09366982	2.17744188
H	5.26516589	-0.04787688	2.13089667
H	1.03078345	-2.96972339	0.17962697
H	2.02205868	-4.33189854	-0.37919156
H	1.60692153	-3.0091685	-1.49632204
H	4.38724306	-2.37326355	1.77181539
H	3.59469155	-3.94115286	1.55255729
H	2.64396781	-2.53864896	2.08919216
H	4.11769734	-2.64554209	-1.98375509
H	4.36573461	-4.05300475	-0.93521842
H	5.26996222	-2.56662512	-0.63320189
H	4.90477055	2.49318374	-1.32835098
H	4.02585928	4.02685092	-1.30649423
H	3.33336214	2.62884498	-2.15140013
H	3.47403873	2.60918515	2.17739225
H	4.10896723	4.01542631	1.30053092
H	4.98889361	2.48253318	1.25521693
H	1.21797557	3.03357964	-0.81273712
H	1.99455122	4.35695019	0.0867626
H	1.25392189	2.9968523	0.96091667
H	-5.34312639	-0.0491718	2.17015023
H	-7.81965433	-0.02562546	2.12878756
H	-9.02981935	0.05104801	-0.04293498
H	-7.74472584	0.09143295	-2.17174732
H	-5.26838599	0.04656602	-2.12885277
H	-1.03194573	2.96967099	-0.1870501
H	-2.02155867	4.33224347	0.37393897
H	-1.6032761	3.01006105	1.4905464
H	-4.39344357	2.37345239	-1.76904136
H	-3.60048528	3.94143083	-1.55203276
H	-2.65119944	2.53923235	-2.09184153
H	-4.111979	2.64558744	1.98579657
H	-4.36385276	4.05298938	0.93807585
H	-5.26858195	2.5663054	0.63896656
H	-4.90316322	-2.49347365	1.32873996
H	-4.02387751	-4.0269029	1.30610561
H	-3.33104809	-2.62875448	2.15049702
H	-3.47516849	-2.60903933	-2.17817989
H	-4.10904167	-4.01546598	-1.30085613
H	-4.98932586	-2.48279892	-1.25479089
H	-1.21662925	-3.03278693	0.81011487
H	-1.9936549	-4.35651938	-0.08850059
H	-1.25409576	-2.99641617	-0.96352867

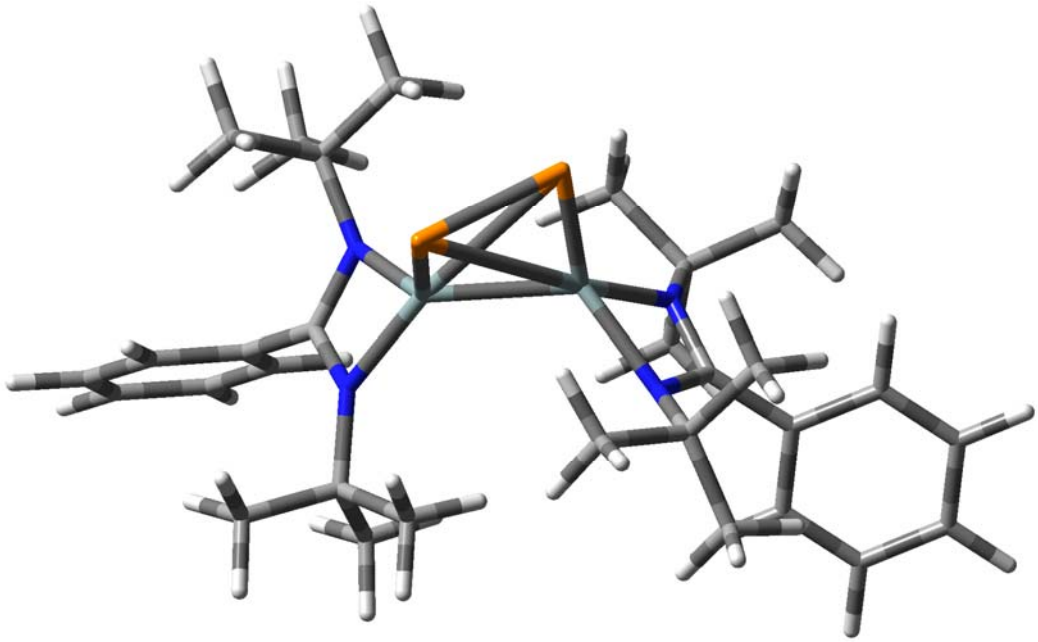


Figure 7. Optimized structure of compound **6**.

Table 7. Cartesian coordinates (x, y, z) for the optimized structure of **6**.

P	-0.83491319	3.44394324	0.44654082	H	5.35370623	0.01865734	-1.39655301
Si	1.09899447	1.22332045	-0.4751348	H	1.69677664	2.87624076	1.92169996
N	2.51242847	0.66176597	0.69949724	H	2.92345161	2.91584462	3.20501755
C	2.92206699	-0.24178107	-0.2022104	H	1.72237399	1.61656661	3.16721623
N	2.07398296	-0.19668045	-1.24689896	H	5.01620301	1.78929535	0.35548522
C	4.10651358	-1.14157042	-0.07339484	H	4.86579802	2.95585235	1.6785653
C	4.0430079	-2.26937578	0.75727331	H	3.74262872	3.03356976	0.30008729
C	5.15216333	-3.10265825	0.8967755	H	3.43766072	-0.26003388	3.10264
C	6.33835697	-2.81061602	0.21966826	H	4.52787264	1.08828003	3.46200503
C	6.40925916	-1.68496759	-0.60276948	H	4.92609126	-0.03483683	2.15927785
C	5.29734695	-0.85550185	-0.7551076	H	2.48382792	-2.99687345	-1.34156164
C	3.32576692	1.41690197	1.70224891	H	1.34083434	-3.23913035	-2.66905909
C	2.35082815	2.25767921	2.54228992	H	0.77102525	-2.57549046	-1.12498895
C	4.29731248	2.35647131	0.9576468	H	3.26825691	-0.11870698	-3.6725889
C	4.1022319	0.48548385	2.65190281	H	2.83239599	-1.75161436	-4.21276024
C	1.86375936	-1.1518226	-2.36439253	H	3.96681677	-1.54428945	-2.87276034
C	1.60468215	-2.57644561	-1.83684232	H	-0.26849883	-0.70093642	-2.48209186
C	3.06275584	-1.1393612	-3.33334107	H	0.44100799	-1.30889506	-3.99166918
C	0.6184223	-0.66624816	-3.12250503	H	0.74744572	0.36407068	-3.46807643
P	0.84140664	3.20422761	-1.24574512	H	-5.39187272	0.29091331	1.32292009
Si	-1.10817414	1.33898826	0.18879141	H	-7.31398429	-1.26915526	1.38270449
N	-2.49691798	0.49942922	-0.83460958	H	-7.09742253	-3.55312708	0.42345996
C	-2.92115568	-0.16224692	0.2539967	H	-4.94797316	-4.26067173	-0.60923871
N	-2.10368323	0.15332769	1.27373793	H	-3.03570944	-2.68639756	-0.69586947
C	-4.08342536	-1.0973327	0.31617085	H	-1.62053215	1.00462853	-3.39211685
C	-5.2946075	-0.70525942	0.90238045	H	-2.93357521	2.12180844	-3.79079479
C	-6.37677186	-1.58635939	0.93432997	H	-1.80938016	2.50318052	-2.46997094
C	-6.25519576	-2.86753473	0.3943772	H	-4.76777159	-0.67564966	-2.19663427
C	-5.04845546	-3.26509924	-0.18616763	H	-4.39653281	0.18428511	-3.69334092
C	-3.96981736	-2.38322495	-0.23224889	H	-3.22236121	-0.96080094	-3.02443719
C	-3.30711148	0.96947668	-2.00362429	H	-3.90063736	2.80651165	-0.99374642
C	-2.35270058	1.69525101	-2.9655131	H	-4.9364523	2.3641819	-2.3688267
C	-3.96459837	-0.19865857	-2.76188395	H	-5.0926501	1.48968717	-0.83893211
C	-4.37547847	1.96853093	-1.51409376	H	-4.05183005	-0.59127064	3.18372
C	-1.93402296	-0.46783628	2.61201283	H	-2.92802482	-0.47141544	4.54380483
C	-3.12675655	-0.12009581	3.524835	H	-3.27681794	0.96395485	3.56046602
C	-1.75401392	-1.99528466	2.51383014	H	-0.92709837	-2.24379989	1.83870196
C	-0.65934169	0.14343466	3.2152379	H	-1.51642414	-2.40157694	3.50366181
H	3.12543004	-2.48640613	1.29613314	H	-2.65680205	-2.49642877	2.15649566
H	5.0913479	-3.97616698	1.53982352	H	-0.7318365	1.23426133	3.26659939
H	7.20429807	-3.45648514	0.3345162	H	-0.50526702	-0.2458353	4.22753993
H	7.33016362	-1.45012283	-1.12897275	H	0.21835747	-0.10914502	2.61194477

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