Supporting Information

for

Assembly of NHC-Stabilized 2-Hydrophosphasilenes from Si(IV) Precursors: A Lewis Acid-Base Complex

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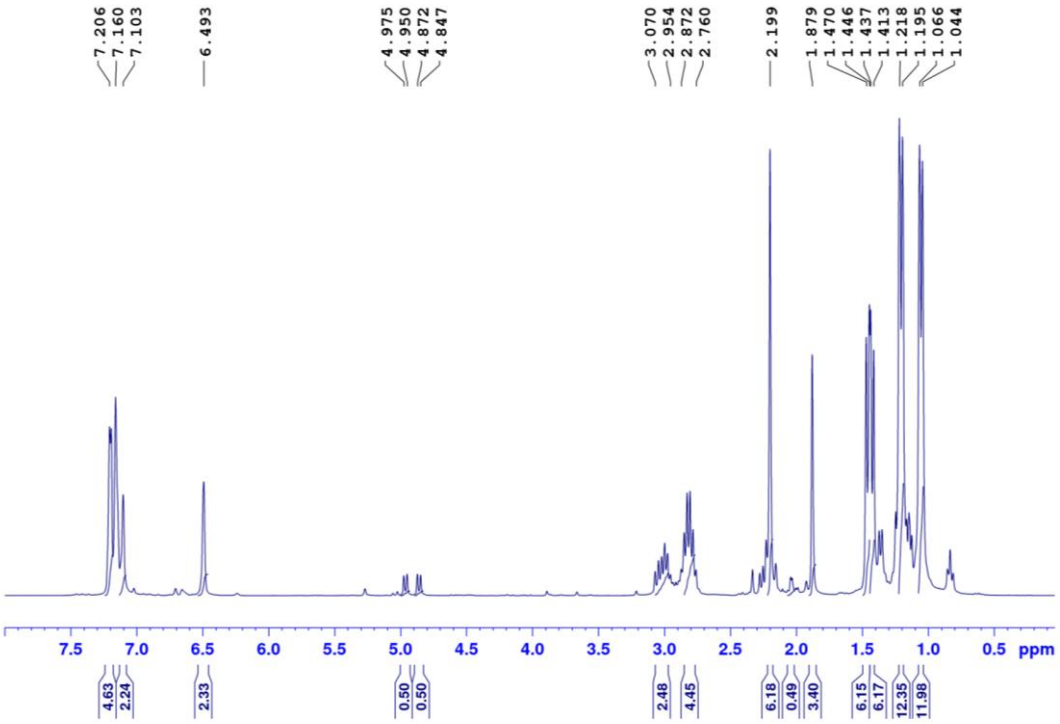


Figure S1 ^{1}H NMR of **2** in [D_6]-benzene at RT.

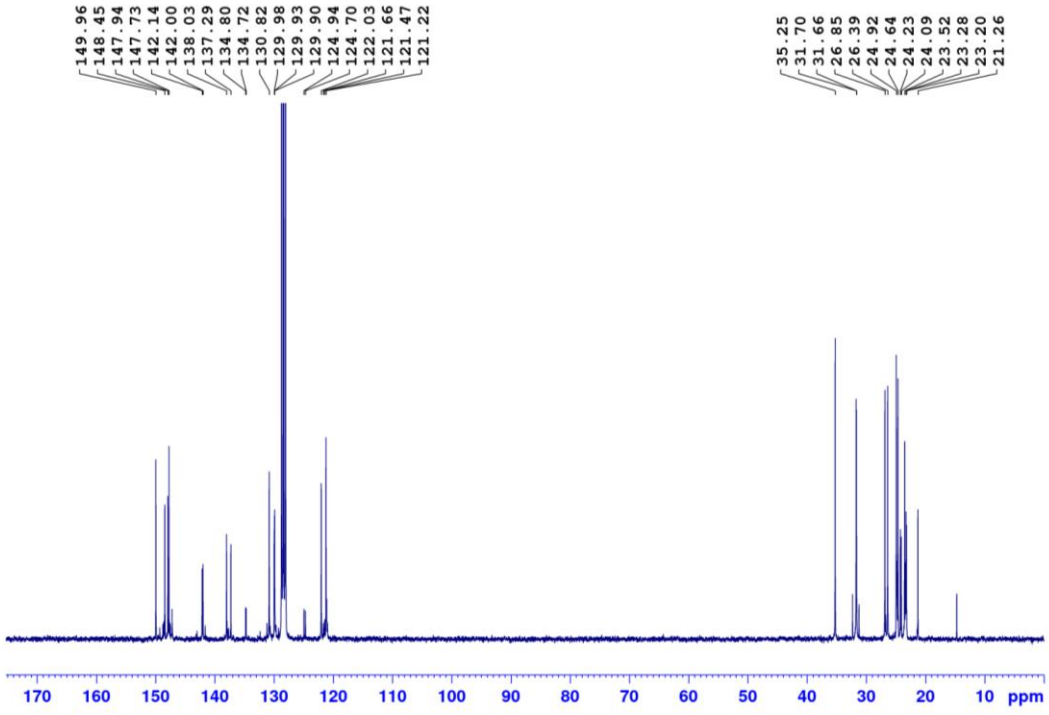


Figure S2 ^{13}C{^{1}H} NMR of **2** in [D_6]-benzene at RT.

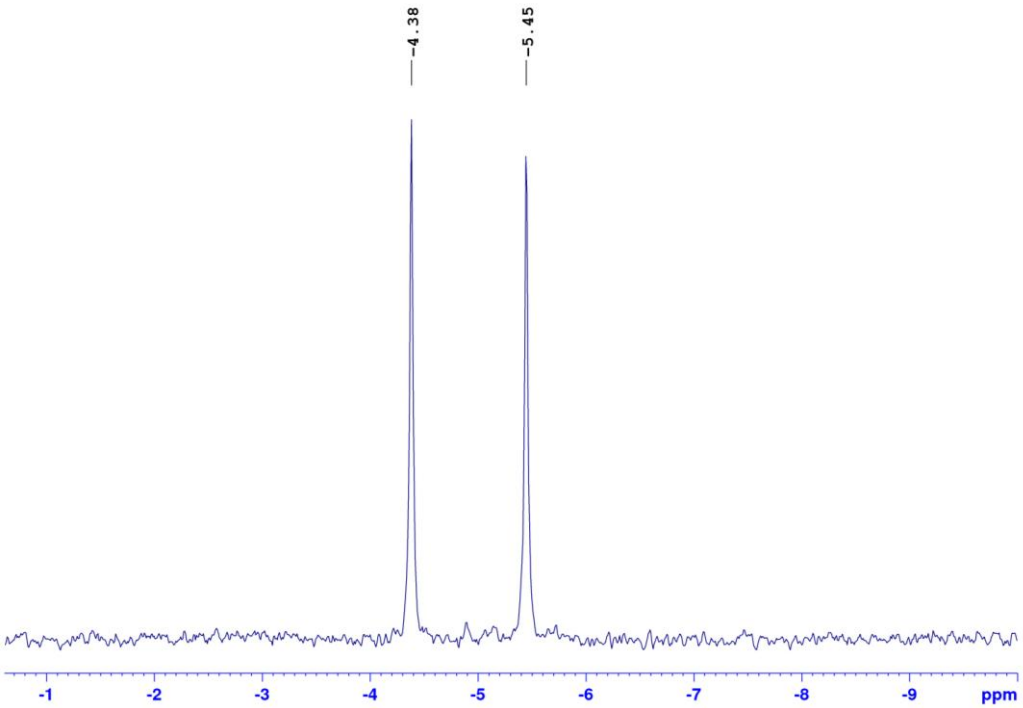


Figure S3 $^{29}Si\{^{1}H\}$ NMR of **2** in $[D_6]$-benzene at RT.

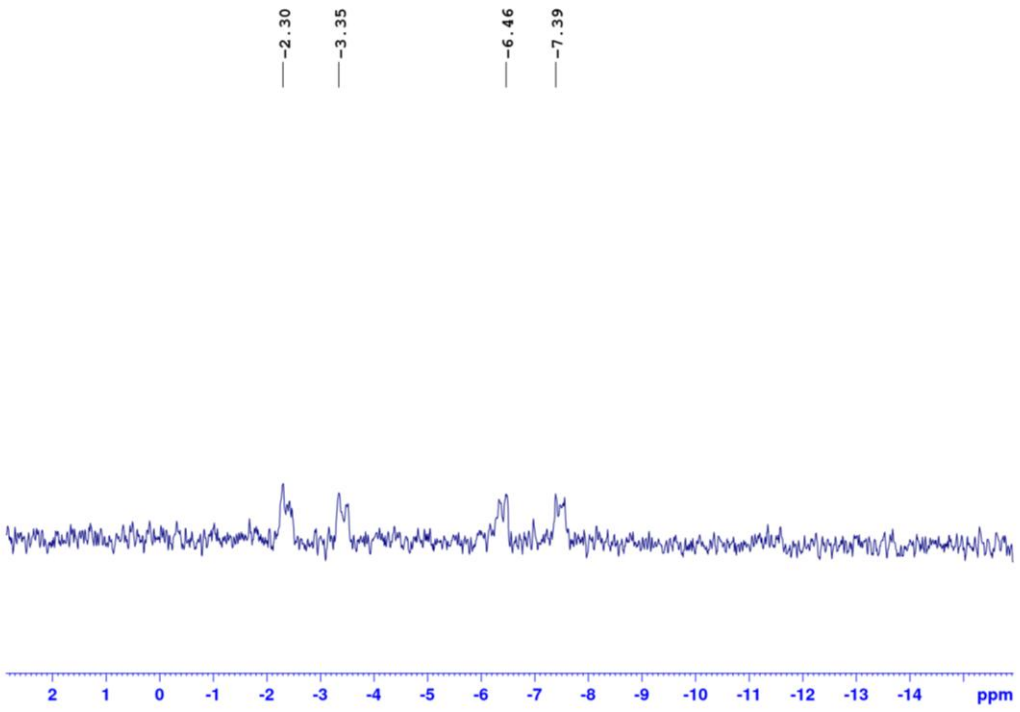


Figure S4 ^{29}Si NMR of **2** in $[D_6]$-benzene at RT.

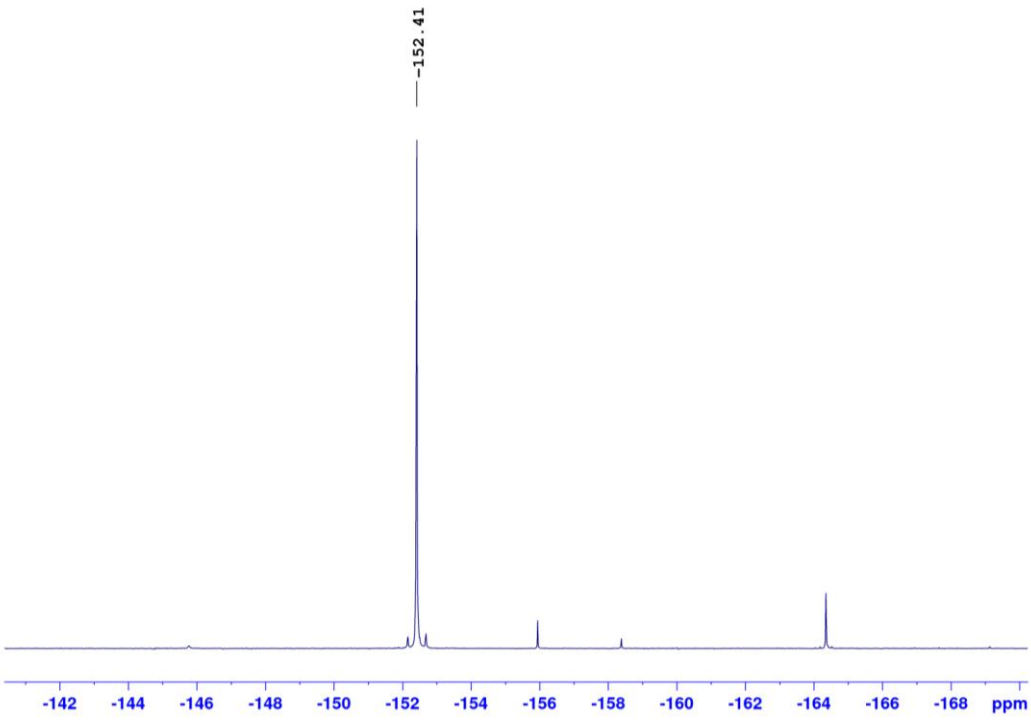


Figure S5 $^{31}P\{^{1}H\}$ NMR of **2** in $[D_6]$-benzene at RT.

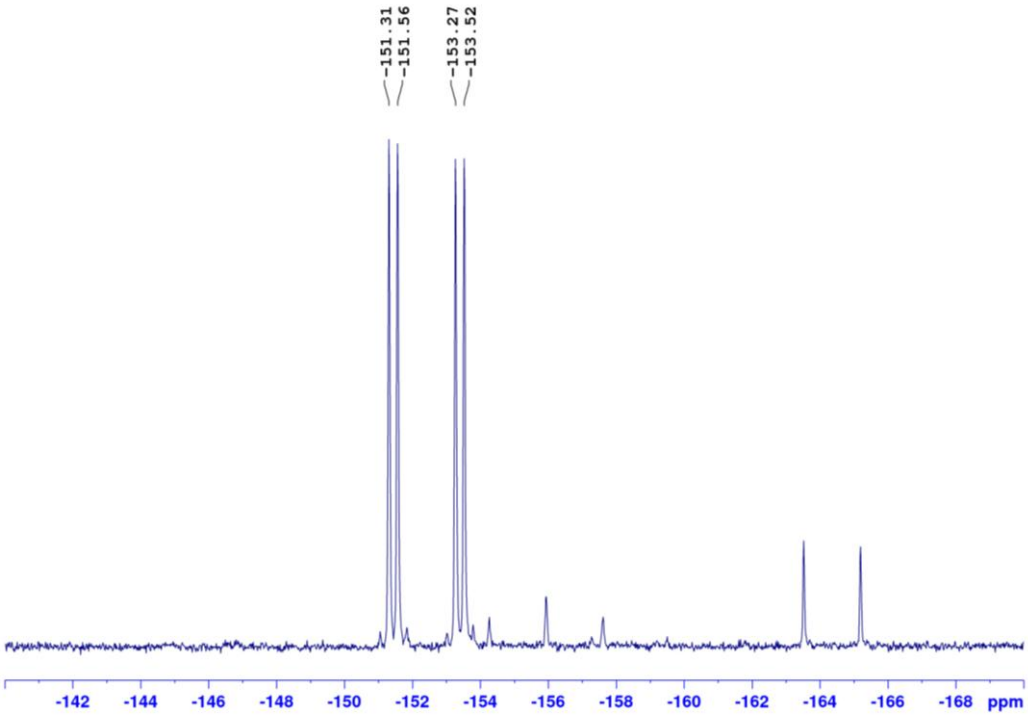


Figure S6 ^{31}P NMR of **2** in $[D_6]$-benzene at RT.

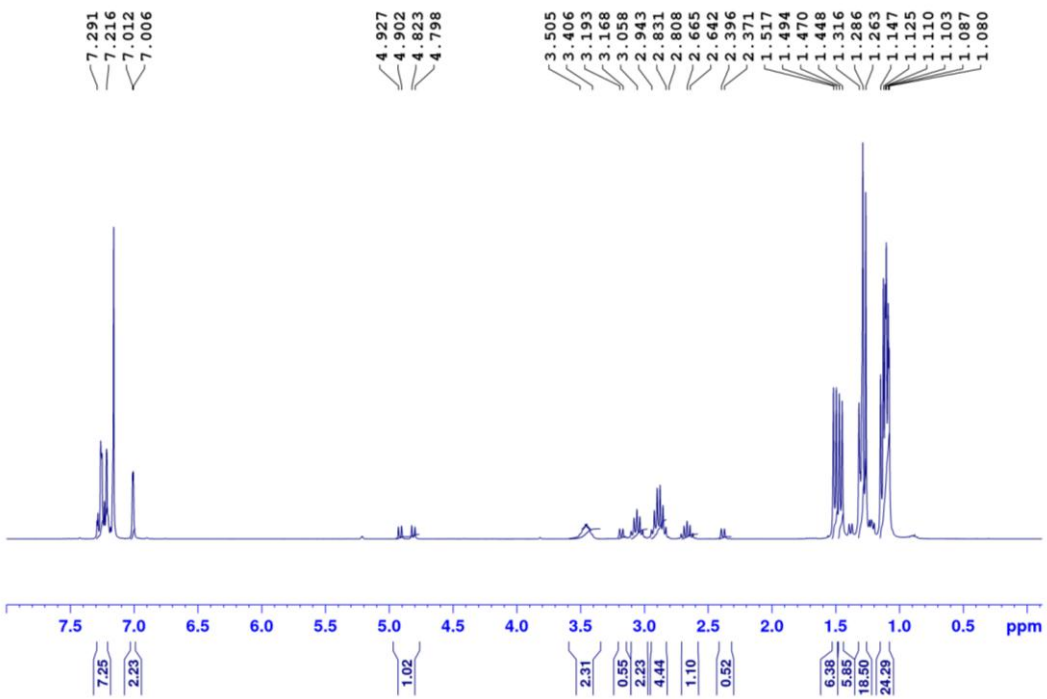


Figure S7 ^{1}H NMR of **3** in [D_6]-benzene at RT.

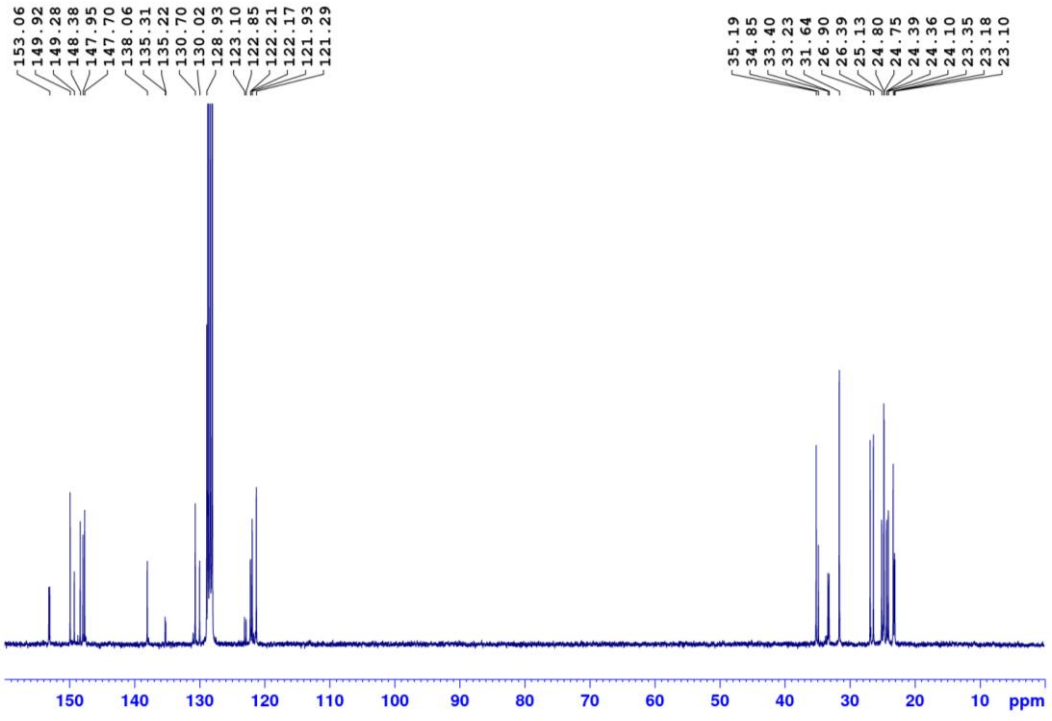


Figure S8 ^{13}C{^{1}H} NMR of **3** in [D_6]-benzene at RT.

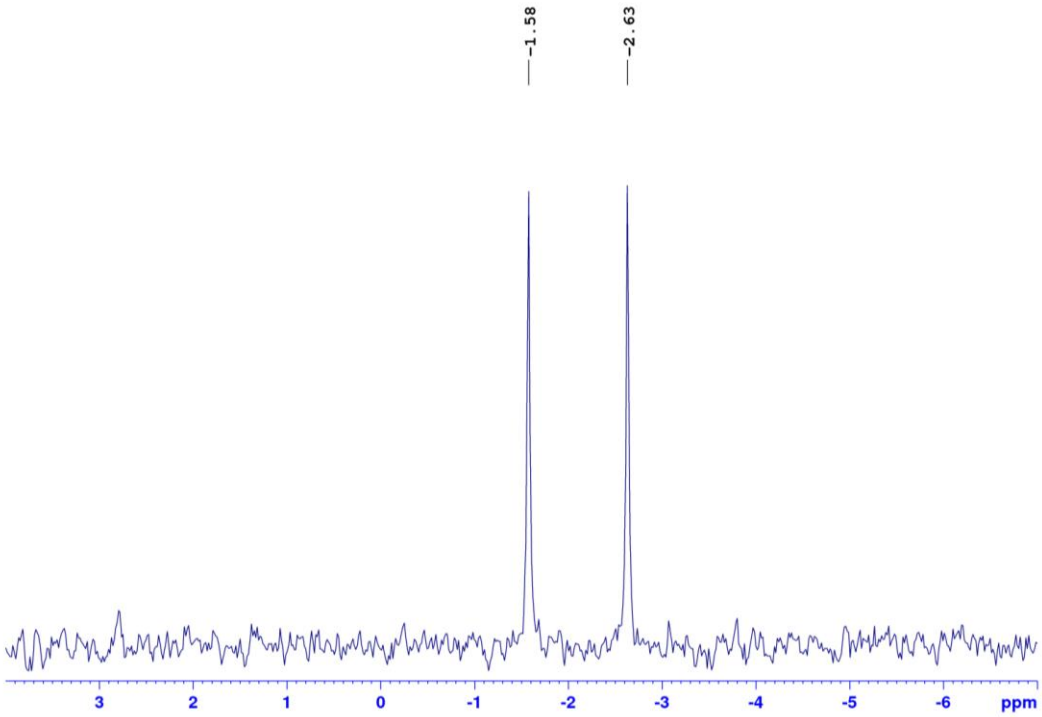


Figure S9 $^{29}Si\{^{1}H\}$ NMR of **3** in $[D_6]$-benzene at RT.

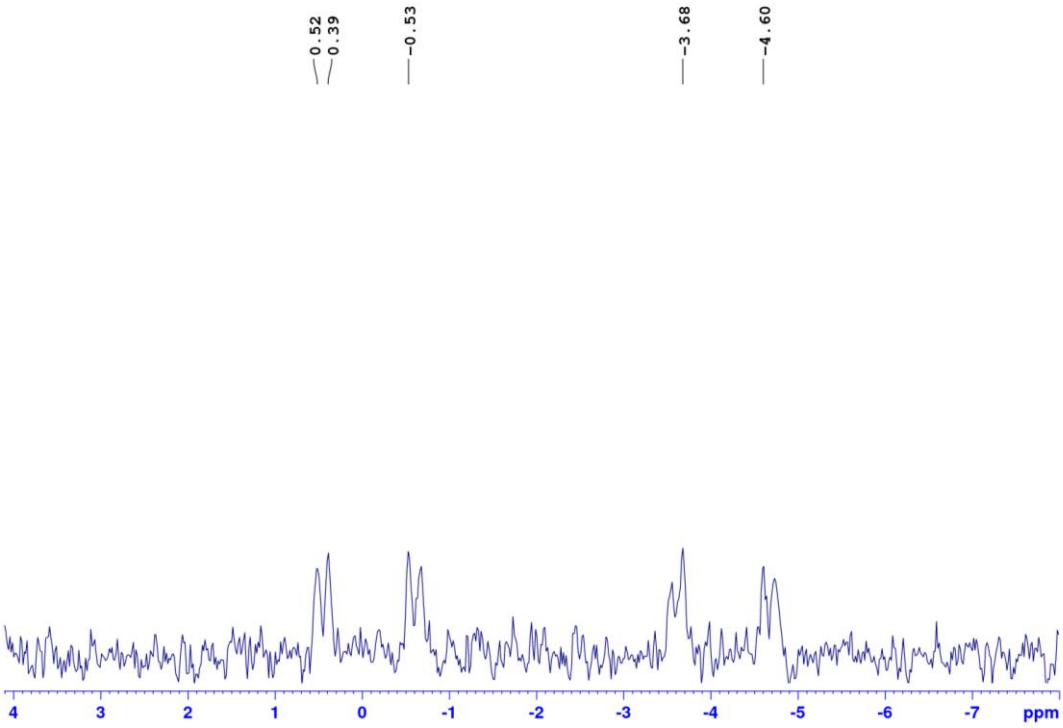


Figure S10 ^{29}Si NMR of **3** in $[D_6]$-benzene at RT.

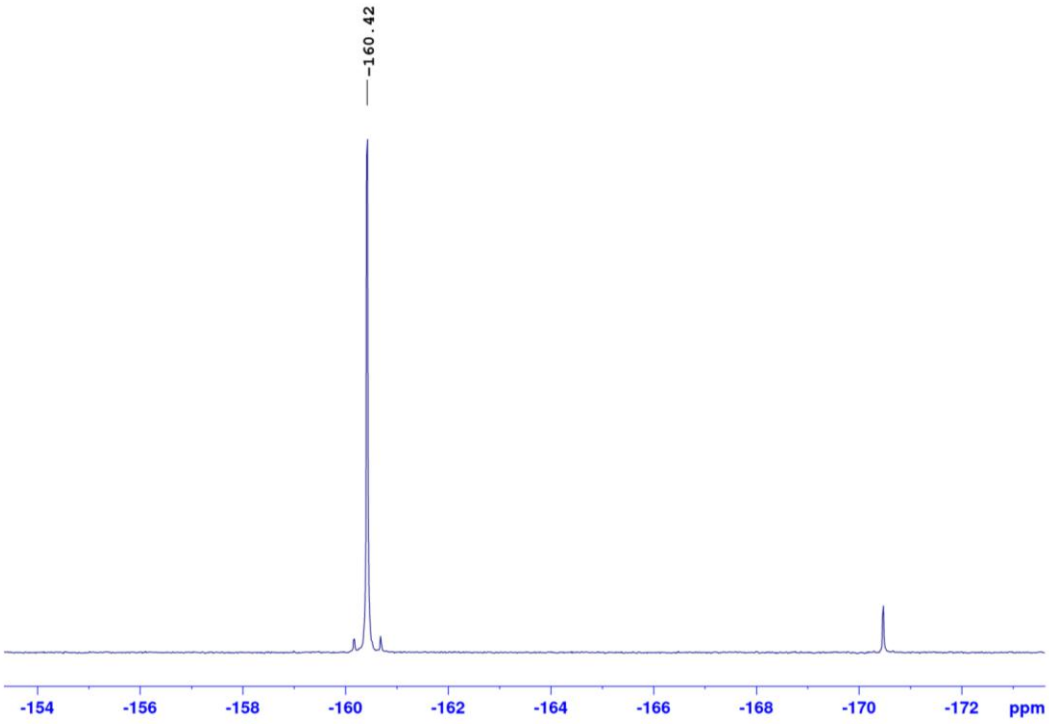


Figure S11 $^{31}P\{^{1}H\}$ NMR of **3** in $[D_6]$-benzene at RT.

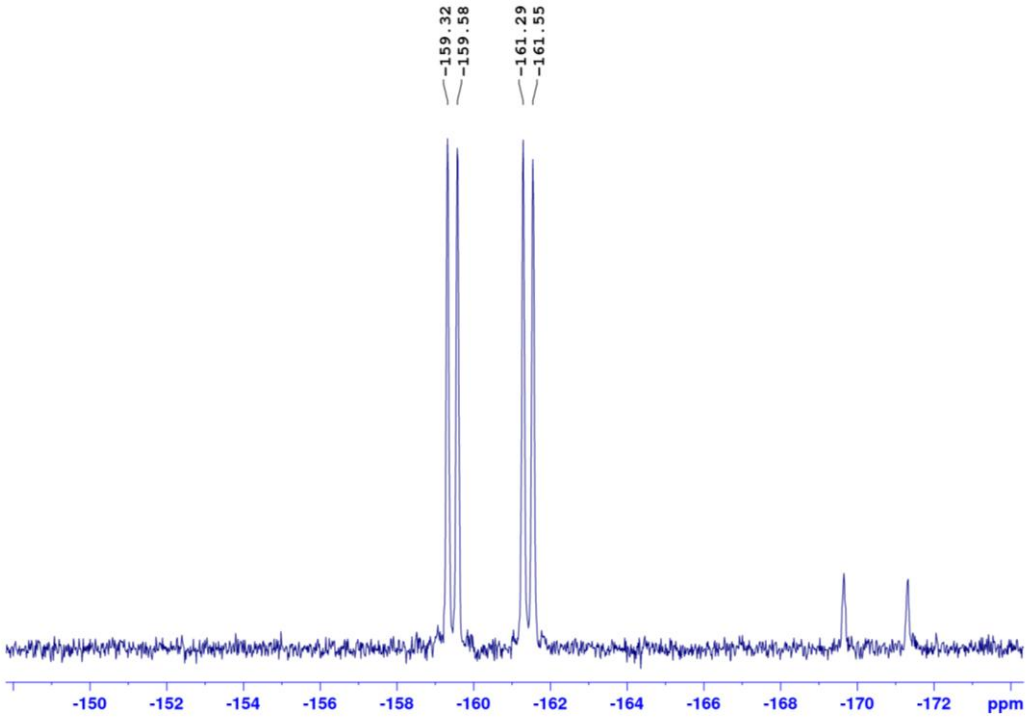


Figure S12 ^{31}P NMR of **3** in $[D_6]$-benzene at RT.

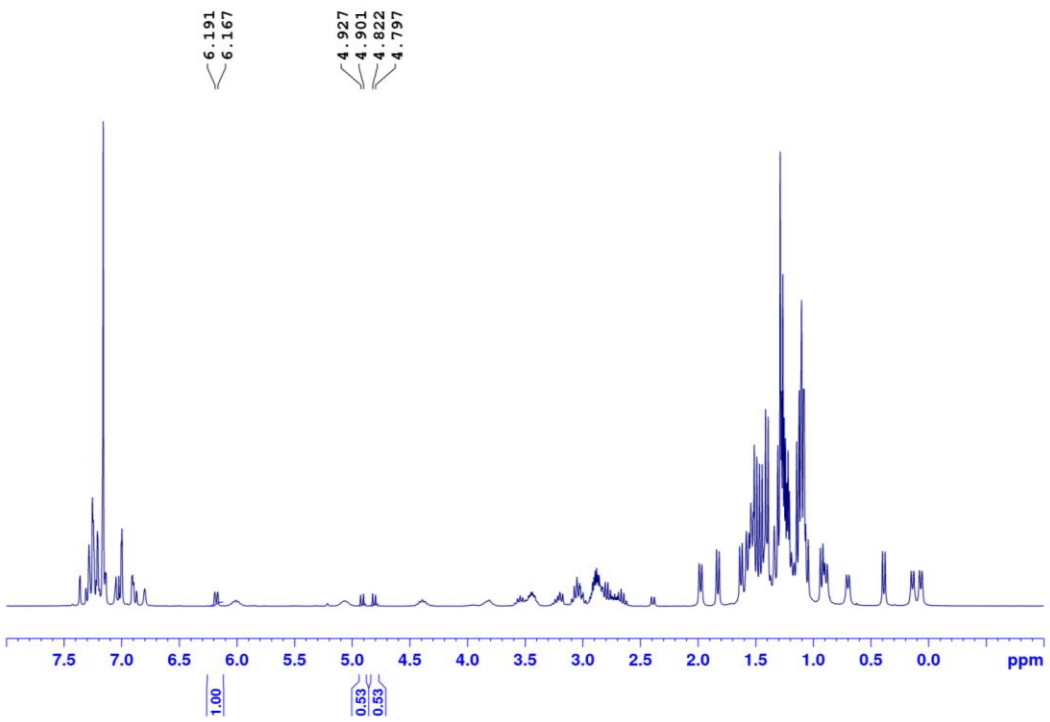


Figure S13 ^{1}H NMR of 1:1 mixture of **3** and NHC^{iPr2Me2} in [D_6]-benzene at RT.

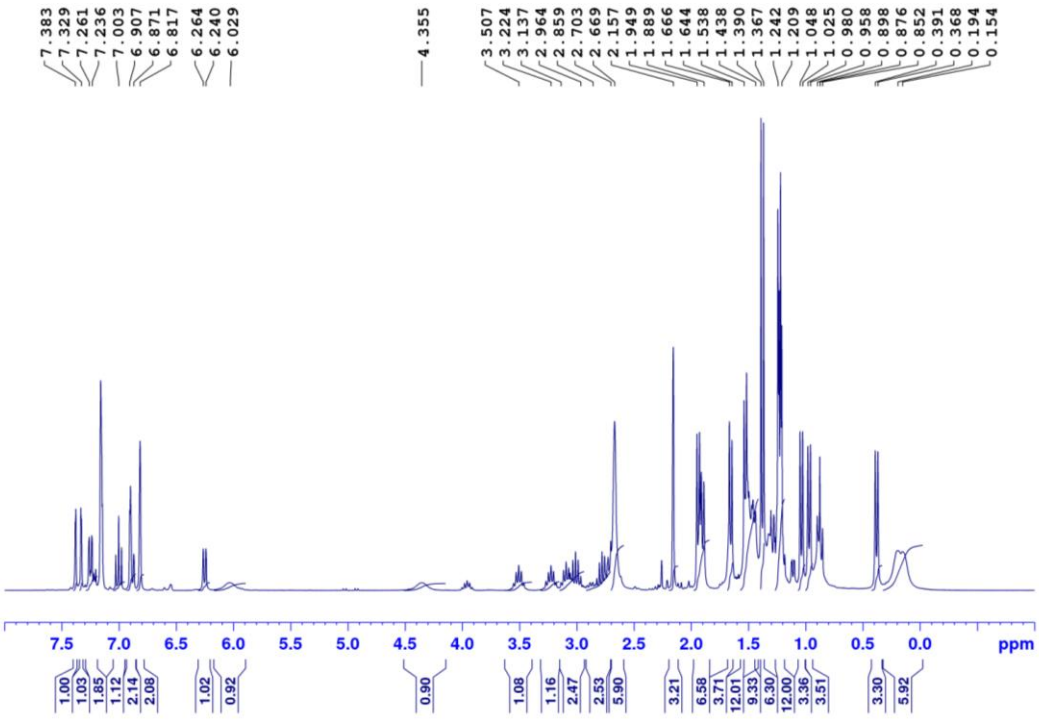


Figure S14 ^{1}H NMR of **4** in [D_6]-benzene at RT.

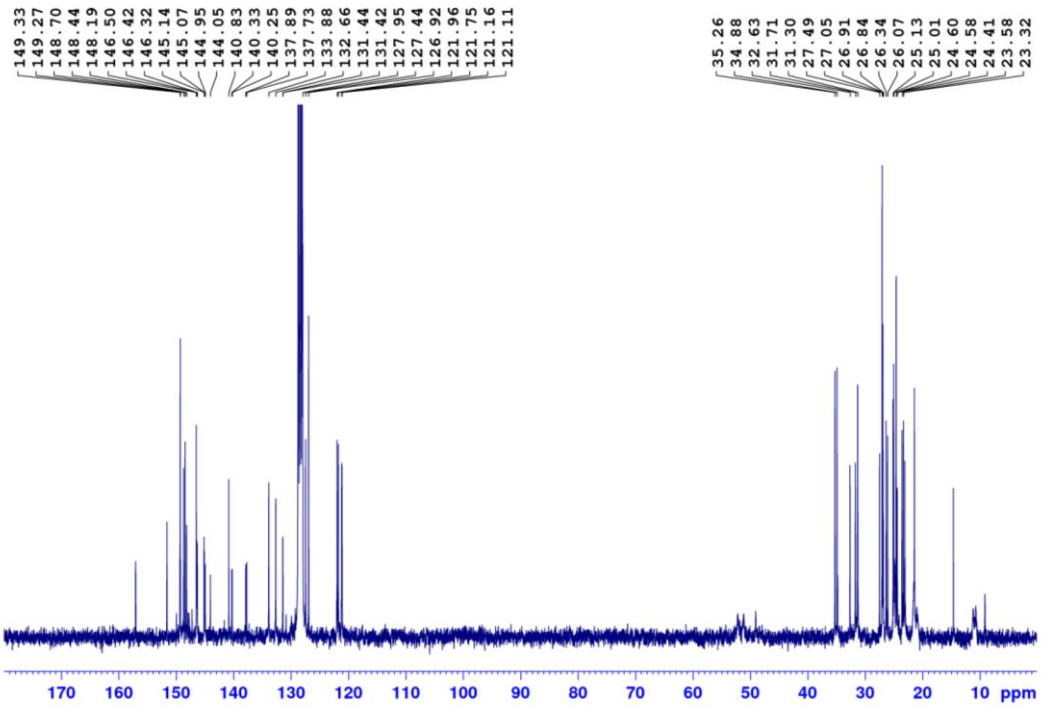


Figure S15 $^{13}C\{^{1}H\}$ NMR of **4** in $[D_6]$-benzene at RT.

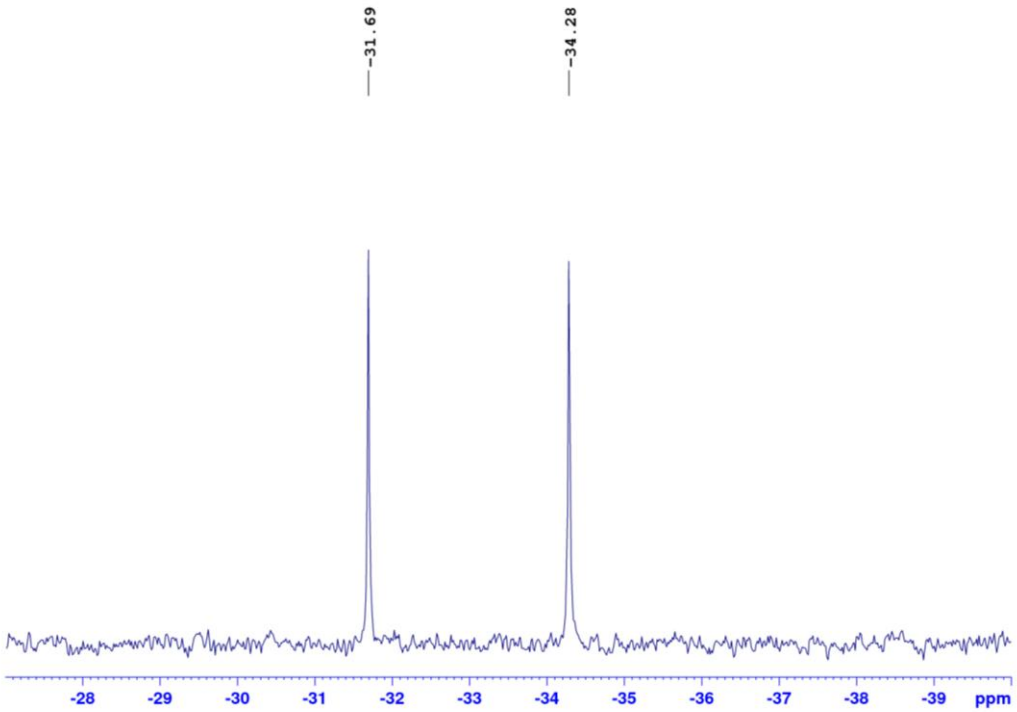


Figure S16 $^{29}Si\{^{1}H\}$ NMR of **4** in $[D_6]$-benzene at RT.

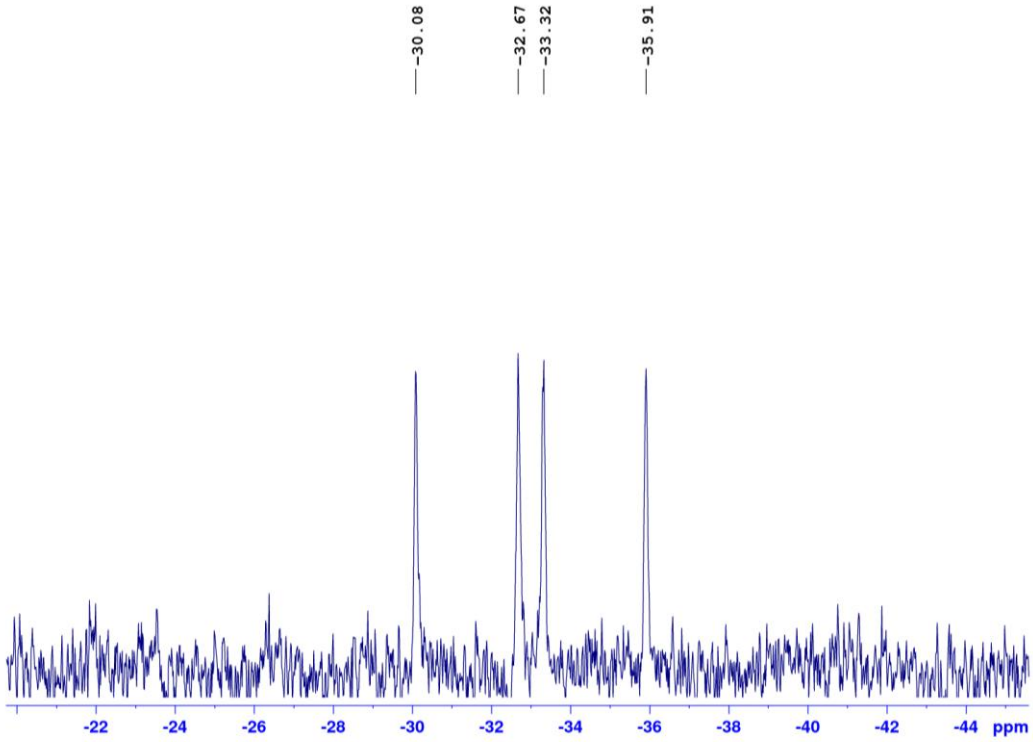


Figure S17 ^{29}Si NMR of **4** in [D_6]-benzene at RT.

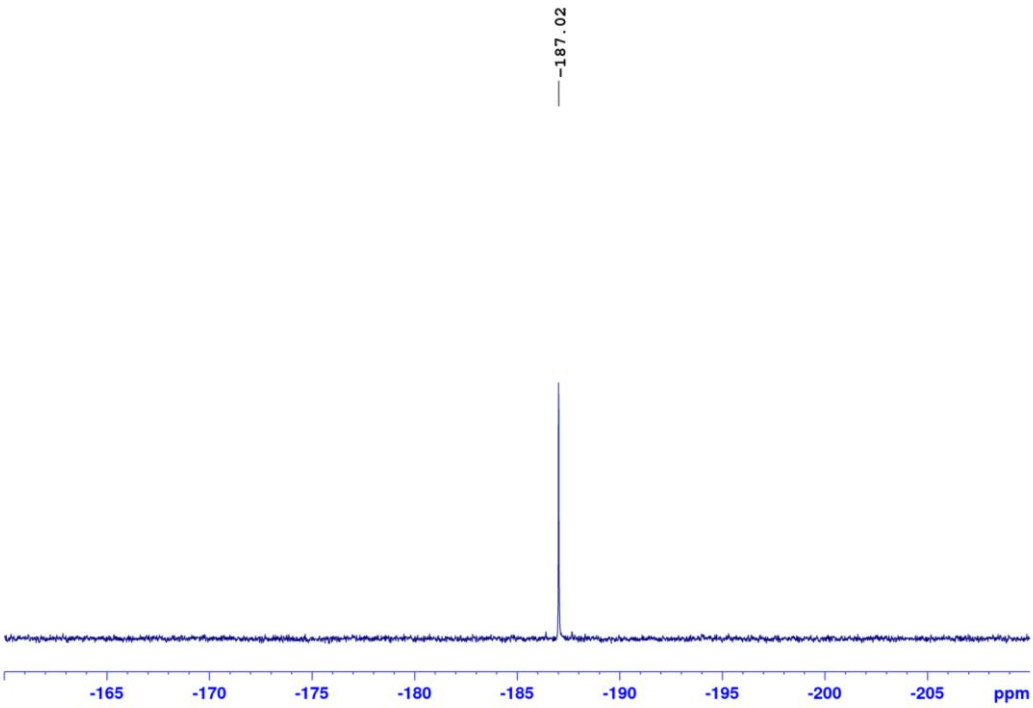


Figure S18 ^{31}P{^{1}H} NMR of **4** in [D_6]-benzene at RT.

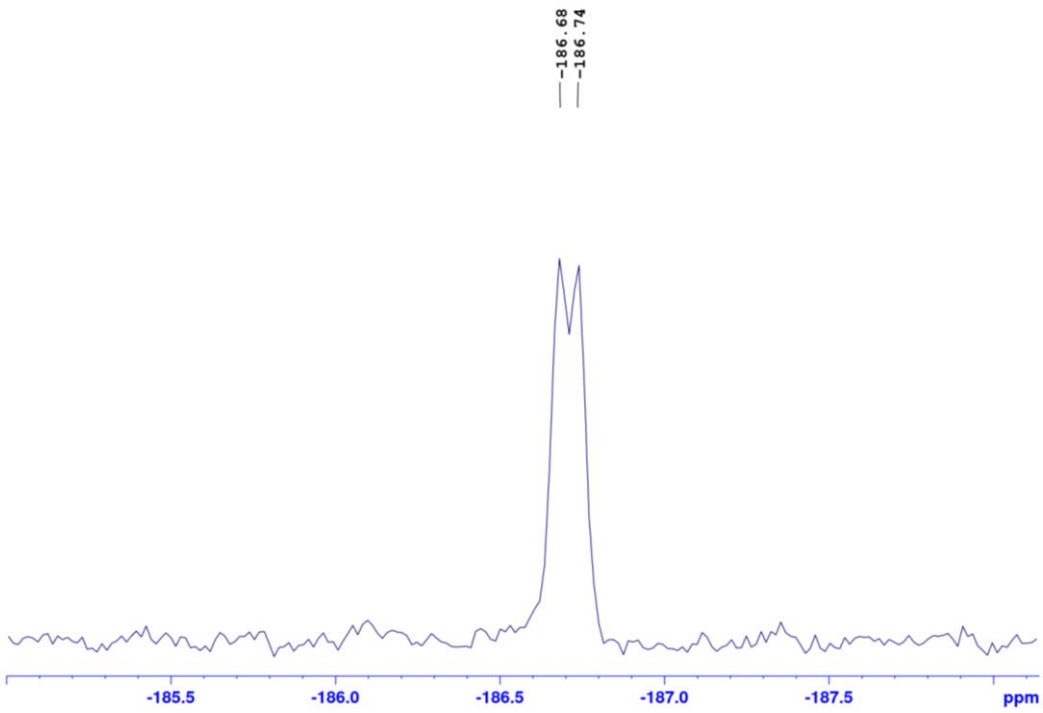


Figure S19 ^{31}P NMR of **4** in [D_6]-benzene at RT.

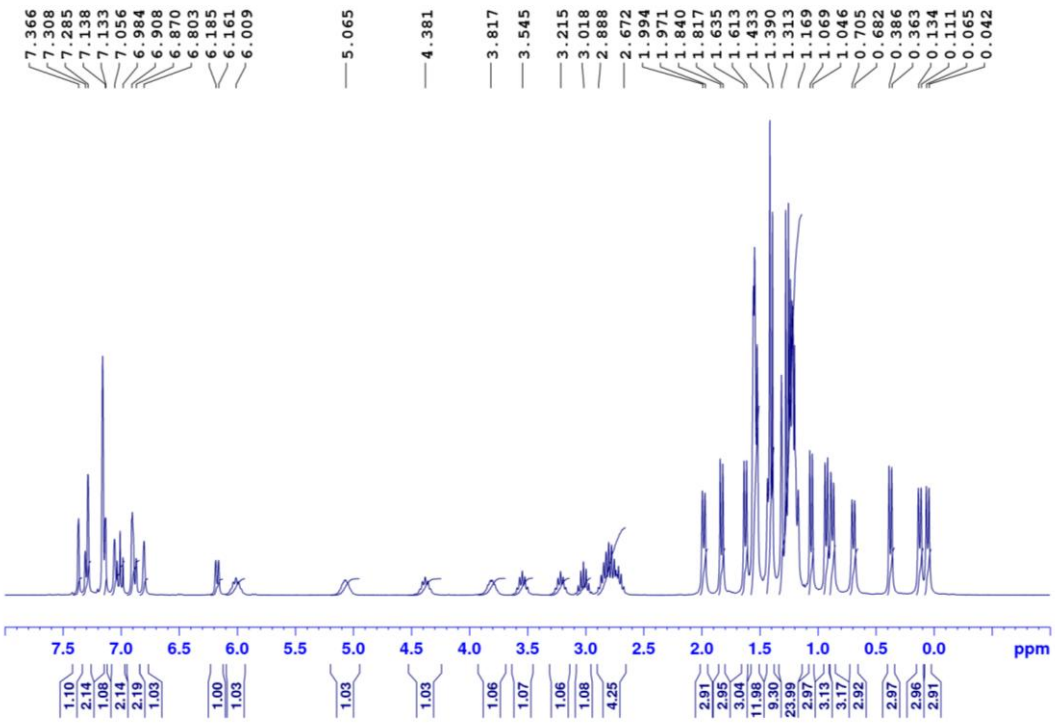


Figure S20 ^{1}H NMR of **5** in [D_6]-benzene at RT.

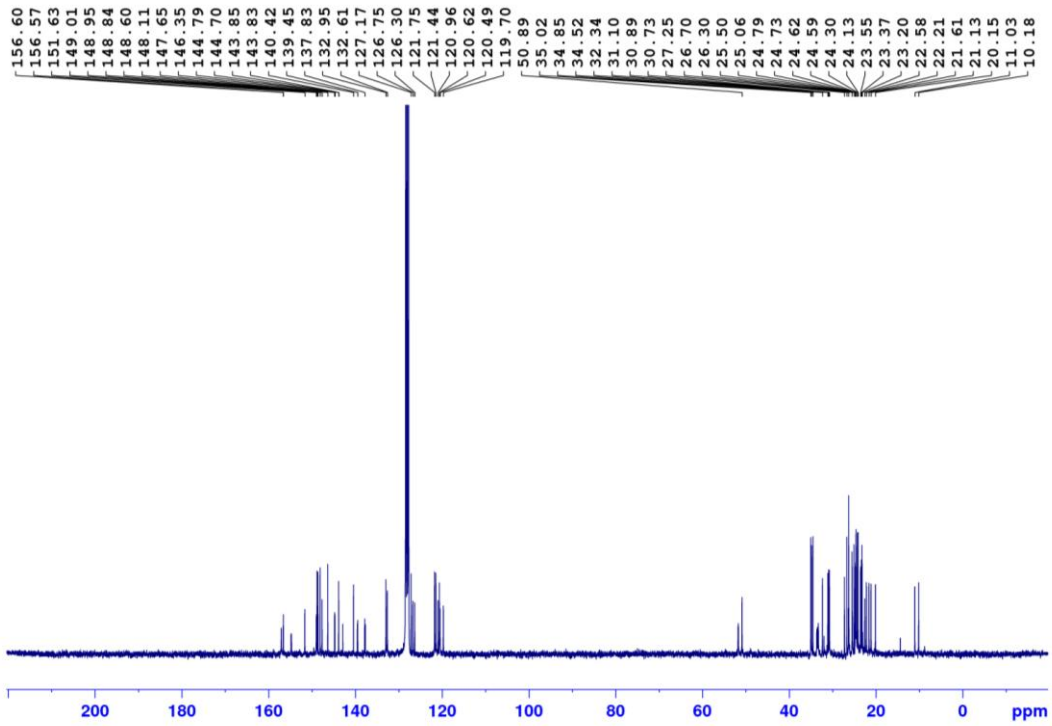


Figure S21 $^{13}C\{^{1}H\}$ NMR of **5** in $[D_6]$-benzene at RT.

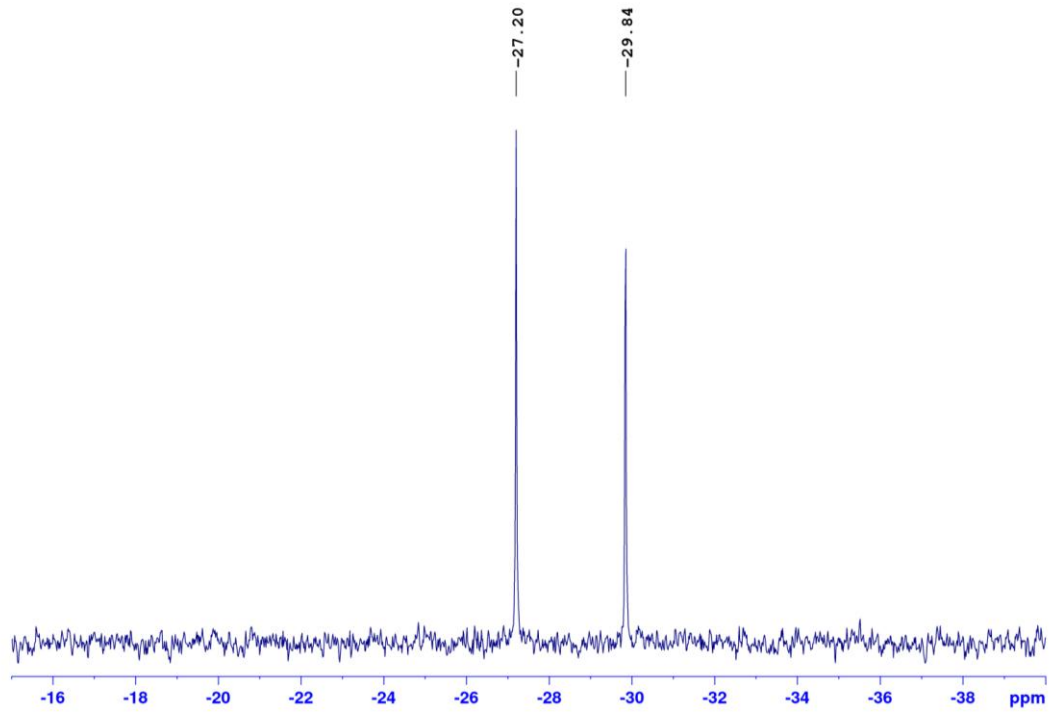


Figure S22 $^{29}Si\{^{1}H\}$ NMR of **5** in $[D_6]$-benzene at RT.

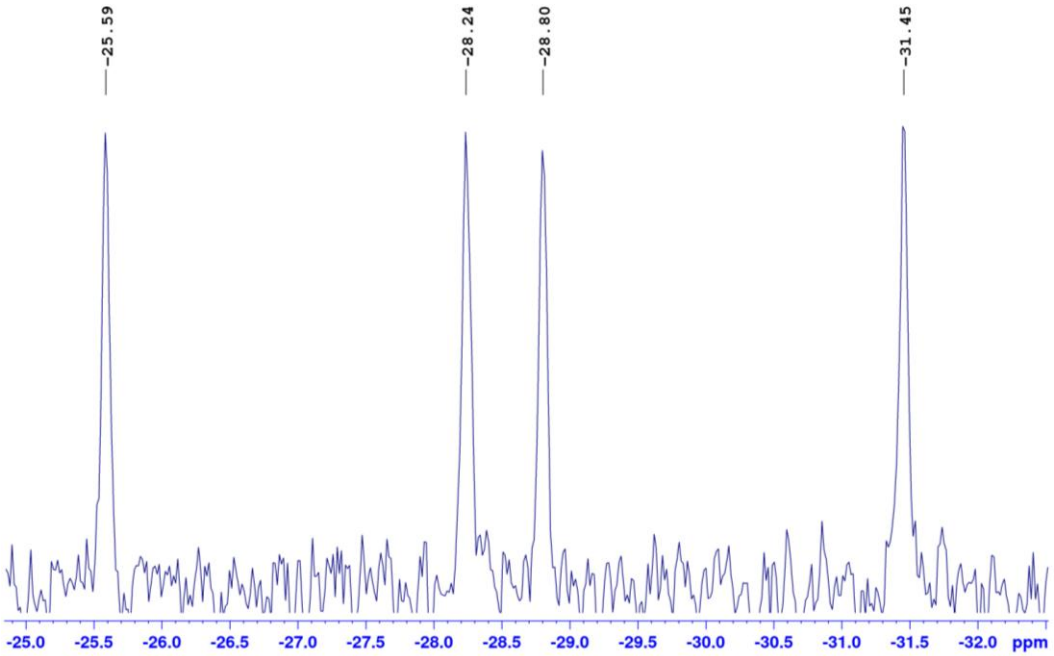


Figure S23 ^{29}Si NMR of **5** in [D_6]-benzene at RT.

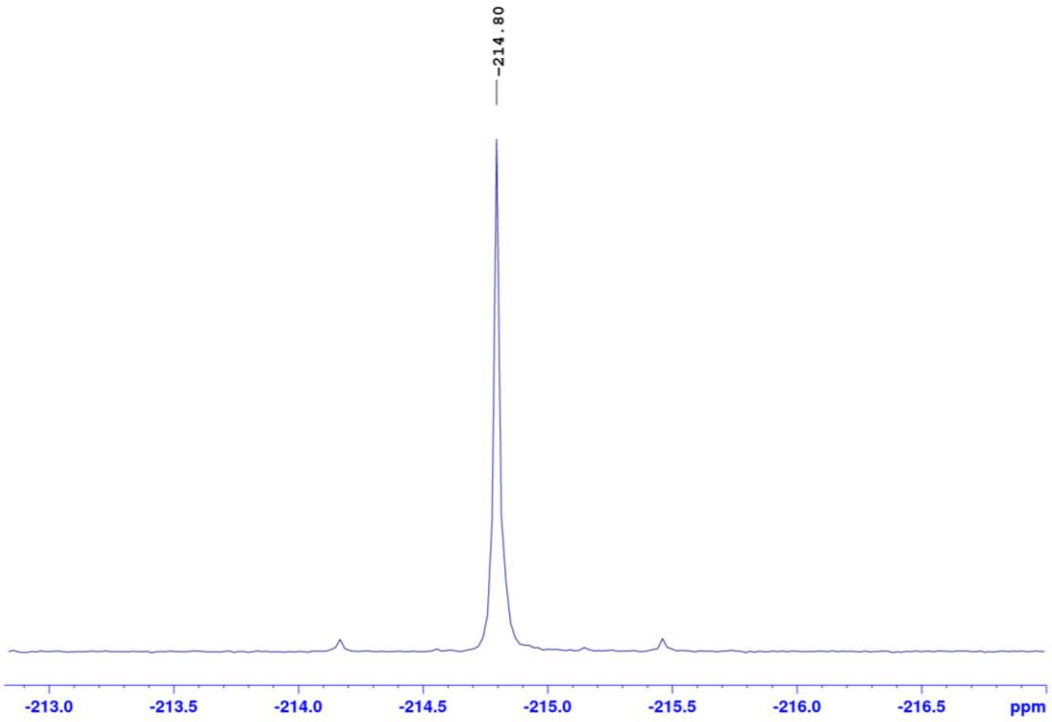


Figure S24 ^{31}P{^{1}H} NMR of **5** in [D_6]-benzene at RT.

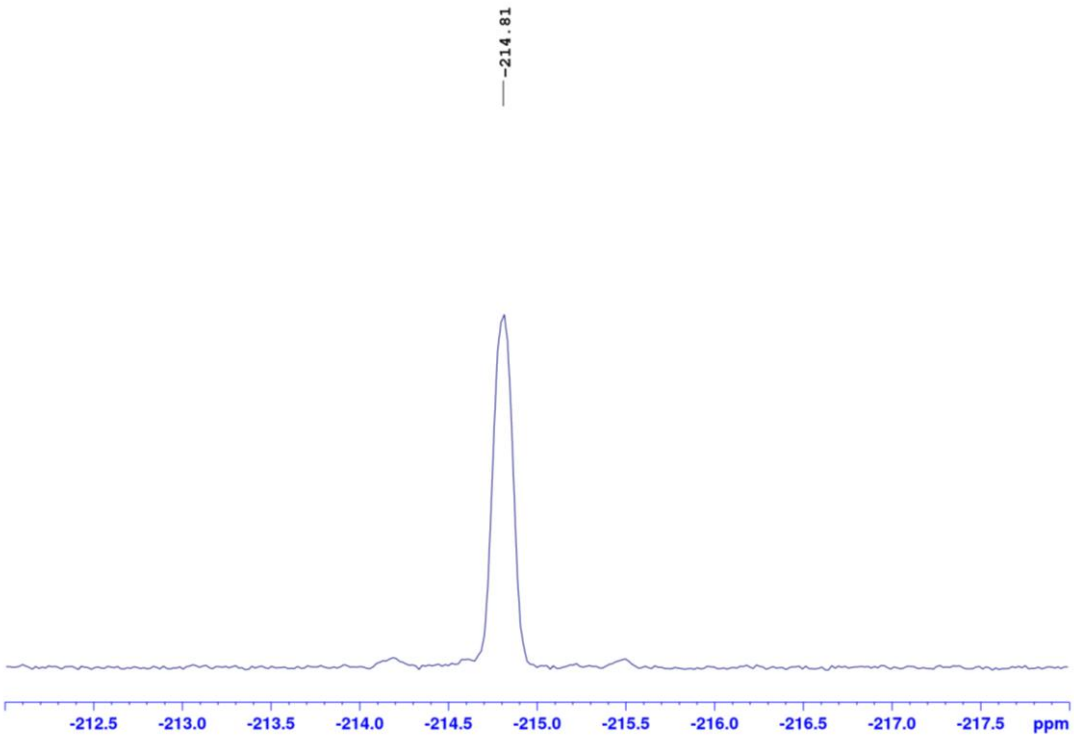


Figure S25 ^{31}P NMR of **5** in [D_6]-benzene at RT.

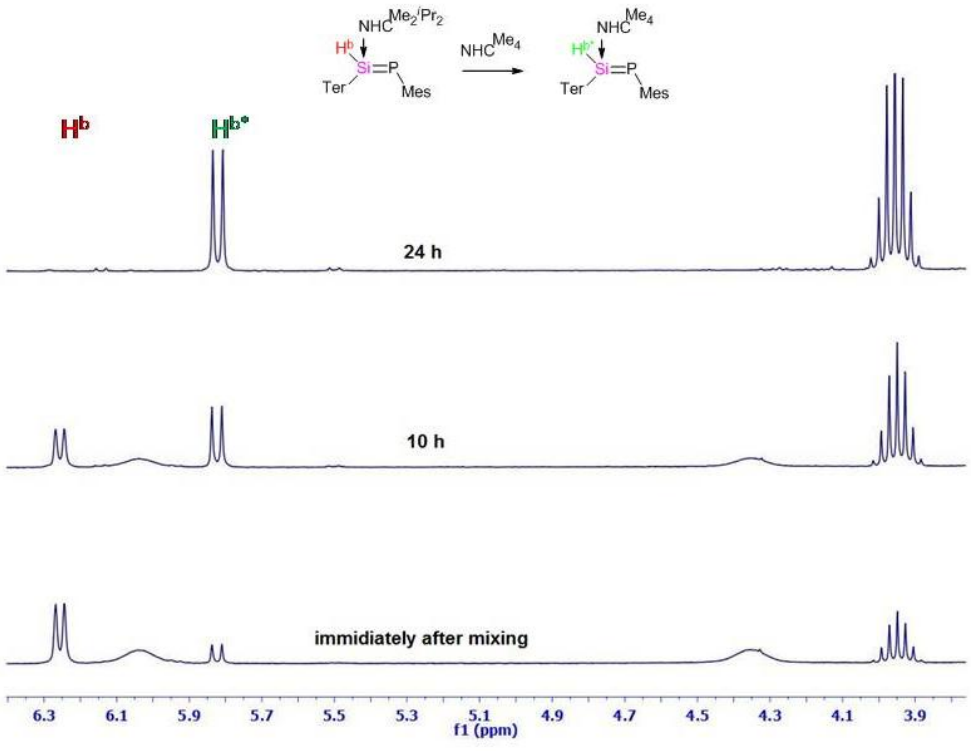


Figure S26 ^{1}H NMR of 1:1 mixture of **4** and NHC^{Me_4} in [D_6]-benzene at RT at different time.

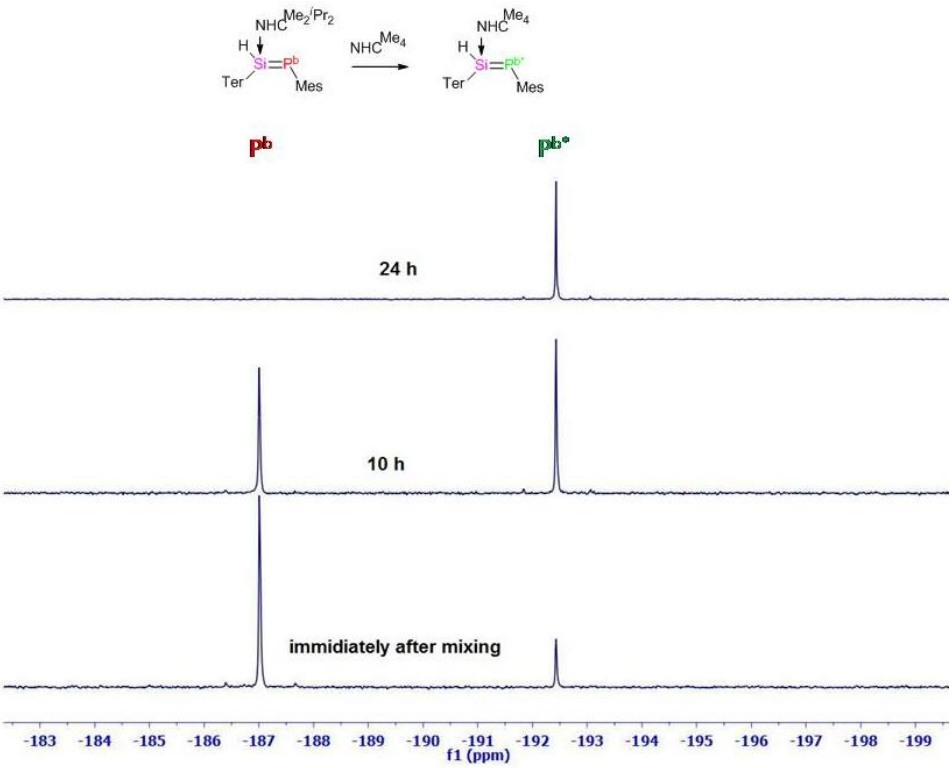


Figure S27 ^{31}P NMR of 1:1 mixture of **4** and NHC^{Me4} in [D_6]-benzene at RT at different time.

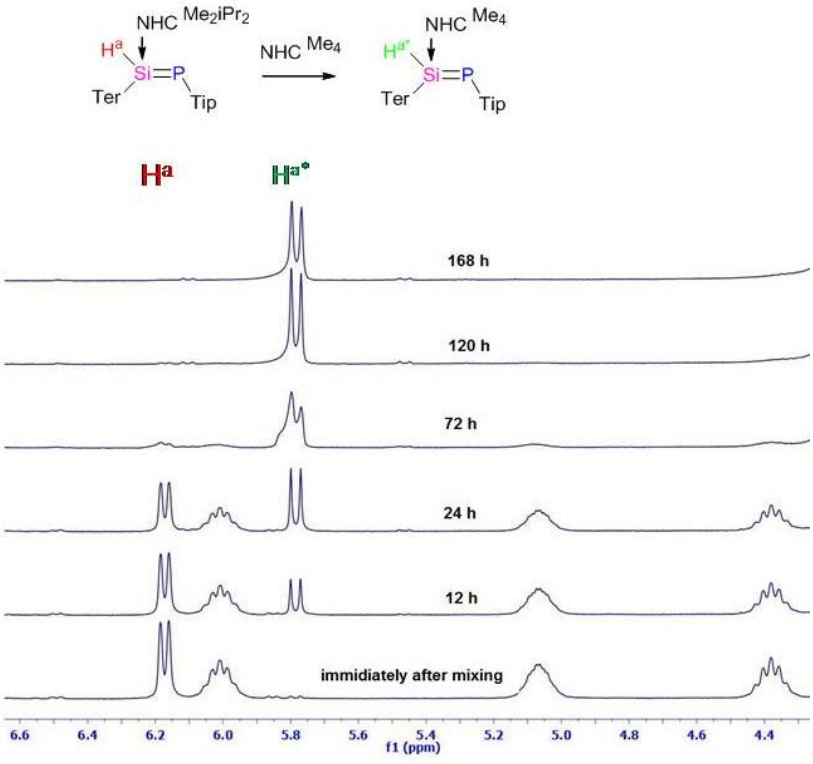


Figure S28 ^{1}H NMR of 1:1 mixture of **5** and NHC^{Me4} in [D_6]-benzene at RT at different time.

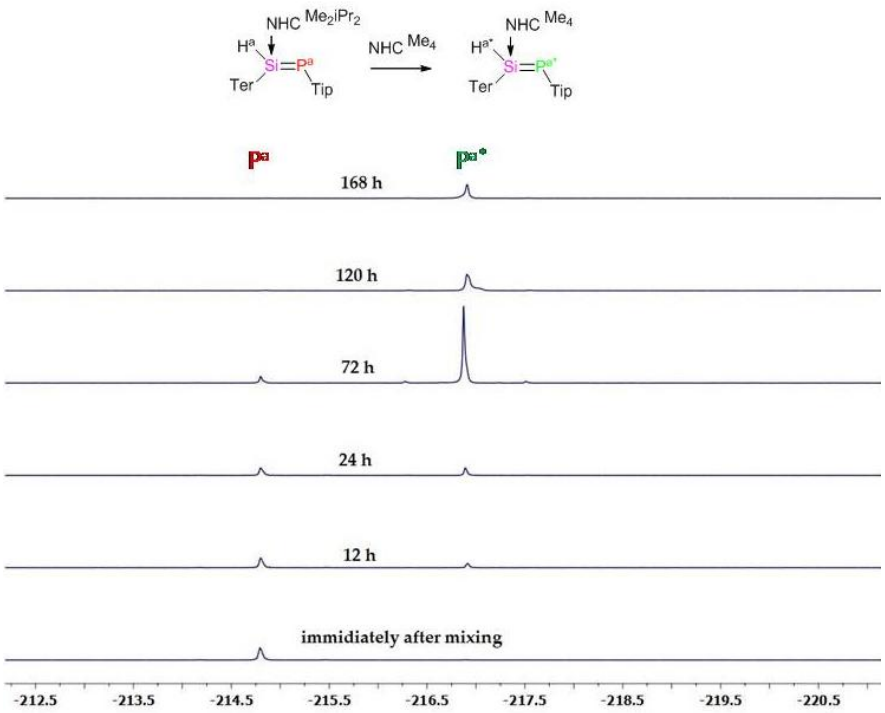


Figure S29 ^{31}P NMR of 1:1 mixture of **5** and NHC^{Me_4} in [D_6]-benzene at RT at different time.

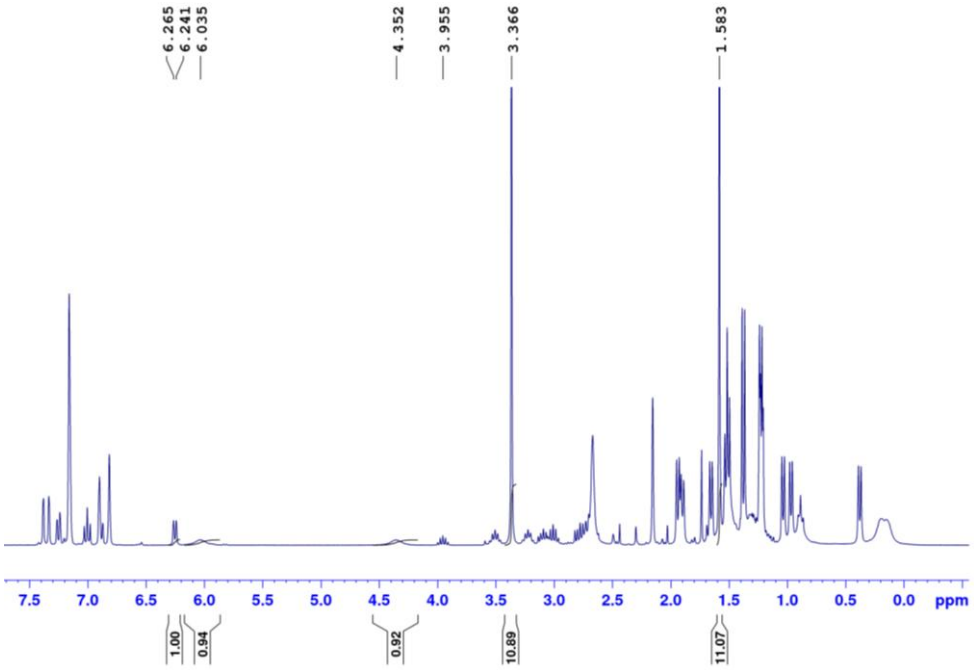


Figure S30 ^{1}H NMR of 1:1 mixture of **4** and NHC^{Me_4} in [D6]-benzene at RT after the addition.

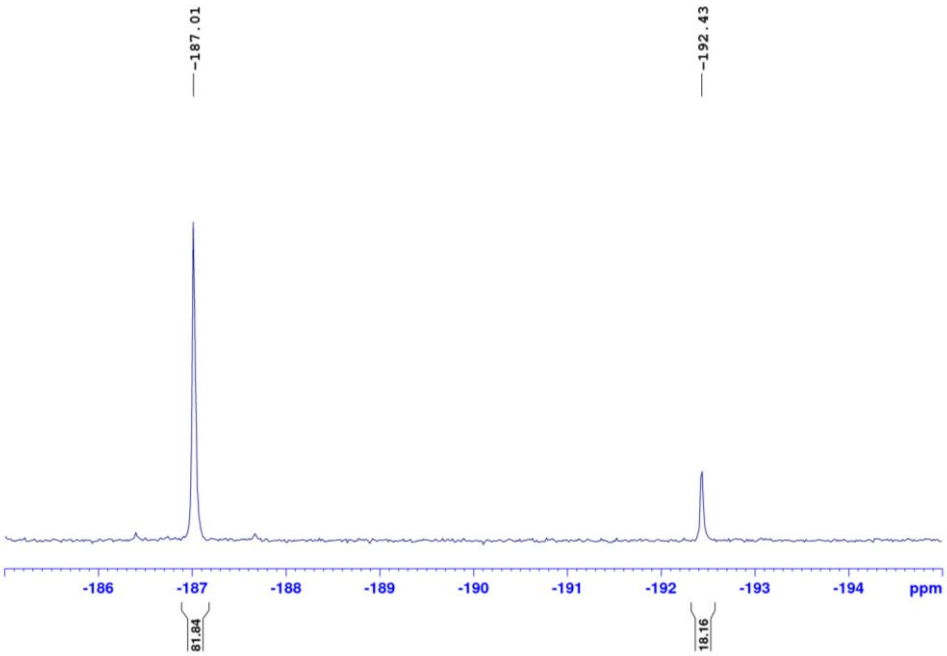


Figure S31 ^{31}P NMR of 1:1 mixture of **4** and NHC^{Me4} in [D6]-benzene at RT after the addition.

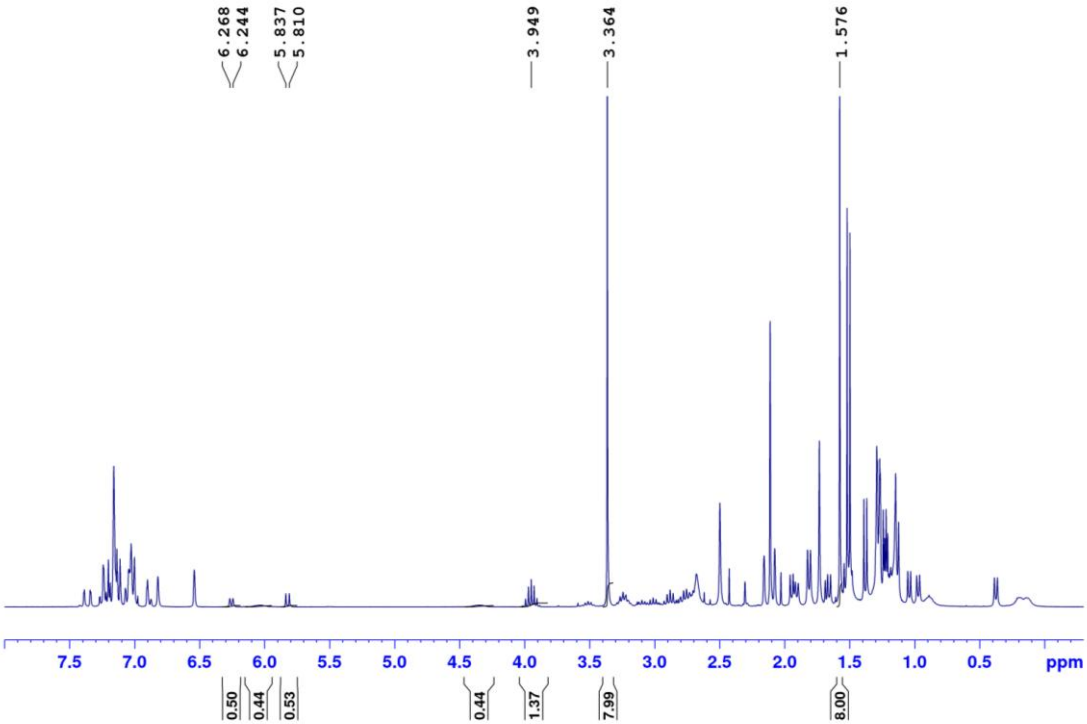


Figure S32 ^{1}H NMR of 1:1 mixture of **4** and NHC^{Me4} in [D6]-benzene at RT after 10 hrs.

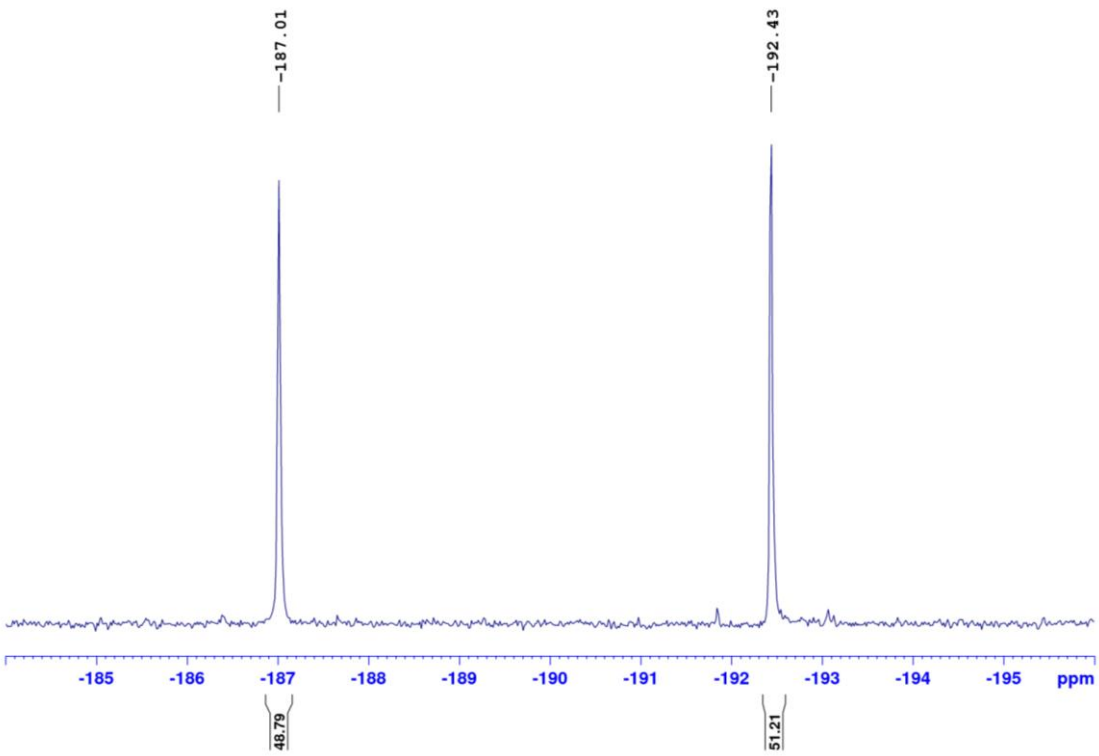


Figure S33 ^{31}P NMR of 1:1 mixture of **4** and NHC^{Me_4} in [D6]-benzene at RT after 10 hrs.

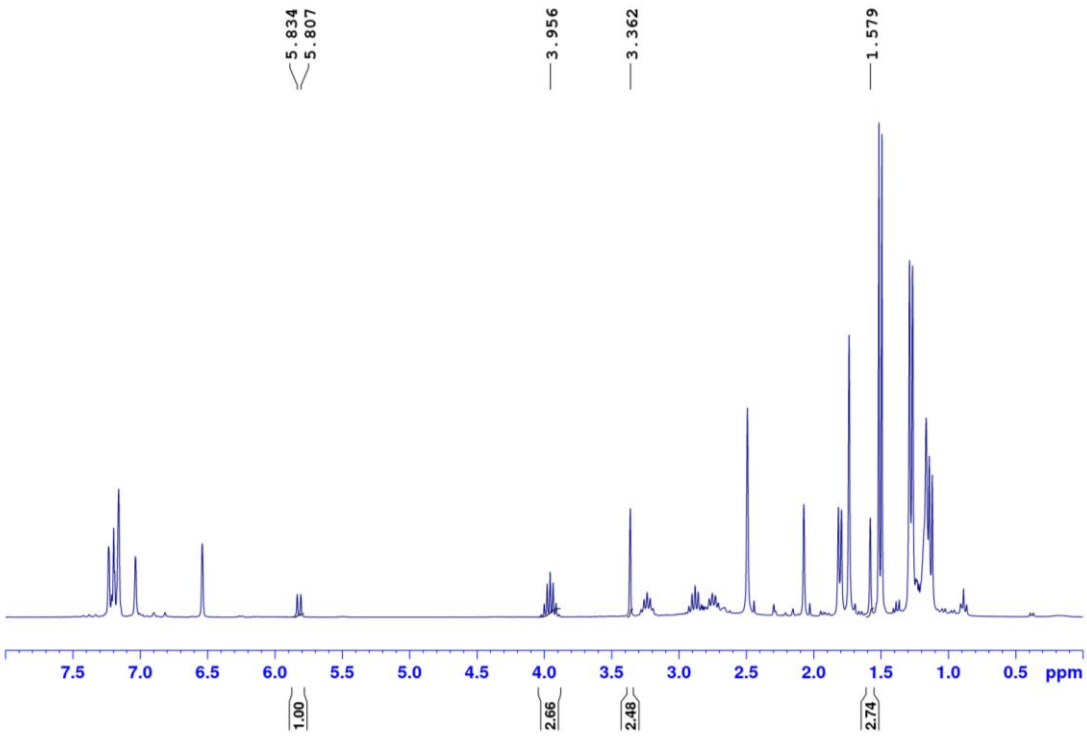


Figure S34 ^{1}H NMR of 1:1 mixture of **4** and NHC^{Me_4} in [D6]-benzene at RT after 24 hrs.

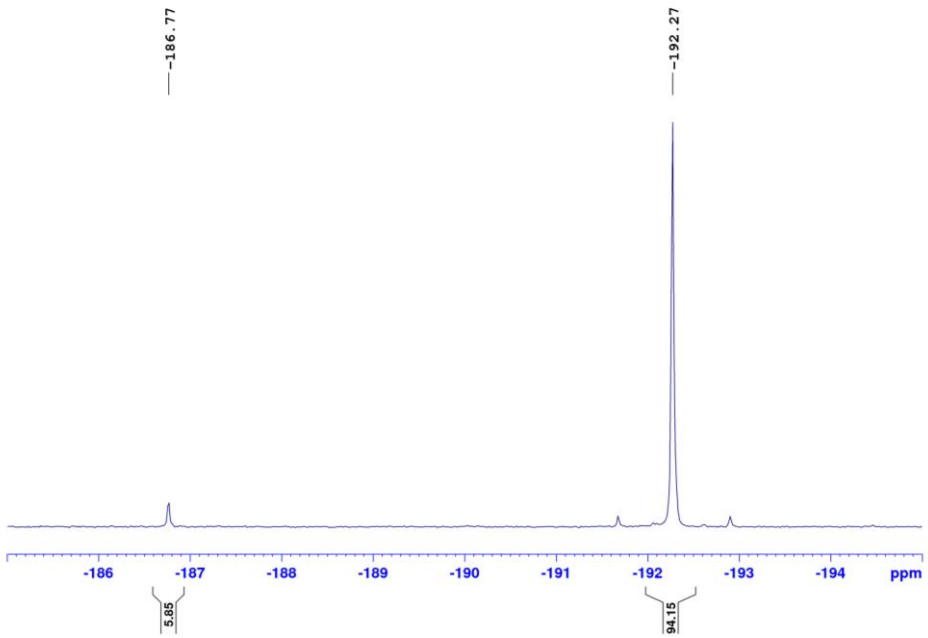


Figure S35 ^{31}P NMR of 1:1 mixture of **4** and NHC^{Me_4} in [D6]-benzene at RT after 24 hrs.

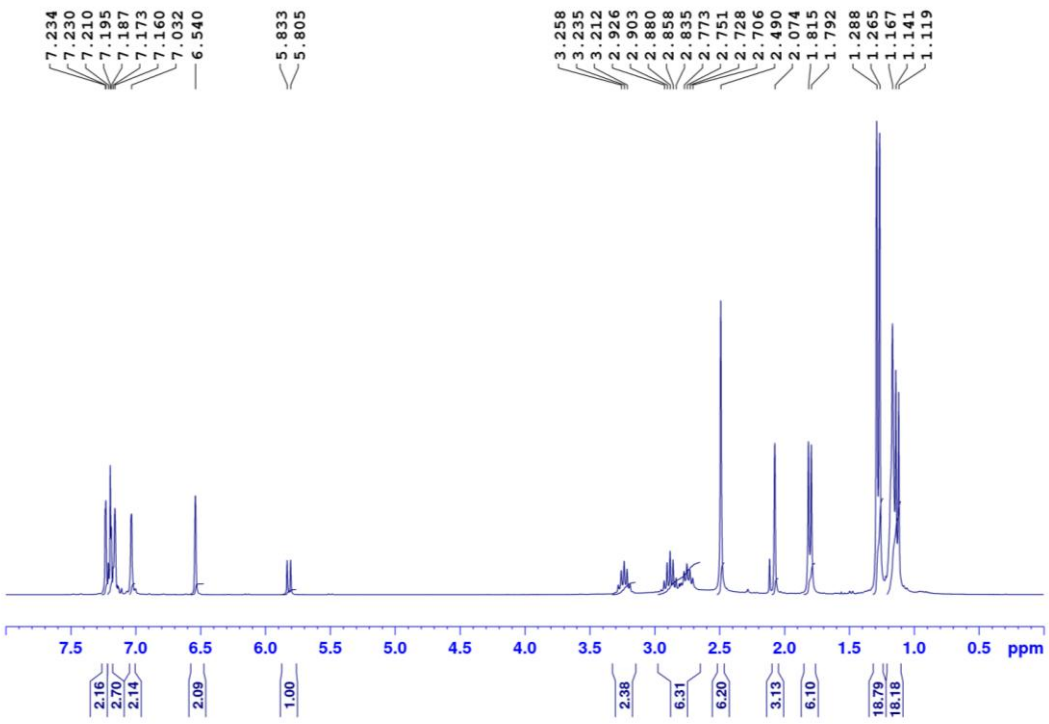


Figure S36 ^{1}H NMR of **6** in [D_6]-benzene at RT.

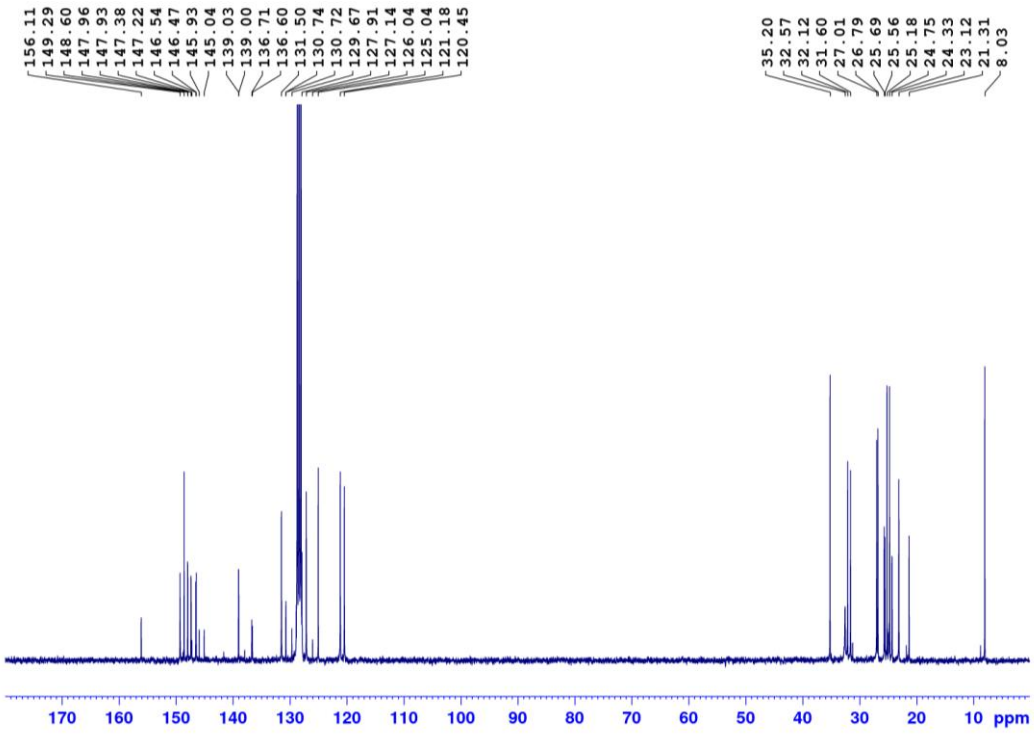


Figure S37 $^{13}C\{^{1}H\}$ NMR of **6** in $[D_6]$-benzene at RT.

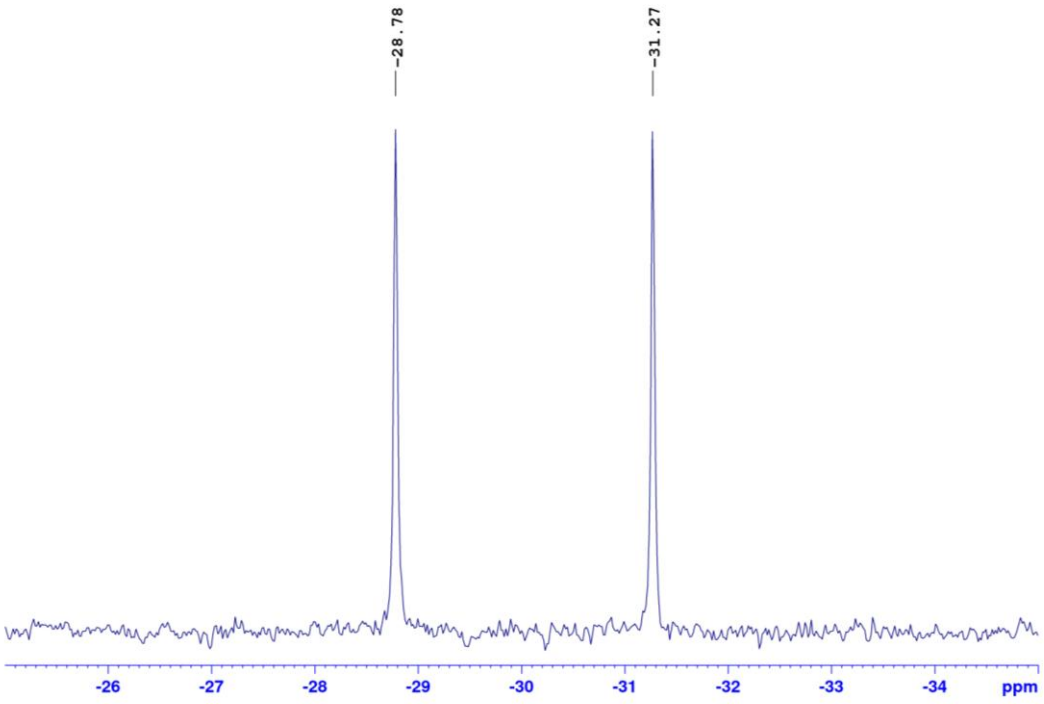


Figure S38 $^{29}Si\{^{1}H\}$ NMR of **6** in $[D_6]$-benzene at RT.

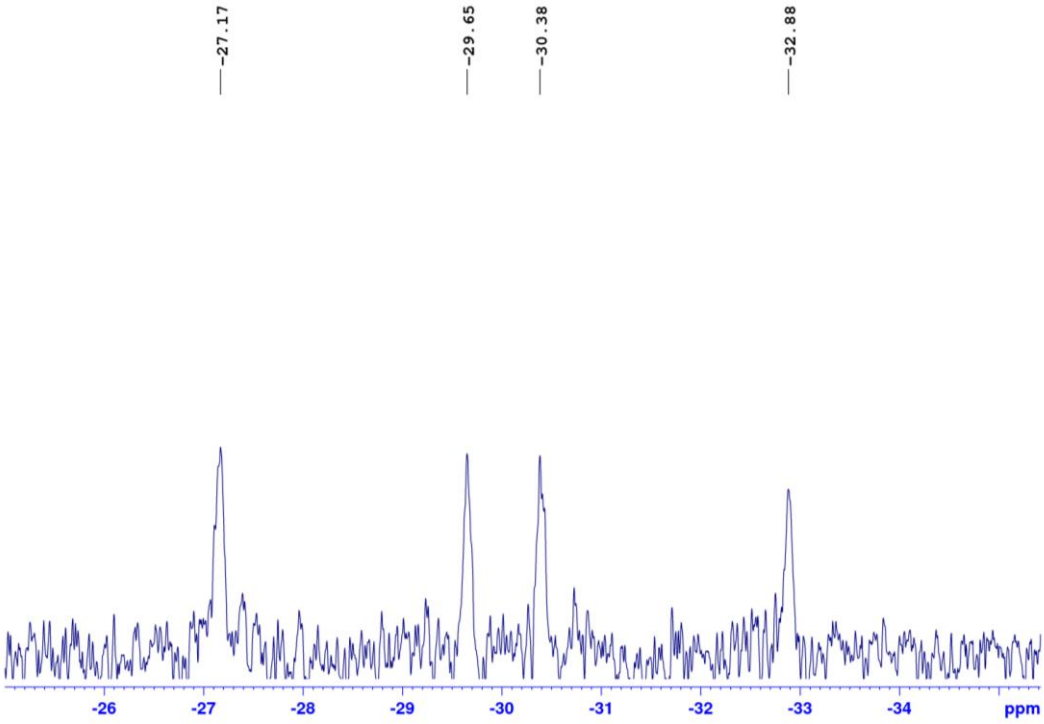


Figure S39 ^{29}Si NMR of **6** in [D_6]-benzene at RT.

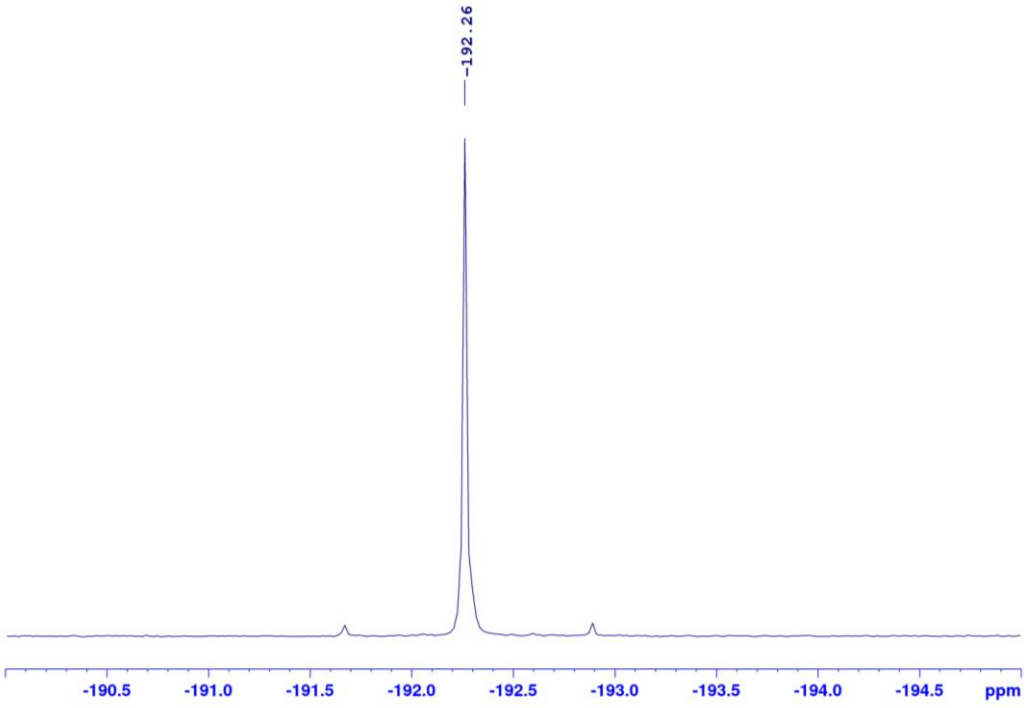


Figure S40 ^{31}P{^{1}H} NMR of **6** in [D_6]-benzene at RT.

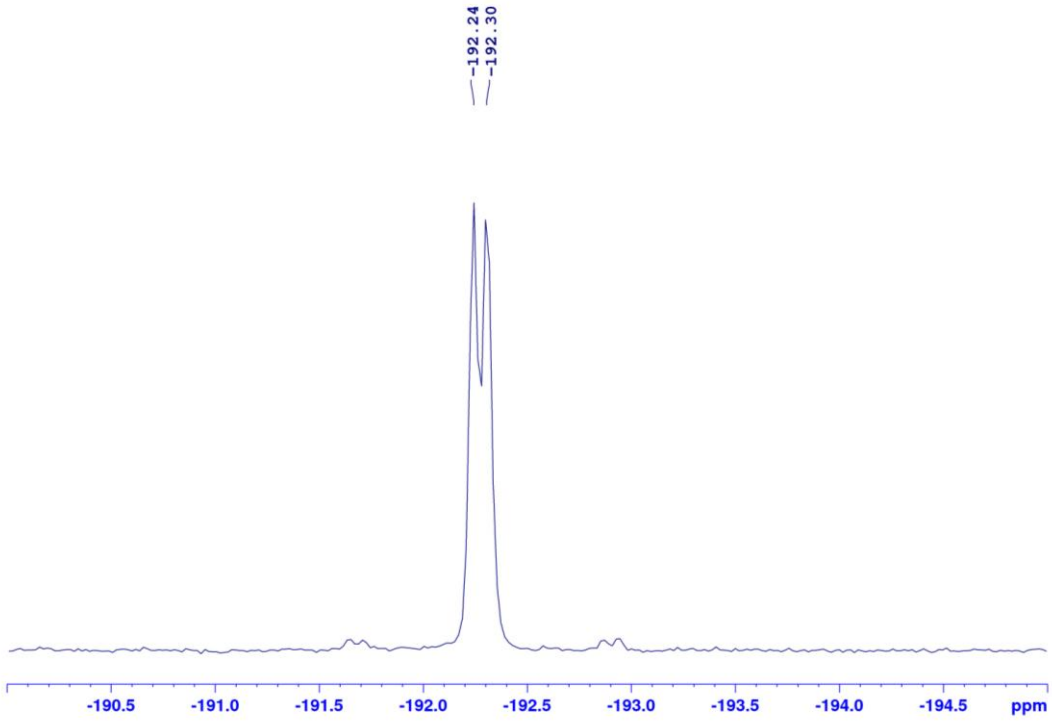


Figure S41 ^{31}P NMR of **6** in [D_6]-benzene at RT.

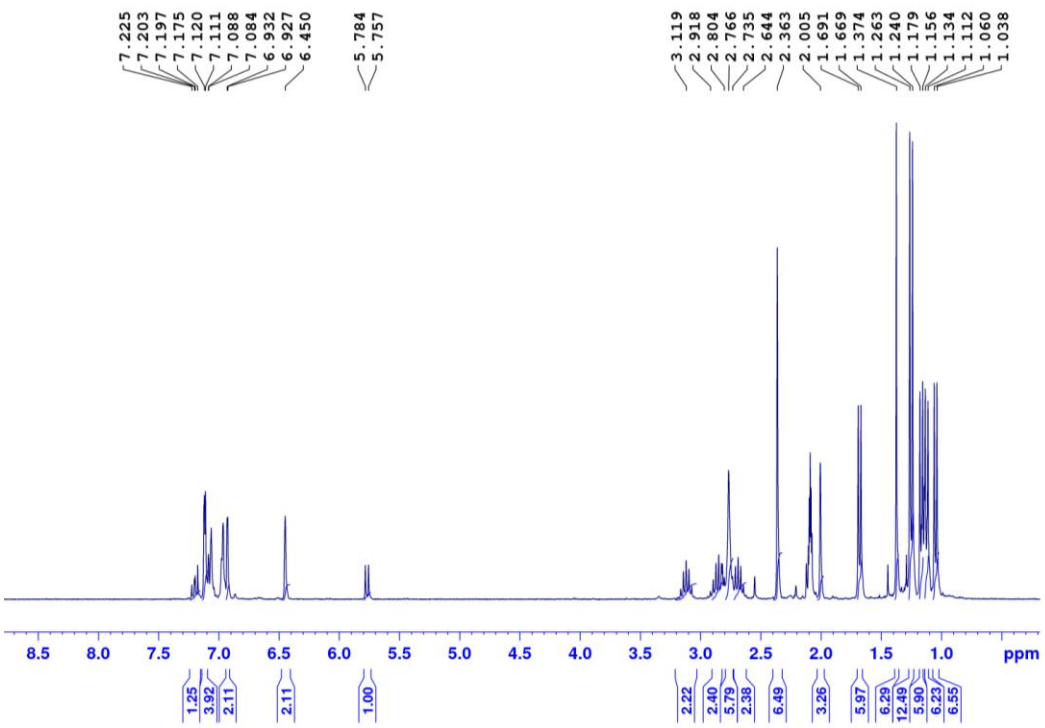


Figure S42 ^{1}H NMR of **6** in [Tol-d_8] at 363 °C.

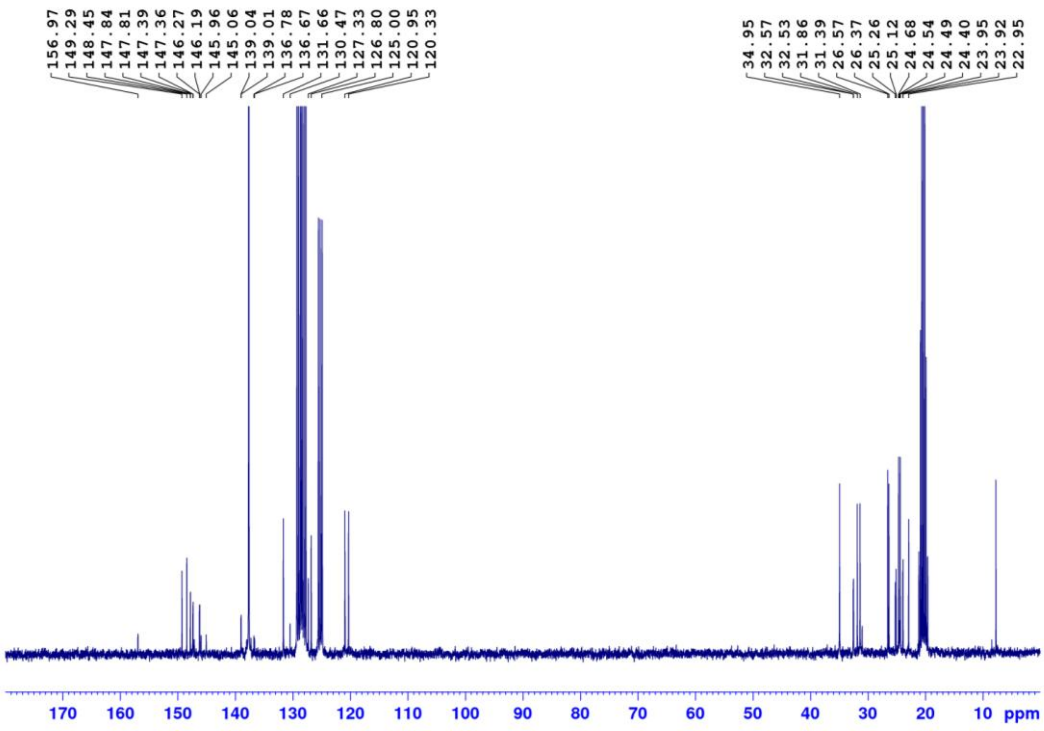


Figure S43 $^{13}C\{^{1}H\}$ NMR of **6** in [Tol-d_8] at 363 °C.

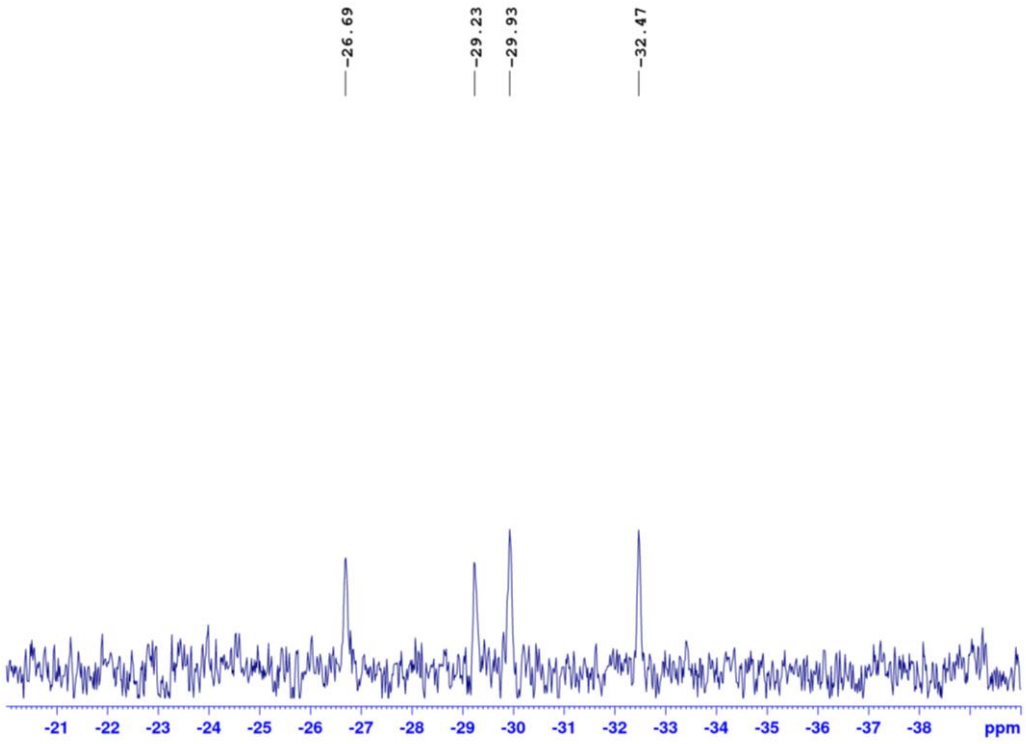


Figure S44 ^{29}Si NMR of **6** in [Tol-d_8] at 363 °C.

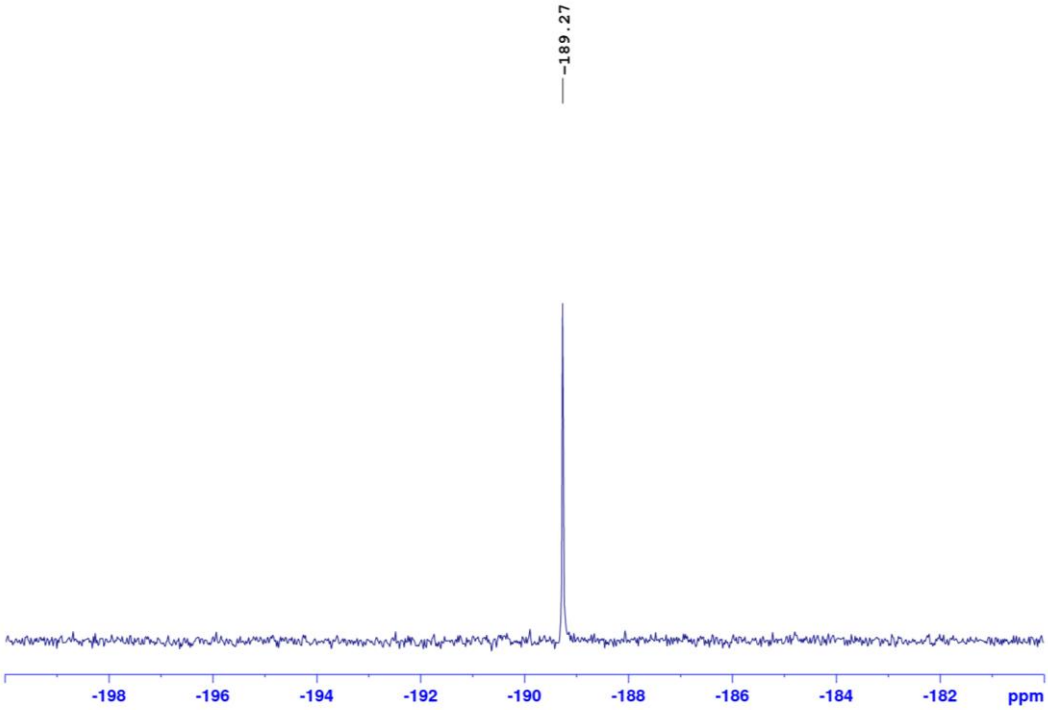


Figure S45 $^{31}P\{^{1}H\}$ NMR of **6** in [Tol-d_8] at 363 °C.

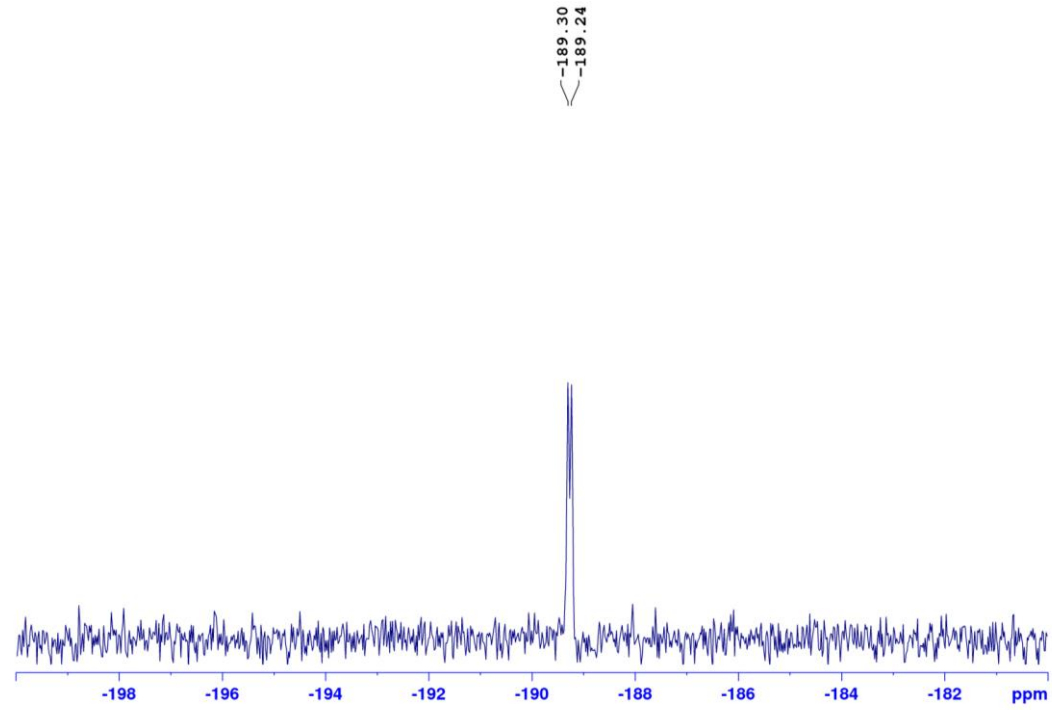


Figure S46 ^{31}P NMR of **6** in [Tol-d_8] at 363 °C.

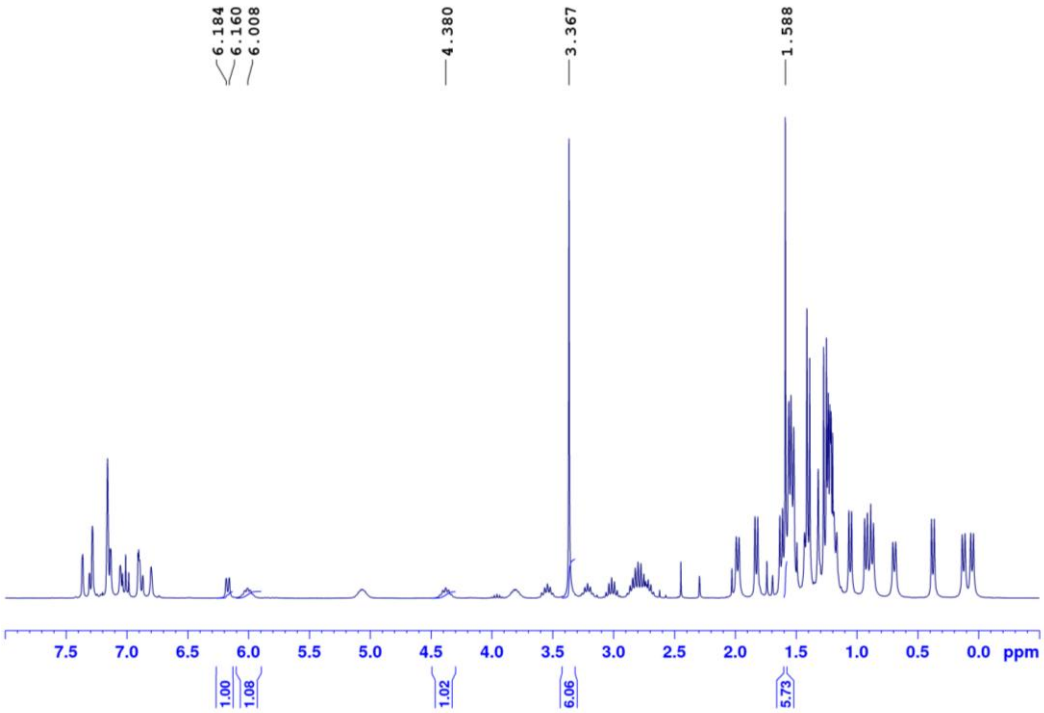


Figure S47 ^{1}H NMR of 1:1 mixture of **5** and NHC^{Me4} in [D_6]-benzene at RT after the addition.

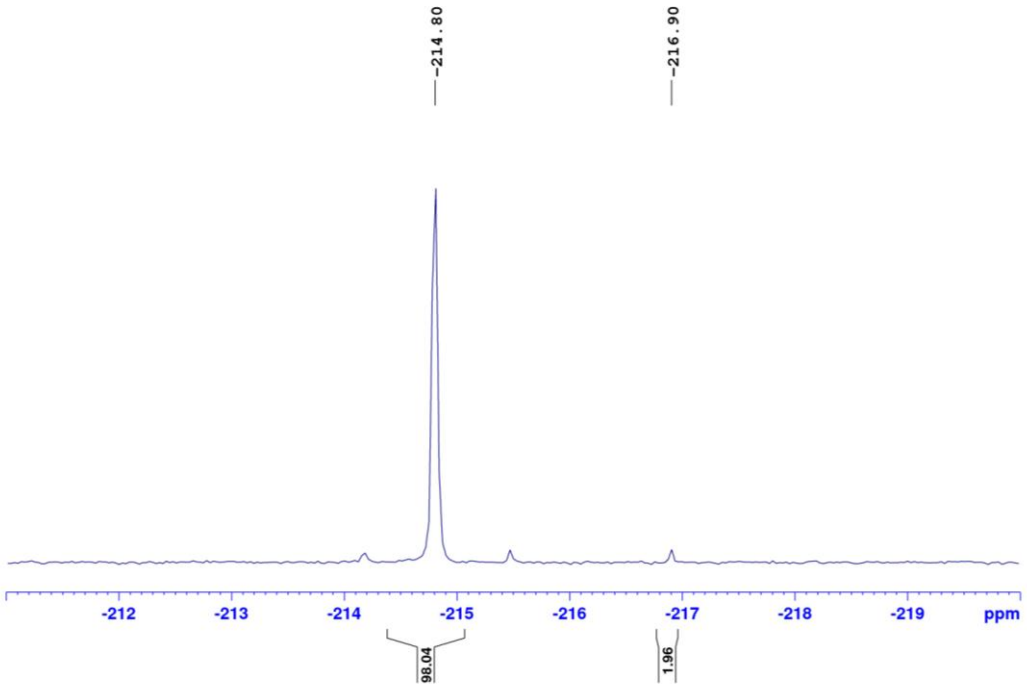


Figure S48 ^{31}P NMR of 1:1 mixture of **5** and NHC^{Me4} in [D6]-benzene at RT after the addition.

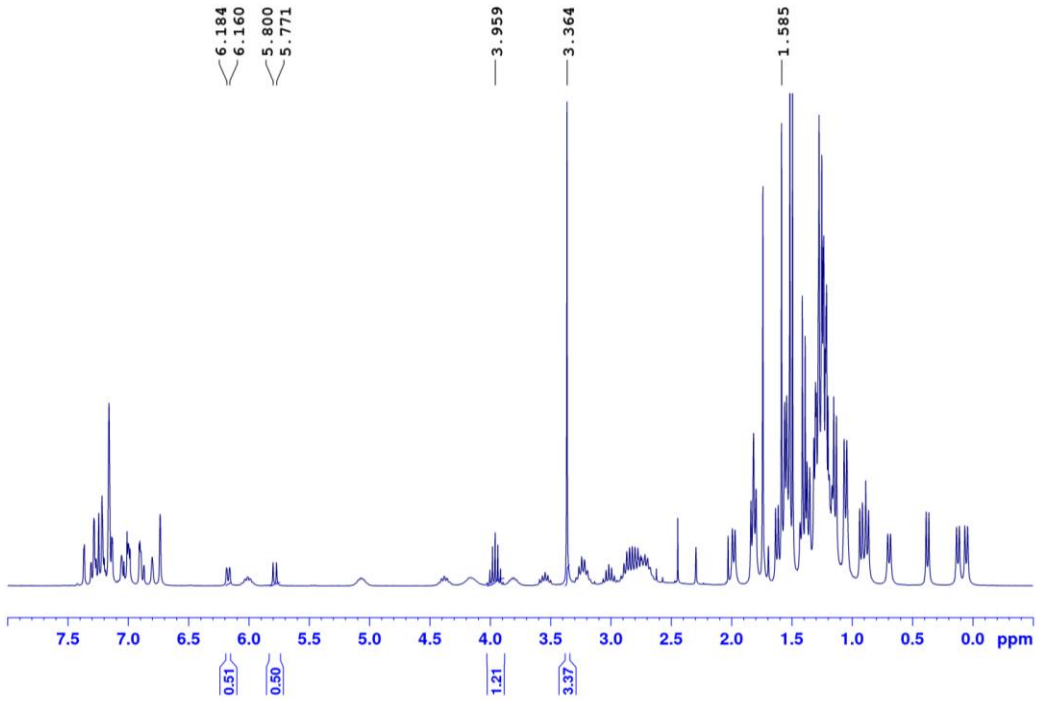


Figure S49 ^{1}H NMR of 1:1 mixture of **5** and NHC^{Me4} in [D_6]-benzene at RT after 24 hrs.

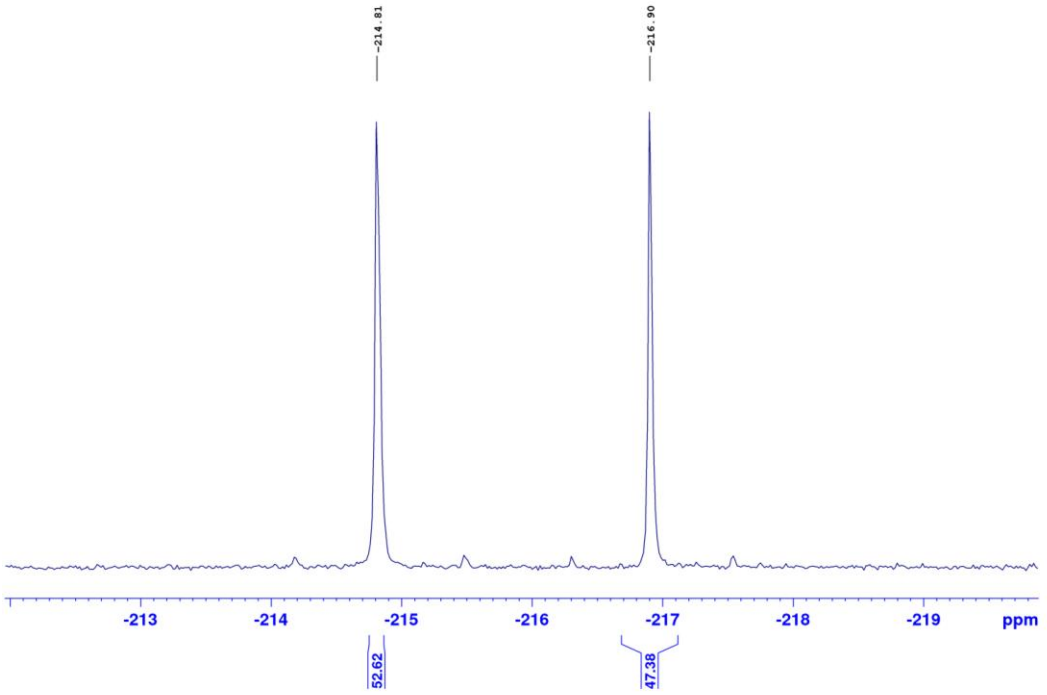


Figure S50 ^{31}P NMR of 1:1 mixture of **5** and NHC^{Me4} in [D6]-benzene at RT after 24 hrs.

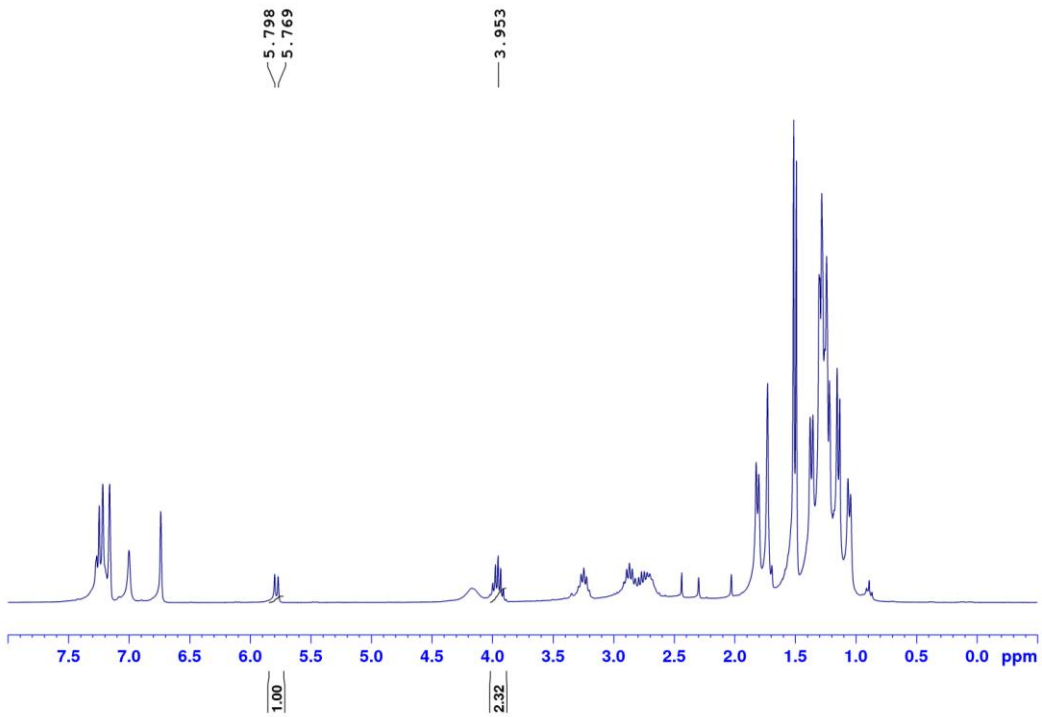


Figure S51 ^{1}H NMR of 1:1 mixture of **5** and NHC^{Me4} in [D_6]-benzene at RT after 168 hrs.

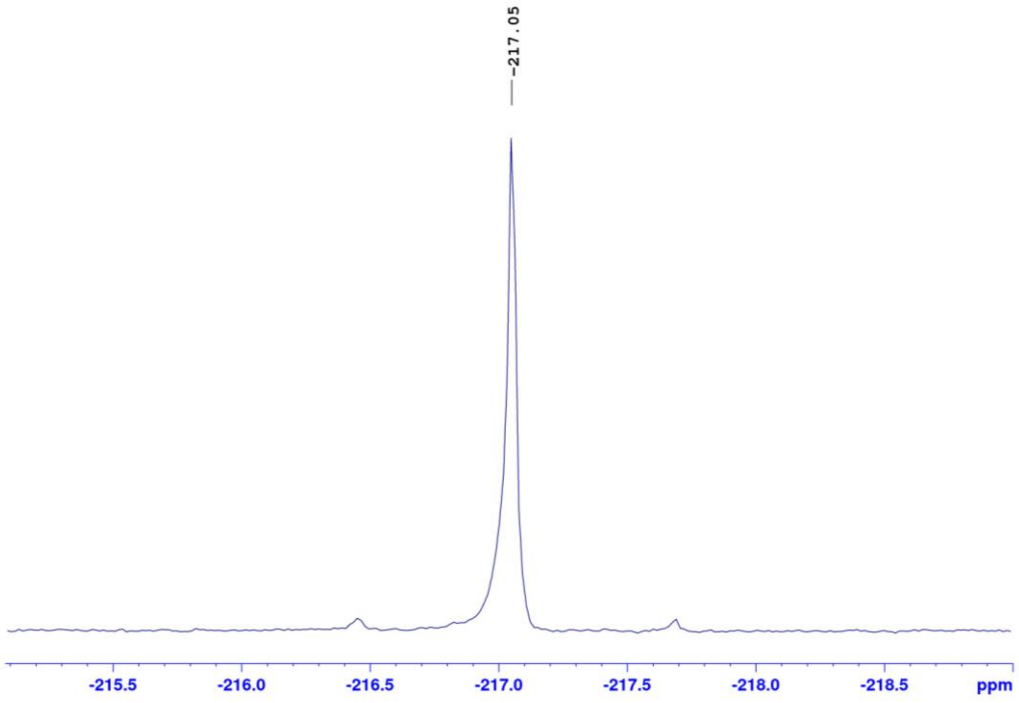


Figure S52 ^{31}P NMR of 1:1 mixture of **5** and NHC^{Me4} in [D6]-benzene at RT after 168 hrs.

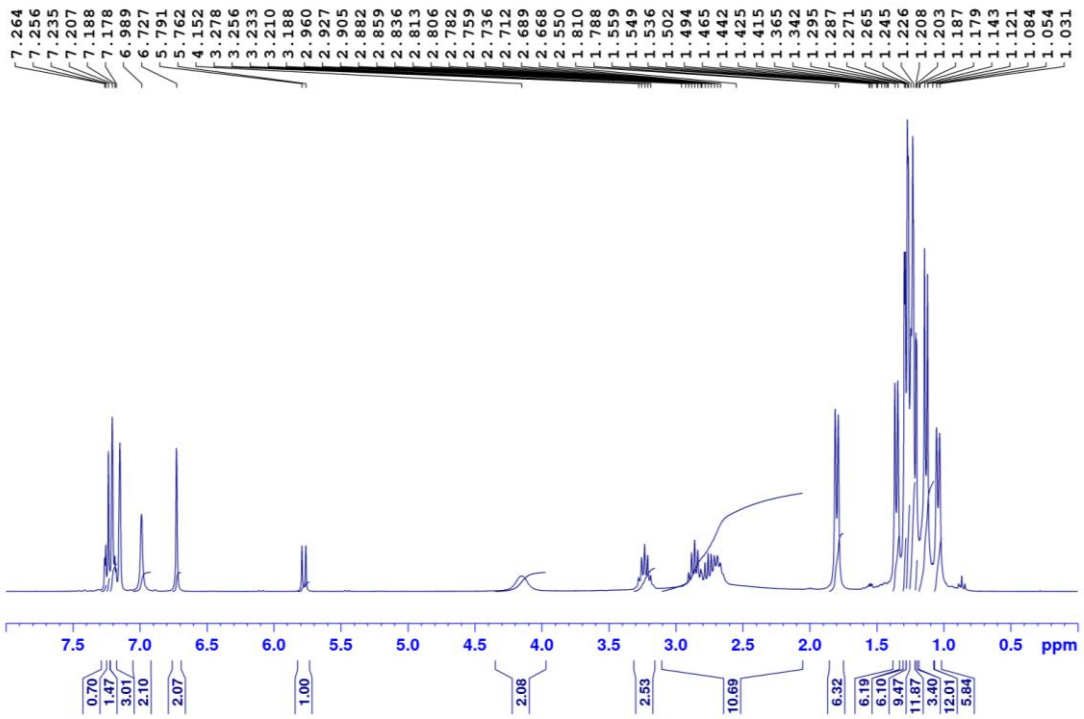


Figure S53 ^{1}H NMR of **7** in [D_6]-benzene at RT.

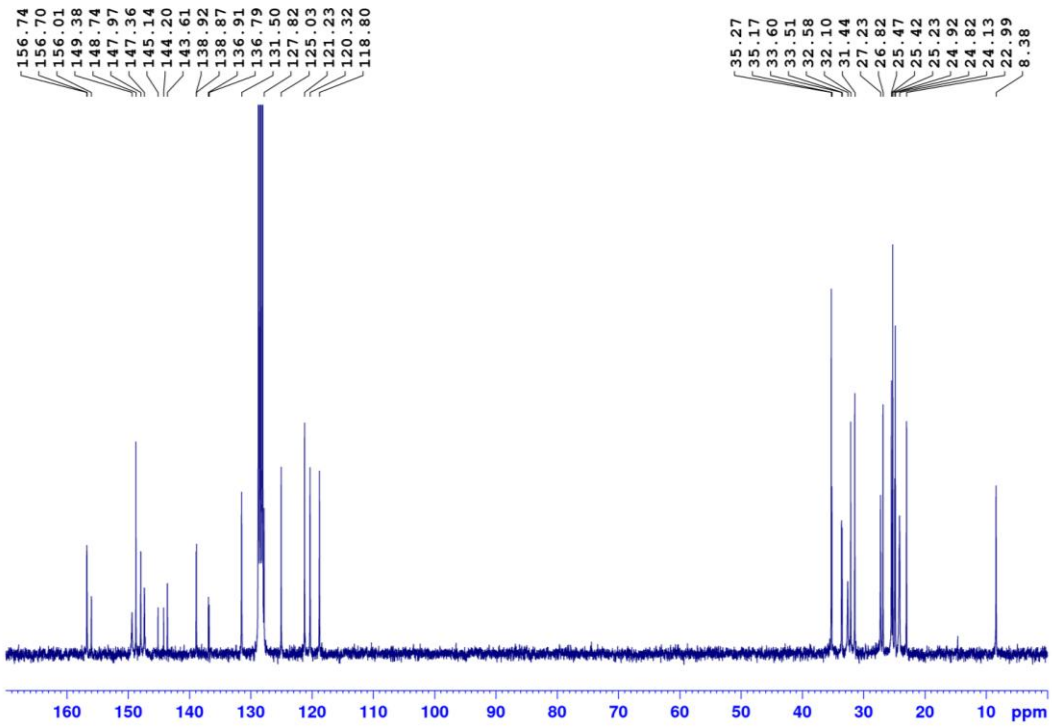


Figure S54 ^{13}C{^{1}H} NMR of **7** in [D_6]-benzene at RT.

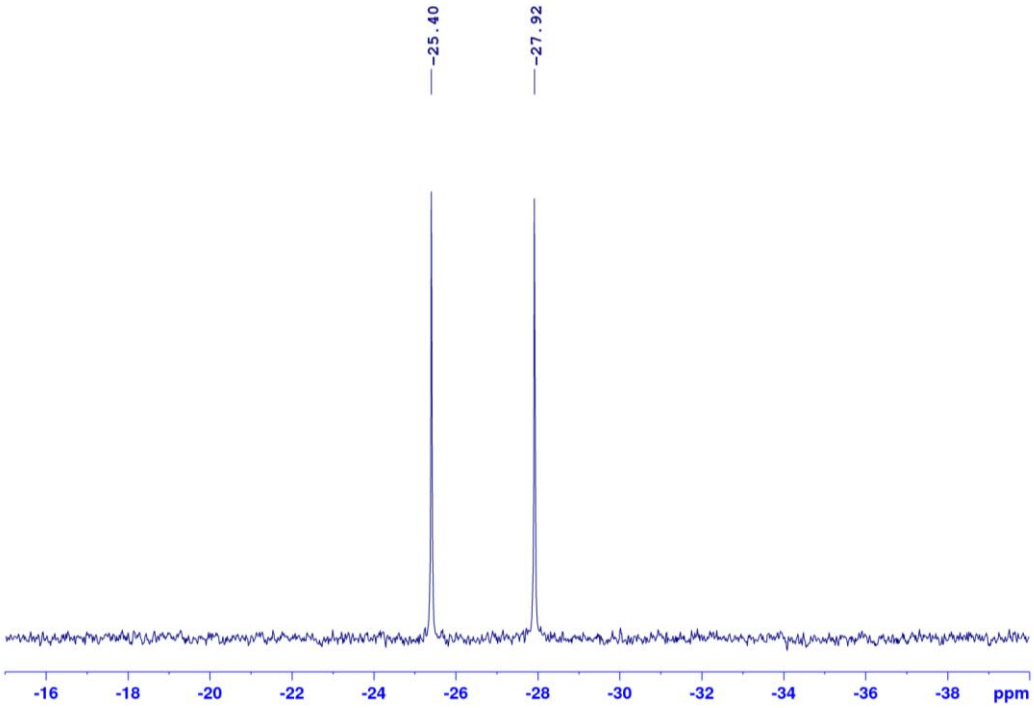


Figure S55 $^{29}Si\{^{1}H\}$ NMR of **7** in $[D_6]$-benzene at RT.

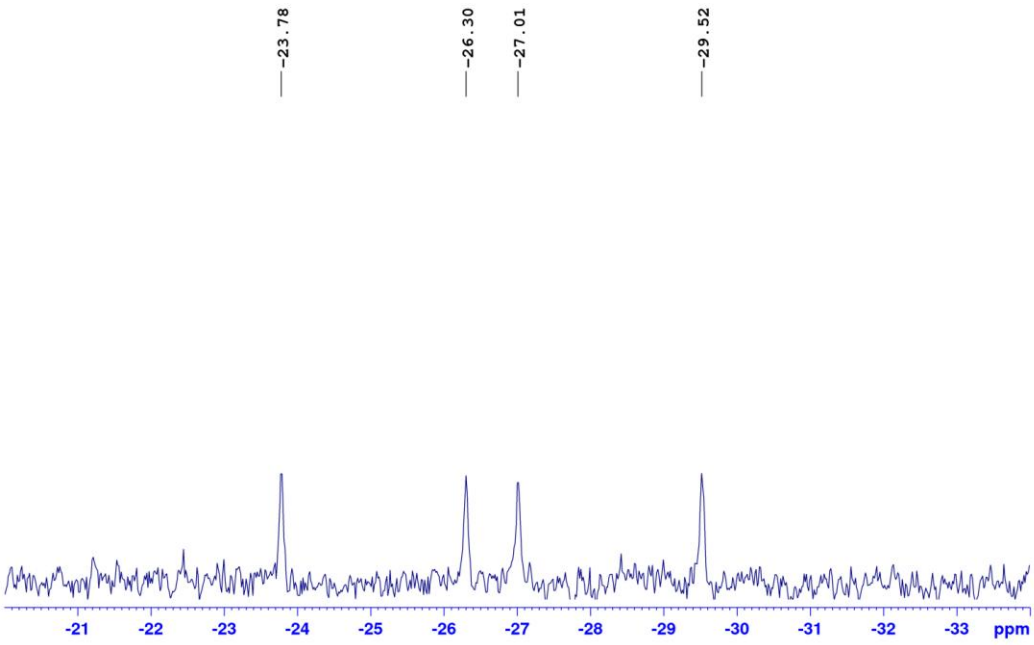


Figure S56 ^{29}Si NMR of **7** in $[D_6]$-benzene at RT.

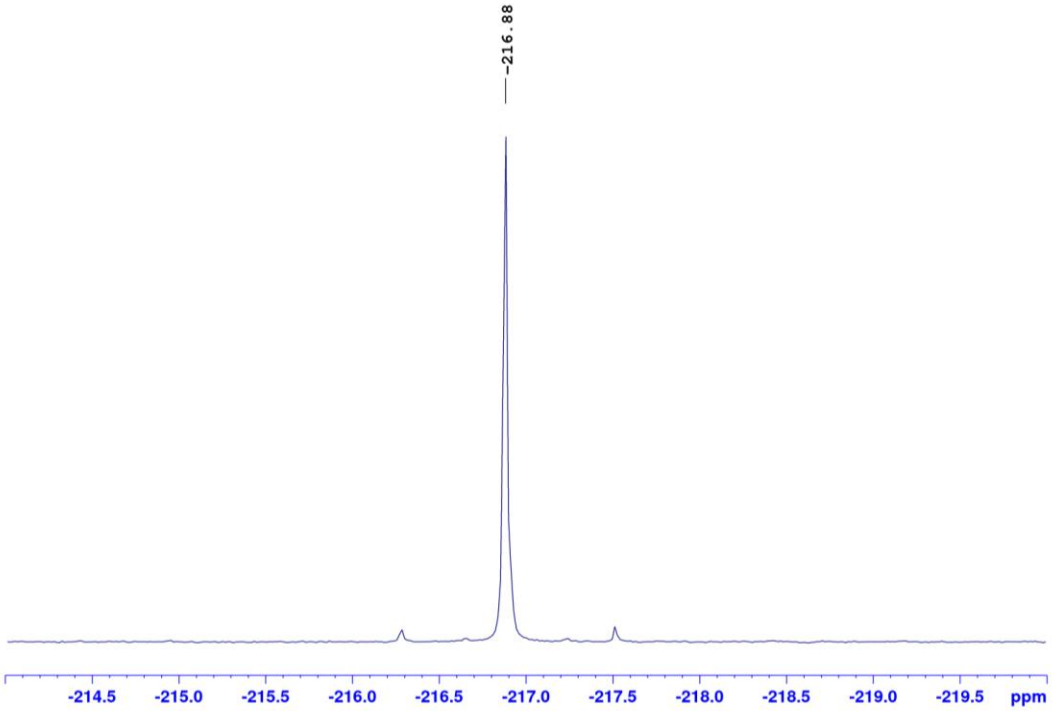


Figure S57 $^{31}P\{^{1}H\}$ NMR of **7** in $[D_6]$-benzene at RT.

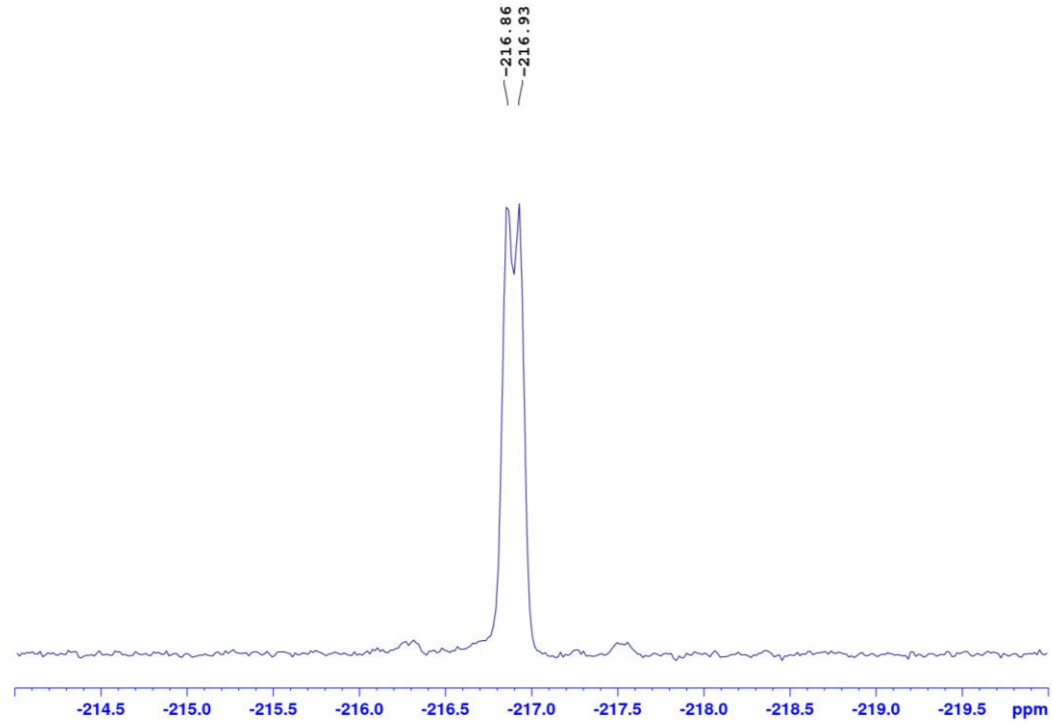


Figure S58 ^{31}P NMR of **7** in $[D_6]$-benzene at RT.

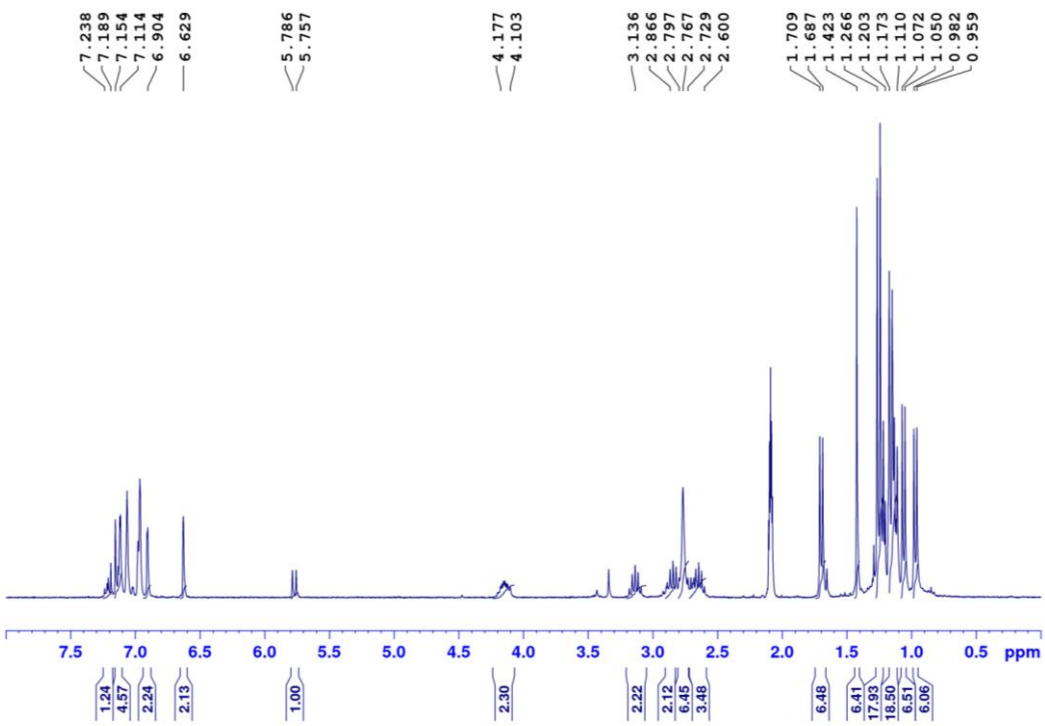


Figure S59 ^{1}H NMR of **7** in [Tol-d8]- at 363 °C.

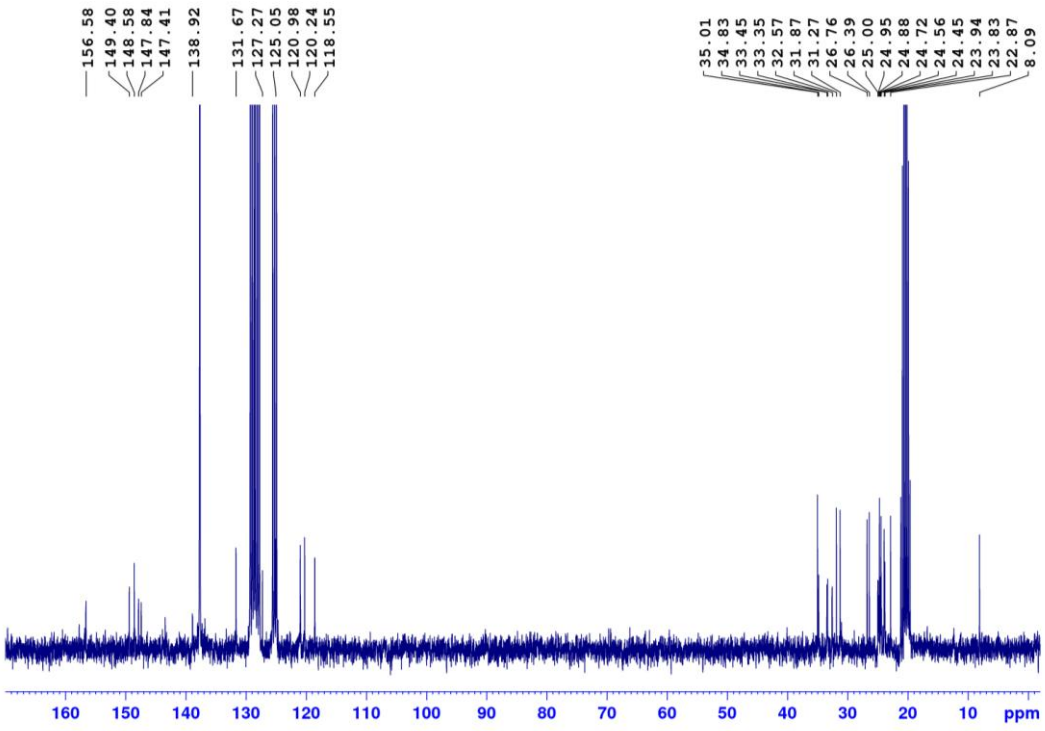


Figure S60 ^{13}C{^{1}H} NMR of **7** in [Tol-d8]- at 363 °C.

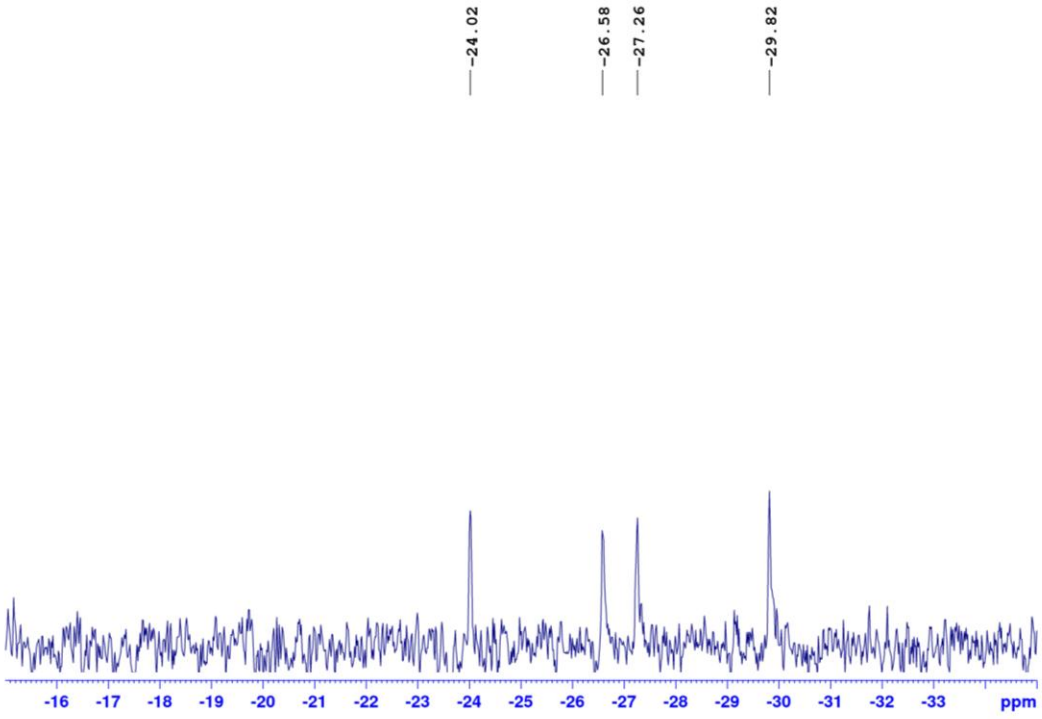


Figure S61 ^{29}Si NMR of **7** in [Tol-d8]- at 363 °C.

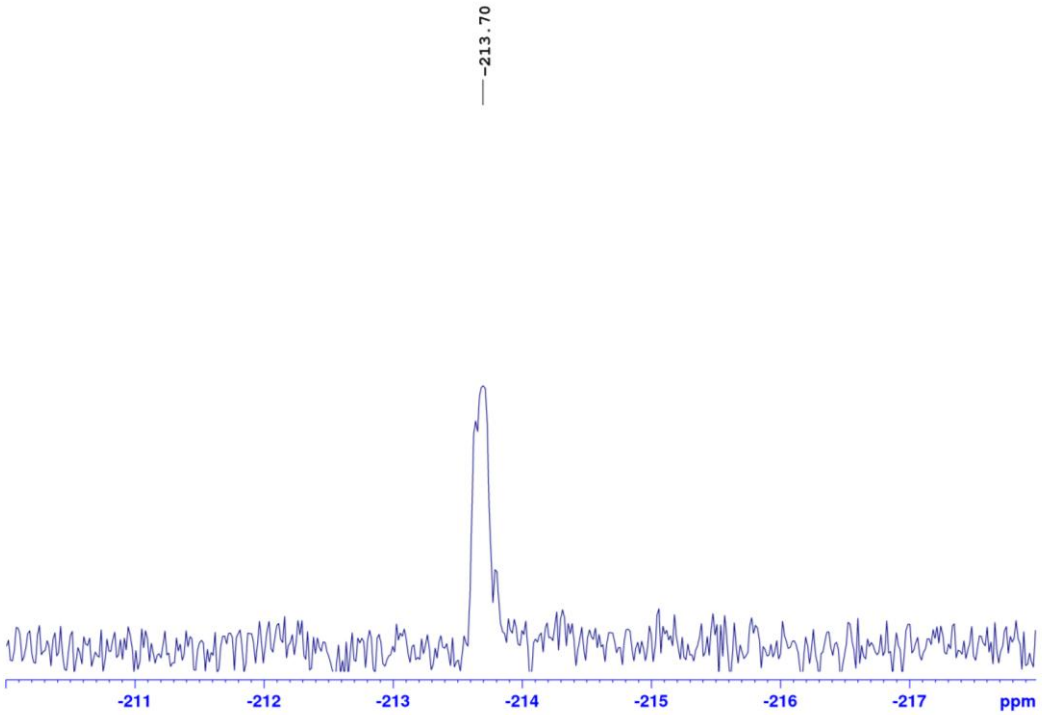


Figure S62 ^{31}P NMR of **7** in [Tol-d8]- at 363 °C.

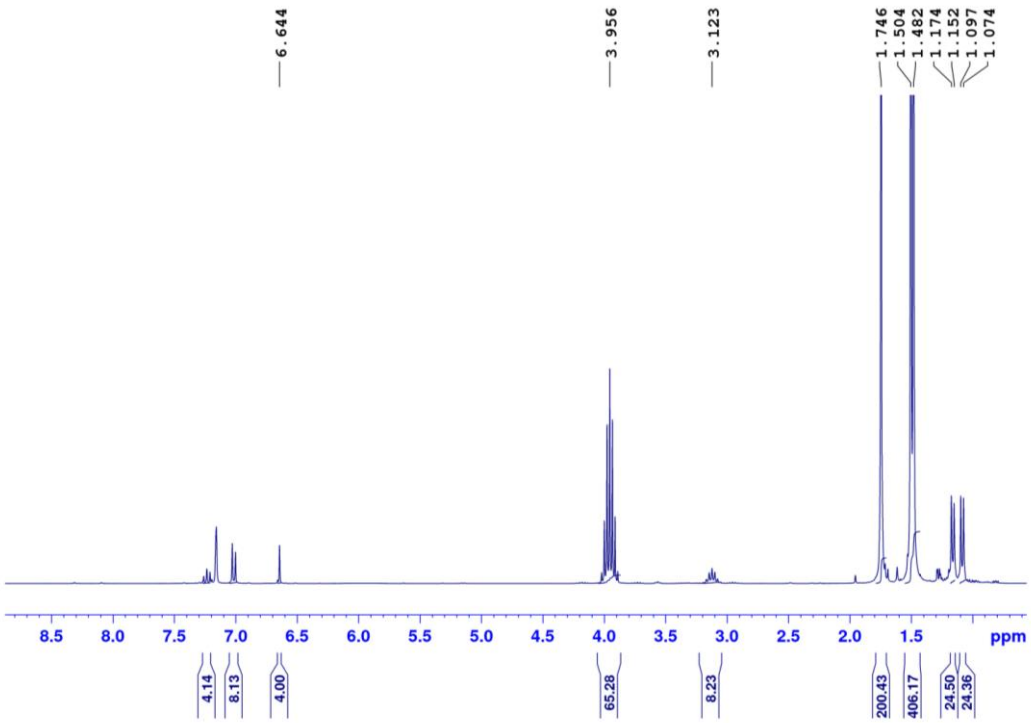


Figure S63 ^{1}H NMR of 1:10 mixture of (NHC^{Dip})Si$_2$ and NHC$^{Me_2{}^{i}Pr_2}$ in [D$_6$]-benzene at RT.

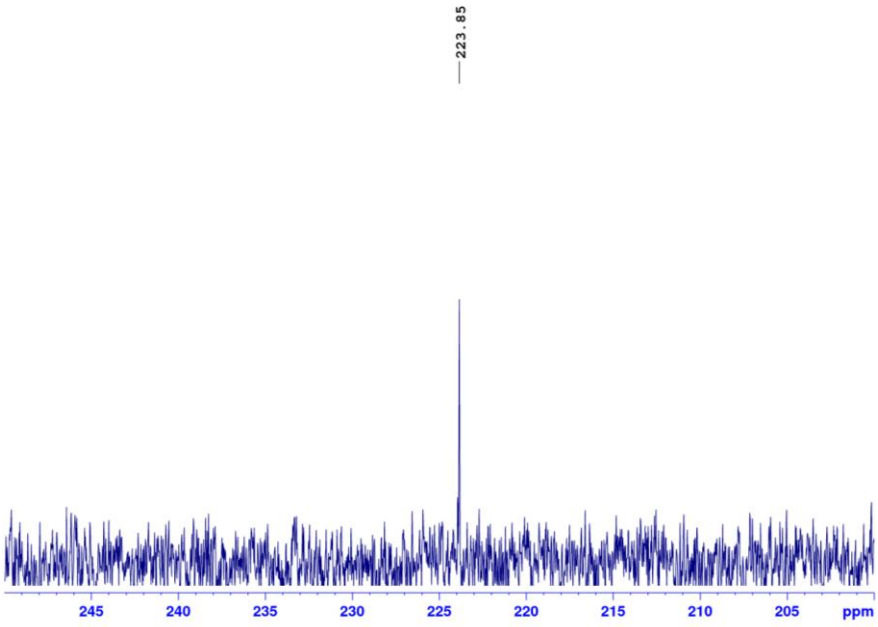


Figure S64 ^{29}Si NMR of 1:10 mixture of (NHC^{Dip})Si$_2$ and NHC$^{Me_2{}^{i}Pr_2}$ in [D$_6$]-benzene at RT.

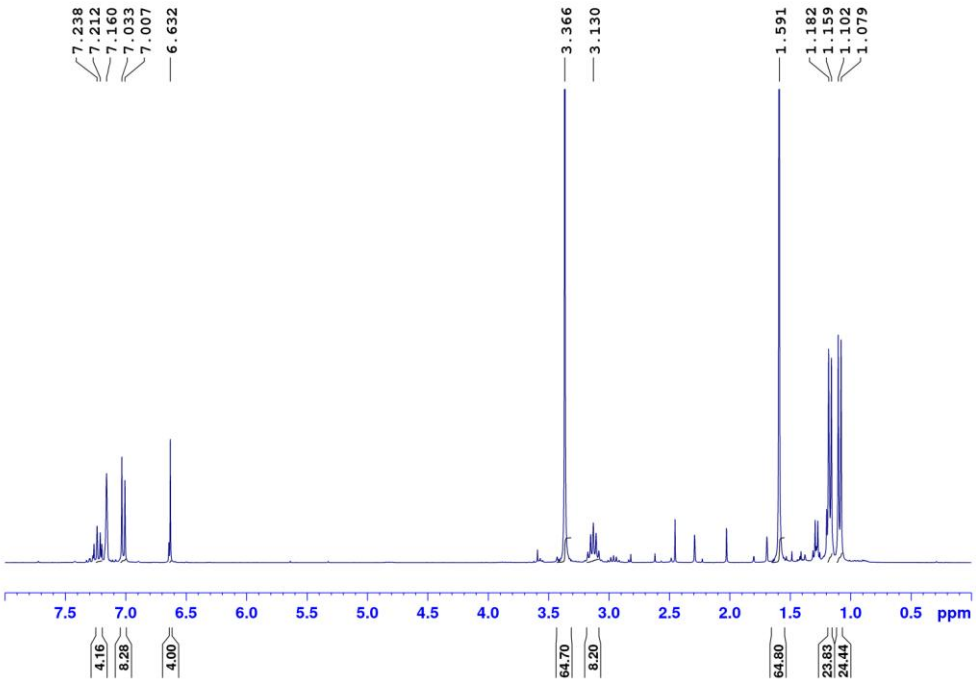


Figure S65 ^{1}H NMR of 1:4.5 mixture of (NHC^{Dip})Si$_2$ and NHC^{Me4} in [D$_6$]-benzene at RT.

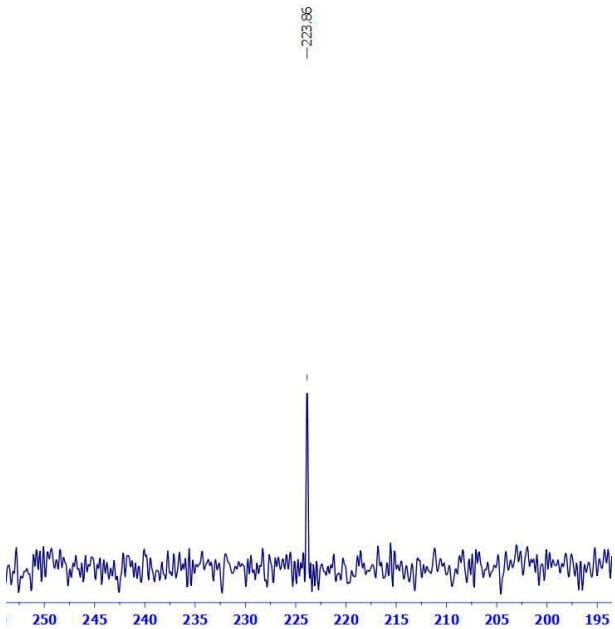


Figure S66 ^{29}Si NMR of 1:4.5 mixture of (NHC^{Dip})Si$_2$ and NHC^{Me4} in [D$_6$]-benzene at RT.

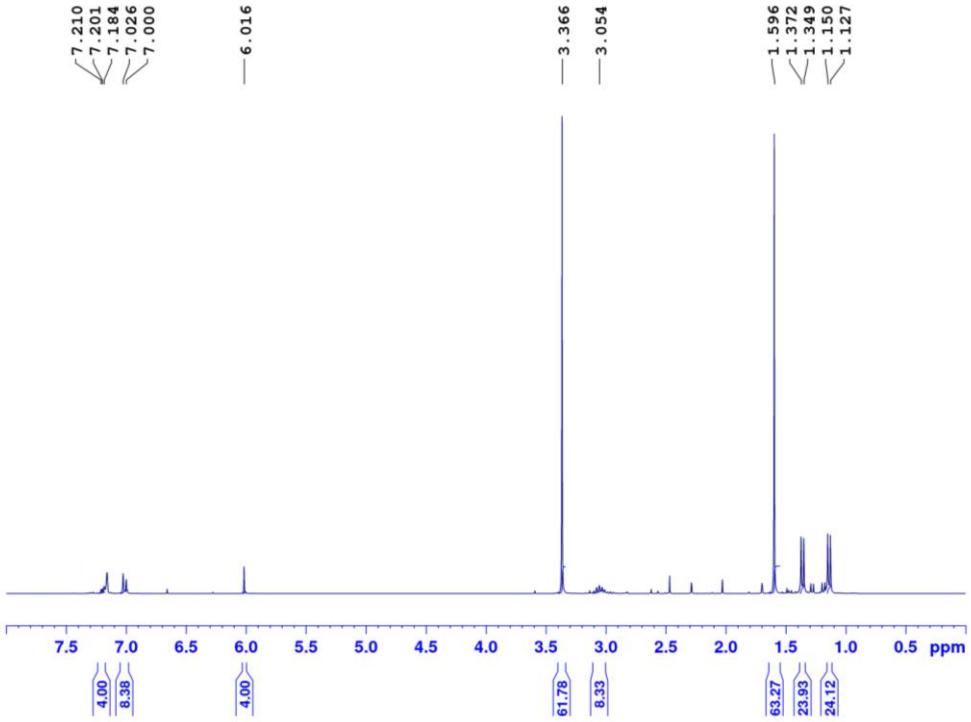


Figure S67 ^{1}H NMR of 1:5 mixture of (NHC^{Dip})P$_2$ and NHC^{Me4} in [D$_6$]-benzene at RT.

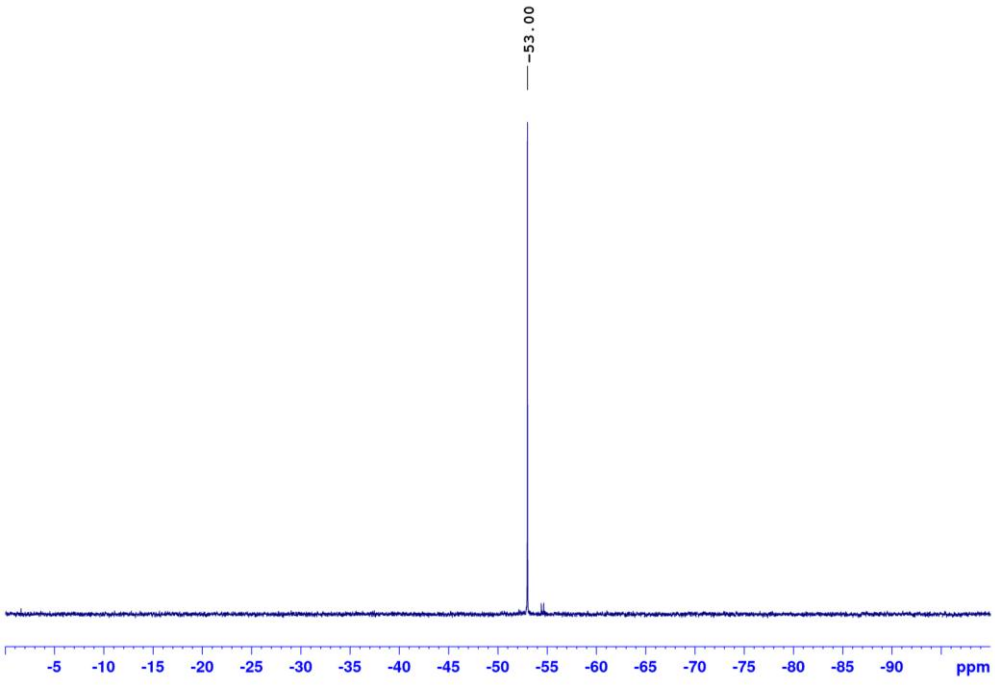


Figure S68 ^{31}P NMR of 1:5 mixture of (NHC^{Dip})P$_2$ and NHC^{Me4} in [D$_6$]-benzene at RT.

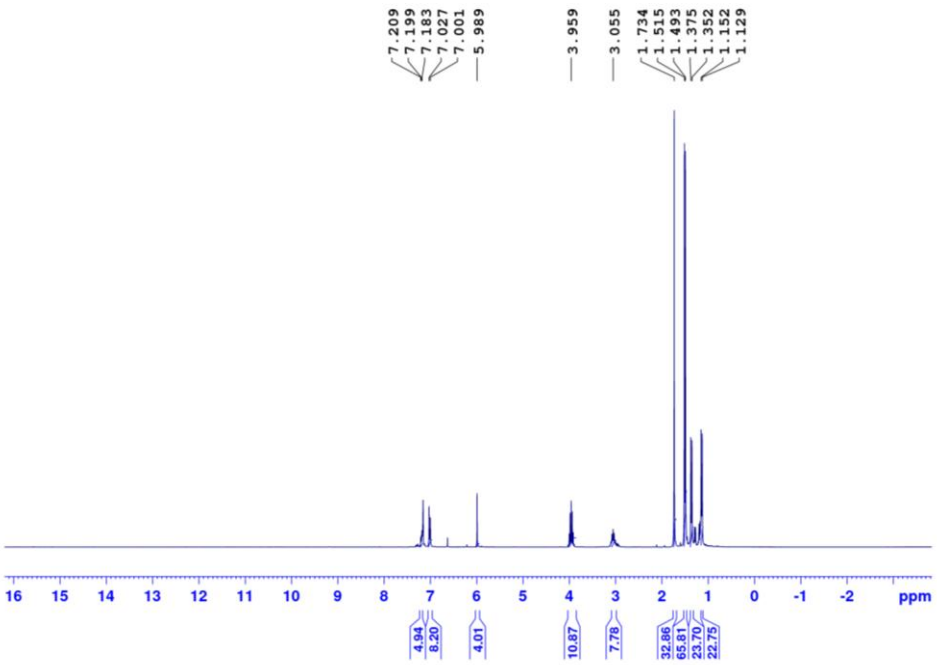


Figure S69 ^{1}H NMR of 1:4.5 mixture of (NHC^{Dip})P_2 and NHC^{Me2iPr2} in [D_6]-benzene at RT.

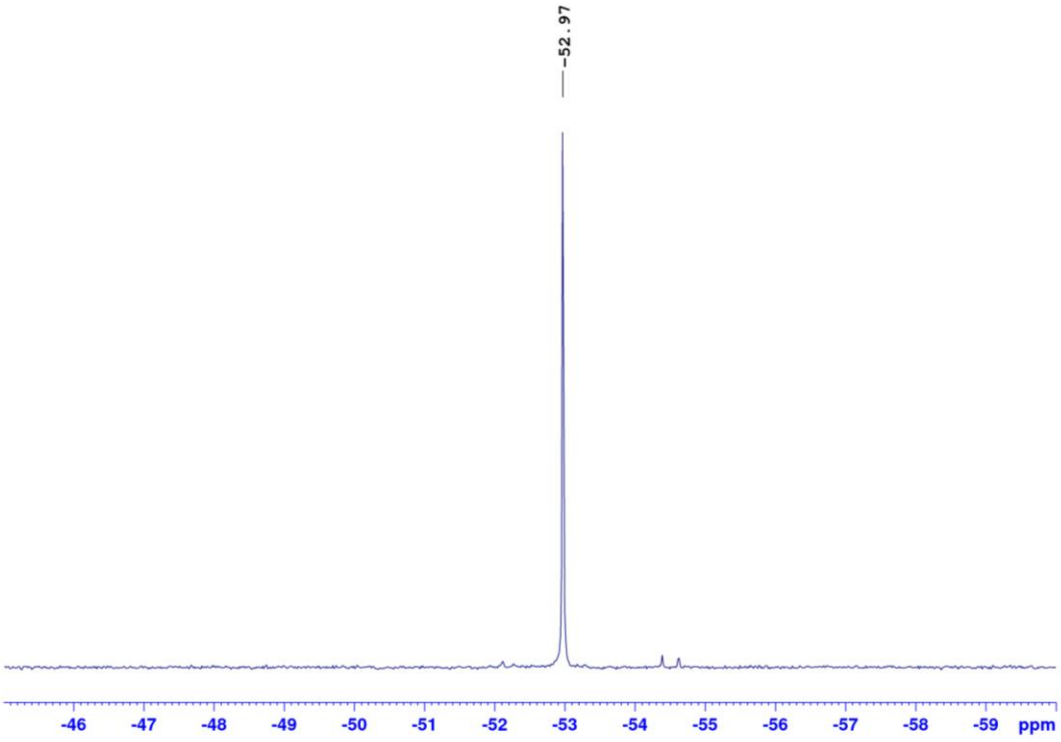


Figure S70 ^{31}P NMR of 1:4.5 mixture of (NHC^{Dip})P_2 and NHC^{Me2iPr2} in [D_6]-benzene at RT.

Absorption Spectra

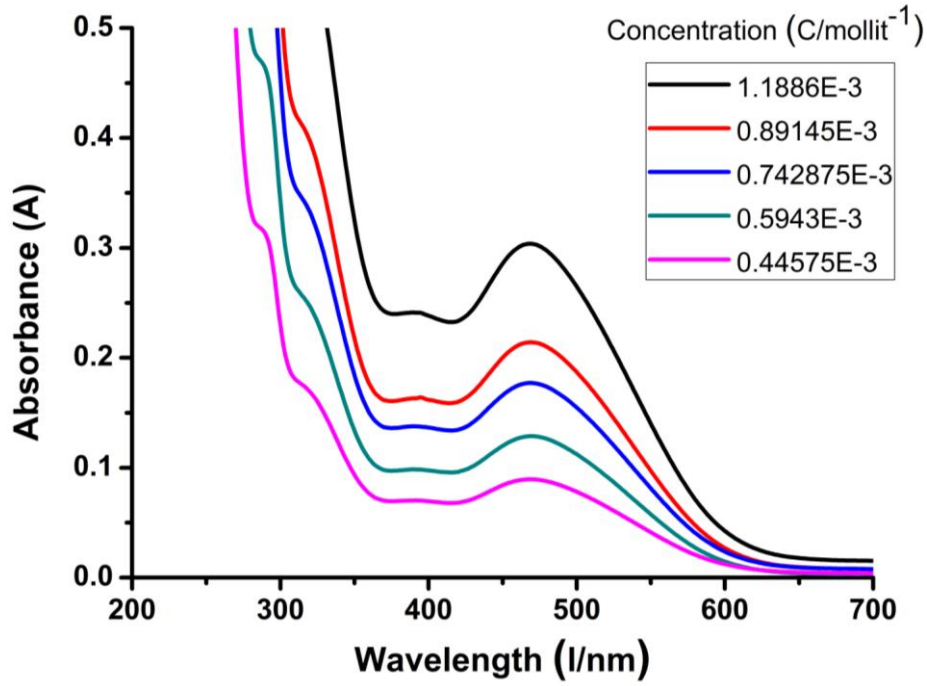


Figure S61 UV-Vis Spectra of **4** in *n*-hexane at different concentrations.

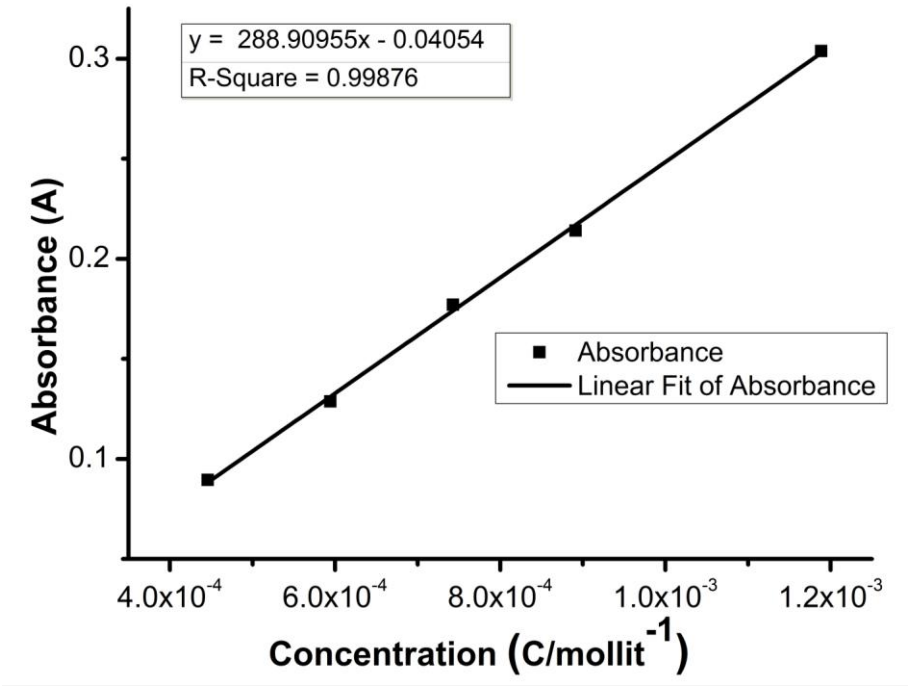


Figure S62 Linear regression of **4** at 469 nm.

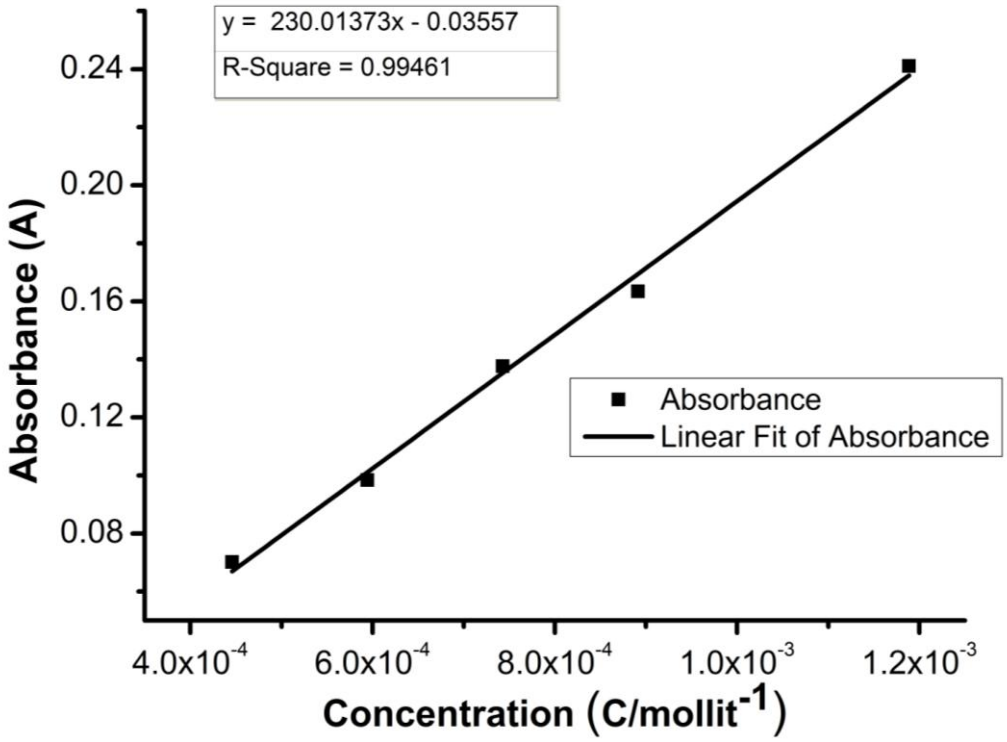


Figure S63 Linear regression of **4** at 393 nm.

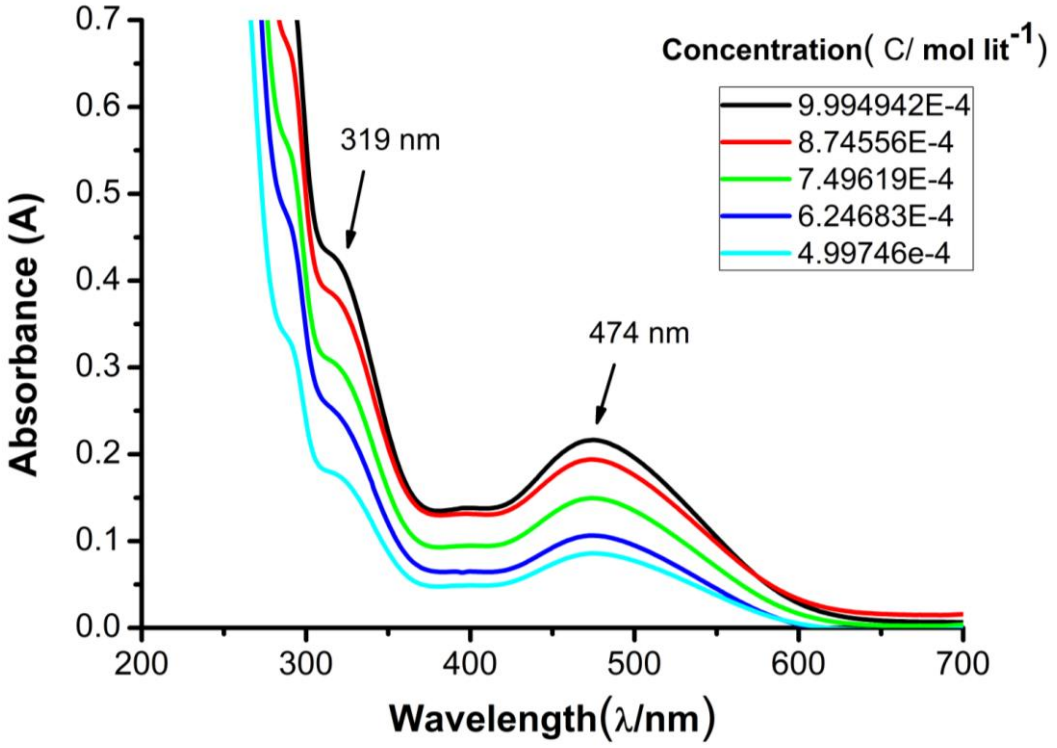


Figure S64 UV-Vis Spectra of **5** in *n*-hexane at different concentrations.

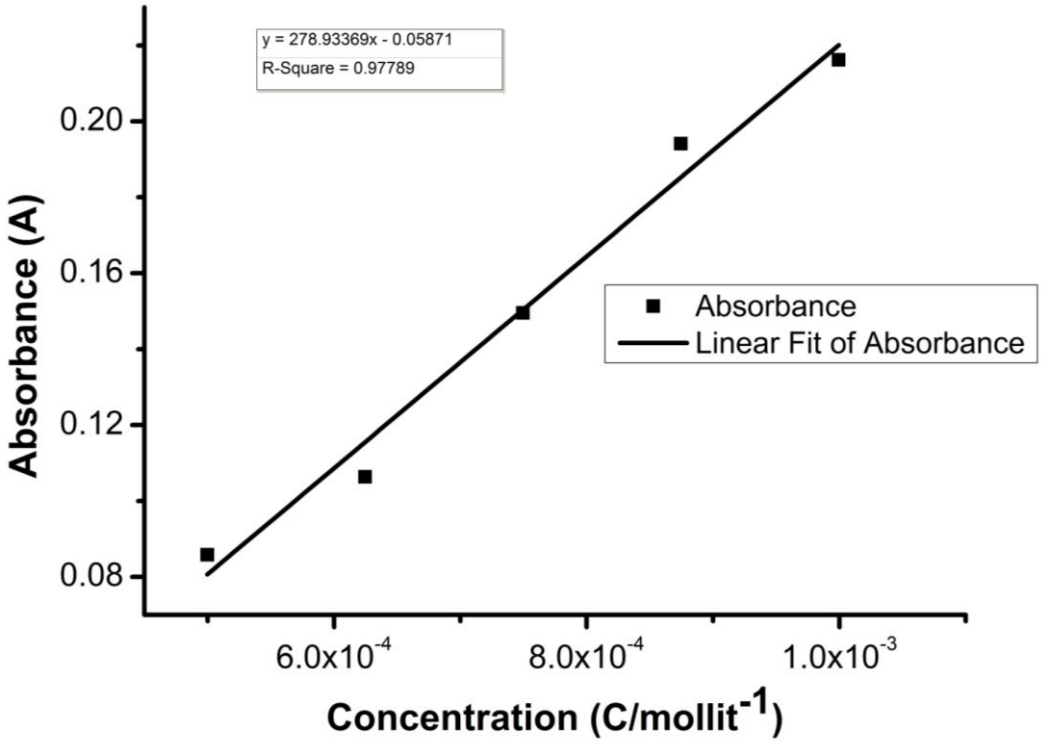


Figure S65 Linear regression of **5** at 474 nm.

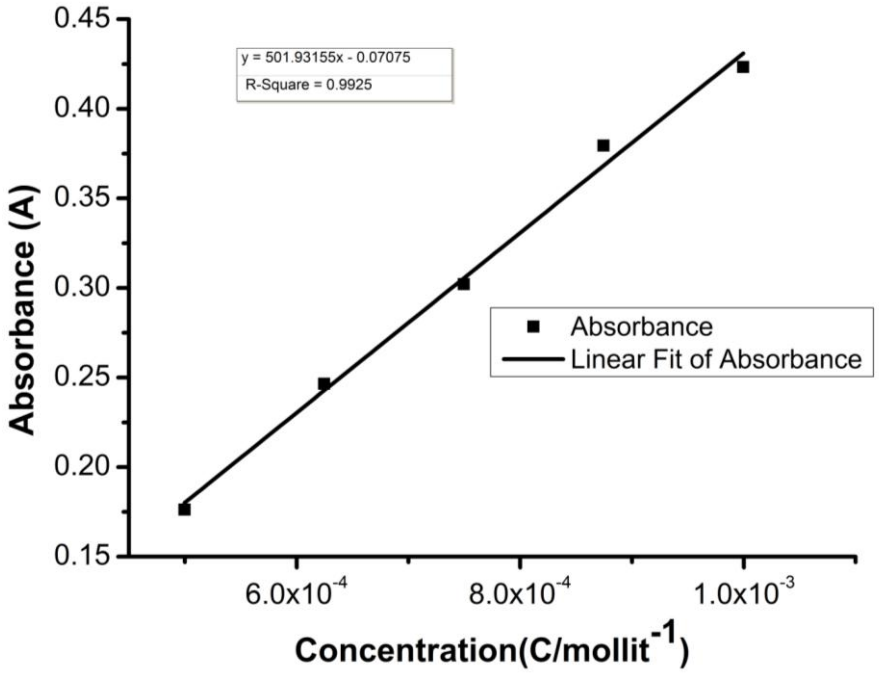


Figure S66 Linear regression of **5** at 319 nm.

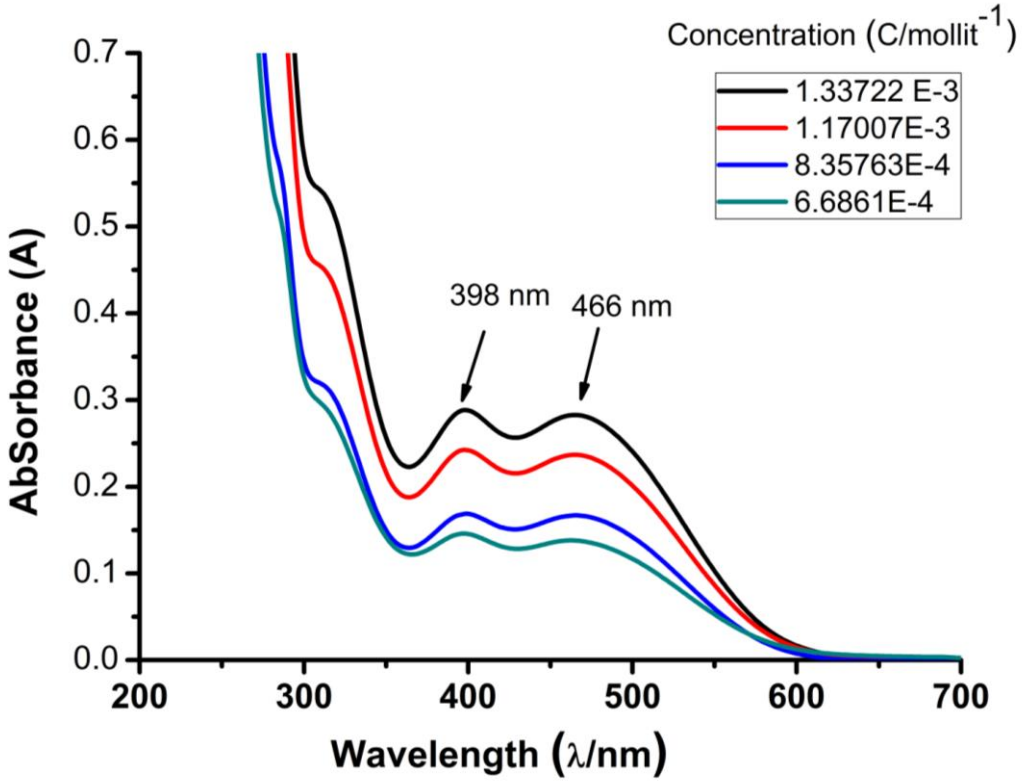


Figure S67 UV-Vis Spectra of **6** in *n*-hexane at different concentrations.

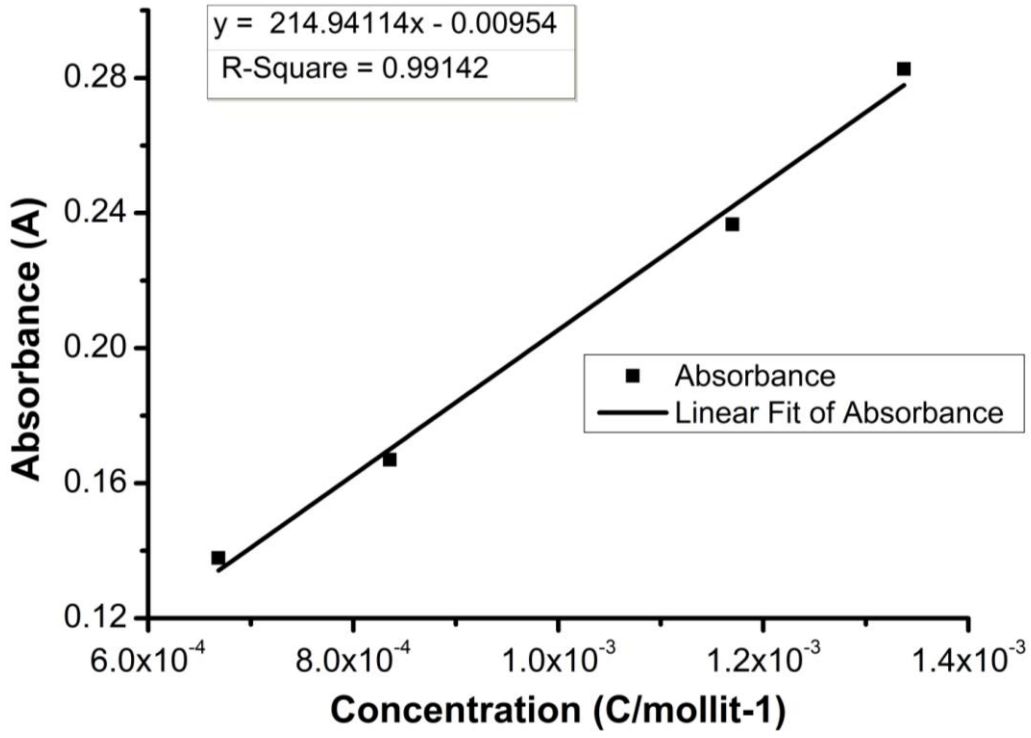


Figure S68 Linear regression of **6** at 466 nm.

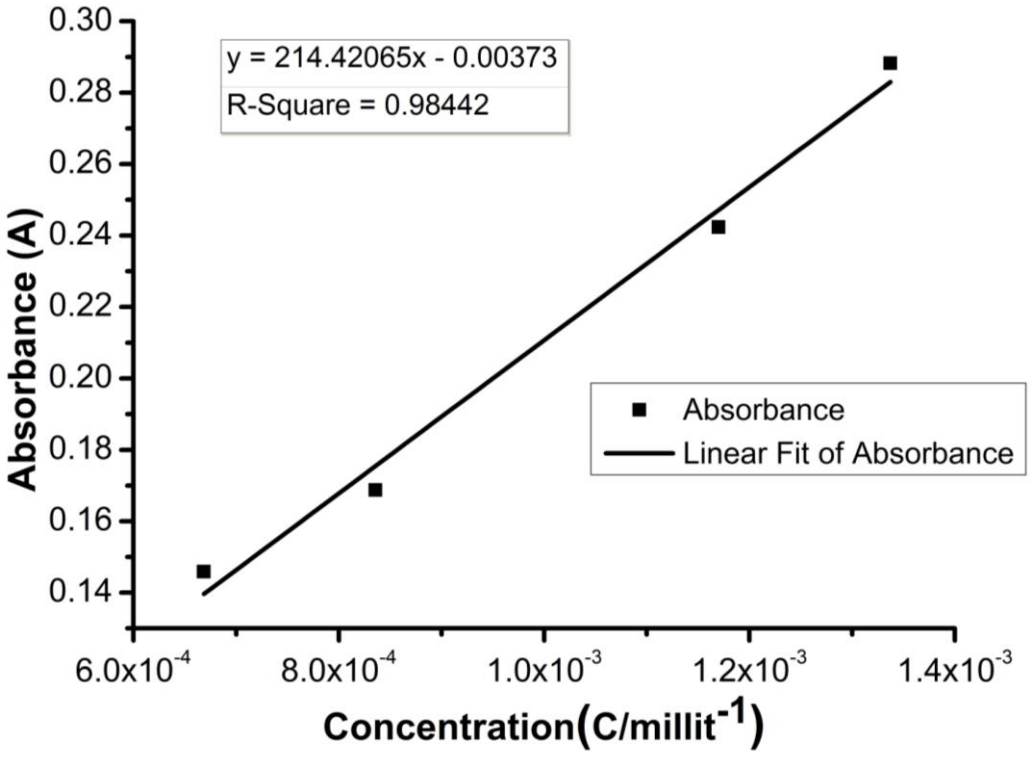


Figure S69 Linear regression of **6** at 398 nm.

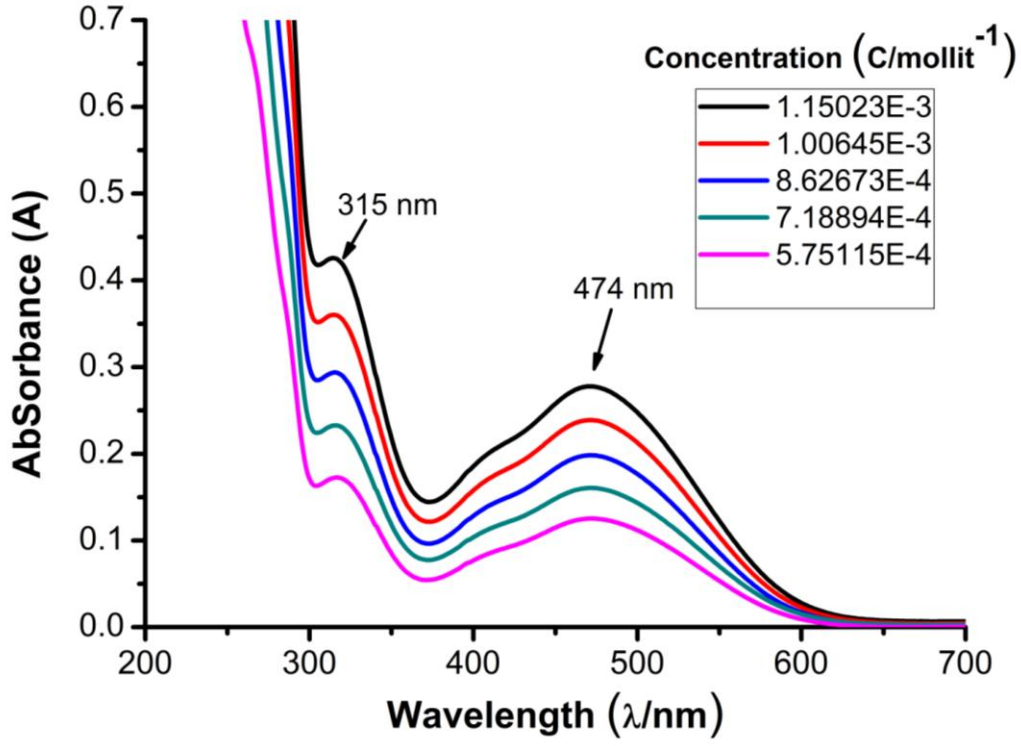


Figure S70 UV-Vis Spectra of **7** in *n*-hexane at different concentrations.

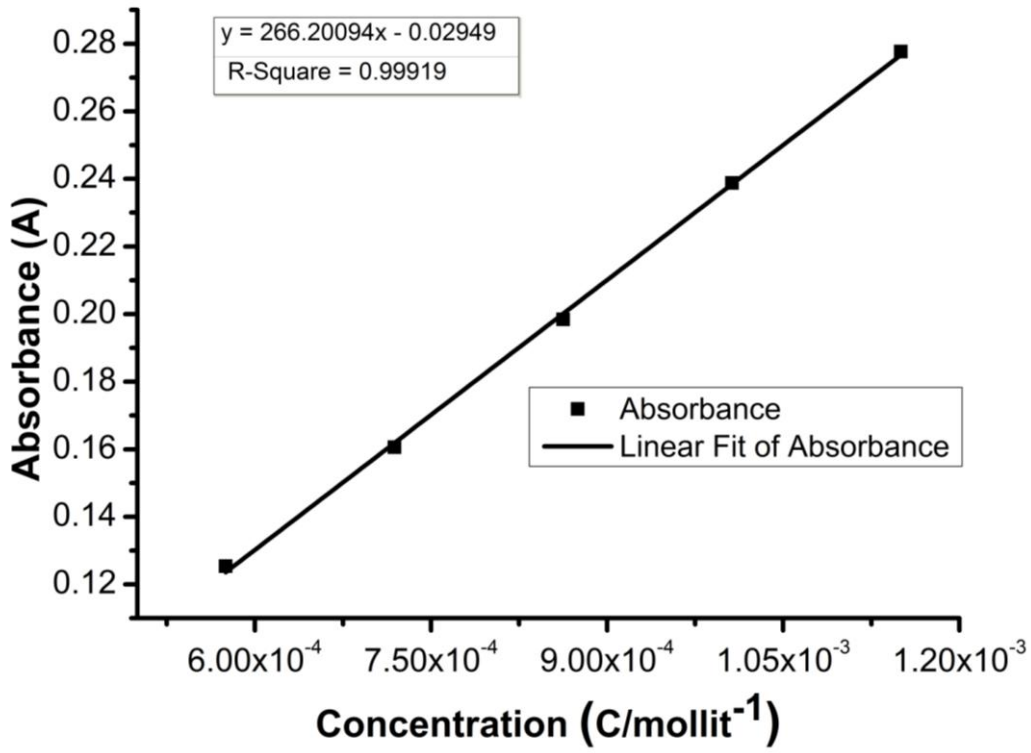


Figure S71 Linear regression of **7** at 474 nm.

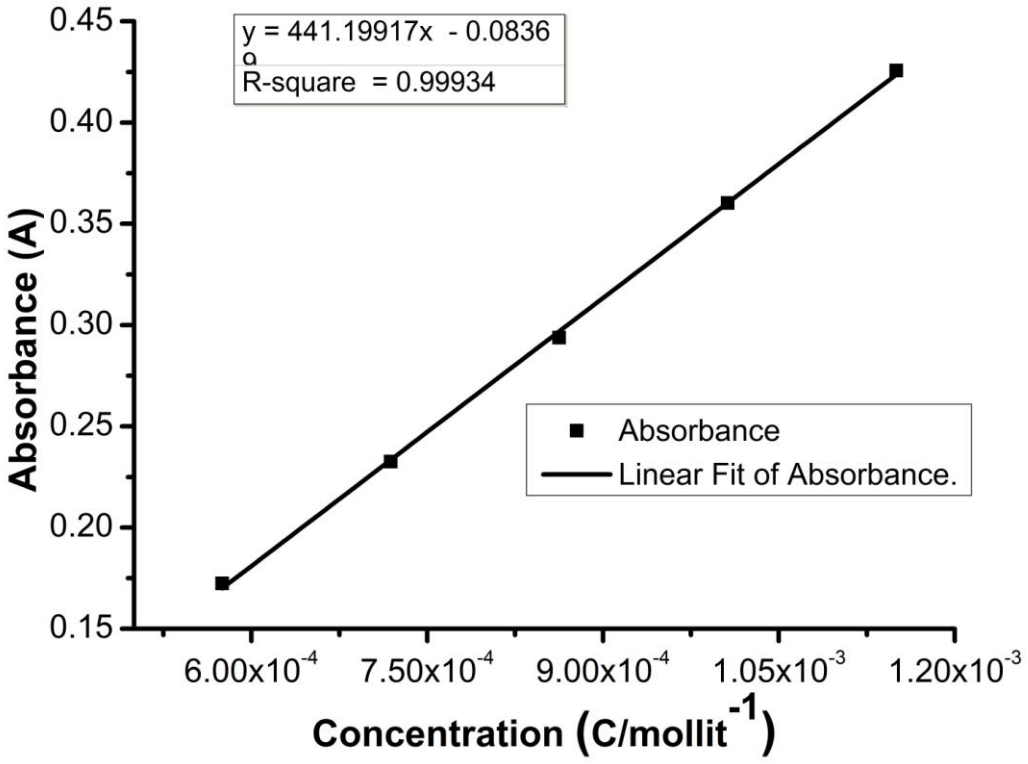


Figure S72 Linear regression of **7** at 315 nm.

Table S1. Crystal data and structure refinement for **3•C_6H_6** (CCDC: 1509722)

Identification code	DD322A
Empirical formula	C51 H74 Cl P Si x C6 H6
Formula weight	859.72
Temperature	170(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	*P*bca
Unit cell dimensions	a = 17.664(4) Å
	b = 21.948(4) Å
	c = 26.612(5) Å
Volume	10317(4) $Å^3$
Z	8
Density (calculated)	1.107 Mg/m^3.
Absorption coefficient	0.163 mm^{-1}
F(000)	3744
Crystal size	0.232 x 0.224 x 0.135 mm^3
Theta range for data collection	3.058 to 20.817°
Index ranges	-17<=h<=17, -21<=k<=21, -26<=l<=26
Reflections collected	34453
Independent reflections	5384 [R(int) = 0.1114]
Completeness to theta = 20.817°	99.7 %
Absorption correction	Numerical
Max. and min. transmission	0.9606 and 0.8284
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5384 / 0 / 567
Goodness-of-fit on F^2	0.785
Final R indices [I>2sigma(I)]	R1 = 0.0405, wR2 = 0.0895
R indices (all data)	R1 = 0.0788, wR2 = 0.1041
Largest diff. peak and hole	0.353 and -0.270 e.$Å^{-3}$

Table S2. Crystal data and structure refinement for **7•2C_6H_6** (CCDC: 1509723)

Identification code	vc_aj_dd_4
Empirical formula	C58 H85 N2 P Si x 2 C6 H6
Formula weight	1025.56
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P21/c
Unit cell dimensions	a = 20.327(4) Å
	b = 14.765(3) Å β= 106.508(10)°.
	c = 21.810(4) Å
Volume	6275.8(19) $Å^3$
Z	4
Density (calculated)	1.085 Mg/m^3
Absorption coefficient	0.104 mm^{-1}
F(000)	2240
Crystal size	0.16 x 0.14 x 0.12 mm^3
Theta range for data collection	1.93 to 26.70°
Index ranges	-25<=h<=25, -18<=k<=18, -27<=l<=27
Reflections collected	76230
Independent reflections	12984 [R(int) = 0.1277]
Completeness to theta = 26.70°	97.7 %
Absorption correction	Multi-scan
Max. and min. transmission	0.9877 and 0.9836
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	12984 / 0 / 689
Goodness-of-fit on F^2	1.028
Final R indices [I>2sigma(I)]	R1 = 0.0569, wR2 = 0.1262
R indices (all data)	R1 = 0.1077, wR2 = 0.1478
Largest diff. peak and hole	0.609 and -0.537 e.$Å^{-3}$

Computational Calculation:

All theoretical calculations, in this paper were carried out using the Gaussian03 suite of programs.[S1] The Full geometry optimizations of **4-7** were performed using Dip (Dip = diisopropylphenyl) groups instead of Tip (Tip = triisopropylphenyl) groups at B3LYP/6-311G(d,p) level of theory. Frequency analyses were performed to determine the energies in solution (CPCM method, Toluene) at B3LYP/6-311G(d,p) level of theory.[S2] Wiberg bond orders (WBI) as a criterion to estimate the bond orders of chemical structures were also calculated within the natural bond orbital (NBO) analysis for **4-Dip-7-Dip**.[S3] The electronic absorption spectrum for **4-Dip-7-Dip** were predicted with the optimized geometry at time-dependent density functional theory (TD-DFT) method in solution (heptane) at B3LYP/6-311G(d,p) level of theory. ^{13}C, ^{29}Si and ^{31}P NMR chemical shifts were calculated by the GIAO method in solution (benzene) at the B3LYP/6-311+2df level of theory. The relative Gibbs free energies are given in kcal/mol. The GaussView 5.0 program was employed for visualization of the final geometries of the optimized structures.[S4]

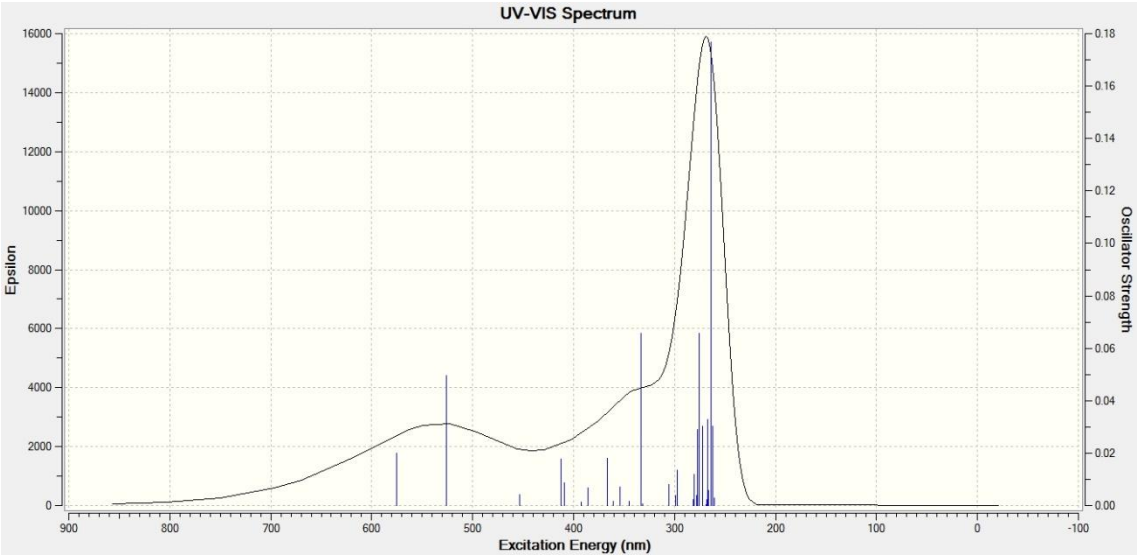


Figure S73 UV/vis spectrun of **4-Dip** at B3LYP/6-311G(d,p) level of theory (solvent = heptane).

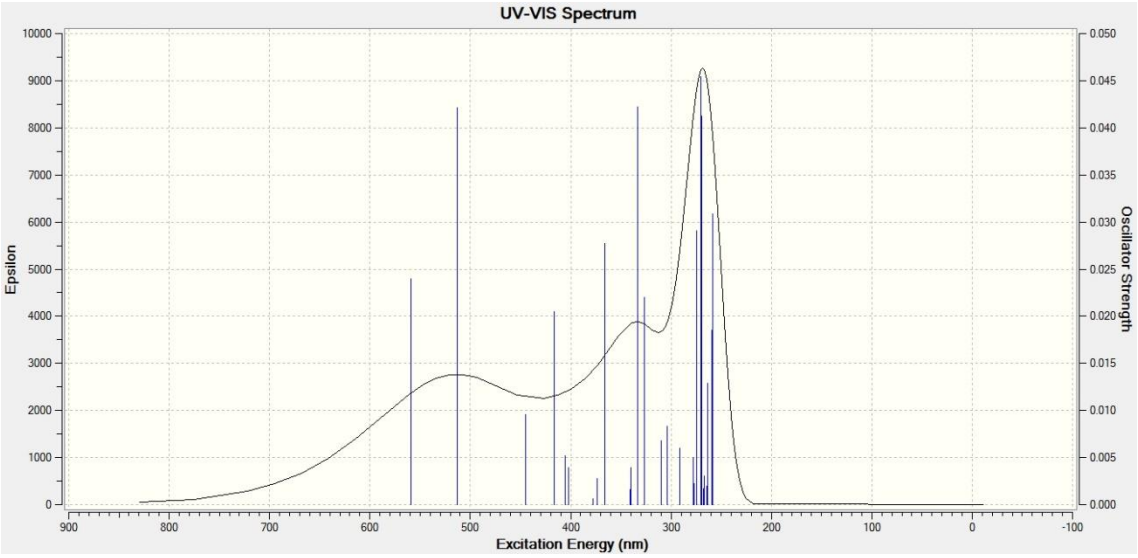


Figure S74 UV/vis spectrum of **5-Dip** at B3LYP/6-311G(d,p) level of theory (solvent = heptane).

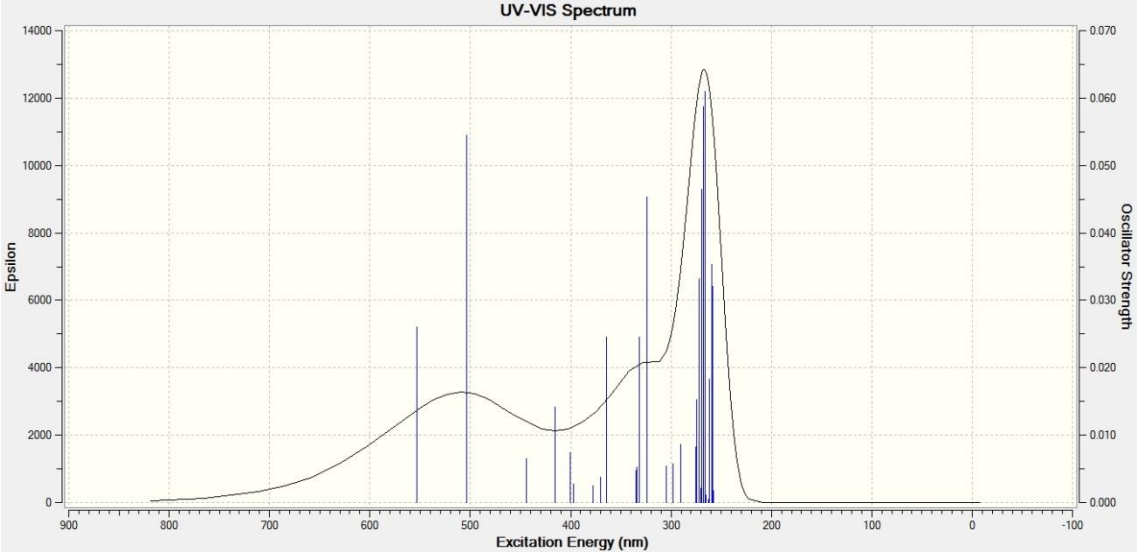


Figure S75 UV/vis spectrum of **6-Dip** at B3LYP/6-311G(d,p) level of theory (solvent = heptane).

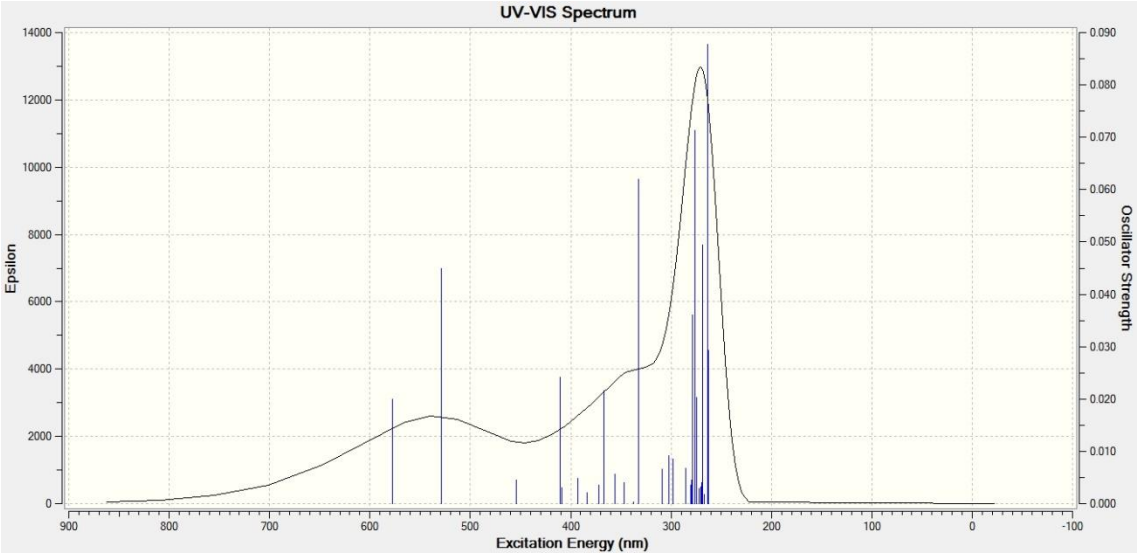


Figure S76 UV/vis spectrum of **7-Dip** at B3LYP/6-311G(d,p) level of theory (Solvent = Heptane).

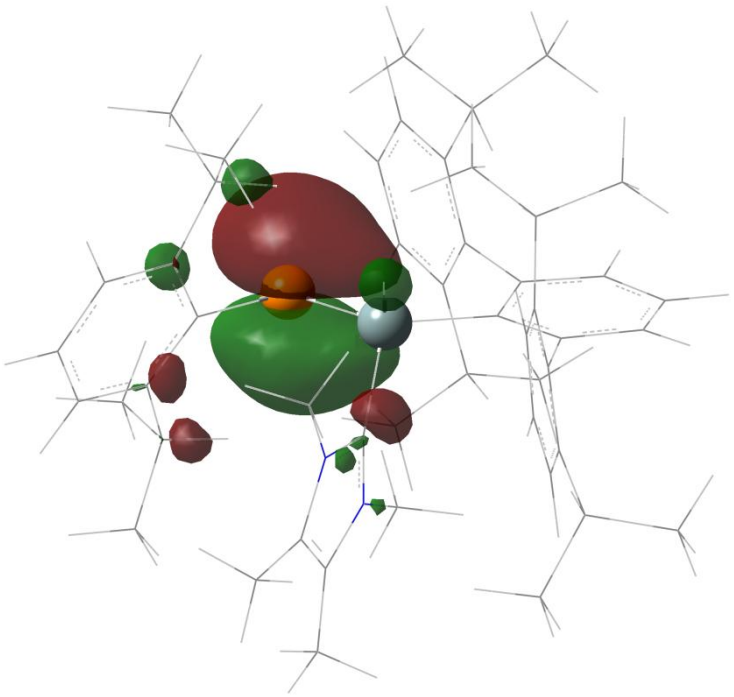
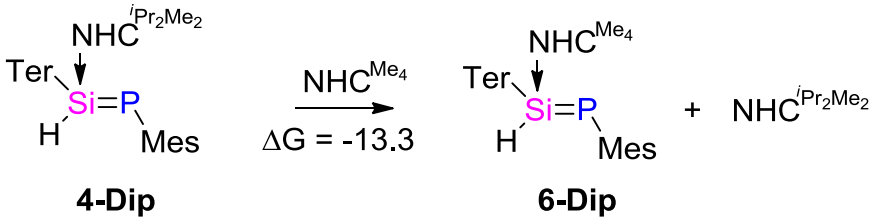
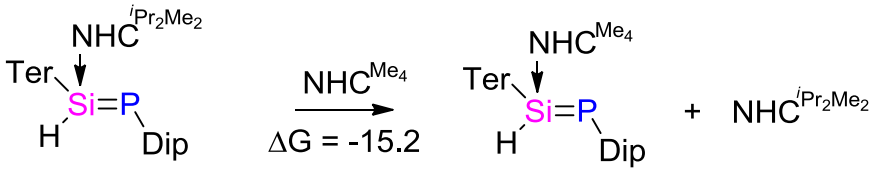


Figure S77 HOMO of model **7-Dip** at an *iso*density *value* of 0.035 au.



4-Dip **6-Dip**

Scheme S1 The relative energy between **4-Dip** and **6-Dip** at B3LYP/6-311G(d,p) levels. ΔG energy values at 298 K are given in kcal mol^{-1}. (Dip instead of Tip, solvent = toluene).



5-Dip **7-Dip**

Scheme S2 The relative energies between **5-Dip** and **7-Dip** at B3LYP/6-311G(d,p) levels. ΔG energy values at 298 K are given in kcal mol^{-1}. (Dip instead of Tip, Solvent = Toluene).

Table S3 The calculated NMR, UV-vis, WBO, and NBO results for the compounds of **4-Dip** – **7-Dip**

	4-Dip		**5-Dip**		**6-Dip**		**7-Dip**	
^{13}C-NMR	171.14		171.18		165.96		167.59	
^{29}Si-NMR	-29.10		-28.17		-29.07		-26.85	
^{31}P-NMR	-172.31		-197.17		-183.23		-209.95	
λ_{max}	526.19, 264.04		528.52, 263.73		503.58, 266.17		512.84, 270.18	
Si-P (WBO)	1.234		1.224		1.210		1.198	
	4-Dip		**5-Dip**		**6-Dip**		**7-Dip**	
BD_{Si-P}	Si	P	Si	P	Si	P	Si	P
Hybrids	$sp^{2.03}$	$sp^{5.31}$	$sp^{2.03}$	$sp^{5.32}$	$sp^{2.08}$	$sp^{5.36}$	$sp^{2.07}$	$sp^{5.34}$
Charges	1.004	-0.284	1.003	-0.296	1.023	-0.272	1.018	-0.559

Table S4 The NBO analaysis for Si-P bonds in the structures H_2Si=PH, **7-Dip'**, and **7-Dip**

	H_2Si=PH		**7-Dip'**		**7-Dip**	
BD_{Si-P}	Si	P	Si	P	Si	P
Hybrids	p	p	$sp^{1.68}$	$sp^{4.68}$	$sp^{2.07}$	$sp^{5.34}$
Charges	0.551	-0.244	0.002	0.861	-0.272	1.023
Polarization	37.5%	62.5%	45.8%	54.2%	48.7%	51.3%
WBO for Si-P	1.996		1.786		1.198	
Bond Length Si-P	2.081		2.099		2.185	

Table S5 Cartesian coordinates and energy values for the **4-Dip**

P,1.5207764779,-1.6516215506,-0.1029496872
Si,0.2098555304,0.0719633351,0.1718171407
H,0.1313788354,0.6570397997,1.5375289315
N,1.2041883705,1.7981021517,-2.0993478108
N,1.6165209611,2.7370928241,-0.1816899578
C,-1.6511509439,-0.0963481887,-0.3828128768
C,-2.1994953558,-1.3211851412,-0.8794144642
C,0.9735160225,1.679856944,-0.7595155086
C,-2.5545640462,1.0065466597,-0.2431499996
C,-4.3454948958,-0.2530231992,-1.3120048191
H,-5.3644886373,-0.3072181318,-1.679379584
C,-1.5773826707,-2.7009336318,-0.7761506128
C,-1.0165691962,-3.3577222831,-1.8935210881
C,-1.7684463928,-3.4179202021,0.4319516144
C,-3.5142475285,-1.3590687258,-1.3663106964
H,-3.8963076721,-2.3009114129,-1.7412331486
C,-2.4903859908,3.6705018836,-1.7042129768
H,-2.4102398123,2.6702371411,-2.1276893507
C,-3.8741277783,0.900311245,-0.7077807982
H,-4.5437267952,1.7389791639,-0.5629210287
C,-2.3465945217,3.5501237878,-0.1870678156
C,-2.3062811237,2.3081993787,0.4992093956
C,-2.2967693524,2.3063175879,1.921136149
C,-1.3110473931,-4.7332228848,0.5219565359
H,-1.4425143049,-5.2816054998,1.4476052528
C,3.0178100921,-1.1023807776,0.9090468166
C,-0.92366605,-2.7046422976,-3.2694703868
H,-1.0482989107,-1.6278941449,-3.1320811392
C,1.9683127518,2.9335153458,-2.3610207598
C,2.244680898,3.5102896917,-1.1565285063
C,-2.2849022097,4.7374631531,1.9320411216
C,-0.7049700132,-5.3598268742,-0.5567235856
C,-2.2717470149,3.5250073166,2.606251526
H,-2.276108556,3.5255307029,3.6894184537
C,-0.5793200763,-4.6787965833,-1.7567711243
H,-0.1325254518,-5.1844928853,-2.6042131429
C,-2.465942563,1.0293431418,2.7436099961
H,-2.1604249755,0.1870101813,2.1256641381
C,-2.5545341289,-2.8494304187,1.6127687999
H,-2.690887441,-1.7812586322,1.4458307464
C,-2.3257453231,4.7418504662,0.5469282605
H,-2.3635467085,5.6900913853,0.0223823283
C,3.0477764166,-1.2445428071,2.3209854987
C,4.2305103729,-0.7440573428,0.2655950411
C,1.7011517553,2.9701905882,1.2913335149
H,0.9535925027,2.2979311762,1.7011408165
C,-1.3863317322,4.5357307997,-2.3380397977
H,-1.4621375466,5.5799448226,-2.0216896815

H,-1.47548643,4.5208924446,-3.4286586329
H,-0.3915325831,4.1771038157,-2.0715531478
C,0.7837830032,0.7721475311,-3.095481032
H,0.6162864016,-0.1186599445,-2.4867590715
C,4.2254815206,-0.9909749122,3.0316351987
H,4.2155815634,-1.1039719116,4.1127418466
C,0.4365017105,-2.9426689417,-3.9472408191
H,1.2570863695,-2.639601799,-3.2937705715
H,0.4945610653,-2.3827397674,-4.886067226
H,0.5798982309,-3.9956309226,-4.2030351269
C,-3.953678602,0.8247318178,3.0973842113
H,-4.3215940082,1.6442137806,3.7225164874
H,-4.090426525,-0.109554879,3.650207261
H,-4.5746839998,0.7800268887,2.2000987806
C,5.4112328994,-0.6204778785,2.4013734185
C,5.3888274214,-0.5088037198,1.0127309326
H,6.3011430069,-0.2330081335,0.4896952175
C,-1.6039515991,0.9890788368,4.0161291655
H,-0.5509869435,1.1760705081,3.7938976213
H,-1.6757652009,0.0021691592,4.4801297537
H,-1.9302999959,1.7196528173,4.7617757067
C,-2.061742319,-3.1835794408,-4.1943235682
H,-2.0037312747,-4.2646948364,-4.3512478501
H,-1.9937496267,-2.698414736,-5.173819257
H,-3.0450330581,-2.95971671,-3.7764418685
C,2.3451565677,3.4428863763,-3.7168214819
H,3.1961565908,2.9086863942,-4.1457338732
H,2.614967642,4.4965496357,-3.6463702184
H,1.5151727807,3.3711971944,-4.4208643523
C,-3.8731597114,4.2277255427,-2.1004382228
H,-4.6868425666,3.616194246,-1.7067954115
H,-3.9728938593,4.2596497487,-3.1897952466
H,-4.0108891019,5.2449586284,-1.7226898065
C,3.0474109536,4.7482510684,-0.9102965744
H,2.4196676505,5.6073601649,-0.6597570611
H,3.6123860398,4.9997306646,-1.8076248397
H,3.7694368726,4.6145900245,-0.1044556058
C,-3.9607604989,-3.4797772922,1.6765380971
H,-4.5101381759,-3.3231501828,0.7452770709
H,-4.543708271,-3.0401014534,2.4921553671
H,-3.8981271931,-4.5581643137,1.8499375272
C,-1.8301657307,-3.0091319023,2.9588896175
H,-1.7202826116,-4.0596502433,3.2424056105
H,-2.3999166305,-2.5184212479,3.7542600792
H,-0.8351561873,-2.5658903883,2.9217635236
H,-0.3486645301,-6.3804231606,-0.4676617444
H,-2.2792583834,5.6713760381,2.4839171056
C,-0.5121723075,1.1588518832,-3.8093542942
H,-1.3412092812,1.2359605502,-3.107270098
H,-0.414823908,2.1068201576,-4.3444339027

H,-0.7636529856,0.3879672815,-4.541343571
C,1.9014901292,0.4195887254,-4.0843767458
H,1.990696957,1.1431075074,-4.8946095435
H,2.8644560861,0.3184601409,-3.5843928407
H,1.6650085113,-0.5441928114,-4.5329655711
C,1.2998688596,4.3916922806,1.6941506788
H,1.1095979694,4.3983953557,2.769763447
H,2.0830683592,5.1248532735,1.4997344999
H,0.381207252,4.7020938206,1.197146422
C,3.067797352,2.556920278,1.8429441834
H,3.0380450447,2.6053828137,2.9343636956
H,3.3205478251,1.5361481652,1.5585995323
H,3.8672568083,3.2209866952,1.5057511876
C,1.841435356,-1.7037639825,3.1020124107
H,1.0160404238,-0.9906703198,3.0355779075
H,1.4658575162,-2.649543249,2.7043379572
H,2.0914911077,-1.8356798548,4.1580685099
C,4.3226434655,-0.6039841775,-1.234852432
H,5.3390903706,-0.3373149249,-1.5374154616
H,4.0369253392,-1.5293610157,-1.7409200074
H,3.6392089362,0.1677190507,-1.5961781189
C,6.6819053082,-0.3969807605,3.1862961907
H,7.2709153451,-1.3186115384,3.2581558334
H,7.3173611209,0.3568742521,2.7135384057
H,6.468591222,-0.0679434547,4.206596625

Zero-point correction= 1.068400 (Hartree/Particle)
Thermal correction to Energy= 1.129068
Thermal correction to Enthalpy= 1.130012
Thermal correction to Gibbs Free Energy= 0.974367
Sum of electronic and zero-point Energies= -2686.737978
Sum of electronic and thermal Energies= -2686.677310
Sum of electronic and thermal Enthalpies= -2686.676366
Sum of electronic and thermal Free Energies= -2686.832011

Table S6. Cartesian coordinates and energy values for the **5-Dip**

P,1.4560866112,-1.7114222976,0.0419145245
Si,0.1931154392,0.0634055514,0.2369383358
H,0.0726992527,0.6808166915,1.5868139571
N,1.2098182319,1.7627473383,-2.0442545122
N,1.671506048,2.6829160141,-0.129532535
C,-1.6546034723,-0.0871269577,-0.3653200849
C,-2.204180154,-1.3064312609,-0.8758969595
C,1.0096128179,1.635546052,-0.701417172
C,-2.5491531874,1.0273267332,-0.2488998501
C,-4.3267760746,-0.2130688391,-1.3623213554
H,-5.336688745,-0.2558614192,-1.7553206905
C,-1.6021553388,-2.6960349355,-0.7691493334
C,-1.0606141212,-3.3642722082,-1.8898706986
C,-1.8034234309,-3.4121664226,0.437561515
C,-3.5083629953,-1.3292528578,-1.3919346002
H,-3.8926400089,-2.2668806299,-1.774534415
C,-2.4254191251,3.7050427648,-1.6940255059
H,-2.3423626873,2.7086171273,-2.1252833632
C,-3.8562011153,0.9364567608,-0.7504416882
H,-4.5187046054,1.783744257,-0.6253905249
C,-2.3137884992,3.572015986,-0.1752315994
C,-2.3104999522,2.3260099773,0.5048347344
C,-2.3496531154,2.3180975929,1.9265275275
C,-1.3794927637,-4.7394215358,0.5214410911
H,-1.5198489663,-5.286461603,1.4464771769
C,3.0296259477,-1.1541940638,0.9548980487
C,-0.9549701581,-2.7140370849,-3.2661107573
H,-1.0742083759,-1.6363953044,-3.1328193429
C,1.9666121456,2.9007696181,-2.3147790384
C,2.2690702162,3.4693841285,-1.1126325019
C,-2.2901799125,4.7481006268,1.9512539645
C,-0.7930647384,-5.3777141274,-0.5608350285
C,-2.3238151918,3.5319918129,2.6189144598
H,-2.3615699398,3.5266820933,3.7012057081
C,-0.6549084011,-4.6958318947,-1.7589592946
H,-0.2261749802,-5.2097857878,-2.6107811929
C,-2.5710013212,1.0396832819,2.7334717178
H,-2.2249607079,0.1989870848,2.1352919217
C,-2.55638719,-2.8251611613,1.6293565231
H,-2.6598244289,-1.7526438665,1.4687477766
C,-2.2908989717,4.7597253143,0.5658873507
H,-2.2965706448,5.7108008854,0.0453239585
C,3.1169083142,-1.1816811968,2.3773336037
C,4.2299942181,-0.9168671662,0.22218048
C,1.814756084,2.8915982677,1.3423994693
H,1.1341825408,2.1634890362,1.7734701484
C,-1.3061359987,4.5705848152,-2.2995585031
H,-1.3879372295,5.6142118794,-1.9827512872

H,-1.3699308717,4.5592291655,-3.3920626909
H,-0.3182012197,4.2100099924,-2.0108961327
C,4.2736995837,-0.994931757,-1.300926269
H,3.2478962664,-0.8394759013,-1.6421330633
C,0.7769690478,0.7400516781,-3.0395288323
H,0.6137893969,-0.1522684277,-2.4316671922
C,4.3403611441,-0.9320616258,3.0091490565
H,4.3952903438,-0.9589725217,4.0916994145
C,1.9389301931,-1.5739776038,3.265781228
H,1.0344567894,-1.4499491707,2.6699597679
C,0.4090959413,-2.9629704262,-3.9325050546
H,1.2269440002,-2.6619307497,-3.2748703891
H,0.4783096187,-2.4089353467,-4.8741056802
H,0.5490999395,-4.0183085203,-4.1800915038
C,-4.0786106832,0.8354281006,2.9914832358
H,-4.484388846,1.6575067157,3.5891493093
H,-4.250510497,-0.096563557,3.5381938605
H,-4.641461909,0.7873526973,2.0570686628
C,5.4939510064,-0.6722473314,2.2840021219
C,5.4319391865,-0.678525063,0.898421276
H,6.3395870008,-0.5047117783,0.331522455
C,-1.7939954324,0.9985016924,4.0586229822
H,-0.73250706,1.2040042847,3.9080194393
H,-1.8802941973,0.0055471383,4.5068484937
H,-2.1819420451,1.7147334137,4.7884857314
C,-2.0878816742,-3.190349922,-4.1989053415
H,-2.033636936,-4.2723168241,-4.3508385851
H,-2.009267919,-2.7093069651,-5.1796036344
H,-3.0739406205,-2.9608963854,-3.7906838303
C,4.6817432795,-2.4093628739,-1.7558597588
H,5.6888346086,-2.6579869768,-1.4057785059
H,4.6752439554,-2.4850508946,-2.8488959554
H,3.9895924459,-3.1555781912,-1.3603800472
C,2.31066694,3.4205762268,-3.6751575386
H,3.1600537354,2.8983914703,-4.1213092443
H,2.5694039115,4.4770807088,-3.6058443394
H,1.4683758123,3.3418784115,-4.3631718724
C,-3.7973985411,4.2736217174,-2.1123344478
H,-4.6227624886,3.6643964166,-1.7401917886
H,-3.8756496261,4.3151706476,-3.2031033397
H,-3.9361321879,5.2884545459,-1.7285214156
C,3.0523815647,4.7221344563,-0.8770421382
H,2.4072116312,5.5718117308,-0.6367077702
H,3.6143213256,4.9749790644,-1.775863197
H,3.7745004105,4.6125810298,-0.0687673687
C,1.7943066898,-0.7129696016,4.531510737
H,2.611041269,-0.8745393643,5.2415950374
H,0.8641056207,-0.9630363464,5.05004296
H,1.7687487337,0.3537961597,4.291800989
C,-3.9812331139,-3.4090214144,1.7119717617

H,-4.5403931591,-3.2247930345,0.7914575767
H,-4.5354750187,-2.9573620709,2.5409756876
H,-3.9524765128,-4.4904522375,1.8751302038
C,5.1741004362,0.0650029882,-1.9569616387
H,4.9125716343,1.0753252716,-1.628425522
H,5.0746470583,0.0235351321,-3.0467140845
H,6.2334993321,-0.0929296955,-1.7352545496
C,-1.8124831798,-3.0126997673,2.9606430003
H,-1.7495259078,-4.0652221218,3.2505249281
H,-2.3365215363,-2.4869486026,3.7648405072
H,-0.7964011226,-2.6234557239,2.8925586816
C,2.0384861592,-3.067545605,3.6325386377
H,2.0317708853,-3.6850952589,2.7317515575
H,1.1958052815,-3.3720671287,4.261601683
H,2.9624314219,-3.2728345237,4.1826344357
H,6.4341145874,-0.4852740714,2.792537276
H,-0.4635047949,-6.4076673124,-0.4764866907
H,-2.2814190751,5.6789578453,2.5081971935
C,-0.5247264397,1.1270888983,-3.7429398102
H,-1.3544372391,1.1804893846,-3.0400375222
H,-0.4383060826,2.0859754397,-4.2596810209
H,-0.7676115888,0.368070535,-4.489965343
C,1.8871966834,0.3944058199,-4.0388358941
H,1.9591888949,1.1141268351,-4.8543503183
H,2.8560986536,0.3114756701,-3.5482740821
H,1.65757391,-0.5744873123,-4.4799904151
C,1.3385998106,4.2758539359,1.788199662
H,1.2251811455,4.26607204,2.8747220283
H,2.0471090868,5.0681238197,1.5435741734
H,0.3674016815,4.5162665312,1.3566186279
C,3.228755096,2.5520170892,1.8219436096
H,3.2476637025,2.5916818736,2.9137514675
H,3.5211191227,1.5471219293,1.5194858775
H,3.9761651213,3.2592518633,1.4561527862

Zero-point correction= 1.154508 (Hartree/Particle)
Thermal correction to Energy= 1.218475
Thermal correction to Enthalpy= 1.219420
Thermal correction to Gibbs Free Energy= 1.058303
Sum of electronic and zero-point Energies= -2804.612090
Sum of electronic and thermal Energies= -2804.548123
Sum of electronic and thermal Enthalpies= -2804.547178
Sum of electronic and thermal Free Energies= -2804.708295

Table S7. Cartesian coordinates and energy values for the **6-Dip**

P,1.448641555,-1.7132877679,-0.0183889727
Si,0.0503122529,-0.0642195561,0.2833619519
H,-0.0793330904,0.4997298597,1.6558910658
N,1.0910970029,1.6579932362,-1.9117872119
N,1.6916144791,2.4030345864,0.0187718198
C,-1.7740393361,-0.2050258177,-0.3393945334
C,-2.3311402588,-1.4203399808,-0.8312406084
C,0.8677790196,1.5062435281,-0.5811973398
C,-2.6502520616,0.9161448373,-0.2093772149
C,-4.4908256588,-0.3479453919,-1.1704141412
H,-5.525572012,-0.402746684,-1.4907206025
C,-1.6581988644,-2.7756093324,-0.8243887866
C,-1.1005075456,-3.3232562817,-2.0000803242
C,-1.7610869626,-3.5694127477,0.3437877151
C,-3.6656860186,-1.4570768685,-1.2624223547
H,-4.0617275081,-2.3938379204,-1.6366386621
C,-2.2367290553,3.3983112935,-1.8726333843
H,-2.1516192761,2.3648957915,-2.216990074
C,-3.9862260081,0.8194807958,-0.6172382513
H,-4.638085197,1.6727630205,-0.475692403
C,-2.081055236,3.3968357555,-0.3507991775
C,-2.2783451427,2.234615423,0.4357663526
C,-2.2720530623,2.337124045,1.8510711943
C,-1.2642478143,-4.8740329257,0.3208184527
H,-1.331565278,-5.4867215083,1.2123647869
C,2.9026703039,-0.9019558451,0.878015763
C,-1.0460966062,-2.5516000225,-3.3157671813
H,-1.2436204424,-1.5021436045,-3.0865949979
C,2.0764714192,2.6128115797,-2.1472281253
C,2.4537608936,3.0852588096,-0.9253966007
C,-1.7404659581,4.7005979259,1.6702056635
C,-0.6875141632,-5.4044134081,-0.8240229494
C,-1.988660868,3.5726782544,2.4408865722
H,-1.9807540905,3.6579970598,3.520834364
C,-0.6162307654,-4.6343389376,-1.9745390367
H,-0.1747708391,-5.058863744,-2.8684891322
C,-2.6781048488,1.1695078194,2.7507667762
H,-2.5209797647,0.2465612711,2.1919796323
C,-2.464171437,-3.079109584,1.6090729866
H,-2.5963437826,-1.9991783659,1.5248400352
C,-1.8013692901,4.6106107301,0.2871806544
H,-1.6436718059,5.5026468396,-0.3074779772
C,2.9901989564,-0.8701369149,2.294731233
C,4.0224235154,-0.4318311868,0.1444636891
C,-1.1649975007,4.2299602077,-2.6010449905
H,-1.3197459643,5.3028521559,-2.4560710342
H,-1.2189816189,4.0450774106,-3.6782787424
H,-0.1586105564,3.9901364323,-2.2579627515

C,4.108177585,-0.307662356,2.9205243858
H,4.1440220903,-0.2901716323,4.0069557206
C,0.3345360305,-2.6352227255,-3.9920761349
H,1.1310229804,-2.3894116693,-3.2860967039
H,0.3844168912,-1.9484963601,-4.8437579327
H,0.5309381569,-3.6383735901,-4.3805016814
C,-4.18240791,1.2556497438,3.0835093944
H,-4.4052434567,2.1700989383,3.641978771
H,-4.4879858653,0.4022960347,3.6964527711
H,-4.793084076,1.2561973361,2.1783553629
C,5.1848701927,0.2058176606,2.1995248331
C,5.1235121584,0.1188779863,0.8091468123
H,5.9655375114,0.475055979,0.220509583
C,-1.8551514494,1.0621992723,4.0452711668
H,-0.7829922907,1.0407363746,3.8387979073
H,-2.112100365,0.1390078336,4.5717632246
H,-2.0554685125,1.8899000569,4.7317146873
C,-2.1457287737,-3.0221938709,-4.2889060591
H,-2.0156988478,-4.0793986307,-4.5382766194
H,-2.1081387555,-2.4497830622,-5.2217017581
H,-3.1423231293,-2.9011477528,-3.8590561429
C,2.55538242,2.9708018751,-3.5131530129
H,2.9834716619,2.1075765414,-4.0313222135
H,3.331035146,3.7337930001,-3.4489287718
H,1.7501237371,3.3720621755,-4.1363614878
C,-3.6314473422,3.9129208051,-2.2888184513
H,-4.4352205173,3.3098382103,-1.8664058767
H,-3.735634109,3.8953643238,-3.3782472056
H,-3.7753236265,4.9443406739,-1.9534222566
C,3.4685561009,4.1118259142,-0.5523176911
H,3.0129289768,4.9797271634,-0.0650197355
H,3.9882134987,4.4680981062,-1.4416728067
H,4.2177624885,3.6988649868,0.1288168946
C,-3.870417917,-3.7002678357,1.7278359445
H,-4.4835990701,-3.4700957544,0.8533087927
H,-4.3870451381,-3.3178784225,2.6140459887
H,-3.8098249813,-4.7891535955,1.8168236886
C,-1.6498374783,-3.3332234488,2.8886745879
H,-1.5575130475,-4.4005374085,3.1088719654
H,-2.1441850025,-2.8679725013,3.7473629811
H,-0.6450565639,-2.918604174,2.8007915123
H,-0.3011503384,-6.4179653355,-0.8210868564
H,-1.525393297,5.6510984203,2.1469732453
C,1.9189609959,-1.4707605089,3.1726399153
H,0.9754873807,-0.9227793807,3.1097060399
H,1.7024815061,-2.4943861664,2.8584254233
H,2.2368435299,-1.4794545754,4.2185835467
C,4.0893243067,-0.535778271,-1.3626109657
H,5.0383190056,-0.1392689954,-1.7342956999
H,3.9969608645,-1.5753155481,-1.6873297343

H,3.2724284963,0.0058364495,-1.8429601792
C,6.4006276285,0.768080489,2.8979011051
H,7.1381706052,-0.0164486326,3.1024637926
H,6.8977099067,1.5275215207,2.2882231633
H,6.1379933394,1.2223996329,3.8569981212
C,0.4901622071,0.8123527806,-2.9350129142
H,0.9718108827,-0.1673596121,-2.9248313069
H,-0.5702114247,0.6863140249,-2.7280776308
H,0.6070381698,1.282818717,-3.9088122014
C,1.8304392831,2.613423089,1.460422212
H,2.6968245386,2.0673682643,1.8380117788
H,1.9431088102,3.6793449648,1.6551879302
H,0.9328873933,2.2617919302,1.9571095647

Zero-point correction= 0.954804 (Hartree/Particle)
Thermal correction to Energy= 1.010660
Thermal correction to Enthalpy= 1.011604
Thermal correction to Gibbs Free Energy= 0.863571
Sum of electronic and zero-point Energies= -2529.571899
Sum of electronic and thermal Energies= -2529.516043
Sum of electronic and thermal Enthalpies= -2529.515099
Sum of electronic and thermal Free Energies= -2529.663132

Table S8 Cartesian coordinates and energy values for the **7-Dip**

P,13.3359661029,9.5293205884,8.8991250436
Si,12.1176168318,8.6770238806,7.2968628298
H,10.8139827762,9.3315682704,6.9898617018
N,14.2571758461,8.6395018324,5.2297262913
N,12.7539851214,10.1039527373,4.7481304207
C,11.6921632157,6.7889477075,7.3346472354
C,12.00295453,5.9499446679,8.4435570063
C,13.0286853877,9.0822382208,5.5972692612
C,10.9326296403,6.2140818072,6.2705487476
C,10.9358353274,4.0442347531,7.365429397
H,10.6489197818,2.9983968728,7.3783024895
C,12.6133660998,6.3869599352,9.7572543099
C,13.9722723503,6.1304262552,10.045168488
C,11.7586214896,6.8812021019,10.7713798724
C,11.6376608052,4.5952643126,8.4247892802
H,11.8858183394,3.9827376713,9.2835053305
C,12.165279695,5.9116102195,3.5385927227
H,12.654113534,5.7182932473,4.496610007
C,10.5671322353,4.8630101994,6.3092298933
H,9.9648919187,4.4624352939,5.5030108866
C,10.9755426793,6.8367844992,3.8012372726
C,10.3876346235,6.9772548127,5.0825476184
C,9.183272131,7.7133869616,5.2251591239
C,12.2891857337,7.1404082811,12.0369648352
H,11.6440991116,7.5270260763,12.8171183671
C,13.411937828,11.3046715948,8.2178161312
C,14.925432998,5.5246697254,9.017752824
H,14.441669778,5.5956165122,8.0406577964
C,14.7573129106,9.3782615684,4.1625998278
C,13.8085954239,10.3114316621,3.864178788
C,9.258874977,8.2777986763,2.8640718002
C,13.6285863556,6.9115841587,12.3157924433
C,8.6495488148,8.3644407927,4.1089604722
H,7.7312439948,8.930423553,4.2100376669
C,14.4578699331,6.4049613263,11.3264943092
H,15.5011882186,6.2202300929,11.5541853775
C,8.3864117366,7.7129704228,6.5297223487
H,9.070829435,7.4591318257,7.3398810834
C,10.2587410965,7.0744662039,10.5544665397
H,10.0702116332,7.0568577847,9.4796958791
C,10.4023564413,7.5063111395,2.7138413909
H,10.847573422,7.4080317812,1.7307385052
C,12.3104415663,12.2032918556,8.3120602921
C,14.6504658761,11.8169958919,7.7297214916
C,11.5451901057,10.9281939096,4.7499314096
H,10.7673444338,10.4111249282,5.3000346088
H,11.2101138447,11.0735497124,3.7236451113
H,11.7488974218,11.8911368999,5.2213499103

C,13.2125717317,6.5117184519,2.5832354069
H,12.8411333897,6.5579688889,1.5555985829
H,14.1083170034,5.8832424736,2.5684639617
H,13.5018354645,7.5207570251,2.8768601117
C,15.9253367074,10.9758775875,7.7554169628
H,15.6108764747,9.935820527,7.6354919328
C,14.9607309013,7.5529425346,5.8999563712
H,14.7894532707,7.65171652,6.9725191166
H,16.0273822611,7.6393059887,5.7054406059
H,14.6049480899,6.5830976988,5.5494977668
C,12.4384731534,13.517727013,7.8469740986
H,11.5941467715,14.1942012349,7.9199150708
C,11.0084811217,11.8216557502,9.0141017469
H,10.9441180222,10.7336283475,9.0045606727
C,16.2650958069,6.2807141306,8.9381842354
H,16.1061223563,7.3563624837,8.8371735
H,16.8534607002,5.924967916,8.0856532113
H,16.8712894506,6.1178664062,9.8334916051
C,7.3013178153,6.6165594117,6.4833843587
H,6.5815766728,6.8164654571,5.6836958558
H,6.7538876037,6.5803042552,7.430074696
H,7.7350474179,5.6302722166,6.3068025723
C,13.633440779,13.9870313608,7.3199955113
C,14.7339584383,13.141117403,7.2848616317
H,15.6772403366,13.5241757603,6.9130072212
C,7.7523547461,9.0695398263,6.8769144597
H,8.4946686151,9.869629336,6.8870317833
H,7.2996972098,9.0232293662,7.8712550473
H,6.9588630053,9.3449179508,6.1760877882
C,15.176652993,4.0284748508,9.2925574768
H,15.6378631747,3.8856223023,10.2742063253
H,15.8499458376,3.6048442395,8.5399902504
H,14.2476159431,3.4550654711,9.2738311058
C,16.603541283,11.0755262914,9.1362833946
H,16.9006071318,12.1078752365,9.3477486045
H,17.5013834954,10.448948878,9.1744020988
H,15.9271220467,10.7443296527,9.9261237184
C,16.0809301458,9.1067887021,3.5316602631
H,16.9059923623,9.2606916642,4.2328189341
H,16.237616646,9.7799395753,2.6888078317
H,16.1453895896,8.0823086916,3.1533785308
C,11.6964352229,4.5539150703,2.9731310825
H,11.0137367788,4.0410143629,3.6506457222
H,12.5537505989,3.8962919874,2.798625205
H,11.1795555688,4.6945947387,2.0191198801
C,13.7959057253,11.388610378,2.8335945198
H,12.9849920644,11.2531033141,2.1111682382
H,14.7346514181,11.3909688337,2.2800044365
H,13.6766947397,12.3751640472,3.2904929273
C,9.7392416497,12.3768948363,8.3482425352

H,9.6600250085,13.4645139639,8.4409921273
H,8.8513165999,11.9507247238,8.8244225462
H,9.6992401682,12.1300064859,7.2835845682
C,9.4611451501,5.9097427624,11.1741434993
H,9.7653920858,4.9489792675,10.7521621097
H,8.3891844564,6.0363901512,10.9914253871
H,9.6157769767,5.8651768197,12.2563561596
C,16.9351620066,11.3092724368,6.646119561
H,16.4626549808,11.3234817782,5.6601225311
H,17.7353664997,10.5618549853,6.6348091699
H,17.4150291228,12.2807515594,6.7990746607
C,9.7461684122,8.4251788166,11.0822245991
H,9.7642106196,8.4682551291,12.1750642195
H,8.7088627441,8.5822628676,10.7702071172
H,10.3546610132,9.2467944448,10.7015614142
C,11.0744522368,12.252605024,10.4927243499
H,11.9272739791,11.7866729103,10.9909026374
H,10.1645862175,11.95647459,11.025132147
H,11.1795486642,13.3389126564,10.5787651789
H,13.7153417682,15.0104374224,6.96817326
H,14.0241334656,7.1230073971,13.3034394021
H,8.8269109183,8.7864185375,2.0085774782

Zero-point correction= 1.039837 (Hartree/Particle)
Thermal correction to Energy= 1.099380
Thermal correction to Enthalpy= 1.100324
Thermal correction to Gibbs Free Energy= 0.944621
Sum of electronic and zero-point Energies= -2647.447193
Sum of electronic and thermal Energies= -2647.387650
Sum of electronic and thermal Enthalpies= -2647.386705
Sum of electronic and thermal Free Energies= -2647.542409

Table S9 Cartesian coordinates and energy values for the **7-Dip'**

P,-2.3638384402,0.0779270849,0.1166680607
Si,-0.3716876382,0.5755967004,0.5553155254
H,0.4372605093,-0.3116739884,1.4163979222
C,0.6117032083,2.0662858367,-0.0415097092
C,-0.0104593948,3.2158272591,-0.5983939037
C,2.0282654829,2.0556118177,0.0928986871
C,2.1534212392,4.2946129243,-0.8325620249
H,2.7438391374,5.1527477491,-1.1343750213
C,-1.4962094573,3.3456369184,-0.7995895814
C,-2.0731911347,2.9656935161,-2.0330100559
C,-2.2869339842,3.9464578469,0.2068781855
C,0.772033863,4.3087008182,-0.9830226064
H,0.2812687633,5.1795233044,-1.4022681272
C,2.9508206261,-0.0428343873,-1.7873077541
H,2.2641205677,0.7894056418,-1.9533805813
C,2.7731450035,3.1714129358,-0.3004012694
H,3.8514056005,3.1440858789,-0.1919488743
C,3.2387333759,-0.1214997286,-0.2889329461
C,2.8026396408,0.8735022353,0.6144272936
C,3.1474729551,0.7999883032,1.982548689
C,-3.649435476,4.13886539,-0.0347554005
H,-4.2683344888,4.5986009893,0.7272072057
C,-2.4783724927,-1.5318327177,1.0911931449
C,-1.2404908333,2.3831392579,-3.1738084221
H,-0.2793606416,2.0701501172,-2.7597681411
C,4.3258528163,-1.2767348749,1.5480432007
C,-4.224878557,3.7588526192,-1.2397308584
C,3.9087043718,-0.2847431259,2.4261466309
H,4.1787907874,-0.3557336224,3.4735696639
C,-3.4400422785,3.1821014471,-2.2282783012
H,-3.8976046183,2.8949107225,-3.1676305563
C,2.7324282769,1.8769242282,2.9828744981
H,2.0344807136,2.5493158222,2.479151505
C,-1.6881460369,4.4384747552,1.5236047468
H,-0.6753143074,4.0372864138,1.6018735911
C,3.994744495,-1.1902578747,0.2026768377
H,4.3350822217,-1.9623723866,-0.4781145063
C,-3.0171635169,-1.5151237501,2.4017105153
C,-2.1774219073,-2.7740578768,0.4738662419
C,2.2643055374,-1.3099128159,-2.3256089533
H,2.9104784821,-2.1885810012,-2.2458825346
H,2.0105718602,-1.1832546853,-3.3822060923
H,1.3424171558,-1.5244513095,-1.7806357755
C,-1.7259361449,-2.882032064,-0.9812240238
H,-1.3508371106,-1.9019911806,-1.2819126737
C,-3.1739613864,-2.7229009052,3.08987263
H,-3.5659385127,-2.7127348843,4.1010419302
C,-3.4498019759,-0.2304552364,3.1044824694

H,-3.367472895,0.5838474625,2.3802237
C,-1.8828285729,1.1415197497,-3.8171881397
H,-2.1281478911,0.3894068379,-3.0647894485
H,-1.1932916542,0.6949681377,-4.5398477817
H,-2.8006279755,1.3913752191,-4.3571429098
C,3.9424358859,2.7252151099,3.4198367807
H,4.6862762776,2.1142286923,3.9398332569
H,3.6278448863,3.5224205244,4.100139991
H,4.4337421041,3.1881356825,2.5605000349
C,-2.845240486,-3.934850441,2.5021036019
C,-2.3655560269,-3.9540792605,1.1995995788
H,-2.1353201073,-4.9068610239,0.7373540201
C,2.0017334217,1.297490973,4.207774083
H,1.1358129995,0.7011641756,3.9112055733
H,1.6509928084,2.1054453135,4.8565185992
H,2.6564659111,0.6579493693,4.8062241621
C,-0.9499638403,3.456856052,-4.2417198467
H,-1.8789166888,3.8196070756,-4.6917413182
H,-0.3256692007,3.0462765943,-5.0413979241
H,-0.4286667862,4.3164263705,-3.8138144936
C,-2.9258967247,-3.2062233727,-1.8926101967
H,-3.3599811349,-4.1774811922,-1.6360866907
H,-2.6167058399,-3.2393163139,-2.9420568299
H,-3.7102109653,-2.451769826,-1.7936656068
C,4.2352417508,0.2652343483,-2.5813299211
H,4.6984231042,1.1950608963,-2.2418415011
H,4.0118751268,0.3675286916,-3.6475793361
H,4.9722374529,-0.5352943405,-2.4681129761
C,-2.5249197935,0.1096501285,4.2857642813
H,-2.543447846,-0.6780096984,5.0448822616
H,-2.8351912196,1.0433100322,4.7645204548
H,-1.4888762084,0.2247960545,3.9561989933
C,-1.5711740062,5.9753132316,1.5351633467
H,-0.9645697001,6.3345935655,0.7005082649
H,-1.1066870877,6.319146397,2.46450969
H,-2.5567188458,6.4440059014,1.457671316
C,-0.5836893423,-3.888323688,-1.198470351
H,0.2609300274,-3.6832973683,-0.5358349589
H,-0.2270034399,-3.8326062317,-2.2310106516
H,-0.9040524259,-4.91928262,-1.0241811622
C,-2.466979648,3.9458372352,2.7557906067
H,-3.4727553976,4.3727809206,2.7986892832
H,-1.9479308515,4.24075501,3.6726541119
H,-2.5638653281,2.8586333858,2.7537898112
C,-4.9235778722,-0.2789061249,3.5465607564
H,-5.5802049553,-0.4905202296,2.6990547039
H,-5.2210617044,0.6829639292,3.9750672911
H,-5.0989922447,-1.0463331737,4.3057575374
H,-2.9739734534,-4.8618871429,3.0503625948
H,-5.2846845213,3.9149942452,-1.4093991267

H,4.9126095684,-2.1133863825,1.9113240028

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