Supplementary information for

Norbornene Based-Sulfide-Stabilized Silylium Ions: Synthesis, Structure and Application in Catalysis.

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Selected spectroscopic data

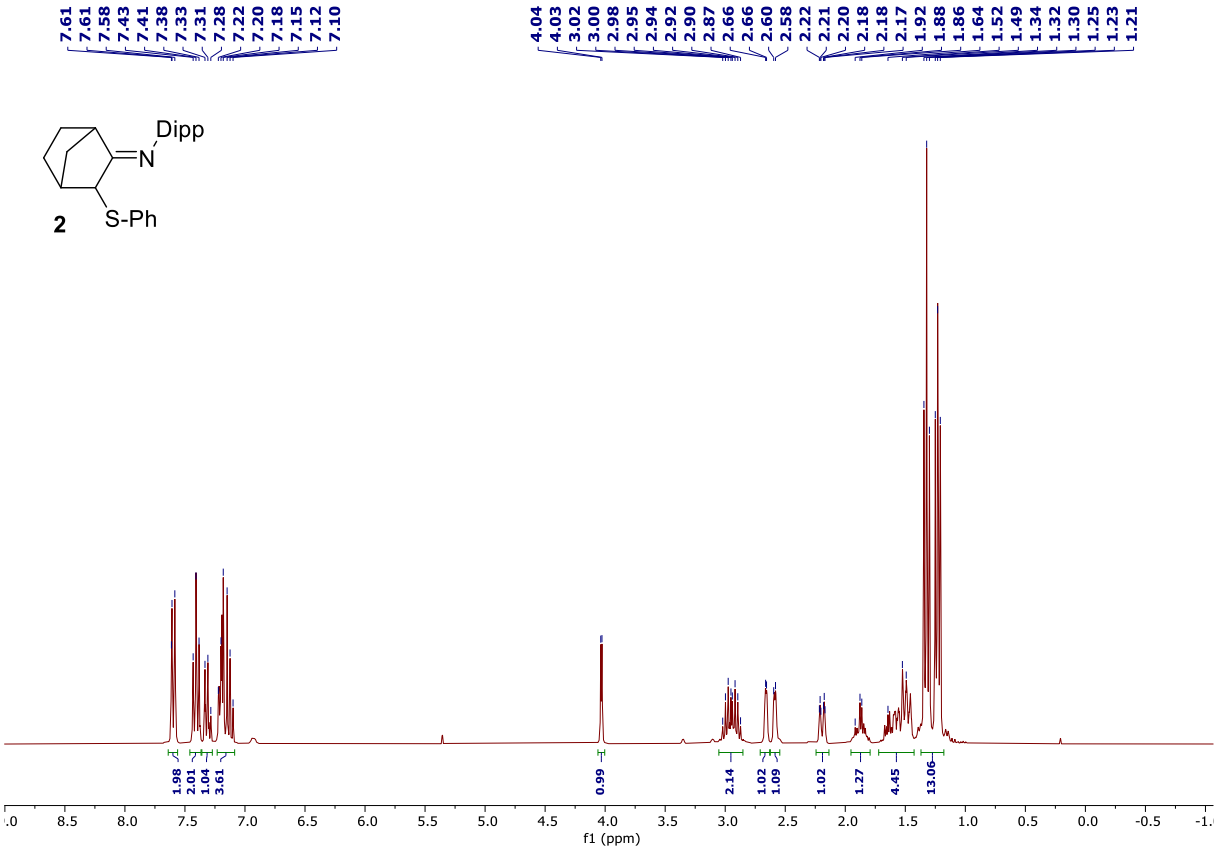


Figure S1: ^{1}H NMR (300 MHz, CD_2Cl_2)

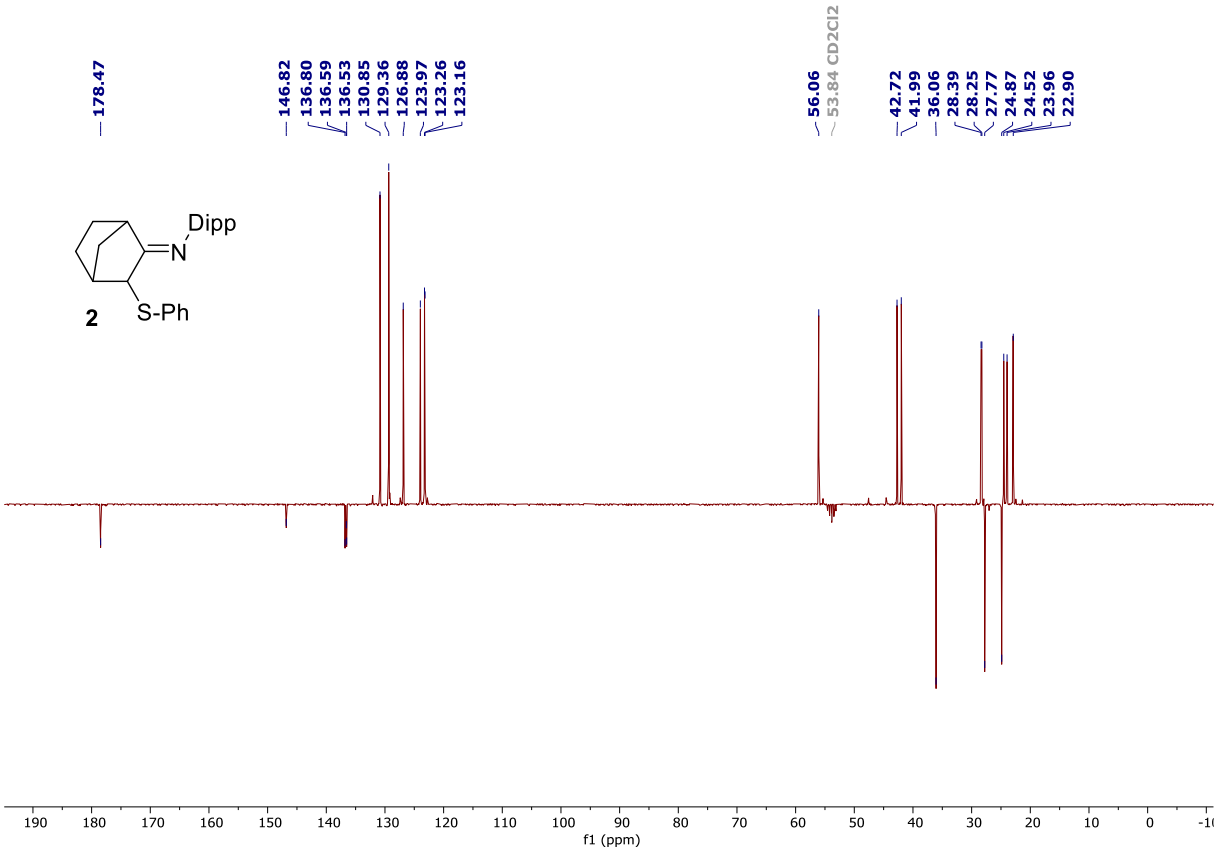


Figure S2: $^{13}C\{^{1}H\}$ NMR (75 MHz, CD_2Cl_2)

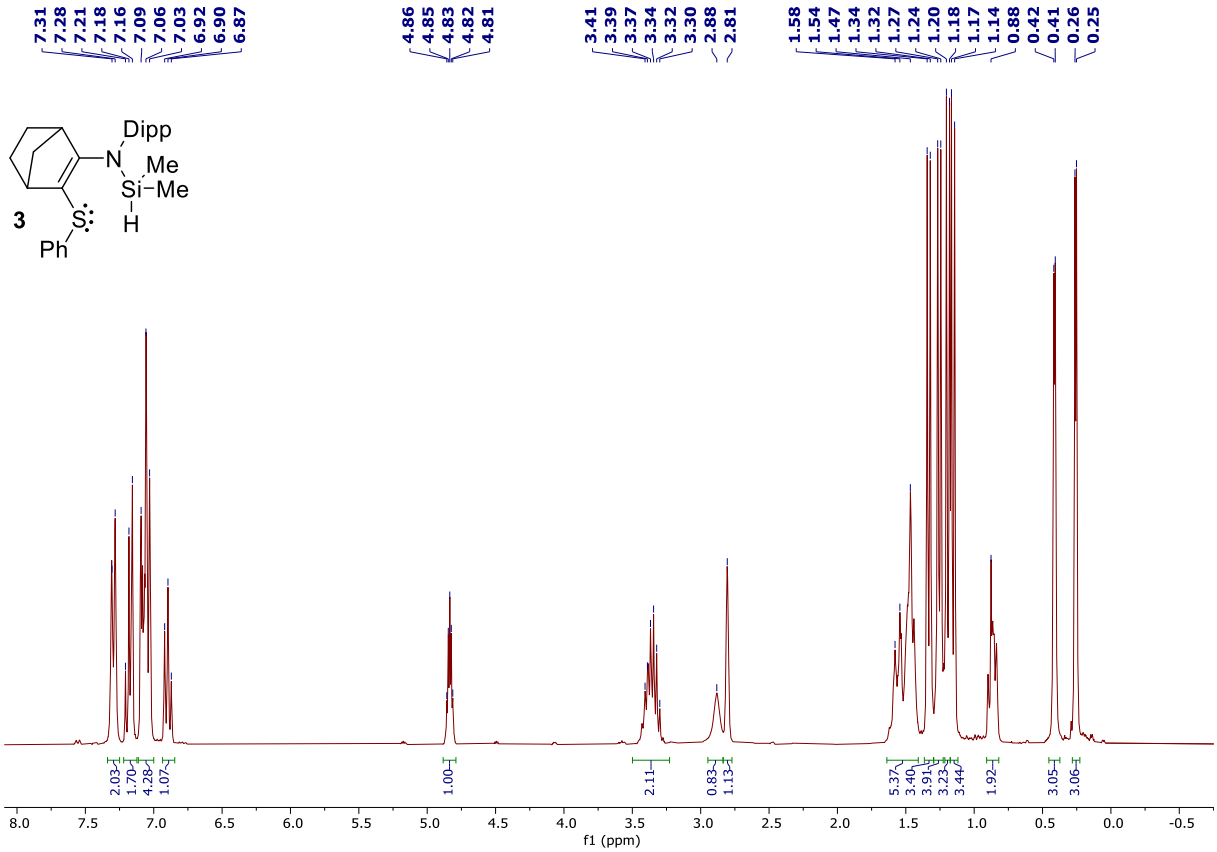


Figure S3: ^{1}H NMR (300 MHz, C_6D_6)

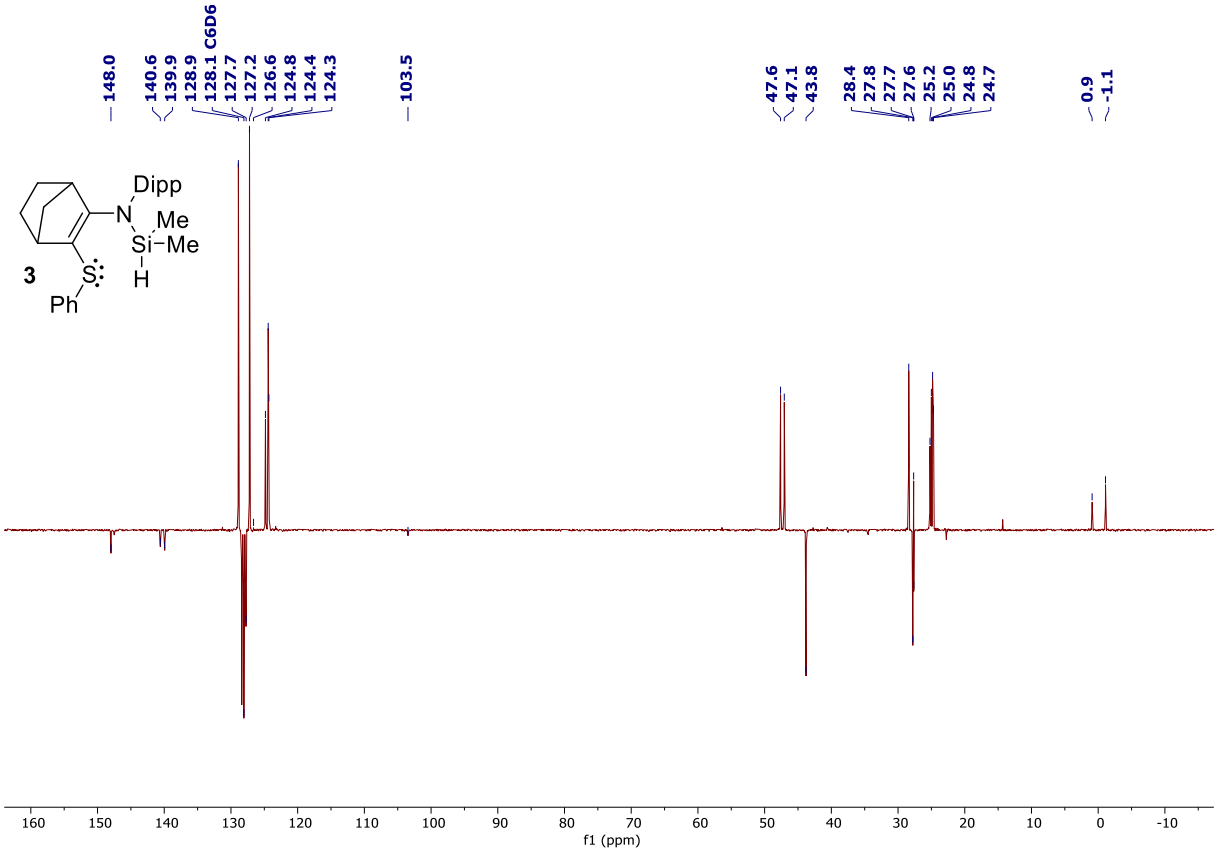


Figure S4: ^{13}C{^{1}H} NMR (75 MHz, C_6D_6)

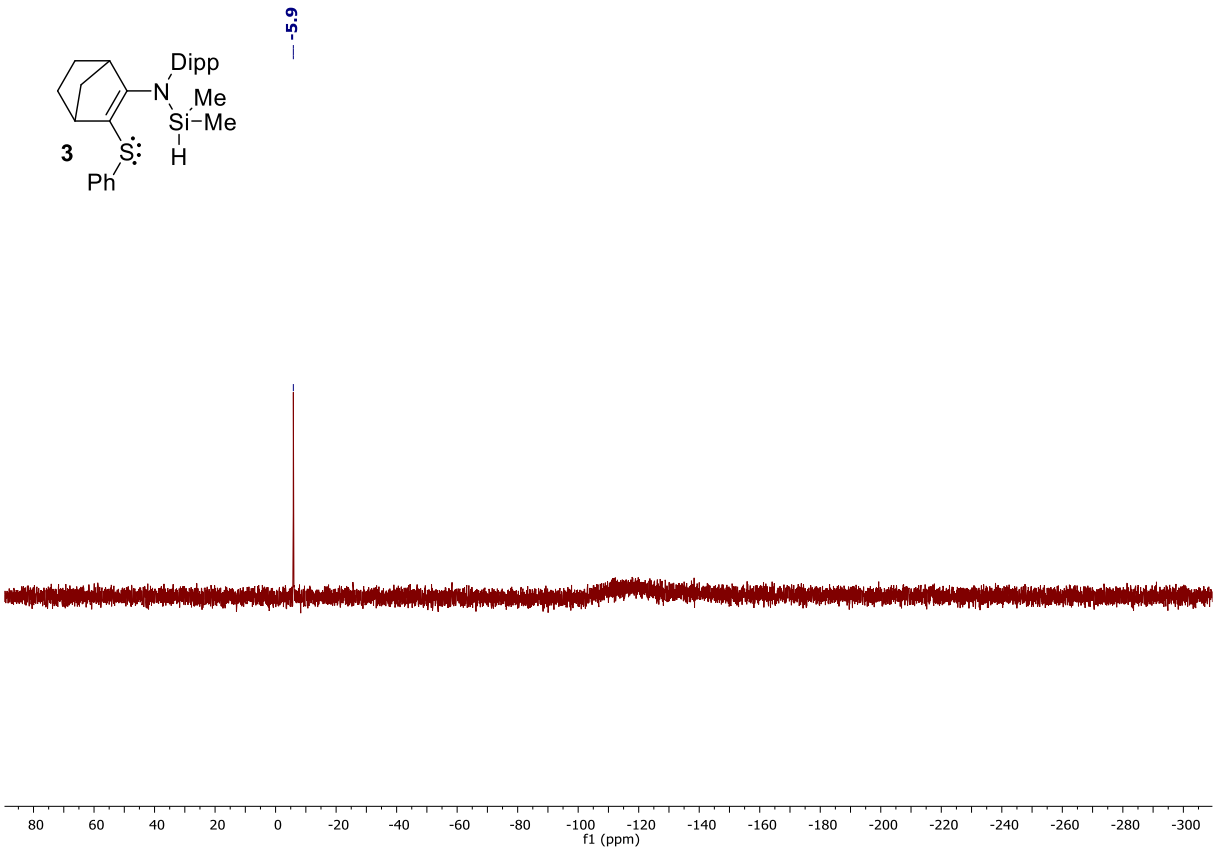


Figure S5: $^{29}Si\{^{1}H\}$ NMR (60 MHz, C_6D_6)

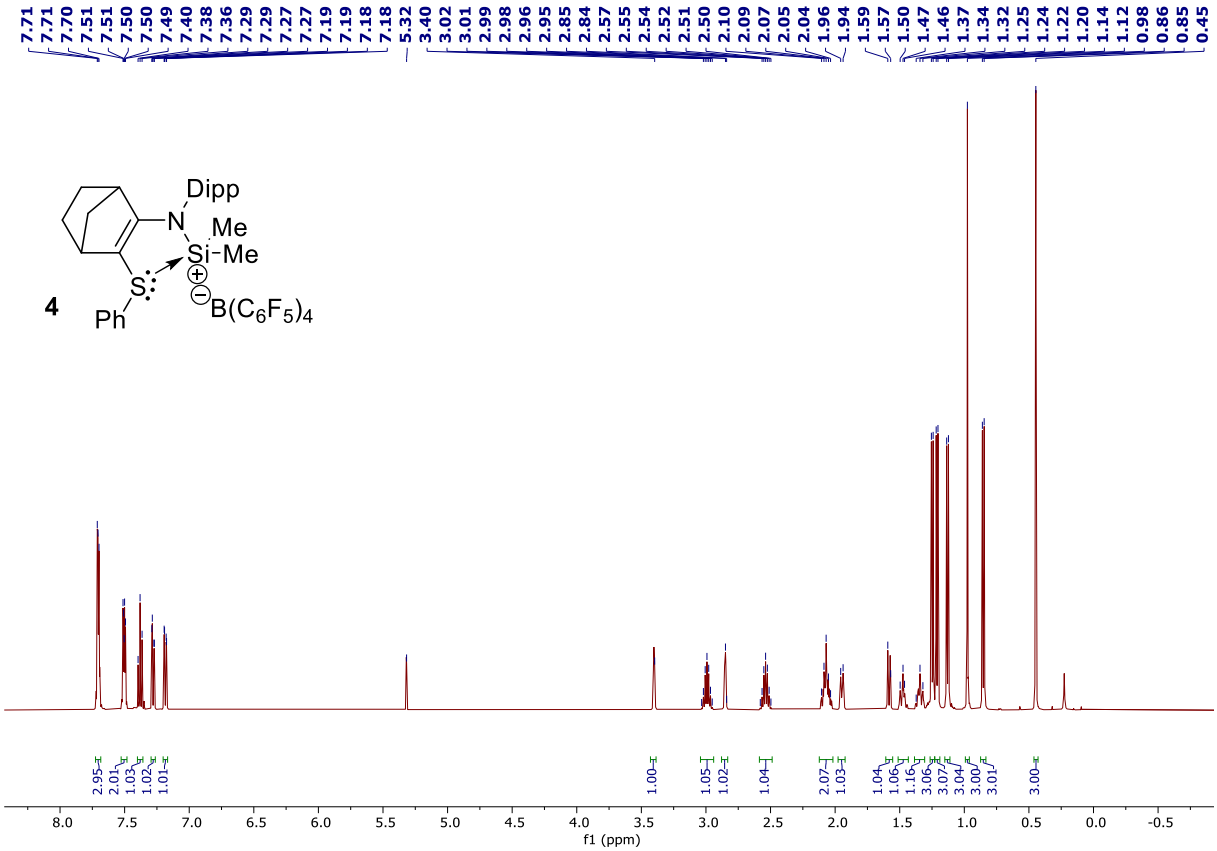


Figure S6: ^{1}H NMR (500 MHz, CD_2Cl_2)

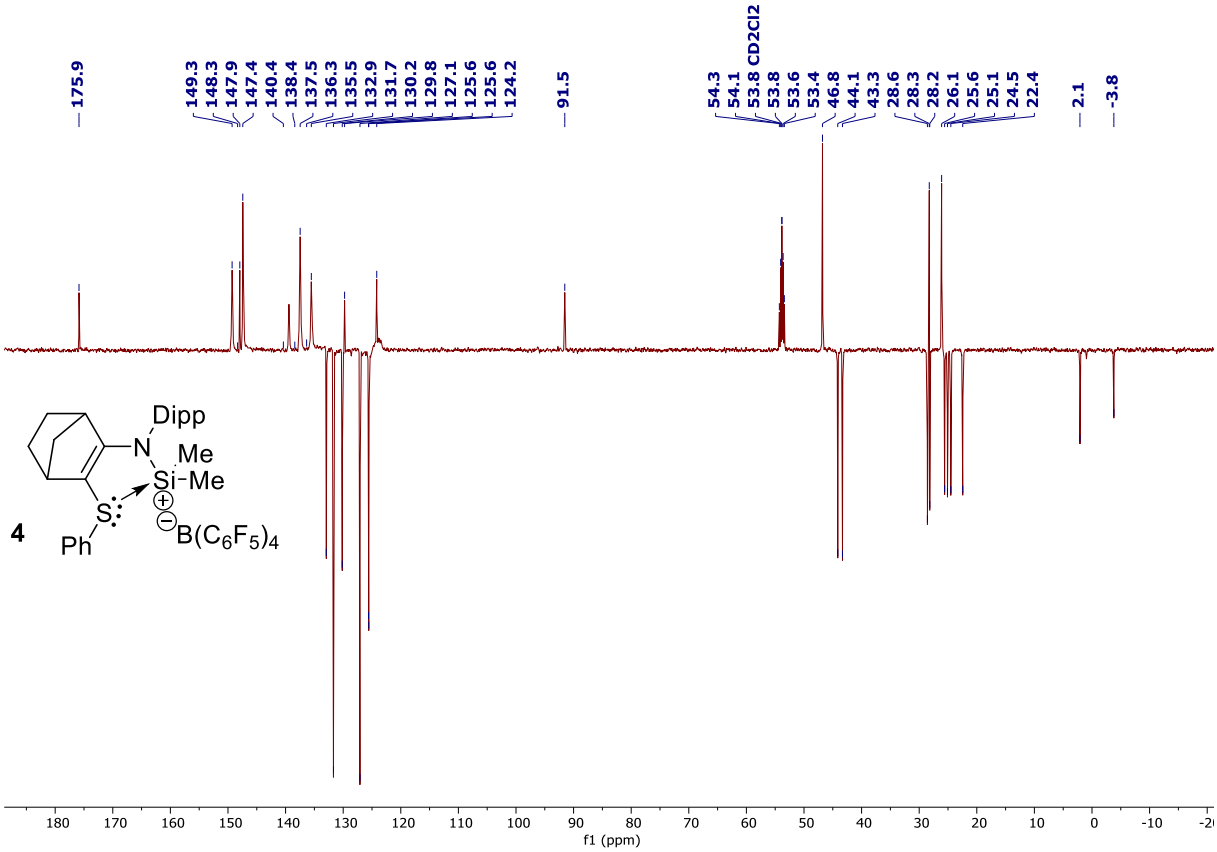


Figure S7: $^{13}C\{^{1}H\}$ NMR (126 MHz, CD_2Cl_2)

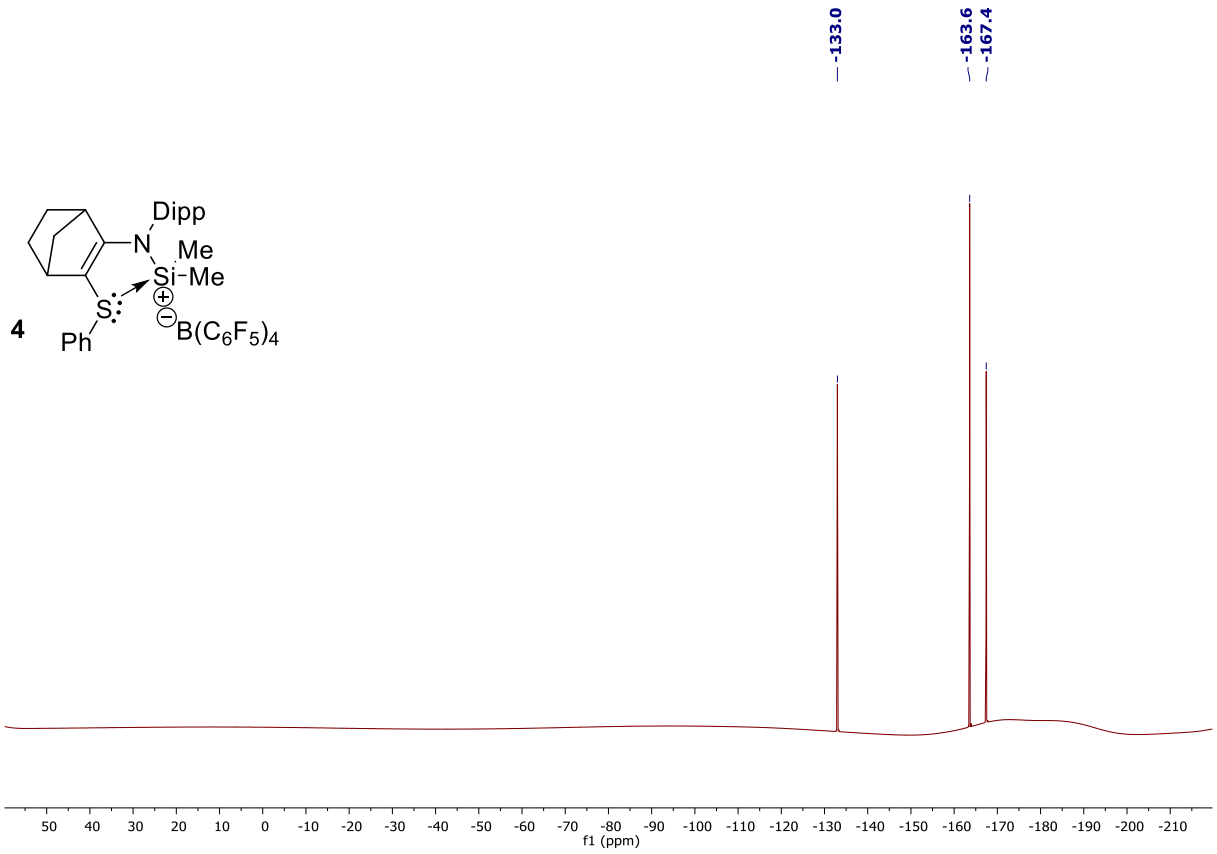


Figure S8: ^{19}F NMR (471 MHz, CD_2Cl_2)

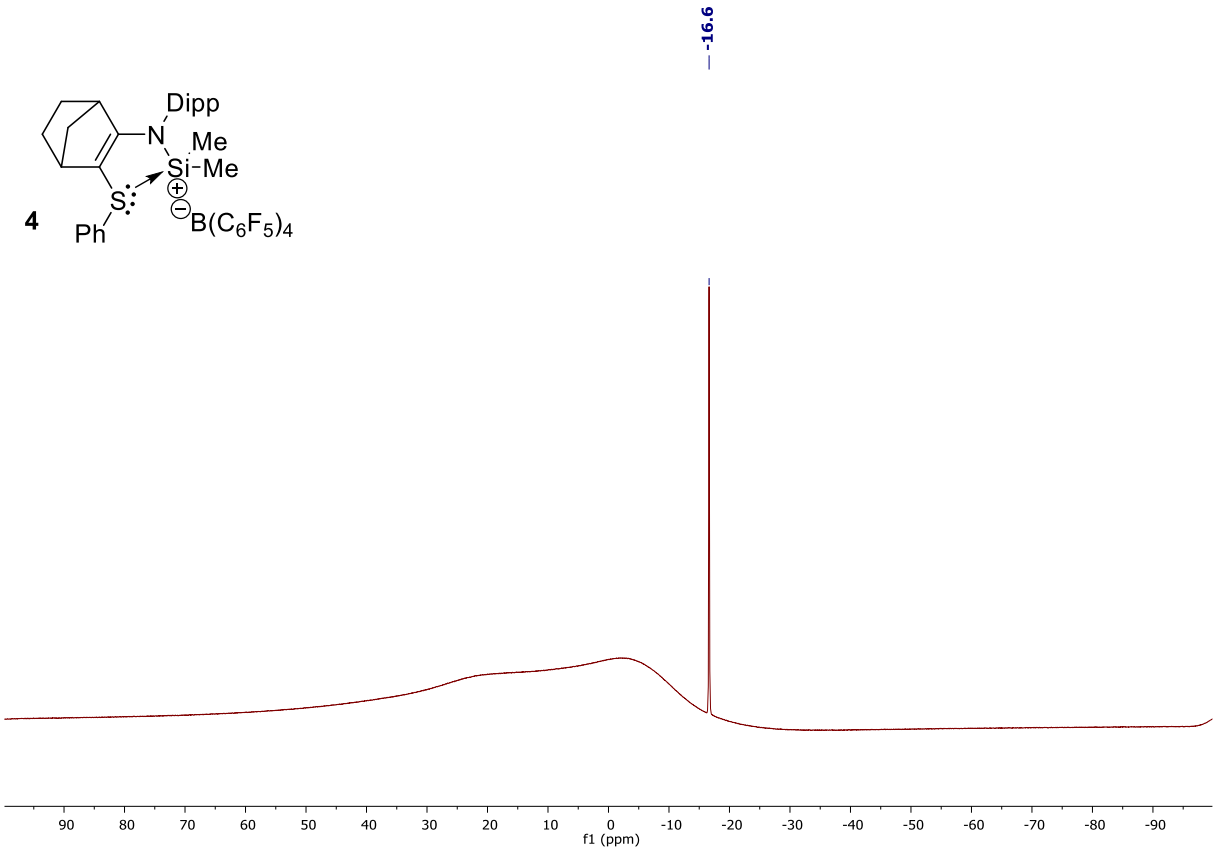


Figure S9: ^{11}B NMR (160 MHz, CD_2Cl_2)

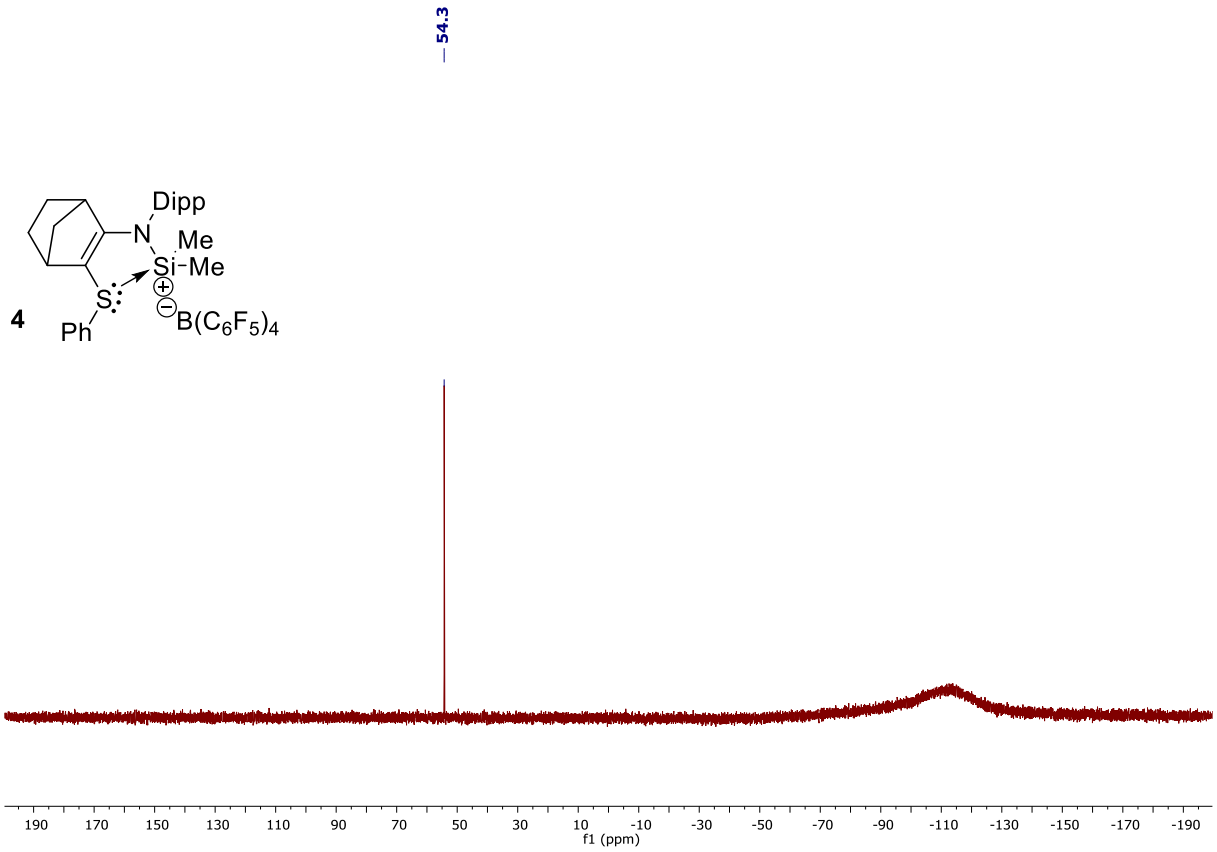
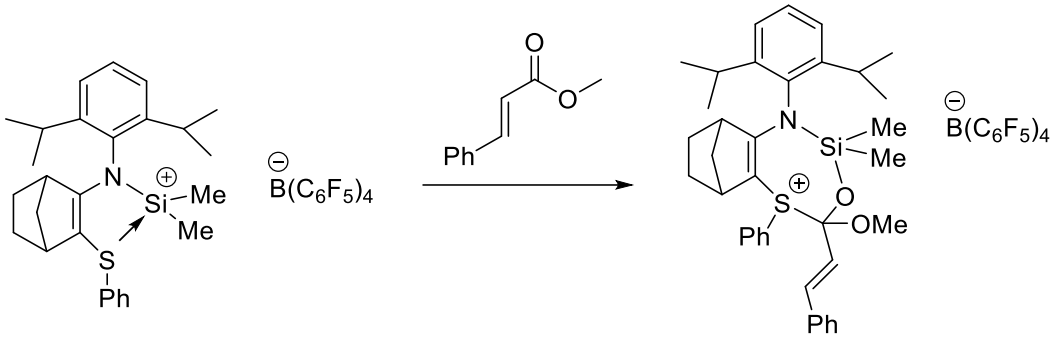


Figure S10: ^{29}Si{^{1}H} NMR (99 MHz, CD_2Cl_2)

1,2-Insertion reactions of 4 into C=O group



To a solution of **4** (50.0 mg, 0.045 mmol) in dichloromethane (0.3 mL) was added (E)-Methyl cinnamate (7.3 mg, 0.045 mmol) at room temperature. After 5 minutes, all volatiles were eliminated under vacuum. The resulting solid was washed with pentane (3 x 0.4 mL) and dried under vacuum for 2h. 1,2-insertion product was obtained as red solid (38 mg, 66 %).

^{1}H NMR (400 MHz, CD_2Cl_2): δ = 7.62-7.54 (m, 1H, C*H*$_{dipp}$), 7.47-7.42 (m, 2H, C*H*$_{dipp}$), 7.42-7.36 (m, 3H, S-C$_6$*H*$_5$), 7.30-7.20 (m, 2H, C$_6$*H*$_5$), 7.14-7.08 (m, 2H, C$_6$*H*$_5$), 7.06-7.01 (m, 2H, S-C$_6$*H*$_5$), 6.94-6.88 (m, 1H, C$_6$*H*$_5$), 6.65 (d, $^{3}J_{H\text{-}H}$ = 16.0 Hz, 1H, PhC*H*), 5.62 (d, $^{3}J_{H\text{-}H}$ = 16.0 Hz, 1H, PhCH=C*H*), 3.36 (m, 1H, C*H*$_{bridgehead}$), 3.30 (s, 3H, OC*H*$_3$), 3.13-3.10 (m, 1H, C*H*$_{bridgehead}$), 2.96-2.90 (m, 2H, C*H*$_{iPr}$ overlapped by 1H C*H*$_2$), 2.80 (sept., $^{3}J_{H\text{-}H}$ = 6.5 Hz, 1H, C*H*$_{iPr}$), 2.76-2.68 (m, 1H, C*H*$_2$), 2.24-2.10 (m, 3H, 2 C*H*$_2$), 2.03-1.92 (m, 1H, C*H*$_2$), 1.41 (d, $^{3}J_{H\text{-}H}$ = 6.7 Hz, 3H, C*H*$_{3iPr}$), 1.39 (d, $^{3}J_{H\text{-}H}$ = 6.5 Hz, 3H, C*H*$_{3iPr}$), 1.26 (d, $^{3}J_{H\text{-}H}$ = 6.7 Hz, 3H, C*H*$_{3iPr}$), 1.22 (d, $^{3}J_{H\text{-}H}$ = 6.5 Hz, 3H, C*H*$_{3iPr}$), 1.17 (s, 3H, Si-C*H*$_3$), 0.50 (s, 3H, Si-C*H*$_3$).

^{13}C NMR (101 MHz, CD_2Cl_2): δ = 213.8 (s, N-*C*), 148.6 (d, $^{1}J_{CF}$ = 240.0 Hz, *C*$_{Ar}$-F), 143.8 (s, *C*$_{dipp}$), 143.2 (s, *C*$_{dipp}$), 138.8 (br d, $J_{C\text{-}F}$ = 246.0 Hz, Ar*C*-F), 137.9 (s, Ph*C*H), 136.6 (br d, $J_{C\text{-}F}$ = 245.5 Hz, Ar*C*-F), 134.7 (s, *i* of *C*$_6$H$_5$), 132.7 (s, N-*C*$_{dipp}$), 132.5 (s, S-*C*$_6$H$_5$), 132.1 (s, *C*H$_{dipp}$), 130.3 (s, S-*C*$_6$H$_5$), 129.6 (s, *i* of S-*C*$_6$H$_5$), 129.5 (s, S-*C*$_6$H$_5$), 129.5 (s, *C*$_6$H$_5$), 128.7 (s, *C*$_6$H$_5$), 127.5 (s, *C*$_6$H$_5$), 127.2 (s, *C*H$_{dipp}$), 127.0 (s, *C*H$_{dipp}$), 121.2 (s, PhCH=*C*H), 107.1 (s, *C*-O), 70.9 (s, *C*-S), 50.9 (s, OCH$_3$), 47.3 (s, *C*H$_{bridgehead}$), 44.2 (s, *C*H$_{bridgehead}$), 40.6 (s, *C*H$_2$), 29.7 (s, *C*H$_2$), 28.7 (s, *C*H$_{iPr}$), 28.3 (s, *C*H$_{iPr}$), 26.2 (s, *C*H$_{3iPr}$), 26.0 (s, *C*H$_{3iPr}$), 25.4 (s, *C*H$_2$), 24.4 (s, *C*H$_{3iPr}$), 24.2 (s, *C*H$_{3iPr}$), 2.3 (s, Si-*C*H$_3$), 0.14 (s, Si-*C*H$_3$).

^{19}F NMR (471 MHz, CD_2Cl_2): δ = -133.1 (br, o of ArC-*F*), -163.7 (t, $J_{F\text{-}F}$ = 20.4 Hz, *p* of ArC-*F*), -167.6 (t, $J_{F\text{-}F}$ = 18.1 Hz, *m* of ArC-*F*).

^{11}B NMR (160 MHz, CD_2Cl_2): δ = -16.7 (s, *B*Ar).

^{29}Si NMR (99 MHz, CD_2Cl_2): δ = 11.0 (s, *Si*Me$_2$).

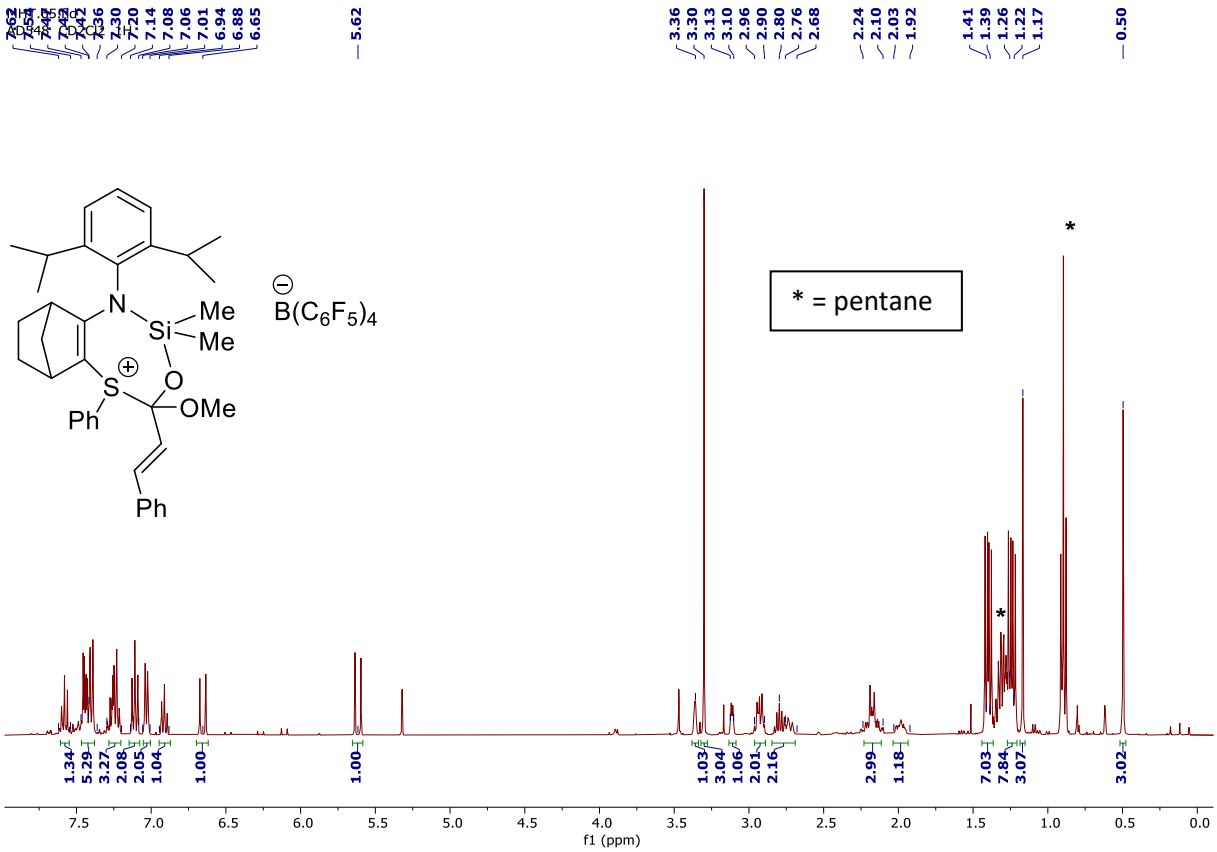


Figure S11: ^{1}H NMR (400 MHz, CD_2Cl_2)

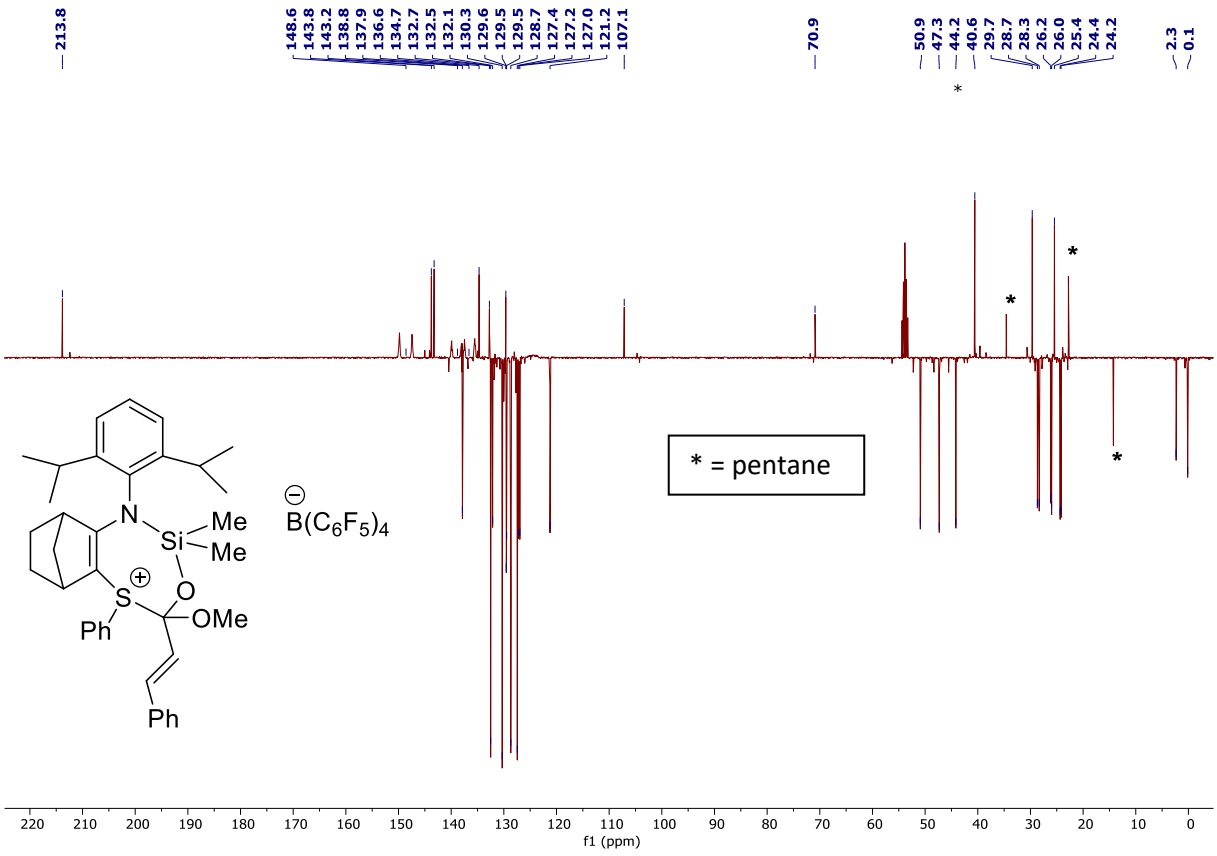


Figure S12: ^{13}C{^{1}H} NMR (101 MHz, CD_2Cl_2)

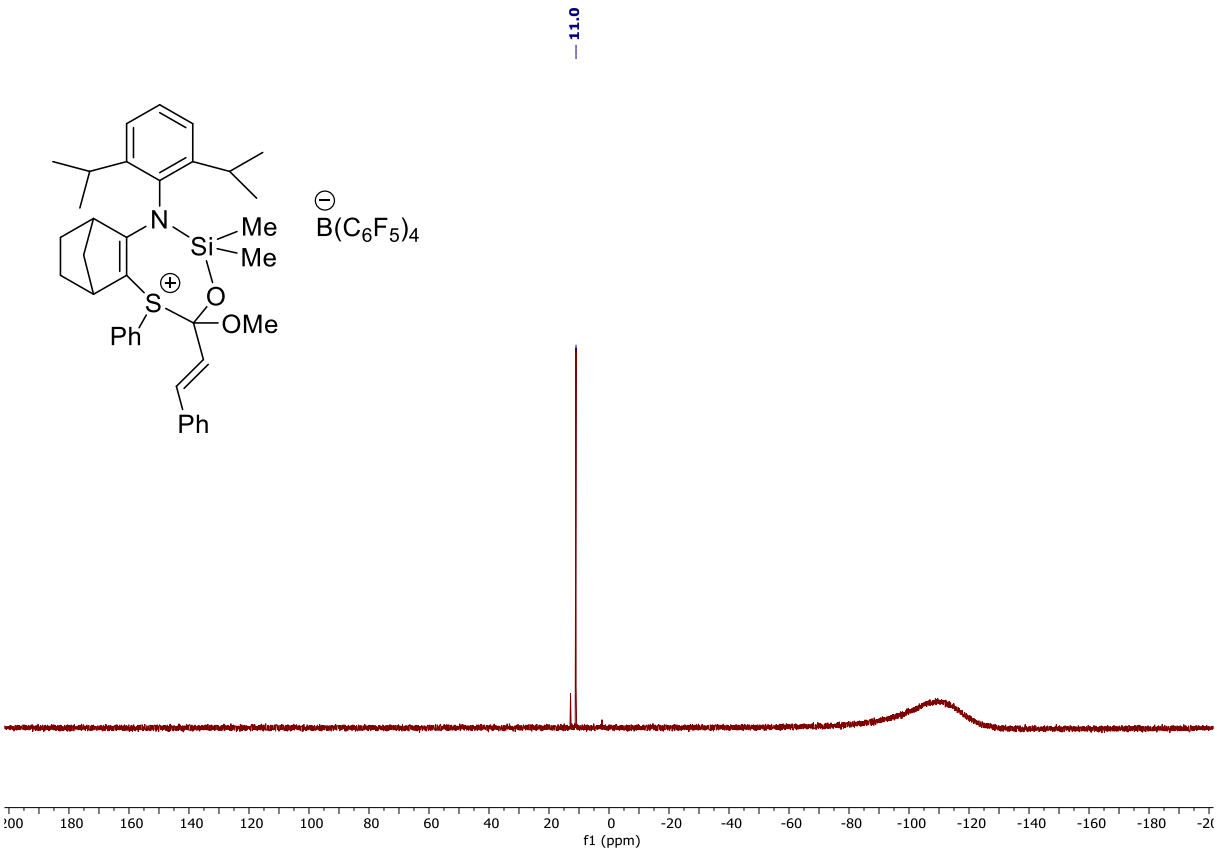


Figure S13: $^{29}Si\{^{1}H\}$ NMR (99 MHz, CD_2Cl_2)

X-ray analysis

Crystallographic data for **4** was collected at 193 K on a Bruker-AXS APEX II CCD Quazar diffractometer equipped with a 30 W air-cooled microfocus source using MoKα radiation (wavelength = 0.71073 Å). Phi- and omega-scans were used. The data were integrated with SAINT, and an empirical absorption correction with SADABS was applied. [1] The structure was solved using an intrinsic phasing method (ShelXT) [2] and refined using the least–squares method on F^2 (ShelXL-2018).[3] All non-H atoms were treated anisotropically. All H atoms attached to C atoms were fixed geometrically and treated as riding on their parent atoms with C-H = 0.95 Å (aromatic), 0.98 Å (CH_3), 0.99 Å (CH_2) or 1.0 Å (CH) with $U_{iso}(H) = 1.2U_{eq}(CH, CH_2)$ or $U_{iso}(H) = 1.5U_{eq}(CH_3)$. The solvent molecule (benzene) was disordered over 2 positions, several restraints (SAME, SIMU, DELU) were applied to refine the disorder.

Supplementary crystallographic data for CCDC- 2115945 (**4**) can be obtained free of charge from The Cambridge Crystallographic Data Centre via https://www.ccdc.cam.ac.uk/structures/.

The details of data collection and crystal structures refinement are summarized in Table S1.

[1] SADABS, Program for data correction, Bruker−AXS.
[2] ShelXT, G. M. Sheldrick, Acta Crystallogr. Sect. A, 2015, 71, 3-8.
[3] ShelXL, G. M. Sheldrick, Acta Crystallogr. Sect. C, 2015, 71, 3-8.

Table S1. Crystallographic data for the compound 4

Compound	**4**
Chemical formula	$C_{27}H_{36}NSSi$, $C_{24}BF_{20}$, C_6H_6
M_r	1191.87
Crystal system	Triclinic
Space group	$P\ \bar{1}$
a [Å]	12.7325(8)
b [Å]	13.4053(9)
c [Å]	16.4281(10)
α [°]	85.829(2)
β [°]	69.6571(17)
γ [°]	89.1970(19)
V [Å^3]	2622.0(3)
Z	2
ρ [g cm^{-3}]	1.510
μ($Mo_{K\alpha}$) [mm^{-1}]	0.197
Reflections collected	63272
Independent reflections	10438 R(int)=0.0587
Data/ restraints/ parameters	10438/234/767
Crystal size [mm^3]	0.360x0.160x0.150
GOOF on F^2	1.025
R ($I > 2\sigma(I)$)	0.0507
wR2 (all data)	0.1242
Largest difference peak and hole, [e Å^{-3}]	0.624 and -0.347
CCDC number	2115945

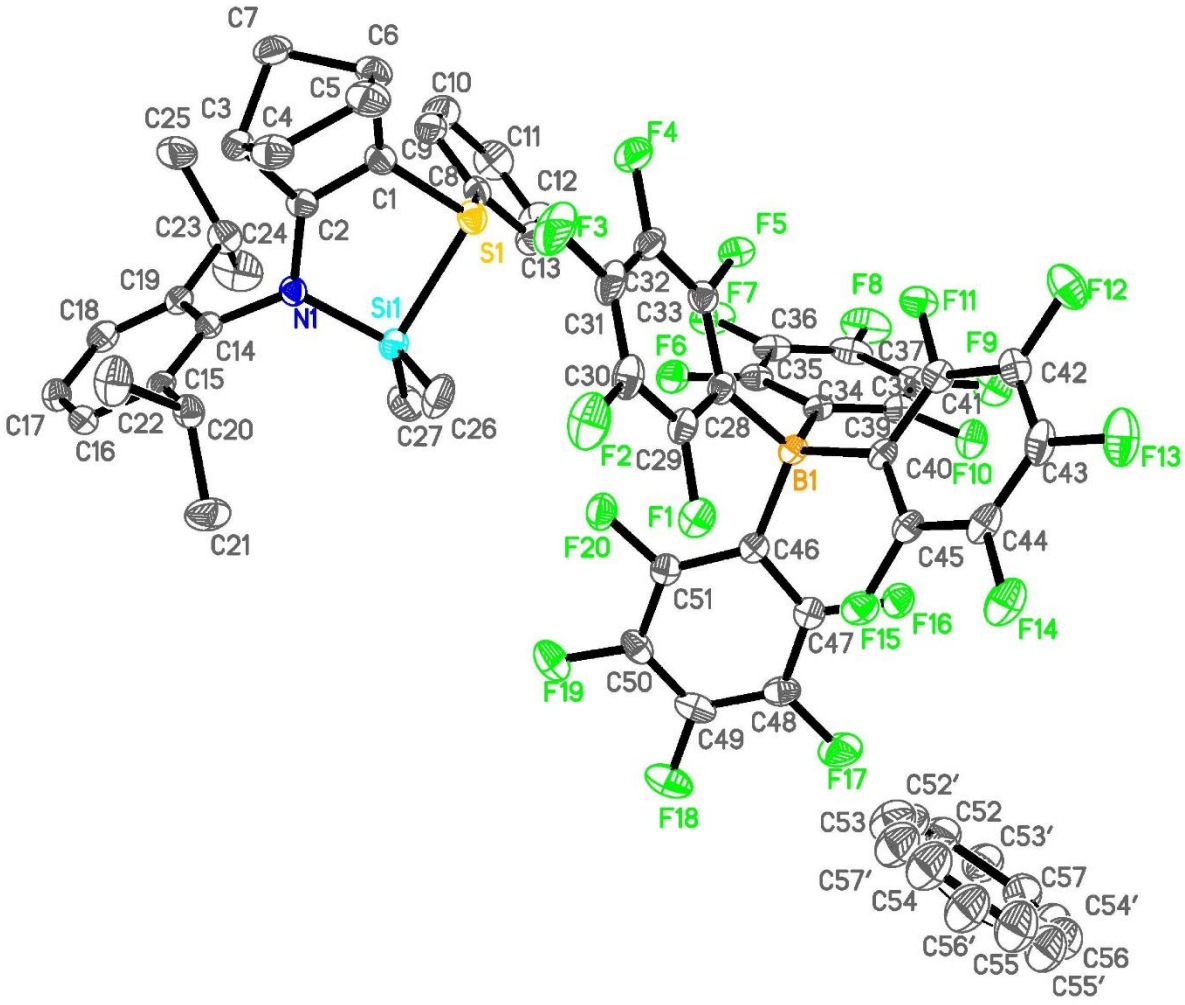


Figure S14: asymmetric unit of **4**

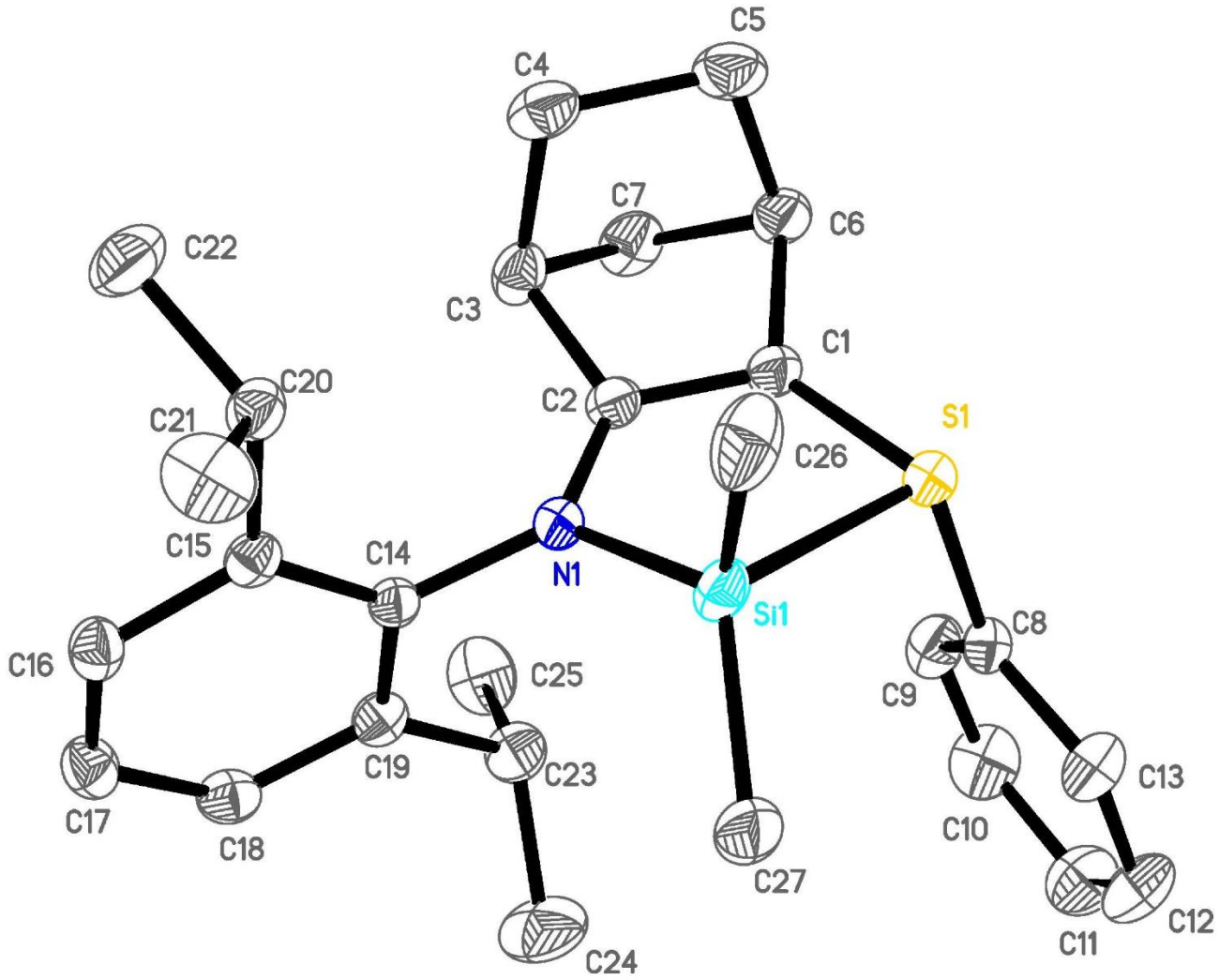


Figure S15 : Molecular view of the cationic part of molecule **4**. Thermal ellipsoids set at 30 % probability. Counterion $^{-}[B(C_6F_5)_4]$ is omitted for clarity. Selected bond lengths [Å] and angles [°]: S1−C1 1.753(3), S1−C8 1.803(3), S1−Si1 2.280(1), Si1−N1 1.737(2), Si1−C27 1.823(3), Si1−C26 1.826(4), N1−C2 1.387(4), N1−C14 1.451(3), C1−C2 1.357(4); C1−S1−C8 106.7(1), C1−S1−Si1 89.1(1), C8−S1−Si1 106.1(1), N1−Si1-C27 116.1(2), N1−Si1−C26 113.2(1), C27−Si1−C26 117.7(2), N1−Si1−S1 94.0(1), C27−Si1−S1 111.5(1), C26−Si1−S1 100.5(1), C2−N1−C14 121.4(2), C2−N1−Si1 112.4(2), C14−N1−Si1 125.7(2), C2−C1−S1 118.0(2), C1−C2−N1 123.0(3).

Computational details

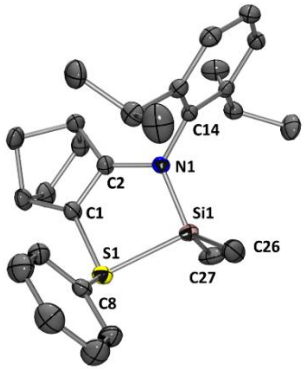
All computations were carried out using Gaussain09[4] and Gaussian16.[5] The structures were optimized at the M06-2X/def-2tzvp level.[6] Frequency computations were also performed to characterize the nature of the local minima (no imaginary frequency) at the same computational level. The natural bond orbital (NBO) analysis of **4'** was done at the M06-2X/def-2tzvp level.

[4] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J.A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian 09, Revision D.01, Inc., Wallingford CT, **2013**.

[5] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman and D. J. Fox, Gaussian 16, Revision A.03, Inc., Wallingford CT, **2016**.

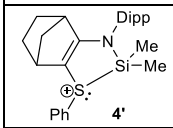
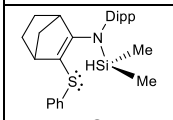
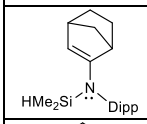
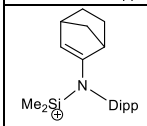
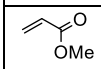
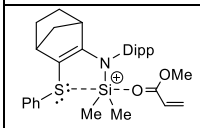
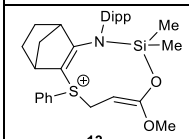
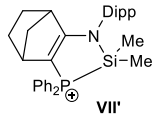
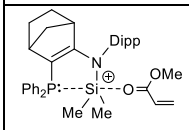
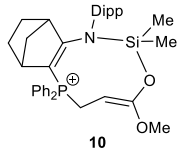
[6] Y. Zhao and D. G. Truhlar, *TheorChemAcc*, 2008, **120**, 215-241.

Table S2. Comparison of calculated geometric parameters of **4'** with the X-Ray data.

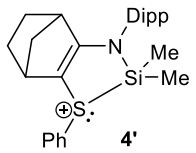


Bonds	**Exp.**	**M06-2X/def-2tzvp**	**Unsigned Error (UE)**
S1-C1	1.753	1.741	0.012
S1-C8	1.803	1.797	0.006
S1-Si1	2.280	2.290	0.010
Si1-N1	1.737	1.740	0.003
Si1-C27	1.823	1.844	0.021
Si1-C26	1.826	1.841	0.015
N1-C2	1.387	1.367	0.02
N1-C14	1.451	1.444	0.007
C1-C2	1.357	1.356	0.001
			(Mean UE) 0.011
Angles			
C1-S1-Si1	89.09	89.56	0.47
C8-S1-Si1	106.11	104.78	1.33
N1-Si1-C27	116.09	115.04	1.05
N1-Si1-C26	113.15	113.68	0.53
C27-Si1-C26	117.65	117.24	0.41
N1-Si1-S1	94.01	93.28	0.73
C27-Si1-S1	111.50	111.33	0.17
C26-Si1-S1	100.49	102.73	2.24
C2-N1-C14	121.4	122.42	1.02
C2-N1-Si1	112.39	113.59	1.20
C14-N1-Si1	125.72	123.61	2.11
C2-C1-S1	118.0	117.95	0.05
C1-C2-N1	123.0	123.50	0.5
			(Mean UE) 0.91

Table S3. Electronic and Gibbs energies (au) and number of imaginary frequencies (NIMAG) for all structures computed with M062x/6-311+G(d,p) computational level.

	E	G	NIMAG
 4'	-1792.155691	-1792.216029	0
 3	-1792.946902	-17923.008021	0
	-1163.798614	-1163.852146	0
 7	-1162.959861	-1163.014274	0
 9	-306.364519	-306.394777	0
 12	-2098.545504	-2098.613603	0
 13	-2098.539703	-2098.606198	0
 VII'	-1966.880436	-1966.947717	0
 11	-2273.254244	-2273.329222	0
 10	-2273.286271	-2273.358959	0

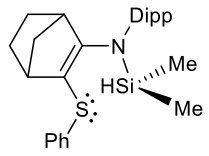
Cartesian Coordinates



4'

S	-1.774500	-1.607800	0.885600
Si	-0.165100	-0.237200	1.766000
N	0.686600	-0.100300	0.255100
C	-0.814800	-1.786600	-0.556100
C	0.299300	-1.022800	-0.676800
C	1.073800	-1.562100	-1.851400
H	1.799000	-0.882100	-2.291700
C	1.658100	-2.917900	-1.332000
H	2.357300	-3.309400	-2.069800
H	2.201500	-2.793700	-0.396200
C	0.408100	-3.828000	-1.194100
H	0.461600	-4.675400	-1.876700
H	0.278400	-4.220000	-0.186300
C	-0.754300	-2.882200	-1.601100
H	-1.694200	-3.372200	-1.838000
C	-0.078400	-2.081300	-2.733500
H	0.277100	-2.719800	-3.541800
H	-0.710300	-1.290000	-3.134000
C	-3.133500	-0.508900	0.466700
C	-3.201200	0.132000	-0.758800
H	-2.438900	-0.039300	-1.508900
C	-4.265400	0.990500	-1.001300
H	-4.338200	1.493100	-1.957000
C	-5.232400	1.200900	-0.027500
H	-6.058300	1.871300	-0.223800
C	-5.150300	0.544400	1.194000
H	-5.910600	0.698400	1.947700
C	-4.099200	-0.324400	1.447200
H	-4.037900	-0.853600	2.390800
C	1.601400	0.974000	-0.052500
C	2.957700	0.838500	0.266900
C	3.805600	1.903300	-0.030600
H	4.860300	1.821700	0.200700
C	3.323800	3.059400	-0.616300
H	3.999100	3.875000	-0.838900
C	1.976000	3.175600	-0.918100
H	1.609800	4.084800	-1.376700
C	1.089600	2.141300	-0.643000
C	3.534600	-0.412200	0.897700
H	2.715600	-1.109800	1.079700
C	4.198800	-0.104500	2.241900
H	4.517600	-1.026800	2.729700

H	3.522800	0.428300	2.913300
H	5.082400	0.520900	2.107200
C	4.525500	-1.094100	-0.049400
H	4.068100	-1.312300	-1.015600
H	4.883600	-2.030100	0.382000
H	5.391900	-0.455400	-0.228000
C	-0.371000	2.267600	-1.026100
H	-0.935600	1.529500	-0.455400
C	-0.963800	3.637900	-0.703100
H	-0.769100	3.925800	0.330900
H	-2.044300	3.617400	-0.856300
H	-0.559400	4.416200	-1.351200
C	-0.554200	1.933800	-2.509000
H	-0.005400	2.644800	-3.129300
H	-1.608600	1.985900	-2.789400
H	-0.179900	0.934400	-2.740800
C	0.673200	-1.330300	2.992500
H	0.967400	-2.276000	2.532800
H	0.012900	-1.541500	3.835400
H	1.573800	-0.845700	3.376000
C	-0.893000	1.332000	2.394900
H	-0.101800	2.087200	2.429300
H	-1.288800	1.208500	3.403300
H	-1.685300	1.702200	1.742600

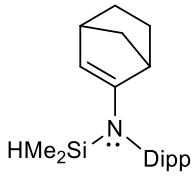


3

S	-2.229800	-0.965700	1.321400
Si	0.788600	0.064200	2.278800
N	0.954500	-0.158900	0.537500
C	-1.175700	-1.331500	-0.020000
C	0.094900	-0.929800	-0.235700
C	0.593100	-1.710900	-1.444600
H	1.439900	-1.265100	-1.959300
C	0.815700	-3.157000	-0.908800
H	1.309400	-3.769000	-1.665300
H	1.441500	-3.159900	-0.015800
C	-0.632000	-3.649900	-0.637300
H	-0.879000	-4.511500	-1.259100
H	-0.798200	-3.924400	0.403500
C	-1.488100	-2.417100	-1.038800
H	-2.548300	-2.616600	-1.178600

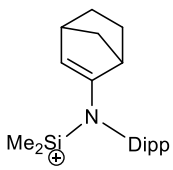
C	-0.698000	-1.902500	-2.246800
H	-0.594000	-2.645100	-3.039800
H	-1.096700	-0.975900	-2.656400
C	-3.632200	-0.258200	0.498700
C	-3.573600	0.265300	-0.788600
H	-2.643000	0.225200	-1.339800
C	-4.702600	0.841400	-1.354600
H	-4.646900	1.243600	-2.358600
C	-5.891900	0.909400	-0.643300
H	-6.769100	1.360600	-1.087700
C	-5.947500	0.390000	0.643900
H	-6.870600	0.434100	1.207700
C	-4.828100	-0.196700	1.212200
H	-4.877200	-0.613600	2.210900
C	1.881600	0.678500	-0.184700
C	3.232100	0.306600	-0.318100
C	4.088100	1.158300	-1.011300
H	5.129800	0.883300	-1.123400
C	3.635500	2.342800	-1.565100
H	4.319500	2.990000	-2.099100
C	2.303100	2.690700	-1.438600
H	1.947400	3.612500	-1.882400
C	1.407300	1.873700	-0.754000
C	3.796100	-0.995800	0.222000
H	3.029400	-1.461000	0.842300
C	5.052800	-0.773600	1.071600
H	5.321200	-1.695800	1.590300
H	4.917100	0.011000	1.813100
H	5.900900	-0.497000	0.442600
C	4.143200	-1.965200	-0.914200
H	3.278900	-2.210700	-1.527400
H	4.542800	-2.895100	-0.504600
H	4.905400	-1.529200	-1.563500
C	-0.054000	2.281700	-0.696500
H	-0.580900	1.597500	-0.030400
C	-0.243200	3.702500	-0.162300
H	0.262300	3.844300	0.792400
H	-1.305700	3.907900	-0.020800
H	0.146400	4.444500	-0.861800
C	-0.684700	2.158100	-2.086600
H	-0.199000	2.837500	-2.790500
H	-1.746500	2.409400	-2.048300
H	-0.578900	1.143900	-2.474300
C	2.473200	0.274200	3.056900

H	3.074300	-0.633300	3.029500
H	2.328400	0.550500	4.104200
H	3.033400	1.080200	2.578600
C	-0.183300	1.580300	2.776800
H	0.411000	2.477300	2.590100
H	-0.377900	1.537000	3.851500
H	-1.137800	1.674200	2.262300
H	0.175400	-1.188700	2.765900



Si	-0.000800	0.205700	2.379700
N	0.164800	-0.108500	0.665400
C	2.327500	-1.291000	0.852100
C	1.327400	-0.698200	0.175800
C	1.790500	-0.546500	-1.266100
H	1.003000	-0.390500	-2.001100
C	2.885100	0.565400	-1.231700
H	3.179200	0.833100	-2.247700
H	2.529000	1.469700	-0.740500
C	4.051800	-0.112400	-0.465200
H	4.936400	-0.206400	-1.097300
H	4.336800	0.432000	0.434100
C	3.462200	-1.511500	-0.126800
H	4.202600	-2.251600	0.167400
C	2.673400	-1.793500	-1.415500
H	3.292200	-1.766100	-2.314700
H	2.115100	-2.726800	-1.369200
C	-0.945800	0.087700	-0.220000
C	-1.159300	1.345300	-0.803100
C	-2.272400	1.521300	-1.621300
H	-2.450400	2.489100	-2.075300
C	-3.150600	0.480700	-1.867000
H	-4.010000	0.634300	-2.506900
C	-2.925100	-0.758900	-1.291300
H	-3.613300	-1.571200	-1.489900
C	-1.831500	-0.975400	-0.459000
C	-0.208500	2.506000	-0.587500
H	0.605400	2.152100	0.045100

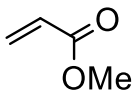
C	-0.888700	3.671600	0.133100
H	-0.179400	4.485900	0.292800
H	-1.280400	3.366900	1.104600
H	-1.721600	4.062600	-0.454800
C	0.393600	2.975000	-1.914200
H	0.859400	2.147000	-2.450100
H	1.152400	3.740100	-1.739200
H	-0.373500	3.405900	-2.560600
C	-1.593800	-2.349800	0.134700
H	-0.846500	-2.252000	0.923800
C	-2.854200	-2.956000	0.751600
H	-3.309700	-2.281700	1.478100
H	-2.608100	-3.889900	1.259300
H	-3.602800	-3.185300	-0.008600
C	-1.018500	-3.282400	-0.934700
H	-1.743700	-3.430100	-1.738600
H	-0.775400	-4.257100	-0.508000
H	-0.113000	-2.860200	-1.371000
C	1.173600	1.569500	2.876700
H	2.168300	1.374700	2.469700
H	1.259600	1.645200	3.962000
H	0.831100	2.533400	2.494100
C	-1.781800	0.634400	2.719000
H	-2.115200	1.491600	2.132900
H	-1.915500	0.867000	3.777200
H	-2.432300	-0.206100	2.470400
H	2.402900	-1.437300	1.920100
H	0.345400	-1.027600	3.129500



7

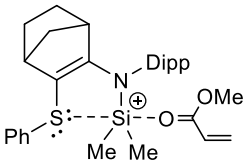
N	0.185200	-0.113400	0.568300
C	2.156800	-1.554000	0.205800
C	1.324700	-0.571800	-0.146100
C	1.894100	0.128800	-1.363100
H	1.188400	0.710000	-1.951800
C	3.131900	0.913100	-0.831200
H	3.542200	1.541900	-1.620300
H	2.877000	1.565000	0.006400
C	4.117600	-0.218700	-0.437300

H	5.022900	-0.179800	-1.041600
H	4.419400	-0.180900	0.608700
C	3.314000	-1.512400	-0.767900
H	3.913100	-2.415600	-0.828600
C	2.584300	-1.060900	-2.047700
H	3.267600	-0.756700	-2.840500
H	1.880300	-1.802400	-2.421200
C	-1.022000	0.129800	-0.209700
C	-1.285400	1.436000	-0.643600
C	-2.454700	1.645100	-1.366600
H	-2.694200	2.638900	-1.720100
C	-3.315300	0.596200	-1.650900
H	-4.218600	0.780200	-2.217300
C	-3.018900	-0.685200	-1.222400
H	-3.693700	-1.497500	-1.460800
C	-1.863600	-0.950500	-0.490800
C	-0.352000	2.592900	-0.332700
H	0.644200	2.184300	-0.156100
C	-0.795100	3.325500	0.937300
H	-0.127100	4.159100	1.156600
H	-0.814400	2.672100	1.816200
H	-1.806500	3.718300	0.818000
C	-0.228200	3.582200	-1.491300
H	0.005100	3.072500	-2.426600
H	0.567000	4.298100	-1.282500
H	-1.146900	4.151700	-1.635200
C	-1.565000	-2.370300	-0.050300
H	-0.672400	-2.362200	0.577800
C	-2.712600	-2.958200	0.773700
H	-2.956300	-2.328600	1.631700
H	-2.444100	-3.949700	1.139400
H	-3.617300	-3.063000	0.174100
C	-1.253300	-3.251300	-1.262900
H	-2.115700	-3.310500	-1.928800
H	-1.003700	-4.263500	-0.943200
H	-0.413200	-2.850900	-1.831400
H	2.077600	-2.204800	1.068500
Si	0.171000	0.108400	2.208800
C	1.747300	0.134000	3.135200
H	2.588900	0.293000	2.461400
H	1.712600	0.923200	3.888800
H	1.894700	-0.814300	3.657800
C	-1.445600	0.265900	3.046900
H	-1.651800	-0.662500	3.588100
H	-1.424500	1.075000	3.778800
H	-2.243700	0.438300	2.325000



9

C	-2.472300	-0.001400	-0.000100
H	-2.486300	1.081800	-0.000200
H	-3.416700	-0.528500	-0.000200
C	-1.317300	-0.647600	0.000100
H	-1.246700	-1.727100	0.000100
C	-0.040100	0.110300	0.000100
O	0.061600	1.307200	0.000000
O	1.012400	-0.720100	0.000000
C	2.286900	-0.082100	-0.000100
H	3.021100	-0.881800	-0.000300
H	2.396900	0.541900	-0.885900
H	2.397200	0.541700	0.885900

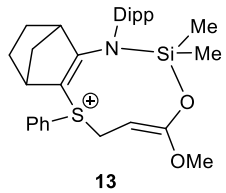


12

S	-2.224700	0.201400	-1.828900
Si	0.416700	-0.665100	-1.343200
N	0.363000	0.518000	-0.072800
C	-1.739800	1.535200	-0.819500
C	-0.591700	1.528100	-0.117000
C	-0.402100	2.921900	0.441900
H	0.263600	2.999500	1.297600
C	-0.006800	3.776700	-0.803400
H	0.295500	4.775100	-0.487700
H	0.829400	3.331800	-1.345100
C	-1.318100	3.816200	-1.634600
H	-1.697000	4.834000	-1.723400
H	-1.197100	3.417700	-2.641300
C	-2.290000	2.948300	-0.785800
H	-3.341300	3.047600	-1.042700
C	-1.862800	3.359600	0.632800
H	-1.958300	4.430700	0.812000
H	-2.379800	2.804100	1.413700
C	-3.502900	-0.617000	-0.897700
C	-3.997400	-0.131700	0.305100
H	-3.603400	0.785200	0.725000
C	-4.997500	-0.834000	0.964600
H	-5.390900	-0.449800	1.897200

C	-5.497100	-2.014700	0.434100
H	-6.277200	-2.556000	0.952100
C	-4.997700	-2.493800	-0.770100
H	-5.386400	-3.410100	-1.194200
C	-4.005000	-1.796500	-1.440800
H	-3.625300	-2.163100	-2.387400
C	1.061400	0.335900	1.176800
C	2.404700	0.732600	1.290800
C	3.057000	0.491500	2.497000
H	4.092000	0.788800	2.610000
C	2.401900	-0.100800	3.565300
H	2.927500	-0.269700	4.496100
C	1.071900	-0.460900	3.442800
H	0.560800	-0.914500	4.283200
C	0.379100	-0.258300	2.250900
C	3.149300	1.454900	0.182300
H	2.558400	1.375500	-0.731900
C	4.535000	0.859000	-0.079600
H	4.969400	1.296200	-0.980300
H	4.511600	-0.226200	-0.192500
H	5.220700	1.077600	0.740000
C	3.299100	2.943200	0.517900
H	3.826400	3.462400	-0.284100
H	3.874500	3.068400	1.437100
H	2.333300	3.425900	0.657000
C	-1.069600	-0.699100	2.160700
H	-1.430800	-0.511500	1.150000
C	-1.231300	-2.196100	2.434000
H	-0.589700	-2.796600	1.785500
H	-2.266300	-2.494300	2.254000
H	-0.987300	-2.441300	3.469200
C	-1.937400	0.116800	3.120600
H	-1.632400	-0.045000	4.156000
H	-2.983200	-0.179700	3.029000
H	-1.856100	1.184700	2.912400
C	0.620100	0.138700	-3.006100
H	0.028600	1.051900	-3.076700
H	0.298500	-0.523400	-3.812100
H	1.663200	0.412100	-3.165100
C	-0.341400	-2.350900	-1.143300
H	-1.232800	-2.305900	-0.516600
H	0.344800	-3.080700	-0.712100
H	-0.654900	-2.716000	-2.124500
C	3.010800	-2.087700	-1.038300
O	2.163000	-1.172700	-1.118700
C	3.156700	-3.026400	0.066200
H	3.869900	-3.822500	-0.096200
C	2.506100	-2.855900	1.212500
H	1.827400	-2.027000	1.367400
H	2.655000	-3.540900	2.037000

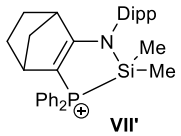
O	3.898100	-2.241900	-1.967200
C	3.894700	-1.347800	-3.095600
H	3.961700	-0.320800	-2.740400
H	4.768800	-1.618800	-3.676100
H	2.984300	-1.495300	-3.672800



13

Si	0.730300	0.244300	-1.862200
O	-0.109600	1.699500	-1.837100
N	0.943400	-0.239300	-0.167700
C	-1.381100	-0.160600	0.794400
C	-0.017500	-0.348400	0.792900
C	2.252200	-0.828600	0.107300
C	3.302400	-0.029200	0.581800
C	4.560300	-0.612300	0.707000
H	5.386100	-0.011400	1.066800
C	4.773100	-1.943800	0.396100
H	5.760600	-2.374300	0.497300
C	3.713100	-2.727000	-0.022900
H	3.875500	-3.775900	-0.237100
C	2.437300	-2.189900	-0.173500
C	3.116700	1.402600	1.043700
H	2.083300	1.692100	0.858400
C	4.012100	2.397000	0.303100
H	5.067800	2.178500	0.470900
H	3.818200	3.407200	0.667600
H	3.836400	2.390300	-0.771600
C	3.393700	1.499400	2.549600
H	2.845900	0.744000	3.112800
H	3.112300	2.484200	2.926400
H	4.456100	1.355500	2.752700
C	1.306100	-3.109300	-0.593700
H	0.402500	-2.514700	-0.726200
C	1.606700	-3.814800	-1.917900
H	1.896800	-3.105800	-2.694900
H	0.730800	-4.366100	-2.263200
H	2.422800	-4.529700	-1.805000
C	1.018300	-4.132500	0.509300
H	1.878100	-4.786400	0.664000
H	0.165000	-4.756400	0.239700
H	0.801800	-3.639200	1.458200
C	-0.344200	-0.915600	-2.838400
H	-1.014000	-1.506900	-2.214400

H	0.271700	-1.607300	-3.414000
H	-0.951000	-0.339000	-3.540000
C	2.381000	0.441800	-2.657800
H	2.238300	0.807700	-3.677700
H	2.898000	-0.518300	-2.712600
H	3.027500	1.135000	-2.123300
C	-1.883500	-0.293800	2.223200
H	-2.941300	-0.520700	2.317900
C	0.332100	-0.619800	2.249500
H	1.298400	-1.089700	2.406500
C	0.146000	0.749900	2.981800
H	0.556900	0.675000	3.987900
H	0.659800	1.561000	2.470700
C	-1.389700	0.944300	3.008100
H	-1.695300	1.882300	2.544200
H	-1.776800	0.932300	4.026800
C	-0.915300	-1.370100	2.728600
H	-0.939700	-1.488000	3.811900
H	-1.058600	-2.331700	2.238500
S	-2.305900	0.466200	-0.512100
C	-3.972600	-0.101100	-0.282100
C	-4.410700	-1.058300	-1.189200
C	-4.807400	0.376500	0.722400
C	-5.702200	-1.553300	-1.080900
H	-3.750800	-1.407200	-1.973400
C	-6.096600	-0.121700	0.816500
H	-4.465200	1.118300	1.431700
C	-6.542000	-1.084600	-0.081600
H	-6.051300	-2.298100	-1.783000
H	-6.754900	0.242800	1.593400
H	-7.550800	-1.466900	-0.002000
C	-0.065000	2.657300	-0.890800
C	-1.129800	2.959100	-0.147900
H	-1.030800	3.749400	0.581100
C	-2.454700	2.289900	-0.288900
H	-3.080500	2.477600	0.579300
H	-3.002500	2.591100	-1.185600
O	1.119800	3.267300	-0.720300
C	1.634600	3.926400	-1.883500
H	0.935600	4.697700	-2.210500
H	2.573200	4.380000	-1.580400
H	1.808600	3.215700	-2.691300

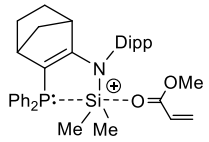


VII'

Si	-0.061000	-0.271300	-1.503400

N	-1.202400	-0.199900	-0.167800
C	0.706900	-0.336400	1.322200
C	-0.638300	-0.334900	1.067400
C	-1.342400	-0.650700	2.362100
H	-2.395400	-0.382700	2.402400
C	-1.031800	-2.162800	2.609700
H	-1.633300	-2.519700	3.444900
H	-1.274500	-2.773900	1.741500
C	0.482700	-2.174300	2.950500
H	0.651700	-2.506200	3.974600
H	1.052000	-2.823100	2.286500
C	0.878000	-0.681400	2.793200
H	1.828700	-0.401500	3.240500
C	-0.377600	-0.000700	3.372100
H	-0.588700	-0.302000	4.398300
H	-0.339800	1.085200	3.302800
C	2.498700	1.608300	0.038200
C	1.832400	2.615400	0.736600
H	0.909100	2.392000	1.259500
C	2.367000	3.893700	0.779200
H	1.855400	4.672800	1.329000
C	3.561600	4.169500	0.126600
H	3.978800	5.167100	0.163000
C	4.228100	3.165700	-0.563100
H	5.165100	3.378800	-1.060100
C	3.700900	1.883600	-0.610300
H	4.235200	1.101800	-1.135100
C	-2.585800	0.170800	-0.340300
C	-3.550700	-0.822300	-0.548000
C	-4.871400	-0.420800	-0.737500
H	-5.636100	-1.171400	-0.894200
C	-5.221700	0.916600	-0.726100
H	-6.253100	1.207600	-0.875600
C	-4.251900	1.885000	-0.521500
H	-4.536400	2.929300	-0.510200
C	-2.920900	1.535200	-0.326600
C	-3.221400	-2.300800	-0.548000
H	-2.142500	-2.408000	-0.421300
C	-3.611800	-2.962800	-1.871900
H	-3.268000	-3.997800	-1.896400
H	-3.188300	-2.435500	-2.728100
H	-4.695300	-2.971300	-1.998800
C	-3.907500	-3.008600	0.624100
H	-3.662700	-2.535400	1.575900
H	-3.602900	-4.055300	0.670300
H	-4.992100	-2.981000	0.508700
C	-1.890900	2.612900	-0.049500
H	-0.898900	2.185600	-0.206100
C	-2.019500	3.820700	-0.977200
H	-2.050500	3.522400	-2.025700

H	-1.169400	4.490200	-0.834700
H	-2.922300	4.394300	-0.764800
C	-1.974200	3.049500	1.415800
H	-2.946200	3.501900	1.621300
H	-1.203600	3.788800	1.645000
H	-1.856600	2.199800	2.090300
C	0.049000	-1.980500	-2.210700
H	0.274300	-2.709900	-1.430000
H	0.821200	-2.048700	-2.977900
H	-0.906000	-2.251200	-2.666000
C	-0.273900	1.089600	-2.735800
H	-1.329700	1.167700	-3.009000
H	0.295300	0.877700	-3.642000
H	0.046800	2.053600	-2.339300
P	1.723300	-0.021800	-0.061600
C	3.004000	-1.245600	-0.372500
C	3.465500	-1.451100	-1.672700
C	3.550400	-1.970900	0.684300
C	4.468600	-2.377000	-1.912900
H	3.047800	-0.885100	-2.498800
C	4.550800	-2.899200	0.437300
H	3.197600	-1.811500	1.695700
C	5.008100	-3.101600	-0.857800
H	4.826400	-2.535800	-2.921300
H	4.974000	-3.464000	1.257000
H	5.788200	-3.827100	-1.046600

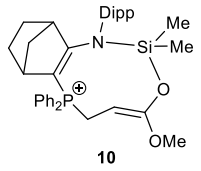


11

Si	-0.114600	0.893300	0.803100
N	-0.850900	-0.167100	-0.420500
C	1.338100	-0.742200	-1.369400
C	-0.022200	-0.743200	-1.364000
C	-0.465800	-1.439000	-2.637200
H	-1.492600	-1.792700	-2.657700
C	-0.082600	-0.466700	-3.798300
H	-0.509700	-0.833900	-4.731200
H	-0.463500	0.539100	-3.633200
C	1.467200	-0.518200	-3.823200
H	1.832300	-0.946600	-4.756600
H	1.914300	0.467600	-3.705500
C	1.790500	-1.456600	-2.631000
H	2.804300	-1.850100	-2.609600
C	0.654300	-2.486600	-2.775500
H	0.643700	-2.981300	-3.747400

H	0.649900	-3.228700	-1.977900
C	2.928000	-1.244000	1.002400
C	2.391700	-2.531600	1.041700
H	1.532800	-2.777300	0.426800
C	2.967400	-3.503000	1.846500
H	2.553500	-4.502900	1.862600
C	4.079100	-3.196500	2.620400
H	4.529800	-3.955500	3.245900
C	4.618100	-1.918500	2.581200
H	5.491700	-1.680000	3.173400
C	4.046700	-0.942900	1.776000
H	4.487700	0.045400	1.740300
C	-2.222000	-0.620000	-0.457900
C	-3.148600	0.030600	-1.285100
C	-4.435500	-0.494200	-1.371400
H	-5.163000	-0.014300	-2.014400
C	-4.804500	-1.615300	-0.644800
H	-5.809700	-2.008000	-0.725400
C	-3.878400	-2.237100	0.175100
H	-4.166600	-3.119500	0.733900
C	-2.571500	-1.762800	0.271100
C	-2.805000	1.278000	-2.074800
H	-1.727800	1.436300	-2.003600
C	-3.498000	2.507400	-1.478400
H	-3.245900	3.403200	-2.047700
H	-3.200600	2.670700	-0.441300
H	-4.583200	2.387600	-1.503800
C	-3.175500	1.135700	-3.553400
H	-2.789000	0.208200	-3.976300
H	-2.770600	1.970800	-4.126700
H	-4.257900	1.140100	-3.689900
C	-1.572900	-2.505200	1.137900
H	-0.600600	-2.026600	1.019800
C	-1.954100	-2.424800	2.616800
H	-2.010500	-1.387400	2.953300
H	-1.213100	-2.937900	3.232400
H	-2.923100	-2.894700	2.797100
C	-1.415300	-3.959000	0.688800
H	-2.338600	-4.522500	0.831700
H	-0.633600	-4.451400	1.270000
H	-1.150100	-4.016000	-0.368400
C	0.196600	2.586100	0.078400
H	0.557100	2.452000	-0.945300
H	0.962700	3.152100	0.608500
H	-0.714600	3.184200	0.042600
C	0.303000	0.368100	2.556200
H	-0.460300	0.588200	3.301000
H	1.236300	0.855600	2.854800
H	0.508700	-0.704600	2.583500
P	2.069800	0.023900	0.019300

C	3.330700	1.243100	-0.422700
C	3.644900	2.261400	0.477300
C	4.013500	1.165400	-1.634500
C	4.627200	3.190400	0.169500
H	3.125900	2.325600	1.428100
C	4.990100	2.101100	-1.944400
H	3.788000	0.371100	-2.334200
C	5.296600	3.112400	-1.044700
H	4.868400	3.975600	0.873600
H	5.515400	2.036900	-2.888000
H	6.059700	3.839600	-1.288200
C	-0.848500	3.661100	2.966800
H	-0.552700	4.585600	3.444400
H	-0.066900	2.949700	2.741800
C	-2.124400	3.416700	2.707000
H	-2.907500	4.109400	2.984700
C	-2.604000	2.151100	2.127000
O	-3.855300	1.940400	2.409800
O	-1.956500	1.343000	1.453200
C	-4.464100	0.713600	1.961400
H	-3.928300	-0.135200	2.380400
H	-5.483300	0.752300	2.328300
H	-4.434700	0.667600	0.876600



10

Si	1.290200	1.802100	-0.132000
O	-0.259700	2.081400	0.425900
N	1.537700	0.060500	-0.136000
C	-0.682800	-0.867800	-0.819400
C	0.684200	-0.789600	-0.807700
C	2.850700	-0.450000	0.229400
C	3.012600	-0.934700	1.538300
C	4.252400	-1.445300	1.907700
H	4.394600	-1.829800	2.908700
C	5.314400	-1.454800	1.020600
H	6.272700	-1.854600	1.324700
C	5.152300	-0.930100	-0.247700
H	5.995400	-0.913800	-0.926500
C	3.929200	-0.413600	-0.669400
C	1.883800	-0.904400	2.552400
H	1.209000	-0.096400	2.262000
C	2.362900	-0.597100	3.971400
H	2.899000	-1.439700	4.410100
H	1.504100	-0.391900	4.612100

H	3.020800	0.272300	3.991700
C	1.102000	-2.223100	2.535700
H	0.592300	-2.378200	1.581500
H	0.356500	-2.241200	3.335000
H	1.778600	-3.064900	2.696500
C	3.852900	0.206500	-2.054700
H	2.804200	0.390900	-2.295100
C	4.596700	1.547200	-2.078400
H	4.215500	2.246000	-1.333500
H	4.512000	2.013900	-3.061600
H	5.656700	1.392600	-1.870600
C	4.429700	-0.702100	-3.146000
H	5.512500	-0.788700	-3.052200
H	4.222500	-0.278500	-4.129300
H	4.016500	-1.710400	-3.113500
C	1.198300	2.486800	-1.853900
H	0.632800	1.807600	-2.496800
H	2.176300	2.643200	-2.305300
H	0.670700	3.442300	-1.837900
C	2.512600	2.550600	1.034300
H	2.458500	3.640200	1.000600
H	3.536300	2.247300	0.816700
H	2.282400	2.239000	2.056800
C	-1.038000	-1.962000	-1.845100
H	-2.049600	-1.914800	-2.240600
C	1.192600	-1.850000	-1.772400
H	2.218800	-1.719100	-2.085000
C	0.894500	-3.248200	-1.171400
H	1.351400	-4.006600	-1.806000
H	1.310900	-3.364400	-0.173000
C	-0.651100	-3.329700	-1.221100
H	-1.098900	-3.475600	-0.241300
H	-0.985900	-4.145600	-1.861500
C	0.102500	-1.767600	-2.851500
H	0.173700	-2.574500	-3.581700
H	0.069300	-0.804100	-3.360900
C	-0.635400	2.346300	1.693900
C	-1.291200	1.454100	2.427400
H	-1.630600	1.753400	3.407700
C	-1.587700	0.062500	1.970600
H	-0.790800	-0.647200	2.207700
H	-2.475700	-0.298200	2.492600
O	-0.323200	3.565900	2.157800
C	-0.554400	4.649400	1.258600
H	-1.565800	4.596300	0.850100
H	-0.435500	5.554700	1.845700
H	0.168200	4.646300	0.441100
P	-1.979700	-0.241100	0.203600
C	-2.823700	1.167500	-0.523200
C	-3.808200	1.824700	0.211900

C	-2.525200	1.572100	-1.819500
C	-4.486000	2.893900	-0.353300
H	-4.047100	1.506900	1.220100
C	-3.210600	2.639100	-2.381800
H	-1.756500	1.055600	-2.382200
C	-4.186600	3.300100	-1.648000
H	-5.248600	3.408800	0.215500
H	-2.983100	2.954000	-3.391400
H	-4.719500	4.133100	-2.087300
C	-3.217000	-1.561800	0.287400
C	-3.058700	-2.594700	1.212400
C	-4.312600	-1.566400	-0.572200
C	-3.986800	-3.621200	1.273600
H	-2.206900	-2.608900	1.883600
C	-5.238400	-2.598600	-0.508500
H	-4.451100	-0.763200	-1.285400
C	-5.076700	-3.623400	0.412100
H	-3.860400	-4.418500	1.993700
H	-6.089800	-2.596400	-1.175800
H	-5.802600	-4.424100	0.462800