Supporting Information

Chemoselective Silyl Transfer in the Mukaiyama Aldol Reaction Promoted by Super Silyl Lewis Acid

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Instrumentation

NMR spectra were recorded on a ECS-400 spectrometer (400 MHz for ^{1}H NMR, 100 MHz for ^{13}C NMR). Chemical shifts were reported in ppm on the δ scale relative to Me_4Si (δ = 0 for ^{1}H NMR), $CDCl_3$ (δ = 77.2 for ^{13}C NMR) as an internal reference. Multiplicities are indicated as: br (broad), s (singlet), d (doublet), t (triplet), q (quartet), or m (multiplet). Coupling constants (*J*) are reported in Hertz (Hz). Infrared (IR) spectra were recorded on a Bruker ALPHA-E using ZnSe ATR. ESI mass spectra were measured on a Bruker Daltonics micrOTOF. For thin-layer chromatography (TLC) analysis throughout this work, Merck precoated TLC plates (silica gel 60 F254 0.25 mm) were used. Visualization was accomplished by UV light (254 nm), anisaldehyde, $KMnO_4$, and phosphomolybdic acid.

Materials

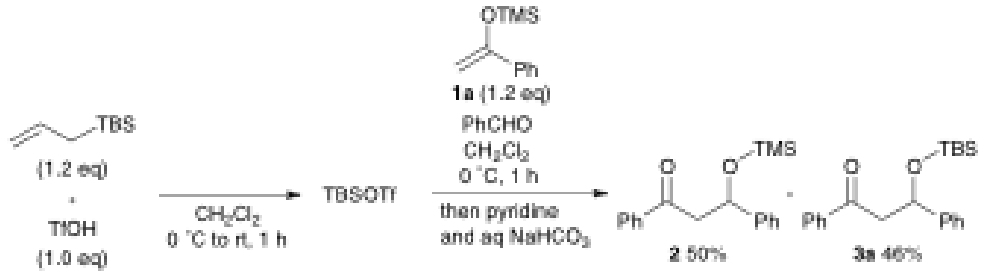
Trifluoromethanesulfonic Acid was purchased from Tokyo Chemical Industry Co. Ltd. Benzaldehyde was purchased from Wako Pure Chemical Co. and distilled before use. CH_2Cl_2 was purchased from Kanto Chemical Co. Ltd. and was purified by passing through a solvent purification system (Glass Contour). Allylsilanes were prepared by the reaction of the corresponding silyl chlorides with allylmagnesium chloride. Silyl enol ethers were prepared from the corresponding ketones and silyl chlorides via classical reaction using LDA as a base. $(TES)_3Si$-aldolates **3d** and **5** were prepared according to the reported method.[1] All other reagents were available from commercial sources and were used without further purification.

Reference

1) M. B. Boxer and H. Yamamoto, *J. Am. Chem. Soc.* 2006, **128**, 48.

Experimental Procedure

Representative Procedure for Silyl Lewis Acid-Promoted Silyl Transfer in the Mukaiyama Aldol Reaction.



Allyl(*tert*-butyl)dimethylsilane (93.8 mg, 0.60 mmol) was placed in an oven-dried test tube with a magnetic stirrer bar. The tube was filled with N_2 and sealed with a rubber septum. To the tube were added CH_2Cl_2 (3.0 mL) and TfOH (75.0 mg, 0.50 mmol) at 0 ˚C. Then the reaction mixture was warmed to room temperature. After stirring for 1 h, to a solution of in situ prepared TBSOTf were added TMS silyl enol ether of acetophenone **1a** (115.4 mg, 0.60 mmol) and freshly distilled benzaldehyde (53.1mg, 0.50 mmol) at 0 ˚C. After stirring for 1 h, pyridine (200 μL) and saturated aqueous $NaHCO_3$ (5 mL) were added. The organic layer was separated and the aqueous layer was extracted twice with CH_2Cl_2 (5 mL). Combined organic layer was dried with Na_2SO_4 and concentrated under reduced pressure. The yields of **2** and **3a** were determined by ^1H NMR analysis using dibenzyl ether as internal standard.

Experimental Data

Chart 1. ^{1}H NMR spectrum of TBSOTf-promoted reaction of benzaldehyde with **1a** at 0 ˚C ($CDCl_3$, 400MHz)

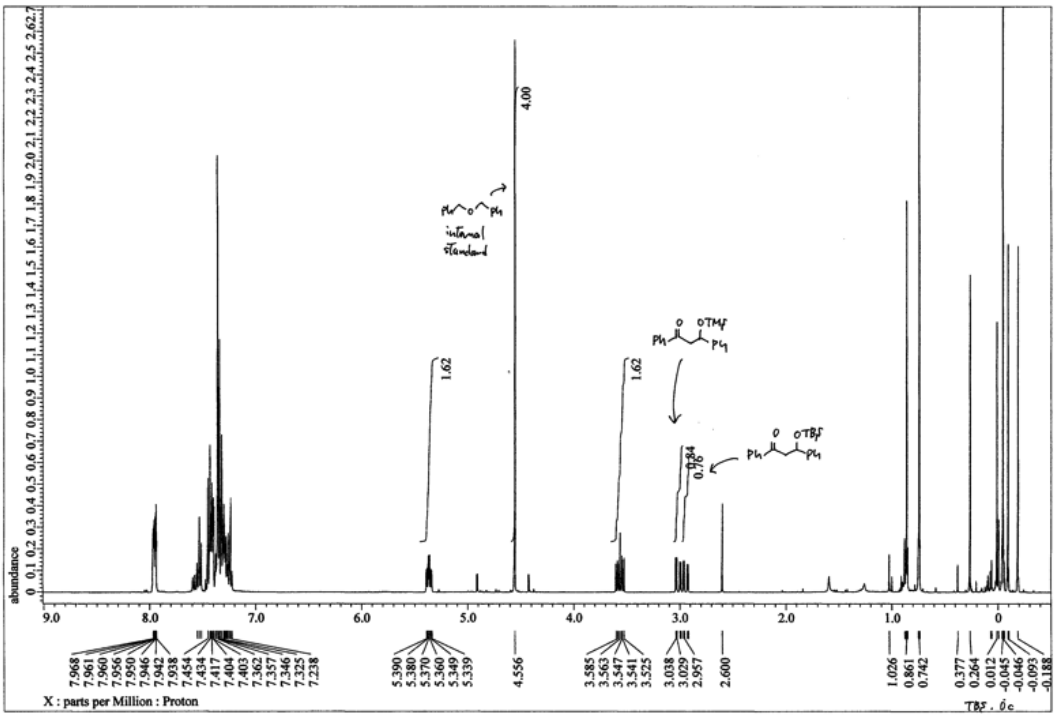


Chart 2. ^{1}H NMR spectrum of TBSOTf-promoted reaction of benzaldehyde with **1a** at -78 ˚C ($CDCl_3$, 400MHz)

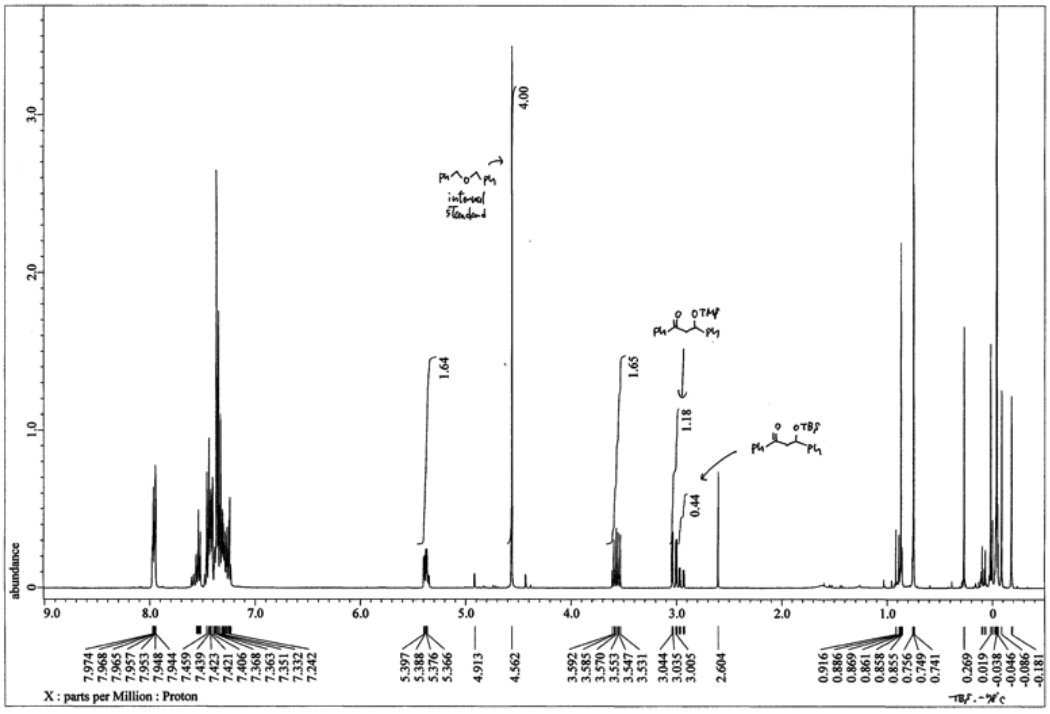


Chart 3. ^{1}H NMR spectrum of TIPSOTf-promoted reaction of benzaldehyde with **1a** at 0 ˚C ($CDCl_3$, 400MHz)

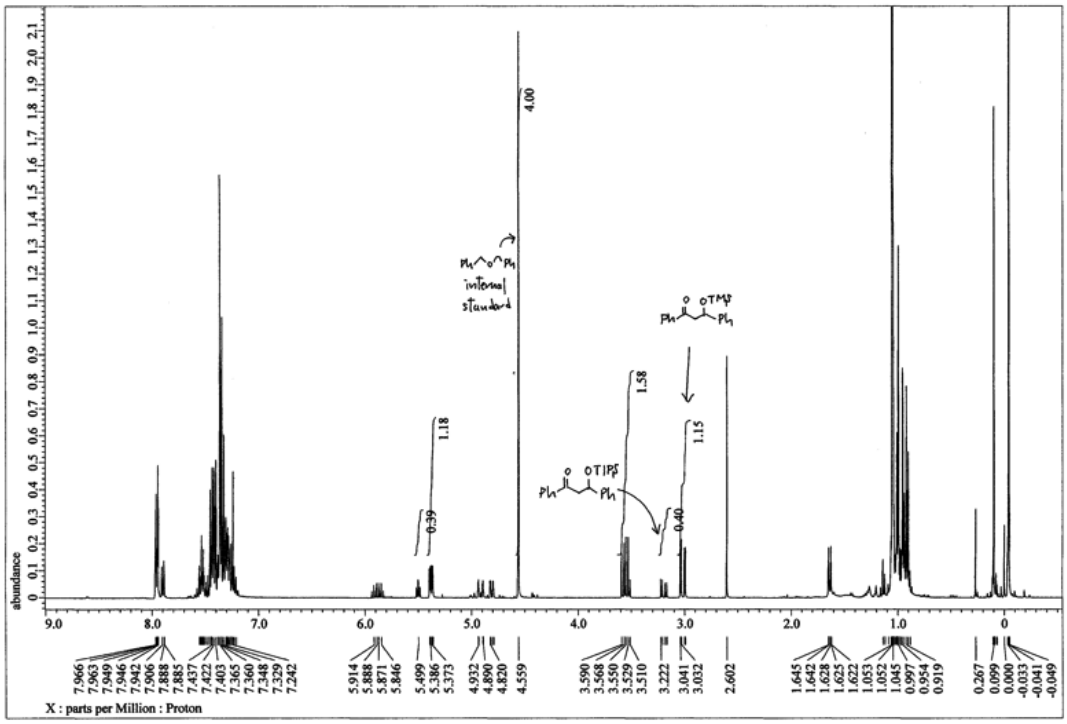


Chart 4. ^{1}H NMR spectrum of TIPSOTf-promoted reaction of benzaldehyde with **1a** at -78 ˚C ($CDCl_3$, 400MHz)

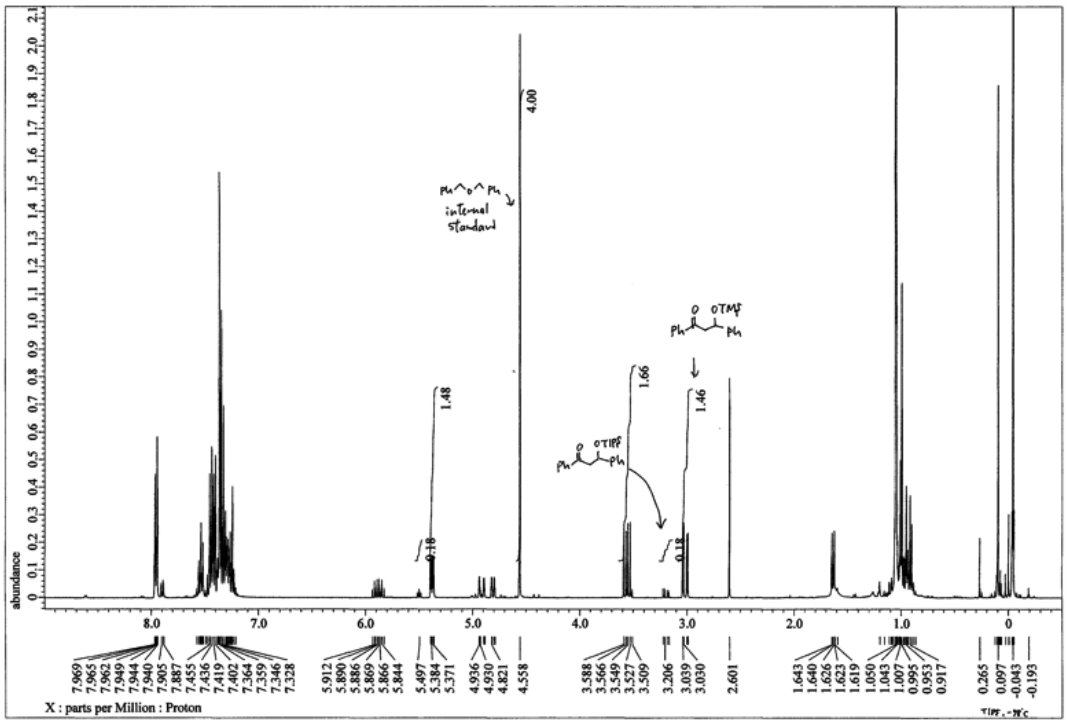


Chart 5. ^{1}H NMR spectrum of $(TMS)_3SiOTf$-promoted reaction of benzaldehyde with **1a** at 0 ˚C ($CDCl_3$, 400MHz)

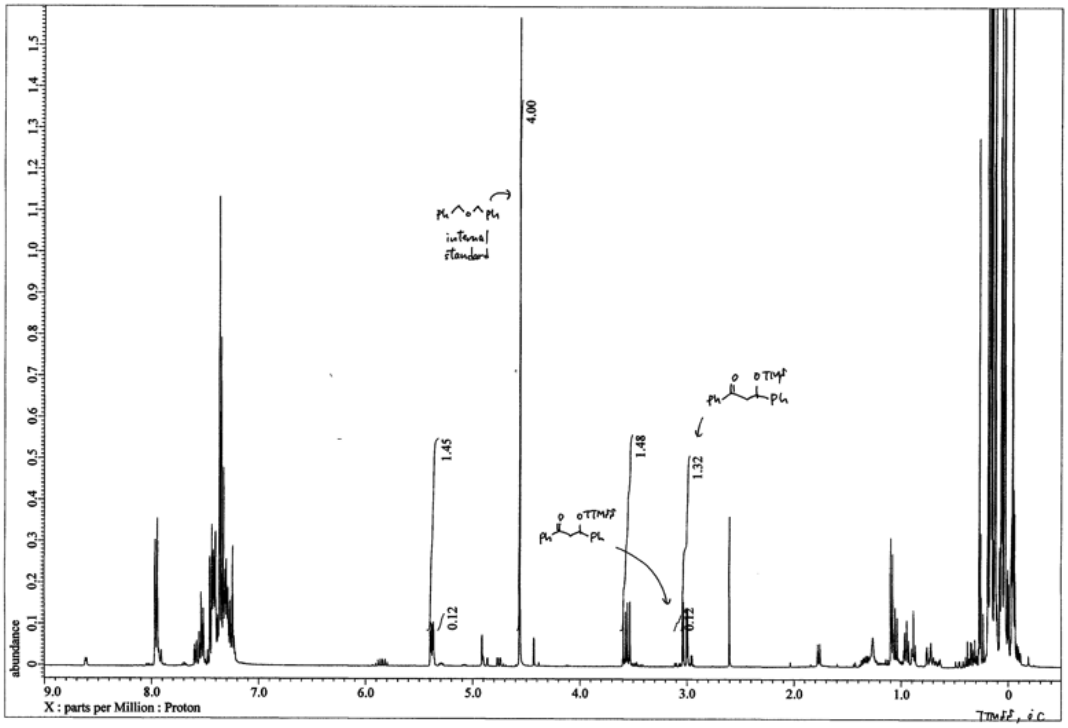


Chart 6. ^{1}H NMR spectrum of $(TMS)_3SiOTf$-promoted reaction of benzaldehyde with **1a** at -78 ˚C ($CDCl_3$, 400MHz)

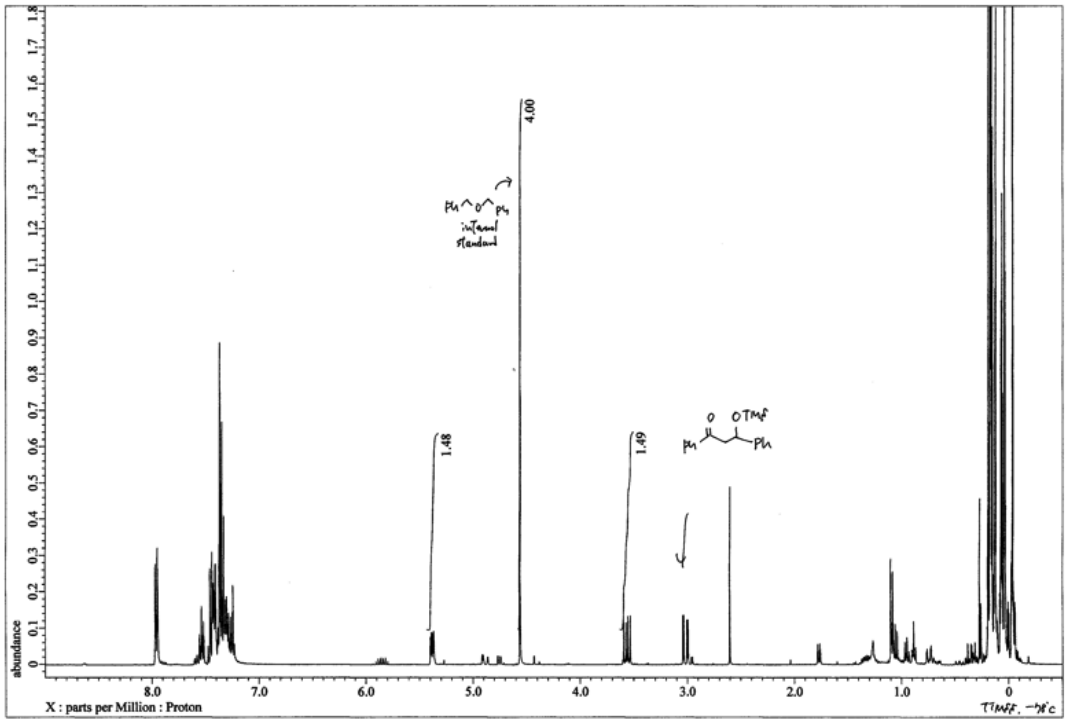


Chart 7. ^{1}H NMR spectrum of $(TES)_3SiOTf$-promoted reaction of benzaldehyde with **1a** at 0 ˚C ($CDCl_3$, 400MHz)

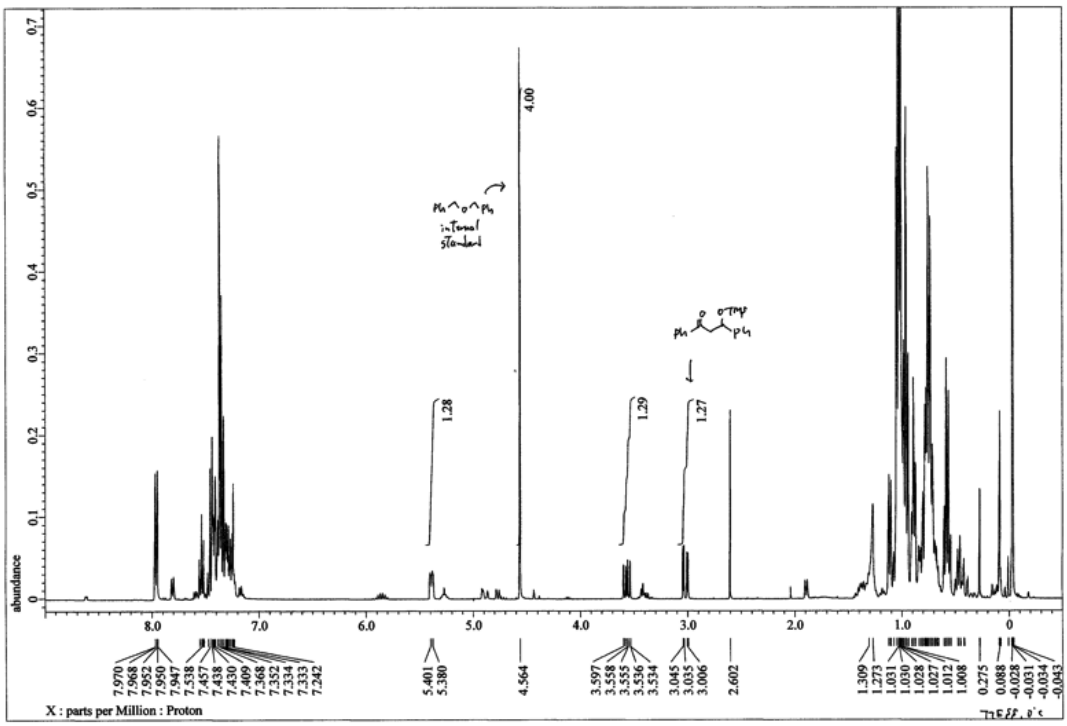


Chart 8. ^{1}H NMR spectrum of $(TES)_3SiOTf$-promoted reaction of benzaldehyde with **1a** at -78 ˚C ($CDCl_3$, 400MHz)

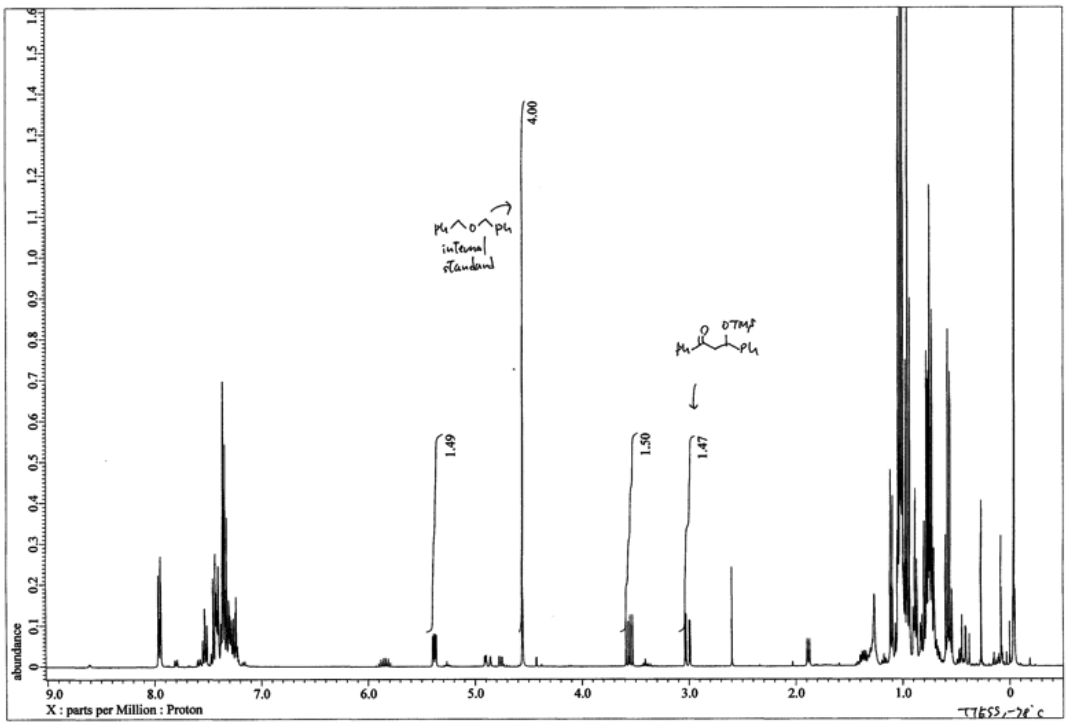


Chart 9. ^{1}H NMR spectrum of $(TES)_3SiOTf$-promoted reaction of benzaldehyde with **1b** at -78 ˚C ($CDCl_3$, 400MHz)

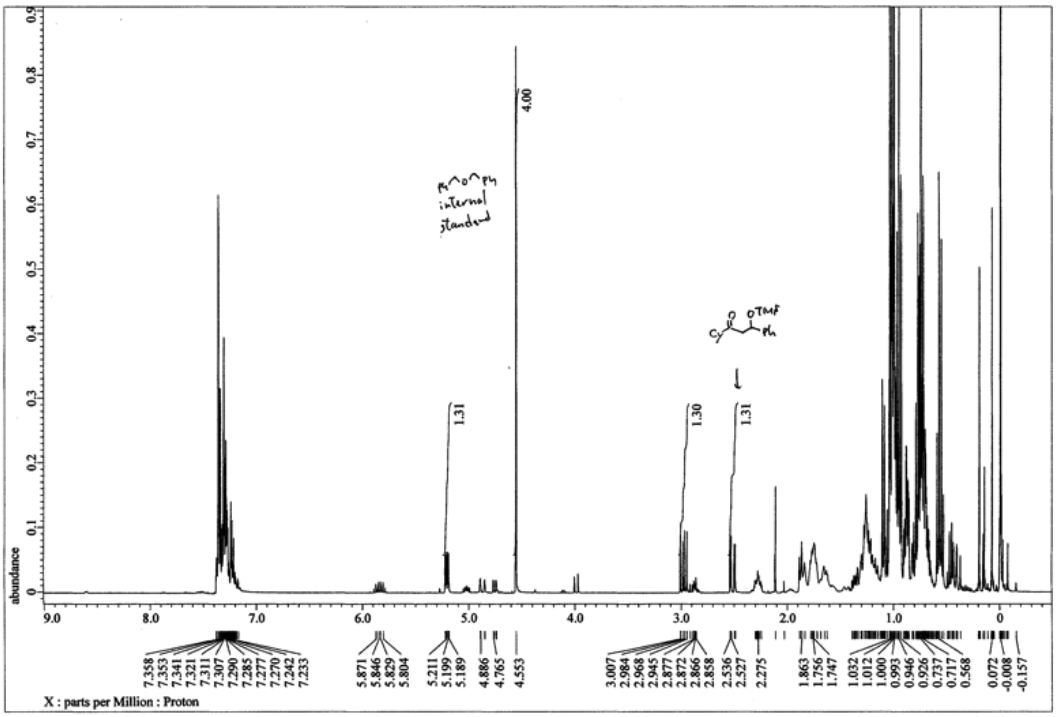
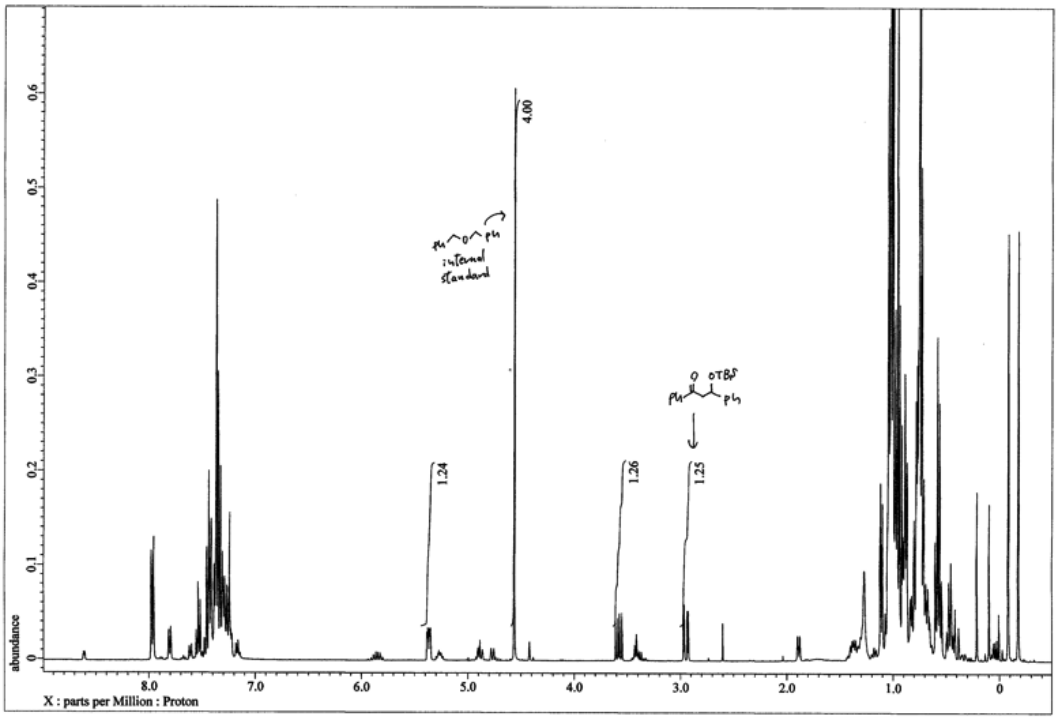


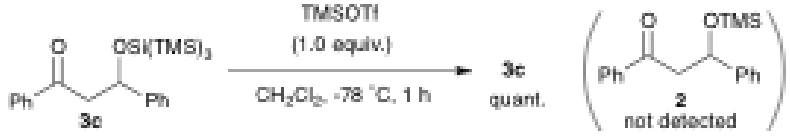
Chart 10. ^{1}H NMR spectrum of $(TES)_3SiOTf$-promoted reaction of benzaldehyde with **1c** at -78 ˚C ($CDCl_3$, 400MHz)



Investigation of Intermolecular Silyl Group Exchange

1. Intermolecular Silyl Group Exchange of the Product

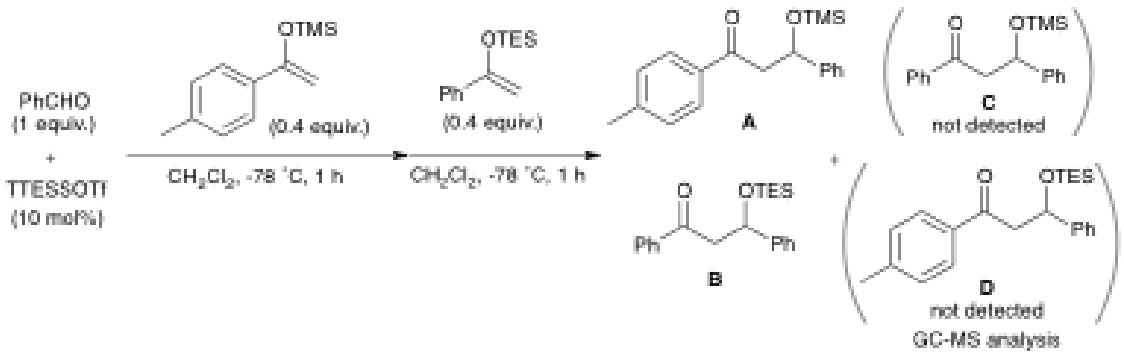
To investigate the intermolecular silyl group exchange of the product, the $(TMS)_3Si$-aldolate **3c** was subjected to the reaction conditions with TMSOTf. In this case, no silyl group exchange was observed and **3c** was recovered quantitatively.



Procedure: An oven-dried test tube was added CH_2Cl_2 (1 mL), allyltrimethylsilane (79.3 μL, 0.50 mmol), and TfOH (21.9 μL, 0.25 mmol). The reaction mixture was stirred for 1 h at room temperature. To a solution of $(TMS)_3Si$-aldolate **3c (**118.2 mg, 0.25 mmol**)** and DTBP (16.9 μL, 0.075 mmol) in CH_2Cl_2 (1 mL) was added the reaction mixture at -78 ˚C. After stirring for 1 h, the reaction mixture was quenched with pyridine (50 μL) and saturated aqueous $NaHCO_3$ (3 mL). The organic layer was separated and the aqueous layer was extracted twice with CH_2Cl_2 (3 mL). Combined organic layer was dried with Na_2SO_4 and concentrated under reduced pressure. The yield of **3c** was determined by ^1H NMR analysis using dibenzyl ether as internal standard.

2. Crossover of Silyl Groups

To test the generation of TMSOTf during the aldol reaction, the crossover experiment was performed. The reaction of TMS-silyl enol ether with benzaldehyde was first performed under $(TES)_3SiOTf$ catalysis. Then TES-silyl enol ether was successively added to the reaction mixture. If the silyl transfer occurred completely in an intramolecular fashion and TMSOTf was not formed during the first aldol reaction, only the products **A** and **B** would be produced. In contrast, if TMSOTf was generated in situ during the first aldol reaction, TMSOTf would promote the reaction of TES-silyl enol ether with benzaldehyde. Thus, the aldolate **C** would be obtained to some extent. As a result, the reaction afforded only **A** and **B** and none of **C** was observed by GC-MS analysis (Chart 1 and 2 as shown below). This result indicates that the silyl transfer occurs in an intramolecular manner and TMSOTf is not generated during the aldol reaction.



Procedure: An oven-dried test tube was added CH_2Cl_2 (2 mL), allyltris(triethylsilyl)silane (20.8 mg, 0.050 mmol), and TfOH (2.2 μL, 0.025 mmol). The reaction mixture was stirred for 1 h at room temperature. Then to the mixture were added benzaldehyde (26.5 mg, 0.25 mmol), TMS-silyl enol ether (20.6 mg, 0.10 mmol), and DTBP (11μL, 0.050 mmol) at -78 ˚C. After stirring for 1 h, TES-silyl enol ether (23.4 mg, 0.10 mmol) was added to the mixture at -78 ˚C. After stirring for another 1 h, the reaction mixture was quenched with pyridine (50 μL) and saturated aqueous $NaHCO_3$ (3 mL). The organic layer was separated and the aqueous layer was extracted twice with CH_2Cl_2 (3 mL). Combined organic layer was dried with Na_2SO_4 and concentrated under reduced pressure. The product composition was determined by GC-MS analysis.

Chart 1. GC-MS spectra of the reaction mixture

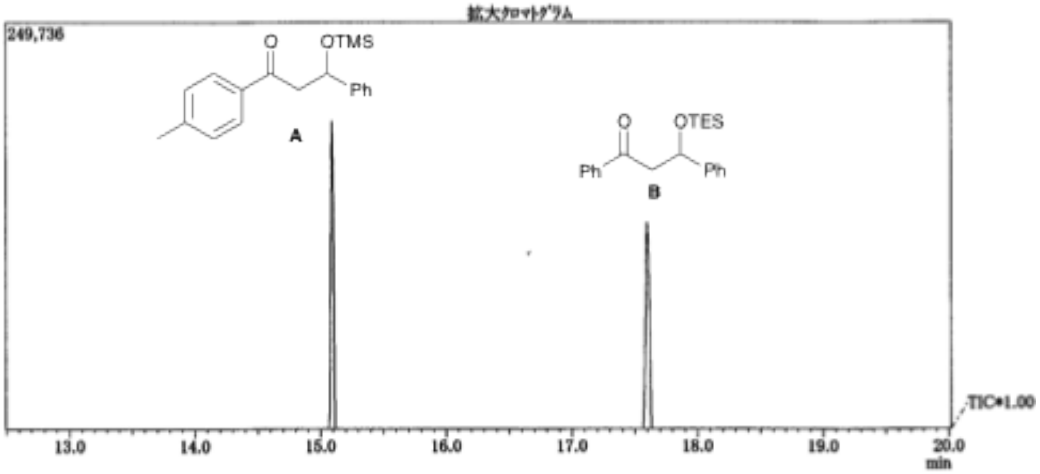
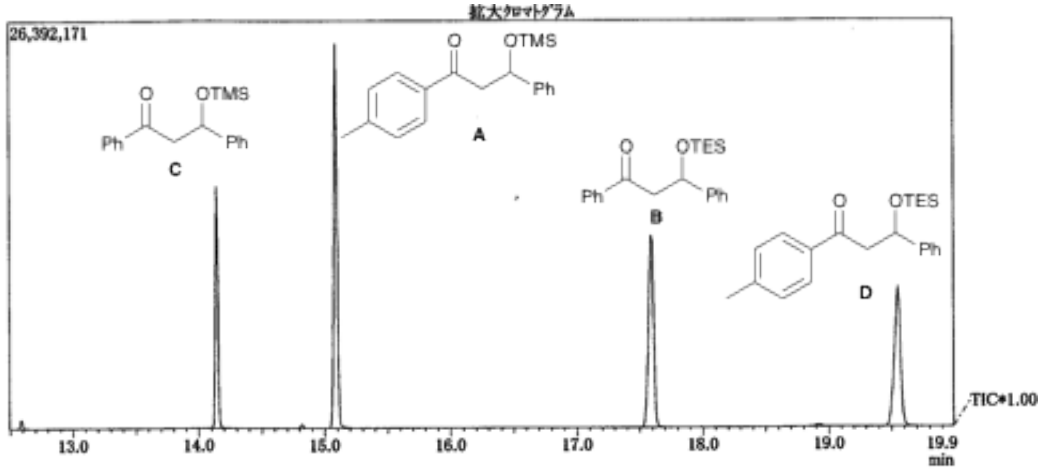
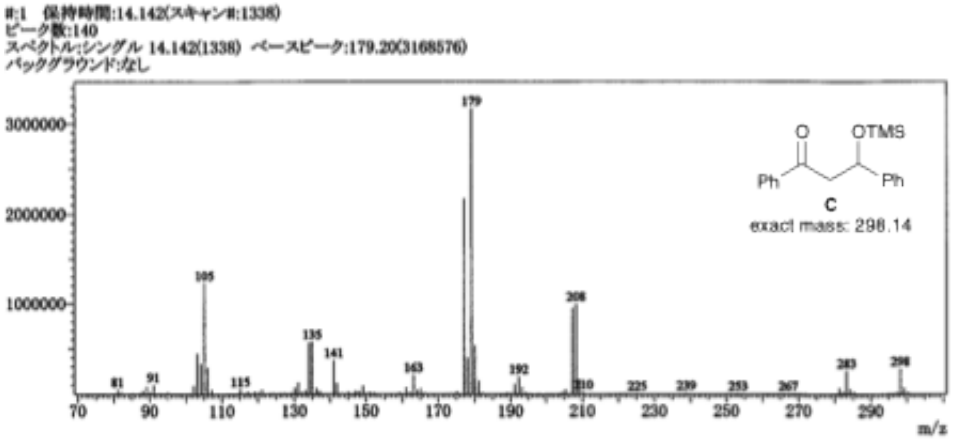
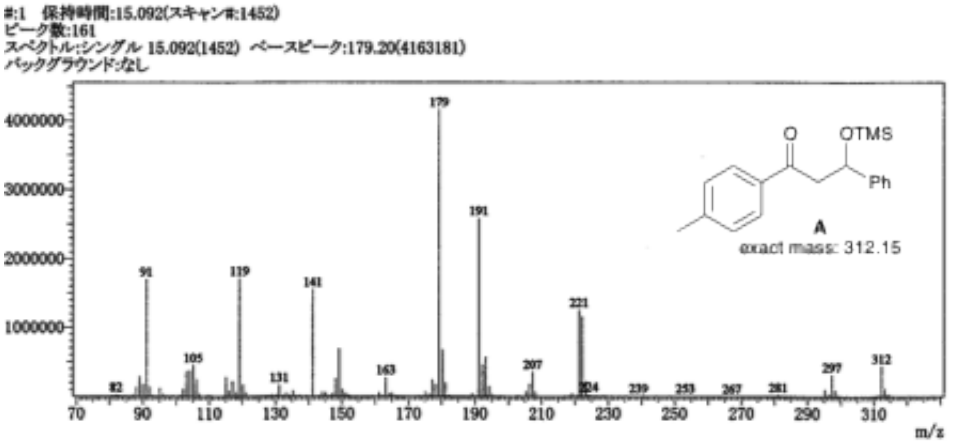


Chart 2. GC-MS spectra of the possible products (**A**, **B**, **C**, and **D)**







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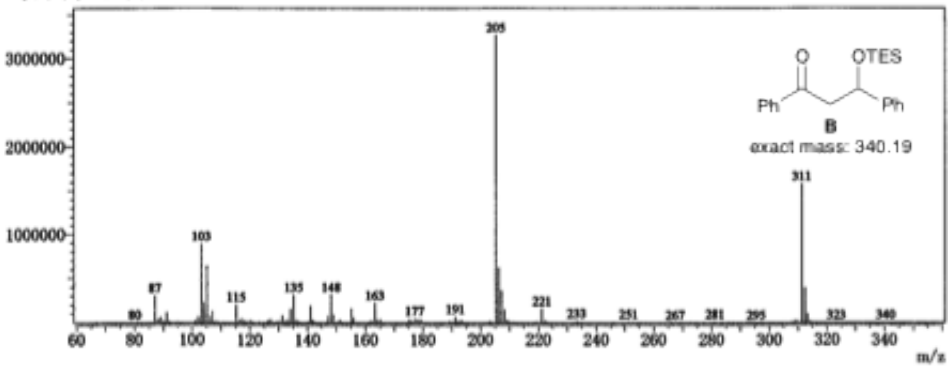

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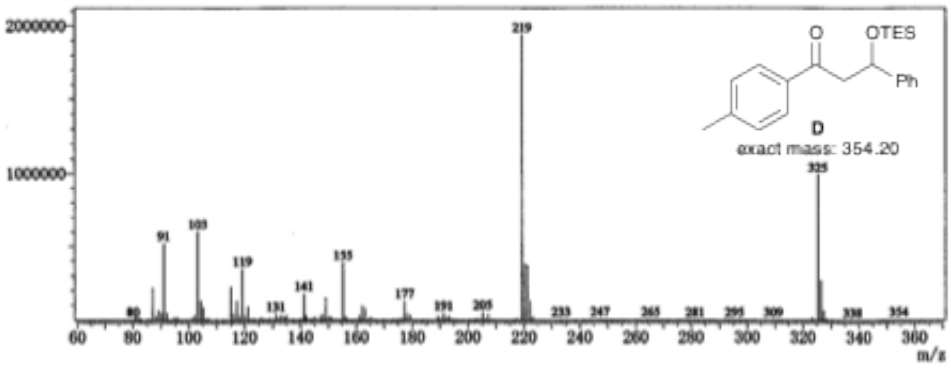
バックグラウンド:なし



Characterization Data of New Compounds

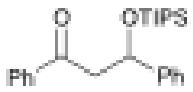
2-allyl-1,1,1,3,3,3-hexamethyl-2-(trimethylsilyl)trisilane:

IR 2949, 2893, 1628, 1420, 1394, 1242 cm^{-1}; ^1H NMR ($CDCl_3$) δ 0.17 (s, 27H), 1.77 (ddd, *J* = 8.0, 1.0, 1.0 Hz, 2H), 4.75 (ddt, *J* = 10.0, 1.0, 1.0 Hz, 1H), 4.88 (ddt, *J* = 17.0, 1.0, 1.0 Hz, 1H), 5.85 (ddt, *J* = 17.0, 10.0, 8.0 Hz, 1H); ^{13}C NMR ($CDCl_3$) δ 1.28, 15.09, 111.98, 138.66 MS (EI) (M^+) 288.

2-allyl-1,1,1,3,3,3-hexaethyl-2-(triethylsilyl)trisilane:

IR 2951, 2874, 1628, 1460, 1235, 1002 cm^{-1}; ^1H NMR ($CDCl_3$) δ 0.76 (q, *J* = 8.0 Hz, 18H), 1.02 (t, *J* = 8.0 Hz, 27H), 1.88 (ddd, *J* = 8.0, 1.0, 1.0 Hz, 2H), 4.76 (ddt, *J* = 10.0, 1.5, 1.0 Hz, 1H), 4.87 (ddt, *J* = 17.0, 1.5, 1.0 Hz, 1H), 5.84 (ddt, *J* = 17.0, 10.0, 8.0 Hz, 1H); ^{13}C NMR ($CDCl_3$) δ 6.26, 9.01, 17.54, 112.33, 139.43 MS (EI) (M^+) 415.

1,3-diphenyl-3-((triisopropylsilyl)oxy)propan-1-one (3b):



IR 2942, 2866, 1686, 1093, 1065 cm^{-1}; ^1H NMR ($CDCl_3$) δ 0.88–1.04 (m, 21H), 3.20 (dd, *J* = 16.0, 6.0 Hz, 1H), 3.54 (dd, *J* = 16.0, 7.0 Hz, 1H), 5.50 (dd, *J* = 7.0, 6.0 Hz, 1H), 7.19–7.24 (m, 1H), 7.27–7.32 (m, 2H), 7.38–7.46 (m, 4H), 7.49–7.55 (m, 1H), 7.88–7.93 (m, 2H); ^{13}C NMR ($CDCl_3$) δ 12.49, 18.06, 18.14, 50.42, 72.29, 126.32, 127.55, 128.35, 128.51, 128.63, 133.16, 137.67, 145.32, 198.55 HRMS (ESI) $[M+Na]^+$ Observed: 405.2220. Calcd for $C_{24}H_{34}O_2SiNa$: 405.2220.

3-((1,1,1,3,3,3-hexamethyl-2-(trimethylsilyl)trisilan-2-yl)oxy)-1,3-diphenylpropan-1-one (3c):

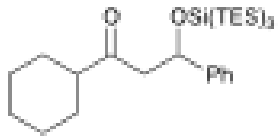
IR 2950, 2893, 1686, 1358, 1244, 1060, 835 cm^{-1}; ^1H NMR ($CDCl_3$) δ 0.03 (s, 27H), 2.96 (dd, *J* = 15.0, 5.0 Hz, 1H), 3.44 (dd, *J* = 15.0, 8.0 Hz, 1H), 5.50 (dd, *J* = 8.0, 5.0 Hz, 1H), 7.21–7.60 (m, 1H), 7.28–7.34 (m, 2H), 7.35–7.46 (m, 4H), 7.50–7.55 (m, 1H), 7.90–7.94 (m, 2H); ^{13}C NMR ($CDCl_3$) δ 0.49, 50.51, 76.37, 126.37, 127.76, 128.52, 128.62, 128.74, 133.12, 137.77, 145.15, 198.43 HRMS (ESI) $[M+Na]^+$ Observed: 495.1986. Calcd for $C_{24}H_{40}O_2Si_4Na$: 495.1998.

3-((1,1,1,3,3,3-hexaethyl-2-(triethylsilyl)trisilan-2-yl)oxy)-1,3-diphenylpropan-1-one

(3d):

IR 2950, 2873, 1686, 1454, 1357, 1055, 1001 cm^{-1}; ^1H NMR ($CDCl_3$) δ 0.70 (q, *J* = 8.0 Hz, 18H), 1.00 (t, *J* = 8.0 Hz, 27H), 3.31 (dd, *J* = 16.0, 5.0 Hz, 1H), 3.39 (dd, *J* = 16.0, 9.0 Hz, 1H), 4.98 (dd, *J* = 9.0, 5.0 Hz, 1H), 7.12–7.16 (m, 1H), 7.18–7.23 (m, 2H), 7.32–7.34 (m, 4H), 7.45–7.48 (m, 1H), 7.73–7.76 (m, 2H); ^{13}C NMR ($CDCl_3$) δ 5.45, 9.02, 50.37, 76.53, 126.78, 127.43, 128.07, 128.22, 128.53, 133.01, 137.45, 144.72, 198.01 HRMS (ESI) $[M+Na]^+$ Observed: 621.3398. Calcd for $C_{33}H_{58}O_2Si_4Na$: 621.3406.

1-cyclohexyl-3-((1,1,1,3,3,3-hexaethyl-2-(triethylsilyl)trisilan-2-yl)oxy)-3-phenylpropan-1-one: (5)



IR 2949, 2873, 1707, 1453, 1056, 1001 cm^{-1}; ^1H NMR ($CDCl_3$) δ 0.69 (q, *J* = 8.0 Hz, 18H), 0.99 (t, *J* = 8.0 Hz, 27H), 1.00–1.17 (m, 5H), 1.35–1.43 (m, 1H), 1.50–1.73 (m, 4H), 1.87–1.96 (m, 1H), 2.80 (dd, *J* = 15.5, 5.0 Hz, 1H), 2.85 (dd, *J* = 15.5, 8.5 Hz, 1H), 4.75 (dd, *J* = 8.5, 5.0 Hz, 1H), 7.14–7.26 (m, 5H); ^{13}C NMR ($CDCl_3$) δ 5.42, 8.99, 25.62, 25.76, 25.96, 27.53, 28.05, 51.75, 52.52, 76.31, 126.67, 127.38, 128.01, 144.75, 211.62 HRMS (ESI) $[M+Na]^+$ Observed: 627.3875. Calcd for $C_{33}H_{64}O_2Si_4Na$: 627.3876.

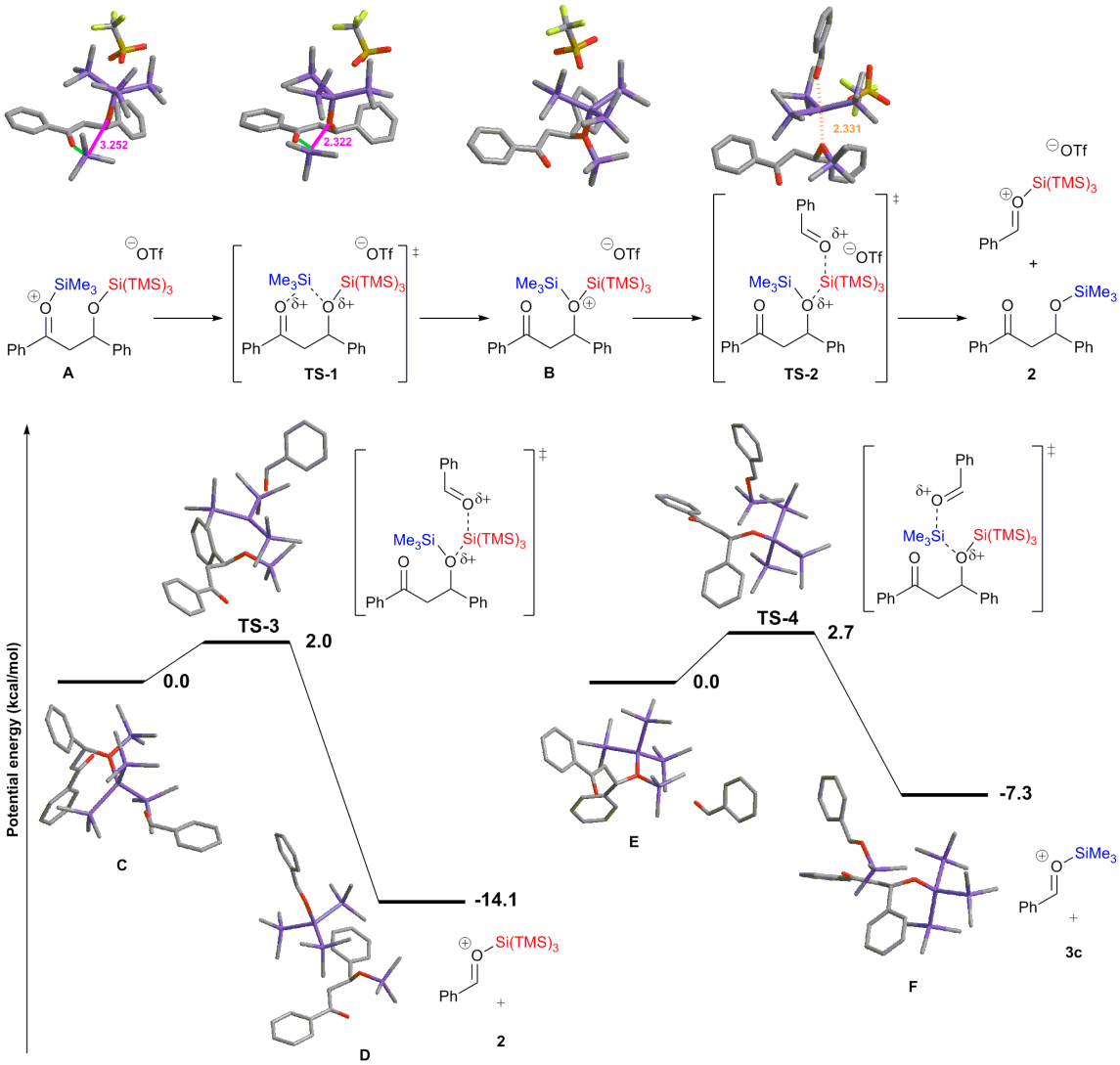
Computational Methods

The quantum chemical calculations were performed using the Gaussian09[1] suites of programs. All the calculations in this paper were performed using density functional theory (DFT) methods employing M06-2X functionals.[2] The standard 6-31G(d) basis set was used for geometry optimizations of the stationary points in the reactions of Scheme 2 and Scheme 3. The optimized geometries are also subjected to full frequency analyses at the same level of theory to verify the nature of the stationary points. Therefore, the energy minimum structures show positive eigenvalues of the Hessian matrix, whereas TSs have one negative eigenvalue. Unscaled vibrational frequencies were used to calculate zero-point energy (ZPE) corrections to total energy. The Gibbs free energies were also calculated employing the usual approximations of statistical thermodynamics (ideal gas, harmonic oscillator, and rigid rotor) at the temperature of 298.15 K and the pressure of 1.00 atm.

References

1) 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, J. 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 Jr., 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, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, in *Gaussian 09, Revision C.01*, Gaussian, Inc., Wallingford CT, 2009.

2) Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.* 2008, **120**, 215-241.



Stable State A

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Method: M06-2X/6-31G(d)
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 Zero-point  correction=                                          0.735501
(Hartree/Particle)
 Thermal correction to Energy=                    0.789842
 Thermal correction to Enthalpy=                  0.790786
 Thermal correction to Gibbs Free Energy=         0.648494
 Sum of electronic and zero-point Energies=          -3616.169050
 Sum of electronic and thermal Energies=             -3616.114709
 Sum of electronic and thermal Enthalpies=           -3616.113765
 Sum of electronic and thermal Free Energies=        -3616.256057
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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.321255	-0.446373	1.756902
2	8	0	1.227012	-1.116692	0.514380
3	6	0	3.054376	1.210329	0.881572
4	6	0	1.727149	1.009031	1.522206

5	8	0	3.898873	0.277462	0.792112
6	14	0	4.473611	-1.372691	0.482400
7	6	0	3.695976	-2.695806	1.528264
8	6	0	6.268455	-1.153864	0.940922
9	6	0	4.166146	-1.470968	-1.340360
10	6	0	0.126575	-0.473919	2.694343
11	6	0	0.200643	-1.256949	3.849047
12	6	0	-0.980147	0.360924	2.507943
13	6	0	-0.800585	-1.192183	4.814790
14	6	0	-1.885040	-0.338397	4.631275
15	6	0	-1.981565	0.428856	3.472624
16	6	0	4.210248	4.990573	-0.647230
17	6	0	4.995451	3.865450	-0.905861
18	6	0	3.058116	4.889406	0.131583
19	6	0	4.627981	2.635612	-0.385904
20	6	0	3.461432	2.521619	0.388162
21	6	0	2.677994	3.658427	0.646070
22	1	0	2.143326	-0.931866	2.297587
23	1	0	0.968484	1.522173	0.920257
24	1	0	1.758196	1.553543	2.479193
25	1	0	2.627653	-2.807037	1.328897
26	1	0	4.195918	-3.637599	1.266916
27	1	0	3.861024	-2.528322	2.597254
28	1	0	6.385539	-0.910210	2.001535
29	1	0	6.814826	-2.084880	0.755224
30	1	0	6.746114	-0.363849	0.353650
31	1	0	4.458039	-2.440720	-1.755148
32	1	0	3.094981	-1.342378	-1.513126
33	1	0	4.704137	-0.682472	-1.877012
34	1	0	1.057742	-1.911419	3.998223
35	1	0	-1.097772	0.958309	1.605883
36	1	0	-0.729784	-1.803023	5.709835
37	1	0	-2.665059	-0.280882	5.384326
38	1	0	-2.833293	1.077804	3.290708
39	1	0	4.498979	5.953244	-1.057782
40	1	0	5.887848	3.951772	-1.516289
41	1	0	2.453863	5.767085	0.332765
42	1	0	5.223494	1.751066	-0.586928
43	1	0	1.779414	3.587398	1.249649
44	14	0	-0.158244	-1.108239	-0.557868
45	14	0	-1.961480	-2.468440	0.168962
46	14	0	-0.389139	1.040941	-1.516929
47	6	0	-2.803004	-2.292746	1.838561
48	6	0	-1.175117	-4.209167	0.251264
49	6	0	-3.292560	-2.420785	-1.179339
50	6	0	-1.556628	0.839645	-2.986621
51	6	0	1.374309	1.430473	-2.194136
52	6	0	-0.824102	2.620023	-0.555845
53	1	0	-3.395020	-1.378878	1.903526
54	1	0	-2.104028	-2.344362	2.677818
55	1	0	-3.491429	-3.144281	1.921856
56	1	0	-0.283683	-4.206930	0.891496
57	1	0	-0.882784	-4.606671	-0.724497
58	1	0	-1.893659	-4.911017	0.691014
59	1	0	-2.980743	-1.874030	-2.074511
60	1	0	-4.161005	-1.895100	-0.770359
61	1	0	-3.592850	-3.430676	-1.481863
62	1	0	-2.556991	0.573095	-2.637201

63	1	0	-1.208103	0.062096	-3.676172
64	1	0	-1.629262	1.777583	-3.549111
65	1	0	2.155954	0.829757	-1.706452
66	1	0	1.627795	2.488293	-2.048450
67	1	0	1.441846	1.218741	-3.265606
68	1	0	0.058344	3.069999	-0.084730
69	1	0	-1.623694	2.521894	0.180994
70	1	0	-1.167116	3.343634	-1.306351
71	14	0	0.628053	-2.433900	-2.392126
72	6	0	-0.798845	-3.257026	-3.330788
73	6	0	1.556523	-1.537660	-3.796406
74	6	0	1.770667	-3.819451	-1.745422
75	1	0	-1.416273	-2.510417	-3.841474
76	1	0	-1.459227	-3.852266	-2.696279
77	1	0	-0.375067	-3.917446	-4.097333
78	1	0	2.427892	-0.951239	-3.496324
79	1	0	0.879434	-0.867644	-4.337213
80	1	0	1.895382	-2.300636	-4.508998
81	1	0	1.188750	-4.705166	-1.475880
82	1	0	2.331286	-3.517552	-0.855289
83	1	0	2.489724	-4.113188	-2.519704
84	6	0	-4.672883	1.892561	-0.995142
85	16	0	-3.975719	1.047414	0.476115
86	9	0	-3.758989	2.706191	-1.541689
87	9	0	-5.743824	2.617940	-0.685358
88	9	0	-5.023198	0.996961	-1.922188
89	8	0	-2.837114	0.312593	-0.120267
90	8	0	-5.063826	0.204020	0.963823
91	8	0	-3.562404	2.155494	1.351173

Transition State 1

Method: M06-2X/6-31G(d)
SCF Done: E(RM062X) = -3616.88939901 A.U. after 6 cycles
Imaginary Frequncy: -146.0872
Zero-point correction= 0.737348
(Hartree/Particle)
Thermal correction to Energy= 0.790897
Thermal correction to Enthalpy= 0.791841
Thermal correction to Gibbs Free Energy= 0.652927
Sum of electronic and zero-point Energies= -3616.152051
Sum of electronic and thermal Energies= -3616.098502
Sum of electronic and thermal Enthalpies= -3616.097558
Sum of electronic and thermal Free Energies= -3616.236472

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.330448	-0.310096	1.889553
2	8	0	1.348447	-1.037200	0.648819
3	6	0	2.961576	1.234789	0.791856
4	6	0	1.715218	1.134759	1.605379
5	8	0	3.595349	0.210744	0.464716

6	14	0	3.573034	-1.702626	0.654129
7	6	0	2.668768	-3.242015	1.243861
8	6	0	4.953137	-1.506694	1.928376
9	6	0	4.243809	-1.885453	-1.074306
10	6	0	0.101122	-0.368438	2.769100
11	6	0	0.142930	-1.162227	3.919800
12	6	0	-0.994907	0.473174	2.560543
13	6	0	-0.887877	-1.109325	4.853010
14	6	0	-1.967910	-0.254994	4.643406
15	6	0	-2.026499	0.528758	3.493855
16	6	0	4.427132	4.977912	-0.573001
17	6	0	5.050548	3.795321	-0.974839
18	6	0	3.334824	4.944402	0.291619
19	6	0	4.579839	2.576035	-0.514165
20	6	0	3.478332	2.534665	0.353416
21	6	0	2.857324	3.725481	0.755584
22	1	0	2.135534	-0.758783	2.492858
23	1	0	0.911461	1.650055	1.067625
24	1	0	1.853057	1.687390	2.543831
25	1	0	1.873324	-3.546851	0.562735
26	1	0	3.408796	-4.049895	1.316786
27	1	0	2.227353	-3.104122	2.236048
28	1	0	4.563575	-1.179543	2.899947
29	1	0	5.431768	-2.478772	2.089696
30	1	0	5.716113	-0.789392	1.614055
31	1	0	4.650054	-2.892340	-1.213771
32	1	0	3.479120	-1.726873	-1.836535
33	1	0	5.046314	-1.160274	-1.236622
34	1	0	1.000071	-1.809285	4.097301
35	1	0	-1.078030	1.085358	1.666500
36	1	0	-0.842549	-1.726789	5.744851
37	1	0	-2.770588	-0.206023	5.372751
38	1	0	-2.870108	1.183114	3.295629
39	1	0	4.793676	5.931434	-0.940258
40	1	0	5.897102	3.829058	-1.652180
41	1	0	2.851576	5.865396	0.599054
42	1	0	5.040014	1.645447	-0.829679
43	1	0	2.000624	3.707473	1.421630
44	14	0	0.016887	-1.088510	-0.555472
45	14	0	-1.861862	-2.398045	0.139798
46	14	0	-0.162819	1.060626	-1.561697
47	6	0	-2.683432	-2.211326	1.816045
48	6	0	-1.207783	-4.191441	0.163175
49	6	0	-3.216908	-2.262055	-1.177946
50	6	0	-1.344221	0.857506	-3.020740
51	6	0	1.587708	1.423289	-2.279895
52	6	0	-0.583652	2.655802	-0.622325
53	1	0	-3.254233	-1.284419	1.880312
54	1	0	-1.992383	-2.286786	2.658974
55	1	0	-3.393864	-3.045649	1.888432
56	1	0	-0.358378	-4.309795	0.846751
57	1	0	-0.909787	-4.563873	-0.820433
58	1	0	-2.009800	-4.844541	0.528208
59	1	0	-2.937966	-1.650613	-2.038922
60	1	0	-4.077029	-1.775046	-0.707638
61	1	0	-3.515263	-3.252980	-1.539116
62	1	0	-2.333397	0.542308	-2.680733
63	1	0	-0.969155	0.133146	-3.751356

64	1	0	-1.456294	1.819408	-3.534581
65	1	0	2.376162	0.781597	-1.864763
66	1	0	1.871972	2.466087	-2.093845
67	1	0	1.596494	1.270438	-3.363713
68	1	0	0.312610	3.136599	-0.212198
69	1	0	-1.352428	2.569464	0.148458
70	1	0	-0.978165	3.346059	-1.378464
71	14	0	0.754739	-2.424442	-2.428449
72	6	0	-0.804332	-2.972029	-3.358016
73	6	0	1.735610	-1.530494	-3.796159
74	6	0	1.690555	-4.039410	-2.055316
75	1	0	-1.411124	-2.123079	-3.685872
76	1	0	-1.450346	-3.636003	-2.778939
77	1	0	-0.477774	-3.514221	-4.254318
78	1	0	2.625566	-0.976614	-3.489993
79	1	0	1.081426	-0.827325	-4.322253
80	1	0	2.046820	-2.290401	-4.524036
81	1	0	1.142675	-4.688292	-1.367038
82	1	0	2.695248	-3.899013	-1.651952
83	1	0	1.790257	-4.577531	-3.006393
84	6	0	-4.457672	1.940959	-1.099680
85	16	0	-3.774616	1.148054	0.406833
86	9	0	-3.544103	2.748646	-1.654173
87	9	0	-5.541307	2.661001	-0.826960
88	9	0	-4.781979	1.013758	-2.004836
89	8	0	-2.621304	0.402392	-0.148903
90	8	0	-4.861286	0.308695	0.906261
91	8	0	-3.381402	2.283693	1.253868

Stable State B

Method: M06-2X/6-31G(d)
SCF Done: E(RM062X) = -3616.91894666 A.U. after 16 cycles
Zero-point correction= 0.740135
(Hartree/Particle)
Thermal correction to Energy= 0.793791
Thermal correction to Enthalpy= 0.794735
Thermal correction to Gibbs Free Energy= 0.656400
Sum of electronic and zero-point Energies= -3616.178811
Sum of electronic and thermal Energies= -3616.125155
Sum of electronic and thermal Enthalpies= -3616.124211
Sum of electronic and thermal Free Energies= -3616.262547

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.472390	-0.242513	1.882099
2	8	0	1.371302	-1.216822	0.743132
3	6	0	3.289309	1.148788	0.800373
4	6	0	1.897960	1.129785	1.396555
5	8	0	3.938631	0.119714	0.719829
6	14	0	2.529413	-2.580715	0.800562
7	6	0	1.408481	-4.058322	0.970377

8	6	0	3.600139	-2.553942	2.336793
9	6	0	3.652020	-2.517086	-0.688675
10	6	0	0.250981	-0.219955	2.763253
11	6	0	0.220383	-1.064482	3.878912
12	6	0	-0.769621	0.716810	2.587610
13	6	0	-0.808914	-0.967666	4.809090
14	6	0	-1.815389	-0.019550	4.631371
15	6	0	-1.800904	0.816775	3.518523
16	6	0	4.926451	4.818034	-0.659867
17	6	0	5.581577	3.607408	-0.886774
18	6	0	3.735459	4.846534	0.061245
19	6	0	5.043269	2.426516	-0.394715
20	6	0	3.843087	2.447147	0.323187
21	6	0	3.192368	3.663532	0.552861
22	1	0	2.295982	-0.639252	2.473469
23	1	0	1.183456	1.564186	0.694837
24	1	0	1.881550	1.794727	2.269890
25	1	0	0.646413	-4.123311	0.195541
26	1	0	1.990722	-4.986705	0.953201
27	1	0	0.896608	-3.995921	1.938693
28	1	0	3.041160	-2.638827	3.273240
29	1	0	4.228222	-3.451971	2.262686
30	1	0	4.264615	-1.688730	2.381467
31	1	0	4.066869	-3.514379	-0.874783
32	1	0	3.164357	-2.183557	-1.605898
33	1	0	4.473876	-1.830815	-0.473450
34	1	0	1.022928	-1.783102	4.034251
35	1	0	-0.781952	1.381343	1.729724
36	1	0	-0.817967	-1.620139	5.676640
37	1	0	-2.615219	0.064151	5.360542
38	1	0	-2.585621	1.547736	3.349587
39	1	0	5.345063	5.741631	-1.047673
40	1	0	6.508146	3.588098	-1.451449
41	1	0	3.227832	5.788614	0.240225
42	1	0	5.530071	1.471314	-0.562891
43	1	0	2.262964	3.699301	1.113302
44	14	0	-0.030736	-1.140421	-0.585341
45	14	0	-2.086075	-2.179573	0.115625
46	14	0	0.119985	1.018275	-1.620266
47	6	0	-2.739694	-1.889683	1.844163
48	6	0	-1.887626	-4.076408	0.039428
49	6	0	-3.382104	-1.728568	-1.188774
50	6	0	-1.046925	0.914703	-3.101490
51	6	0	1.930139	1.137580	-2.240472
52	6	0	-0.211554	2.687364	-0.783398
53	1	0	-3.187576	-0.901133	1.946521
54	1	0	-1.975829	-2.035263	2.612784
55	1	0	-3.527200	-2.636816	2.007144
56	1	0	-1.405253	-4.479912	0.934487
57	1	0	-1.366148	-4.465440	-0.839884
58	1	0	-2.906409	-4.484169	0.012811
59	1	0	-3.014288	-1.055204	-1.965177
60	1	0	-4.185766	-1.194882	-0.670940
61	1	0	-3.789067	-2.627744	-1.663357
62	1	0	-2.084770	0.908599	-2.756603
63	1	0	-0.878163	0.055270	-3.754834
64	1	0	-0.900075	1.819892	-3.703728
65	1	0	2.614272	0.418677	-1.771616

66	1	0	2.324453	2.140949	-2.044317
67	1	0	1.985211	0.975082	-3.320545
68	1	0	0.723204	3.217294	-0.572759
69	1	0	-0.848141	2.674743	0.103046
70	1	0	-0.755973	3.282811	-1.525456
71	14	0	0.524577	-2.535249	-2.503286
72	6	0	-1.134575	-2.827444	-3.377756
73	6	0	1.617314	-1.724869	-3.825307
74	6	0	1.207859	-4.298338	-2.295828
75	1	0	-1.684310	-1.917643	-3.628592
76	1	0	-1.804159	-3.469448	-2.799128
77	1	0	-0.906139	-3.346988	-4.317022
78	1	0	2.615058	-1.422869	-3.497736
79	1	0	1.129118	-0.846111	-4.254770
80	1	0	1.738844	-2.459131	-4.631078
81	1	0	0.496368	-4.969883	-1.807833
82	1	0	2.162533	-4.376758	-1.772933
83	1	0	1.358989	-4.677033	-3.314469
84	6	0	-4.168237	2.336692	-1.050913
85	16	0	-3.437406	1.567714	0.445706
86	9	0	-3.255506	3.077155	-1.692404
87	9	0	-5.199883	3.115948	-0.746243
88	9	0	-4.584648	1.388028	-1.895645
89	8	0	-2.382251	0.712068	-0.149547
90	8	0	-4.546538	0.830557	1.049129
91	8	0	-2.908916	2.700685	1.216060

Transition State 2

Method: M06-2X/6-31G(d)
SCF Done: E(RM062X) = -3962.34669905 A.U. after 6 cycles
Imaginary Frequncy: -155.3389
Zero-point correction= 0.852345
(Hartree/Particle)
Thermal correction to Energy= 0.913402
Thermal correction to Enthalpy= 0.914347
Thermal correction to Gibbs Free Energy= 0.757103
Sum of electronic and zero-point Energies= -3961.494354
Sum of electronic and thermal Energies= -3961.433297
Sum of electronic and thermal Enthalpies= -3961.432353
Sum of electronic and thermal Free Energies= -3961.589596

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.630317	0.069282	1.139520
2	8	0	1.332060	-0.416791	1.602369
3	6	0	4.109207	-1.545232	-0.176125
4	6	0	2.998851	-0.501270	-0.231797
5	8	0	4.668449	-1.830722	0.865096
6	14	0	1.466104	-0.777423	3.307393
7	6	0	-0.200857	-1.171359	4.034317
8	6	0	2.220518	0.683427	4.200864

9	6	0	2.557055	-2.288265	3.518137
10	6	0	2.727841	1.576563	1.220274
11	6	0	4.000087	2.152562	1.265500
12	6	0	1.602878	2.391043	1.258498
13	6	0	4.137107	3.534136	1.345607
14	6	0	3.004494	4.347483	1.384975
15	6	0	1.736213	3.776602	1.337919
16	6	0	5.271460	-3.532917	-3.786646
17	6	0	5.774363	-3.945470	-2.552580
18	6	0	4.386640	-2.460299	-3.858290
19	6	0	5.391311	-3.286352	-1.392401
20	6	0	4.499061	-2.211355	-1.456909
21	6	0	3.999963	-1.799874	-2.696127
22	14	0	-0.590116	-0.676953	0.303090
23	14	0	-2.190643	0.503017	1.676322
24	14	0	-0.089966	0.195056	-1.902909
25	6	0	-1.448234	1.828738	2.793978
26	6	0	-3.236272	-0.739903	2.671597
27	6	0	-3.520547	1.302455	0.597375
28	6	0	-1.638588	0.754572	-2.826390
29	6	0	0.439833	-1.341367	-2.909341
30	6	0	1.276460	1.482833	-2.109734
31	14	0	-0.264107	-3.046364	0.401704
32	6	0	-1.061749	-3.969168	-1.046355
33	6	0	1.569547	-3.499773	0.328936
34	6	0	-1.013984	-3.840883	1.954793
35	6	0	-7.257209	-3.407550	-0.484257
36	6	0	-6.076314	-3.849650	0.117466
37	6	0	-7.272040	-2.247897	-1.256724
38	6	0	-4.902890	-3.130670	-0.053083
39	6	0	-4.914846	-1.967305	-0.833769
40	6	0	-6.097600	-1.525981	-1.433672
41	6	0	-3.694984	-1.179306	-1.028346
42	8	0	-2.622356	-1.474019	-0.513253
43	1	0	3.384112	-0.340253	1.823982
44	1	0	2.128829	-0.951224	-0.722430
45	1	0	3.337486	0.306443	-0.888999
46	1	0	-0.816983	-1.763097	3.358918
47	1	0	-0.023643	-1.779572	4.930400
48	1	0	-0.765133	-0.286037	4.333664
49	1	0	1.683485	1.616522	4.008749
50	1	0	2.168967	0.475507	5.276785
51	1	0	3.270279	0.850858	3.942601
52	1	0	2.844829	-2.346178	4.575144
53	1	0	2.020126	-3.210837	3.273949
54	1	0	3.474846	-2.261189	2.923209
55	1	0	4.883127	1.514710	1.248933
56	1	0	0.611043	1.960932	1.188046
57	1	0	5.128388	3.975906	1.385461
58	1	0	3.113250	5.425903	1.447207
59	1	0	0.839852	4.391137	1.342002
60	1	0	5.570899	-4.049119	-4.693758
61	1	0	6.463852	-4.782061	-2.498943
62	1	0	3.997624	-2.134615	-4.817754
63	1	0	5.767456	-3.587266	-0.420021
64	1	0	3.313835	-0.961145	-2.765393
65	1	0	-1.355875	2.763162	2.228986
66	1	0	-0.470204	1.591722	3.218553

67	1	0	-2.144606	1.999962	3.624756
68	1	0	-2.755860	-1.253145	3.503908
69	1	0	-3.661317	-1.491812	1.995782
70	1	0	-4.081115	-0.169238	3.078929
71	1	0	-4.440246	0.704705	0.613840
72	1	0	-3.218874	1.501851	-0.429575
73	1	0	-3.756634	2.284651	1.024122
74	1	0	-2.224459	1.516722	-2.307406
75	1	0	-2.264933	-0.096142	-3.111484
76	1	0	-1.282369	1.209745	-3.759663
77	1	0	1.157552	-2.013640	-2.425231
78	1	0	0.894742	-1.000627	-3.849085
79	1	0	-0.440397	-1.934130	-3.177274
80	1	0	2.144941	1.055547	-2.623257
81	1	0	1.594981	1.961217	-1.182969
82	1	0	0.871207	2.277275	-2.742110
83	1	0	-0.642613	-3.683143	-2.012989
84	1	0	-2.146376	-3.845110	-1.089276
85	1	0	-0.848798	-5.035678	-0.899963
86	1	0	2.186149	-2.906257	1.006802
87	1	0	1.967386	-3.386945	-0.686952
88	1	0	1.688874	-4.554493	0.605557
89	1	0	-1.981491	-3.404794	2.228181
90	1	0	-0.356973	-3.777084	2.827231
91	1	0	-1.174168	-4.905027	1.744155
92	1	0	-8.174472	-3.971741	-0.345382
93	1	0	-6.079215	-4.752135	0.719600
94	1	0	-8.194890	-1.909115	-1.715474
95	1	0	-3.972060	-3.449728	0.408694
96	1	0	-6.091403	-0.616836	-2.029941
97	1	0	-3.777809	-0.287562	-1.665000
98	6	0	-0.483182	4.663515	-1.773676
99	16	0	-1.553631	3.810061	-0.550593
100	9	0	0.798502	4.624938	-1.404073
101	9	0	-0.843611	5.935463	-1.912207
102	9	0	-0.581334	4.070844	-2.972372
103	8	0	-0.901632	2.482858	-0.416284
104	8	0	-2.855314	3.775307	-1.218687
105	8	0	-1.445004	4.635802	0.655749

Stable State 2

Method: M06-2X/6-31G(d)
SCF Done: E(RM062X) = -3962.38328894 A.U. after 16 cycles
Zero-point correction= 0.850579
(Hartree/Particle)
Thermal correction to Energy= 0.913356
Thermal correction to Enthalpy= 0.914300
Thermal correction to Gibbs Free Energy= 0.750994
Sum of electronic and zero-point Energies= -3961.532710
Sum of electronic and thermal Energies= -3961.469933
Sum of electronic and thermal Enthalpies= -3961.468989
Sum of electronic and thermal Free Energies= -3961.632295

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.717271	1.362522	-0.066389
2	8	0	3.261999	0.867553	1.185348
3	6	0	4.617432	-0.863056	-0.851479
4	6	0	3.585134	0.230461	-1.077127
5	8	0	5.474949	-0.753208	0.000802
6	14	0	3.962403	1.462328	2.598341
7	6	0	3.068966	0.591704	3.993849
8	6	0	3.699666	3.318310	2.707343
9	6	0	5.793906	1.062269	2.641675
10	6	0	2.940286	2.593842	-0.484511
11	6	0	3.602195	3.729059	-0.952257
12	6	0	1.548876	2.609118	-0.395528
13	6	0	2.884303	4.866567	-1.314501
14	6	0	1.496529	4.879973	-1.198457
15	6	0	0.826934	3.748508	-0.736382
16	6	0	4.485944	-4.415179	-3.250840
17	6	0	5.398684	-4.296819	-2.202508
18	6	0	3.614719	-3.368239	-3.539392
19	6	0	5.434907	-3.135620	-1.441682
20	6	0	4.560397	-2.082146	-1.723257
21	6	0	3.654112	-2.201788	-2.780090
22	14	0	-0.831677	-1.157372	0.570505
23	14	0	-1.072417	0.360224	2.408052
24	14	0	-0.844976	-0.809479	-1.804505
25	6	0	-0.195549	2.013292	2.328648
26	6	0	-0.407656	-0.569947	3.918391
27	6	0	-2.910960	0.600713	2.791546
28	6	0	-2.643713	-0.973057	-2.370341
29	6	0	0.048531	-2.296307	-2.579634
30	6	0	-0.040596	0.709023	-2.565326
31	14	0	0.380099	-3.117988	1.114401
32	6	0	-0.156559	-4.535058	-0.028555
33	6	0	2.213383	-2.732906	0.873329
34	6	0	0.066401	-3.741728	2.873394
35	6	0	-7.440567	-2.879050	0.666351
36	6	0	-6.338500	-3.709291	0.904290
37	6	0	-7.274377	-1.528733	0.366717
38	6	0	-5.059780	-3.185840	0.842866
39	6	0	-4.892177	-1.823374	0.541339
40	6	0	-5.995170	-0.988651	0.302004
41	6	0	-3.586074	-1.225329	0.466239
42	8	0	-2.540878	-1.899377	0.663465
43	1	0	4.784763	1.623170	-0.005412
44	1	0	2.575622	-0.199588	-1.002118
45	1	0	3.690994	0.617482	-2.099237
46	1	0	3.059076	-0.492333	3.836632
47	1	0	3.564396	0.786481	4.951172
48	1	0	2.033791	0.937476	4.076775
49	1	0	2.637290	3.571813	2.619553
50	1	0	4.064485	3.701097	3.667348
51	1	0	4.227937	3.851657	1.910192
52	1	0	6.231110	1.423336	3.579689
53	1	0	5.961399	-0.015751	2.567912
54	1	0	6.340183	1.531151	1.817284

55	1	0	4.688595	3.727024	-1.018987
56	1	0	1.021031	1.723897	-0.047731
57	1	0	3.410692	5.746490	-1.672400
58	1	0	0.935032	5.770120	-1.464706
59	1	0	-0.254782	3.750488	-0.638150
60	1	0	4.454991	-5.324719	-3.843087
61	1	0	6.078049	-5.113572	-1.979083
62	1	0	2.901381	-3.457945	-4.352894
63	1	0	6.131071	-3.019710	-0.617164
64	1	0	2.969224	-1.391528	-3.015746
65	1	0	-0.637844	2.664883	1.570847
66	1	0	0.874229	1.898615	2.129751
67	1	0	-0.310221	2.492803	3.309223
68	1	0	0.630480	-0.890594	3.793313
69	1	0	-1.012686	-1.451716	4.151955
70	1	0	-0.443069	0.097430	4.788594
71	1	0	-3.424542	-0.351634	2.971737
72	1	0	-3.471370	1.178115	2.051978
73	1	0	-2.952923	1.160929	3.733986
74	1	0	-3.306189	-0.199667	-1.972923
75	1	0	-3.051309	-1.963452	-2.135265
76	1	0	-2.654428	-0.871078	-3.462444
77	1	0	1.021360	-2.503046	-2.120324
78	1	0	0.224887	-2.084477	-3.642283
79	1	0	-0.551627	-3.209132	-2.519807
80	1	0	1.047314	0.712697	-2.446387
81	1	0	-0.433760	1.643209	-2.166069
82	1	0	-0.255628	0.671095	-3.641120
83	1	0	0.401693	-4.531848	-0.967629
84	1	0	-1.224413	-4.482174	-0.269684
85	1	0	0.024714	-5.494810	0.467792
86	1	0	2.504218	-1.765001	1.301366
87	1	0	2.455113	-2.711067	-0.195518
88	1	0	2.839996	-3.508249	1.328593
89	1	0	-1.002316	-3.777258	3.110720
90	1	0	0.562463	-3.136329	3.634304
91	1	0	0.456706	-4.763478	2.948563
92	1	0	-8.441731	-3.296920	0.717453
93	1	0	-6.490282	-4.758110	1.136114
94	1	0	-8.138783	-0.899673	0.183626
95	1	0	-4.185835	-3.804010	1.024977
96	1	0	-5.824315	0.060842	0.070163
97	1	0	-3.507169	-0.158464	0.231916
98	6	0	-3.083250	3.039490	-2.114139
99	16	0	-3.144460	2.419740	-0.385992
100	9	0	-1.959554	3.728635	-2.324041
101	9	0	-4.119062	3.831106	-2.364513
102	9	0	-3.107328	2.020905	-2.978802
103	8	0	-1.998869	1.479134	-0.320925
104	8	0	-4.440607	1.718093	-0.328080
105	8	0	-3.000860	3.612679	0.437652

Stable State C

Method: M06-2X/6-31G(d)
SCF Done: E(RM062X) = -3000.95492378 A.U. after 8 cycles
Zero-point correction= 0.822233 (Hartree/Particle)

Thermal correction to Energy= 0.874641
Thermal correction to Enthalpy= 0.875585
Thermal correction to Gibbs Free Energy= 0.738986
Sum of electronic and zero-point Energies= -3000.132691
Sum of electronic and thermal Energies= -3000.080283
Sum of electronic and thermal Enthalpies= -3000.079339
Sum of electronic and thermal Free Energies= -3000.215938

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.475735	1.311365	0.337221
2	8	0	1.177219	0.863063	0.926439
3	6	0	3.782788	-0.836496	0.525065
4	6	0	3.139445	0.174275	-0.418219
5	8	0	3.785796	-0.620127	1.723512
6	14	0	0.999050	1.254539	2.686674
7	6	0	-0.770681	1.751048	3.027739
8	6	0	2.081464	2.731719	3.060914
9	6	0	1.514441	-0.164527	3.777540
10	6	0	2.357534	2.589143	-0.456400
11	6	0	3.146997	3.681695	-0.087971
12	6	0	1.557068	2.693087	-1.593632
13	6	0	3.124967	4.857342	-0.834923
14	6	0	2.315710	4.951466	-1.963539
15	6	0	1.531801	3.864025	-2.343127
16	6	0	5.608146	-4.365460	-1.037251
17	6	0	5.455628	-4.195719	0.338816
18	6	0	5.162661	-3.384667	-1.921340
19	6	0	4.860018	-3.043099	0.832012
20	6	0	4.406279	-2.056064	-0.050404
21	6	0	4.559489	-2.232613	-1.430688
22	1	0	3.110038	1.506175	1.201677
23	1	0	2.447737	-0.328679	-1.096702
24	1	0	3.923642	0.603075	-1.055788
25	1	0	-1.542831	1.133954	2.568065
26	1	0	-0.899682	1.661665	4.114547
27	1	0	-0.952772	2.795645	2.762641
28	1	0	1.951436	3.559380	2.357986
29	1	0	1.764293	3.091589	4.047748
30	1	0	3.145357	2.487599	3.136482
31	1	0	1.506395	0.242457	4.797749
32	1	0	0.841421	-1.022529	3.761377
33	1	0	2.526945	-0.507106	3.557317
34	1	0	3.789239	3.613679	0.786948
35	1	0	0.939011	1.857075	-1.894560
36	1	0	3.742593	5.697622	-0.535212
37	1	0	2.299816	5.865708	-2.547779
38	1	0	0.900597	3.925404	-3.225179
39	1	0	6.076512	-5.265788	-1.422471
40	1	0	5.805329	-4.961515	1.023267
41	1	0	5.287156	-3.517993	-2.990914
42	1	0	4.736512	-2.883905	1.898435
43	1	0	4.211145	-1.476008	-2.129157
44	14	0	-0.370194	0.175027	-0.046603
45	14	0	-1.714615	2.146444	-0.227628

46	14	0	0.164190	-0.881908	-2.173174
47	6	0	-0.788881	3.718618	0.308566
48	6	0	-3.314510	2.020328	0.788237
49	6	0	-2.147987	2.344715	-2.057662
50	6	0	-1.455620	-1.253356	-3.067088
51	6	0	1.043037	-2.533240	-1.881196
52	6	0	1.174590	0.059652	-3.474656
53	14	0	-0.883613	-1.757827	1.267984
54	6	0	-1.932204	-3.010737	0.318421
55	6	0	0.781904	-2.595446	1.623517
56	6	0	-1.855720	-1.447528	2.861369
57	1	0	-0.560891	4.335635	-0.565263
58	1	0	0.160417	3.538417	0.819915
59	1	0	-1.429004	4.305574	0.976339
60	1	0	-3.335111	2.775726	1.579421
61	1	0	-3.455394	1.037831	1.245489
62	1	0	-4.178332	2.195855	0.136650
63	1	0	-2.834212	1.566277	-2.401277
64	1	0	-1.260809	2.323857	-2.701197
65	1	0	-2.638250	3.313623	-2.208183
66	1	0	-2.011276	-0.338677	-3.294803
67	1	0	-2.109790	-1.929117	-2.514535
68	1	0	-1.193829	-1.730552	-4.019218
69	1	0	1.911089	-2.488385	-1.217639
70	1	0	1.395076	-2.906267	-2.850855
71	1	0	0.359405	-3.283845	-1.474473
72	1	0	1.297252	-0.639682	-4.311097
73	1	0	2.171303	0.392149	-3.173384
74	1	0	0.634728	0.929269	-3.864803
75	1	0	-1.675613	-3.112892	-0.738057
76	1	0	-2.995909	-2.769489	0.386527
77	1	0	-1.774302	-3.987835	0.791646
78	1	0	1.623239	-1.902937	1.716578
79	1	0	1.015042	-3.306464	0.824892
80	1	0	0.721350	-3.165016	2.558682
81	1	0	-2.775119	-0.887708	2.655789
82	1	0	-1.315290	-0.920198	3.649904
83	1	0	-2.151609	-2.426313	3.258394
84	6	0	-7.925760	-1.502273	0.464646
85	6	0	-6.790653	-1.464780	1.278611
86	6	0	-7.829642	-1.245704	-0.901623
87	6	0	-5.554824	-1.165864	0.725320
88	6	0	-5.454632	-0.905896	-0.646796
89	6	0	-6.591709	-0.948096	-1.458823
90	6	0	-4.159517	-0.582503	-1.256526
91	8	0	-3.107079	-0.495052	-0.647071
92	1	0	-8.892209	-1.734262	0.901381
93	1	0	-6.878609	-1.668956	2.340559
94	1	0	-8.715972	-1.277494	-1.526086
95	1	0	-4.657291	-1.133563	1.336158
96	1	0	-6.501525	-0.746548	-2.523701
97	1	0	-4.177561	-0.412879	-2.351595

Transition State 3

Method: M06-2X/6-31G(d)
SCF Done: E(RM062X) = -3000.94712046 A.U. after 7 cycles
Zero-point correction= 0.820809 (Hartree/Particle)
Thermal correction to Energy= 0.873958
Thermal correction to Enthalpy= 0.874902
Thermal correction to Gibbs Free Energy= 0.734376
Sum of electronic and zero-point Energies= -3000.126312
Sum of electronic and thermal Energies= -3000.073162
Sum of electronic and thermal Enthalpies= -3000.072218
Sum of electronic and thermal Free Energies= -3000.212745

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.469232	-1.298289	0.381059
2	8	0	-1.155944	-0.997181	0.945958
3	6	0	-3.757177	0.886414	0.560175
4	6	0	-3.026808	-0.088040	-0.357416
5	8	0	-3.907469	0.625408	1.738410
6	14	0	-0.972035	-1.532894	2.603038
7	6	0	0.834179	-1.892977	2.968833
8	6	0	-1.931982	-3.122839	2.863186
9	6	0	-1.641063	-0.265801	3.802003
10	6	0	-2.445117	-2.533324	-0.490393
11	6	0	-3.366291	-3.556922	-0.266205
12	6	0	-1.570105	-2.639624	-1.570510
13	6	0	-3.408305	-4.668352	-1.105774
14	6	0	-2.531046	-4.763429	-2.182148
15	6	0	-1.609981	-3.743529	-2.414784
16	6	0	-5.311067	4.544455	-1.015161
17	6	0	-5.260814	4.327366	0.361777
18	6	0	-4.852282	3.568666	-1.897394
19	6	0	-4.754685	3.132976	0.856321
20	6	0	-4.285724	2.151116	-0.023663
21	6	0	-4.337050	2.374840	-1.403992
22	1	0	-3.150933	-1.481370	1.217816
23	1	0	-2.233014	0.439485	-0.895699
24	1	0	-3.736200	-0.431347	-1.121232
25	1	0	1.554238	-1.180912	2.563512
26	1	0	0.941704	-1.863969	4.060706
27	1	0	1.117175	-2.897415	2.643252
28	1	0	-1.770134	-3.878851	2.089856
29	1	0	-1.589465	-3.548610	3.814474
30	1	0	-3.009067	-2.953848	2.960906
31	1	0	-1.632804	-0.729545	4.796601
32	1	0	-1.054433	0.653304	3.861244
33	1	0	-2.672697	0.004184	3.562259
34	1	0	-4.056247	-3.486090	0.571511
35	1	0	-0.843579	-1.852361	-1.745349
36	1	0	-4.128189	-5.458486	-0.918431
37	1	0	-2.565035	-5.627320	-2.837907
38	1	0	-0.924102	-3.810300	-3.255196
39	1	0	-5.711132	5.476486	-1.401908
40	1	0	-5.620944	5.088704	1.045927
41	1	0	-4.899164	3.736893	-2.968344
42	1	0	-4.712404	2.935719	1.922718

43	1	0	-3.979571	1.621620	-2.101423
44	14	0	0.747542	-0.069109	-0.105635
45	14	0	1.787340	-2.215045	-0.316788
46	14	0	0.067311	0.988541	-2.186413
47	6	0	0.808938	-3.751984	0.194363
48	6	0	3.454975	-2.182538	0.593721
49	6	0	2.116753	-2.360731	-2.176892
50	6	0	1.617873	1.480827	-3.153607
51	6	0	-0.854879	2.604282	-1.846784
52	6	0	-0.954894	-0.005714	-3.428918
53	14	0	0.824845	1.741457	1.443160
54	6	0	1.858343	3.089331	0.602244
55	6	0	-0.909642	2.421021	1.737687
56	6	0	1.698075	1.384689	3.080613
57	1	0	0.616270	-4.367156	-0.690225
58	1	0	-0.161403	-3.537632	0.643913
59	1	0	1.395764	-4.349128	0.899826
60	1	0	3.641211	-3.156750	1.057060
61	1	0	3.510461	-1.424631	1.381100
62	1	0	4.278639	-1.993466	-0.103779
63	1	0	2.617374	-1.489101	-2.609478
64	1	0	1.183882	-2.514468	-2.730119
65	1	0	2.753923	-3.233104	-2.364295
66	1	0	2.165632	0.613960	-3.537046
67	1	0	2.302463	2.123260	-2.592656
68	1	0	1.277111	2.053145	-4.024744
69	1	0	-1.737664	2.510612	-1.209977
70	1	0	-1.195872	2.999612	-2.812009
71	1	0	-0.204070	3.360758	-1.398343
72	1	0	-1.092719	0.646321	-4.300513
73	1	0	-1.945187	-0.309598	-3.080671
74	1	0	-0.431399	-0.902508	-3.776592
75	1	0	1.736258	3.130398	-0.483732
76	1	0	2.924572	2.957754	0.810427
77	1	0	1.556854	4.063153	1.005881
78	1	0	-1.661336	1.645752	1.897383
79	1	0	-1.231717	3.046824	0.899214
80	1	0	-0.897843	3.056207	2.631918
81	1	0	2.664323	0.891105	2.927162
82	1	0	1.120283	0.774477	3.777840
83	1	0	1.894008	2.349182	3.564733
84	6	0	7.685530	1.523367	0.403832
85	6	0	6.599902	1.522932	1.285208
86	6	0	7.514867	1.205833	-0.942851
87	6	0	5.335014	1.205449	0.819058
88	6	0	5.158654	0.887744	-0.536230
89	6	0	6.248981	0.884895	-1.415344
90	6	0	3.846065	0.545204	-1.057213
91	8	0	2.821687	0.555208	-0.372860
92	1	0	8.675031	1.773011	0.774068
93	1	0	6.751158	1.768991	2.330742
94	1	0	8.365193	1.208766	-1.615812
95	1	0	4.475367	1.193951	1.482366
96	1	0	6.098671	0.634890	-2.462810
97	1	0	3.794509	0.266782	-2.120045

Stable State D

Method: M06-2X/6-31G(d)
SCF Done: E(RM062X) = -3000.96329757 A.U. after 6 cycles
Zero-point correction= 0.816738 (Hartree/Particle)
Thermal correction to Energy= 0.872434
Thermal correction to Enthalpy= 0.873378
Thermal correction to Gibbs Free Energy= 0.724816
Sum of electronic and zero-point Energies= -3000.146560
Sum of electronic and thermal Energies= -3000.090864
Sum of electronic and thermal Enthalpies= -3000.089919
Sum of electronic and thermal Free Energies= -3000.238481

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.217704	1.226609	-0.534371
2	8	0	2.609894	1.263546	0.748599
3	6	0	4.111560	-1.105551	-0.179944
4	6	0	3.233563	-0.209495	-1.041704
5	8	0	4.785964	-0.635788	0.715902
6	14	0	3.372313	1.801823	2.162975
7	6	0	2.347011	3.232887	2.819458
8	6	0	5.110688	2.412449	1.826966
9	6	0	3.355269	0.409917	3.415086
10	6	0	2.488580	2.188963	-1.456578
11	6	0	2.853571	3.536662	-1.427690
12	6	0	1.442926	1.798675	-2.296153
13	6	0	2.199092	4.476326	-2.217971
14	6	0	1.166878	4.074453	-3.063811
15	6	0	0.795029	2.733221	-3.103357
16	6	0	4.102100	-5.338357	-0.828164
17	6	0	4.723673	-4.791957	0.294375
18	6	0	3.485890	-4.507216	-1.760935
19	6	0	4.726444	-3.416233	0.485561
20	6	0	4.102873	-2.576762	-0.442552
21	6	0	3.485349	-3.129200	-1.568560
22	1	0	4.260219	1.560993	-0.457088
23	1	0	2.218345	-0.626762	-1.041229
24	1	0	3.591169	-0.241192	-2.079676
25	1	0	1.334274	2.924663	3.100882
26	1	0	2.820654	3.657578	3.711670
27	1	0	2.257410	4.030813	2.073935
28	1	0	5.133857	3.264011	1.137957
29	1	0	5.545061	2.756980	2.772559
30	1	0	5.752568	1.621755	1.430591
31	1	0	3.808727	0.745291	4.354599
32	1	0	2.331569	0.090535	3.641070
33	1	0	3.917044	-0.455650	3.052487
34	1	0	3.670044	3.849147	-0.780000
35	1	0	1.141559	0.753959	-2.346198
36	1	0	2.502998	5.517923	-2.185732
37	1	0	0.666246	4.798985	-3.698339
38	1	0	0.010754	2.413256	-3.784119
39	1	0	4.103339	-6.413442	-0.978911

40	1	0	5.206983	-5.441418	1.017208
41	1	0	3.014401	-4.931465	-2.641874
42	1	0	5.206297	-2.967029	1.349255
43	1	0	3.015139	-2.488664	-2.308737
44	14	0	-1.515670	-0.108841	-0.090628
45	14	0	-1.798695	2.249650	0.013662
46	14	0	-1.533910	-1.328615	-2.128117
47	6	0	-0.202468	3.156077	0.399101
48	6	0	-3.039737	2.501758	1.421515
49	6	0	-2.601533	2.860934	-1.582698
50	6	0	-2.856255	-2.666630	-1.902901
51	6	0	0.129035	-2.157013	-2.439816
52	6	0	-1.975409	-0.237856	-3.602032
53	14	0	-0.497747	-1.205404	1.746795
54	6	0	-1.552747	-2.745413	2.036926
55	6	0	1.277897	-1.724731	1.447175
56	6	0	-0.623010	-0.018163	3.204145
57	1	0	0.136445	3.722912	-0.474632
58	1	0	0.611159	2.482144	0.684338
59	1	0	-0.372465	3.860475	1.220979
60	1	0	-3.203723	3.578636	1.546190
61	1	0	-2.657814	2.116849	2.372170
62	1	0	-4.018675	2.046687	1.237176
63	1	0	-3.572586	2.391131	-1.778924
64	1	0	-1.956783	2.696600	-2.450353
65	1	0	-2.777464	3.939958	-1.499167
66	1	0	-3.878852	-2.281197	-1.984022
67	1	0	-2.764023	-3.181621	-0.941037
68	1	0	-2.741361	-3.416416	-2.693532
69	1	0	0.900513	-1.427092	-2.705862
70	1	0	0.030611	-2.849220	-3.284431
71	1	0	0.483435	-2.732481	-1.578037
72	1	0	-2.025209	-0.842733	-4.514400
73	1	0	-1.217387	0.536629	-3.757872
74	1	0	-2.941332	0.265302	-3.483483
75	1	0	-1.411605	-3.472224	1.229366
76	1	0	-2.621097	-2.521803	2.113452
77	1	0	-1.243014	-3.230482	2.969609
78	1	0	1.921861	-0.852650	1.303029
79	1	0	1.378918	-2.394096	0.585641
80	1	0	1.639314	-2.270049	2.327859
81	1	0	-1.666090	0.210144	3.447391
82	1	0	-0.106911	0.924389	2.984913
83	1	0	-0.161224	-0.454040	4.097180
84	6	0	-8.188024	-0.911854	1.280774
85	6	0	-7.094172	-1.099230	2.133895
86	6	0	-8.010470	-0.536467	-0.051662
87	6	0	-5.809893	-0.913867	1.655863
88	6	0	-5.625971	-0.535582	0.312141
89	6	0	-6.727309	-0.343923	-0.539767
90	6	0	-4.312186	-0.320427	-0.216037
91	8	0	-3.272747	-0.506109	0.455294
92	1	0	-9.192959	-1.058413	1.664483
93	1	0	-7.256275	-1.386451	3.166988
94	1	0	-8.869089	-0.393440	-0.698188
95	1	0	-4.943930	-1.045167	2.297488
96	1	0	-6.567986	-0.047679	-1.573660
97	1	0	-4.211698	0.033328	-1.252586

Stable State E

Method: M06-2X/6-31G(d)
SCF Done: E(RM062X) = -3000.96190620 A.U. after 7 cycles
Zero-point correction= 0.820800 (Hartree/Particle)
Thermal correction to Energy= 0.875178
Thermal correction to Enthalpy= 0.876122
Thermal correction to Gibbs Free Energy= 0.730981
Sum of electronic and zero-point Energies= -3000.141106
Sum of electronic and thermal Energies= -3000.086729
Sum of electronic and thermal Enthalpies= -3000.085784
Sum of electronic and thermal Free Energies= -3000.230926

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.965100	0.725193	1.104215
2	8	0	-0.215457	-0.394298	0.498965
3	6	0	-1.527871	3.091282	0.478288
4	6	0	-1.540978	1.627599	0.024803
5	8	0	-0.840422	3.423660	1.424482
6	6	0	-1.922084	0.217625	2.155790
7	6	0	-3.060114	0.953398	2.493959
8	6	0	-1.592389	-0.910933	2.911452
9	6	0	-3.860017	0.558076	3.563997
10	6	0	-3.526421	-0.568993	4.311275
11	6	0	-2.390492	-1.304462	3.980547
12	6	0	-3.880195	5.986160	-1.601411
13	6	0	-3.199982	6.328428	-0.432704
14	6	0	-3.798378	4.691257	-2.108845
15	6	0	-2.437713	5.376036	0.228883
16	6	0	-2.359286	4.070683	-0.270288
17	6	0	-3.042847	3.732216	-1.443219
18	14	0	-1.080354	-1.581248	-0.638908
19	14	0	-0.381728	-3.799753	-0.089425
20	14	0	-3.456976	-1.621701	-0.416982
21	6	0	0.027060	-3.940828	1.749578
22	6	0	1.065658	-4.429628	-1.139316
23	6	0	-1.806134	-4.985515	-0.466809
24	6	0	-3.905186	-2.638727	-1.953987
25	6	0	-4.505737	-0.060451	-0.607759
26	6	0	-4.014580	-2.491913	1.160066
27	14	0	-0.548627	-1.037678	-2.890671
28	6	0	-1.080892	-2.536726	-3.917437
29	6	0	-1.537081	0.472081	-3.455968
30	6	0	1.278796	-0.745839	-3.277578
31	1	0	-0.212885	1.321037	1.627868
32	1	0	-0.910958	1.562684	-0.871638
33	1	0	-2.547259	1.327038	-0.269526
34	1	0	-3.323551	1.851479	1.940714
35	1	0	-0.703581	-1.481700	2.662203
36	1	0	-4.739573	1.140140	3.819014

37	1	0	-4.146988	-0.869954	5.148907
38	1	0	-2.121965	-2.183967	4.557791
39	1	0	-4.474601	6.732371	-2.119300
40	1	0	-3.265390	7.338349	-0.041476
41	1	0	-4.324300	4.429708	-3.021039
42	1	0	-1.893877	5.619000	1.135915
43	1	0	-2.978854	2.728079	-1.853787
44	1	0	-0.866479	-3.787747	2.364198
45	1	0	0.796060	-3.235391	2.082421
46	1	0	0.399876	-4.951745	1.951244
47	1	0	0.924306	-5.505015	-1.296524
48	1	0	2.035485	-4.292106	-0.656220
49	1	0	1.116460	-3.962908	-2.129437
50	1	0	-1.914676	-5.145142	-1.544716
51	1	0	-2.777499	-4.686008	-0.065249
52	1	0	-1.546980	-5.955380	-0.024518
53	1	0	-4.910626	-3.052357	-1.811072
54	1	0	-3.236858	-3.472650	-2.177913
55	1	0	-3.944282	-1.988111	-2.835056
56	1	0	-4.511562	0.578579	0.278108
57	1	0	-5.534248	-0.412633	-0.758359
58	1	0	-4.245853	0.541532	-1.484620
59	1	0	-4.923168	-3.068312	0.950479
60	1	0	-4.254232	-1.750720	1.928968
61	1	0	-3.270980	-3.174428	1.581688
62	1	0	-2.148467	-2.522642	-4.148222
63	1	0	-0.853553	-3.494045	-3.435608
64	1	0	-0.535519	-2.513302	-4.868046
65	1	0	-1.118738	1.414320	-3.085616
66	1	0	-2.583741	0.410268	-3.135617
67	1	0	-1.528222	0.522579	-4.550795
68	1	0	1.853140	-1.676972	-3.233239
69	1	0	1.775566	-0.010577	-2.638806
70	1	0	1.336783	-0.378290	-4.309304
71	14	0	1.582473	-0.137011	0.722439
72	6	0	2.405080	-1.579288	-0.105752
73	6	0	1.808465	-0.141603	2.572711
74	6	0	1.868658	1.512842	-0.100332
75	6	0	9.175437	1.324410	-0.859550
76	6	0	7.933065	1.236150	-1.492810
77	6	0	9.287617	1.126016	0.514742
78	6	0	6.798488	0.948754	-0.749399
79	6	0	6.907760	0.750062	0.631518
80	6	0	8.150813	0.839024	1.262395
81	6	0	5.714746	0.447014	1.435528
82	8	0	4.588541	0.336764	0.984977
83	1	0	1.928294	-1.892882	-1.035331
84	1	0	3.430149	-1.271947	-0.336003
85	1	0	2.457626	-2.438393	0.568844
86	1	0	1.681207	-1.146382	2.988111
87	1	0	2.839408	0.169972	2.765848
88	1	0	1.141281	0.536590	3.112447
89	1	0	2.948696	1.674958	-0.162800
90	1	0	1.463220	1.539450	-1.117343
91	1	0	1.432234	2.344545	0.463223
92	1	0	10.061648	1.551404	-1.443952
93	1	0	7.858843	1.393341	-2.563894
94	1	0	10.255934	1.197663	0.998557

95	1	0	5.820859	0.873868	-1.216120
96	1	0	8.223347	0.683830	2.336407
97	1	0	5.891734	0.316987	2.520970

Transition State 4

Method: M06-2X/6-31G(d)
SCF Done: E(RM062X) = -3000.95845391 A.U. after 7 cycles
Zero-point correction= 0.819778 (Hartree/Particle)
Thermal correction to Energy= 0.873336
Thermal correction to Enthalpy= 0.874280
Thermal correction to Gibbs Free Energy= 0.731785
Sum of electronic and zero-point Energies= -3000.138676
Sum of electronic and thermal Energies= -3000.085118
Sum of electronic and thermal Enthalpies= -3000.084174
Sum of electronic and thermal Free Energies= -3000.226669

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.684800	0.578868	1.176848
2	8	0	-0.252365	-0.466405	0.298022
3	6	0	-1.108624	3.053038	0.744267
4	6	0	-1.557126	1.619856	0.458884
5	8	0	-0.195188	3.271043	1.519343
6	6	0	-1.310487	0.039826	2.450226
7	6	0	-1.980891	0.912131	3.314184
8	6	0	-1.184104	-1.300631	2.814771
9	6	0	-2.545625	0.442082	4.495118
10	6	0	-2.441029	-0.905480	4.836852
11	6	0	-1.750057	-1.772652	3.998273
12	6	0	-3.087904	6.342143	-1.141413
13	6	0	-2.121062	6.559715	-0.159580
14	6	0	-3.420992	5.044514	-1.522220
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91	1	0	1.575636	2.268289	-0.091050

92	1	0	10.080478	1.255696	-0.162548
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Stable State F

```
Method: M06-2X/6-31G(d)
SCF Done:  E(RM062X) =  -3000.96869931    A.U. after    5 cycles
 Zero-point correction=                          0.817839 (Hartree/Particle)
 Thermal correction to Energy=                   0.873262
 Thermal correction to Enthalpy=                 0.874206
 Thermal correction to Gibbs Free Energy=        0.726106
 Sum of electronic and zero-point Energies=          -3000.150860
 Sum of electronic and thermal Energies=             -3000.095437
 Sum of electronic and thermal Enthalpies=           -3000.094493
 Sum of electronic and thermal Free Energies=        -3000.242593
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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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3	6	0	-1.635845	1.742625	-0.887700
4	6	0	-0.249762	1.345018	-0.424002
5	8	0	-2.497958	0.896264	-1.097386
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9	6	0	0.338496	-0.674851	-4.236157
10	6	0	1.072009	-1.857543	-4.286748
11	6	0	1.496004	-2.454016	-3.100363
12	6	0	-2.598594	5.874848	-1.395888
13	6	0	-3.499100	4.885141	-1.790425
14	6	0	-1.371821	5.525621	-0.835910
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16	6	0	-1.941613	3.188271	-1.058025
17	6	0	-1.039308	4.185706	-0.671077
18	14	0	2.539891	0.061657	0.741282
19	14	0	3.825618	-1.856306	1.215816
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21	6	0	2.676173	-3.135578	2.002318
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23	6	0	4.608952	-2.601231	-0.338141
24	6	0	5.359776	1.383358	-0.336785
25	6	0	2.921004	2.971838	-1.311013
26	6	0	3.714981	0.340084	-2.681039
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47	1	0	5.795662	-2.336457	2.655050
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49	1	0	5.915008	-0.701685	1.993130
50	1	0	5.334193	-1.911410	-0.782916
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52	1	0	5.143608	-3.523738	-0.084330
53	1	0	5.847520	0.404445	-0.265998
54	1	0	5.397838	1.848678	0.653007
55	1	0	5.961142	1.998400	-1.016230
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66	1	0	1.336594	3.421409	1.763828
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75	6	0	-6.482573	0.414214	2.918496
76	6	0	-6.238885	-0.955332	3.088629
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78	6	0	-5.359616	-1.605088	2.244152
79	6	0	-4.724058	-0.871614	1.221310
80	6	0	-4.971022	0.505063	1.053151
81	6	0	-3.812340	-1.483524	0.313379
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83	1	0	-2.584609	-5.896546	-1.494802
84	1	0	-3.317382	-5.716863	0.104061
85	1	0	-4.170794	-5.133308	-1.339529
86	1	0	-1.467055	-2.945848	-2.889465
87	1	0	-3.226903	-2.739153	-2.840163
88	1	0	-2.141722	-1.526248	-2.121219

89	1	0	-1.006738	-4.161186	1.284472
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91	1	0	-0.368636	-2.672284	0.554897
92	1	0	-7.175442	0.916084	3.587318
93	1	0	-6.740746	-1.499453	3.880996
94	1	0	-6.055514	2.204020	1.795824
95	1	0	-5.151597	-2.664883	2.351633
96	1	0	-4.462896	1.044634	0.256952
97	1	0	-3.351089	-0.862956	-0.462720

^{1}H and ^{13}C NMR Spectra

Chart 1. ^{1}H NMR spectrum of 2-allyl-1,1,1,3,3,3-hexamethyl-2-(trimethylsilyl)trisilane ($CDCl_3$, 400MHz)

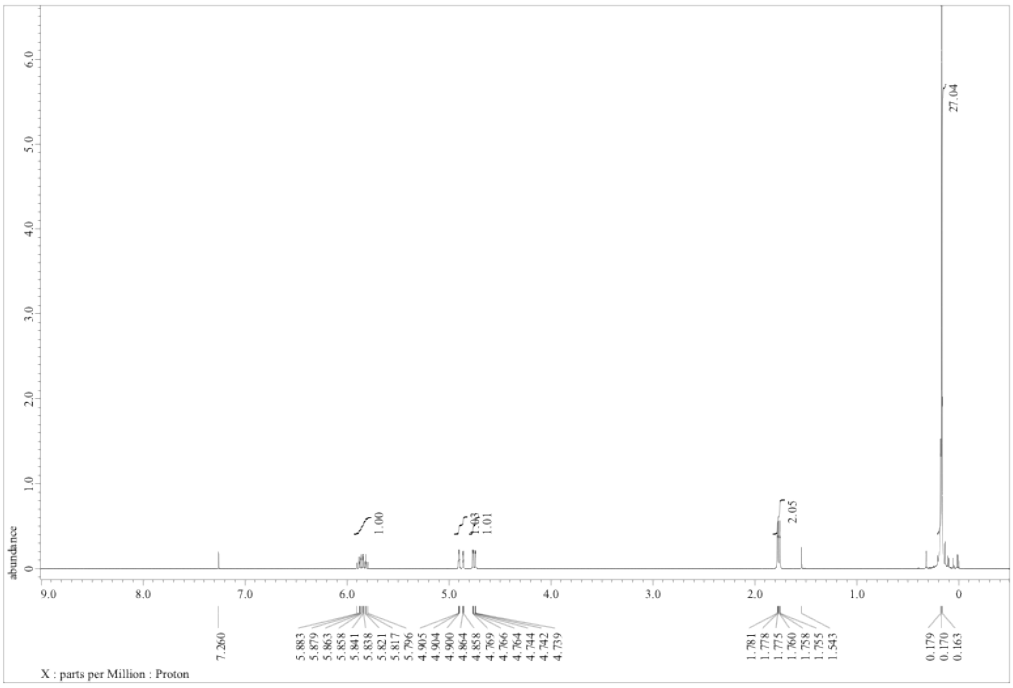

Chart 2. ^{13}C NMR spectrum of 2-allyl-1,1,1,3,3,3-hexamethyl-2-(trimethylsilyl)trisilane ($CDCl_3$, 100MHz)

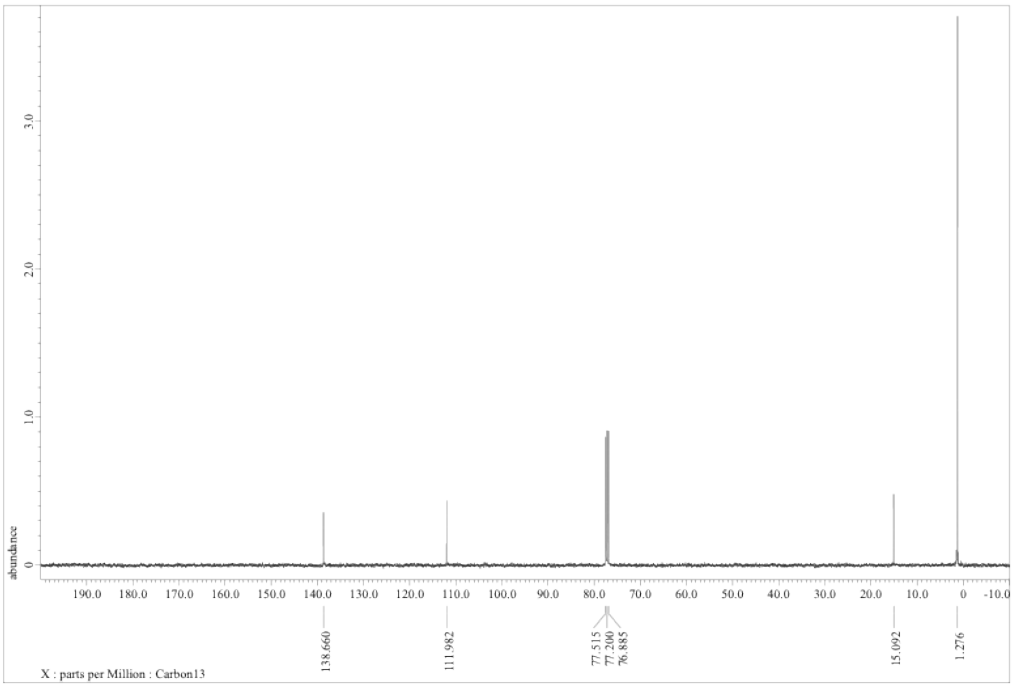

Chart 3. ^{1}H NMR spectrum of 2-allyl-1,1,1,3,3,3-hexaethyl-2-(triethylsilyl)trisilane ($CDCl_3$, 400MHz)

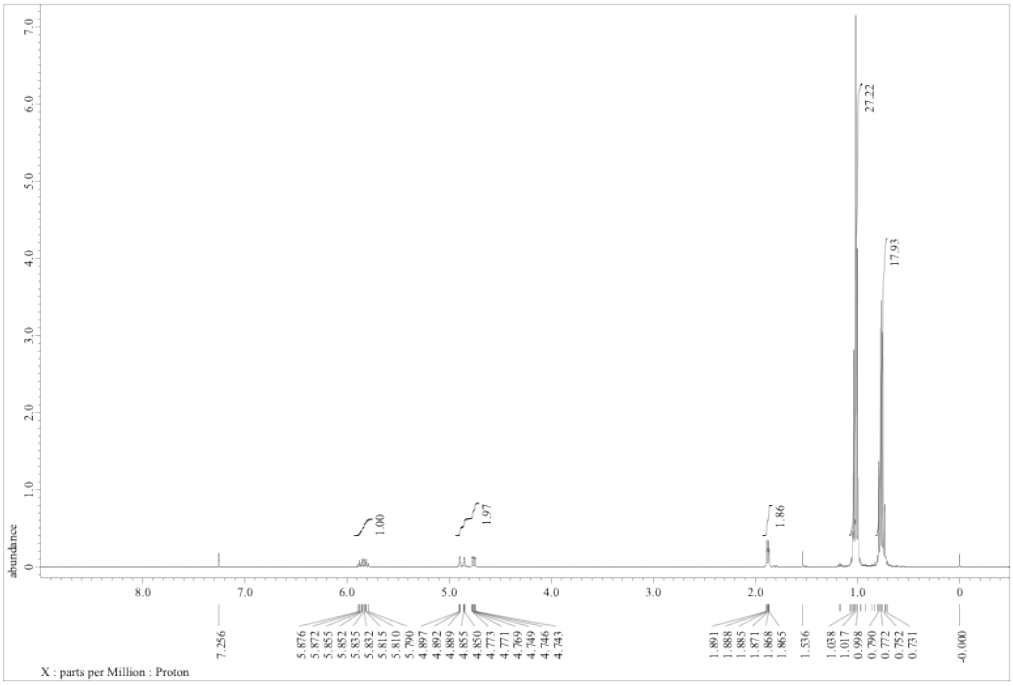

Chart 4. ^{13}C NMR spectrum of 2-allyl-1,1,1,3,3,3-hexaethyl-2-(triethylsilyl)trisilane ($CDCl_3$, 100MHz)

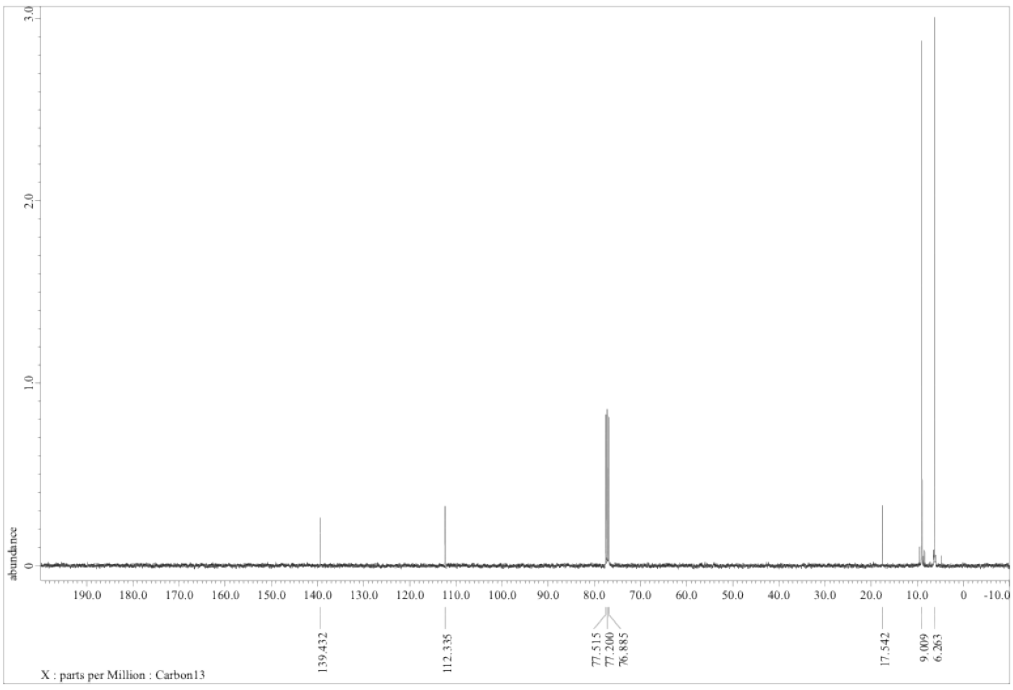

Chart 5. ^{1}H NMR spectrum of **3b** ($CDCl_3$, 400MHz)

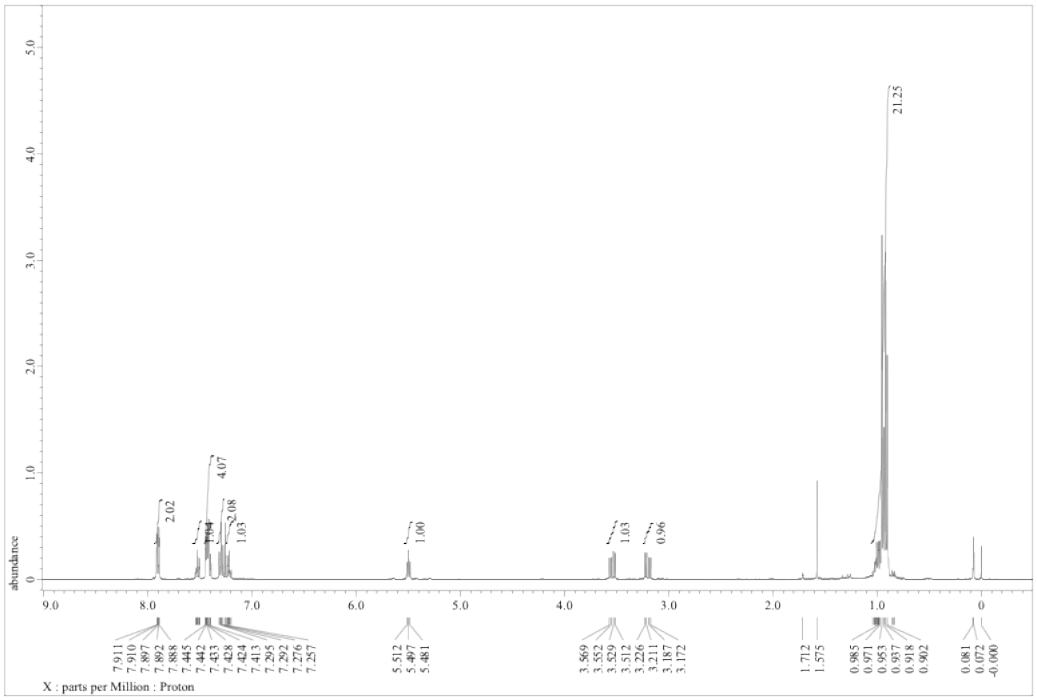

Chart 6. ^{13}C NMR spectrum of **3b** ($CDCl_3$, 100MHz)

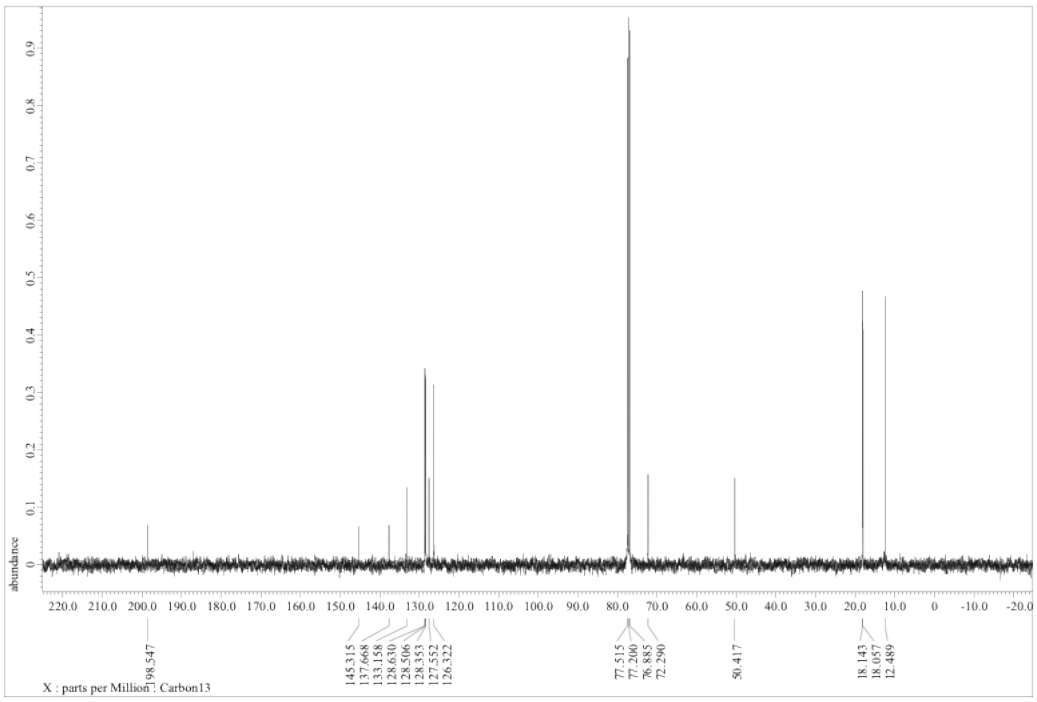

Chart 7. ^{1}H NMR spectrum of **3c** ($CDCl_3$, 400MHz)

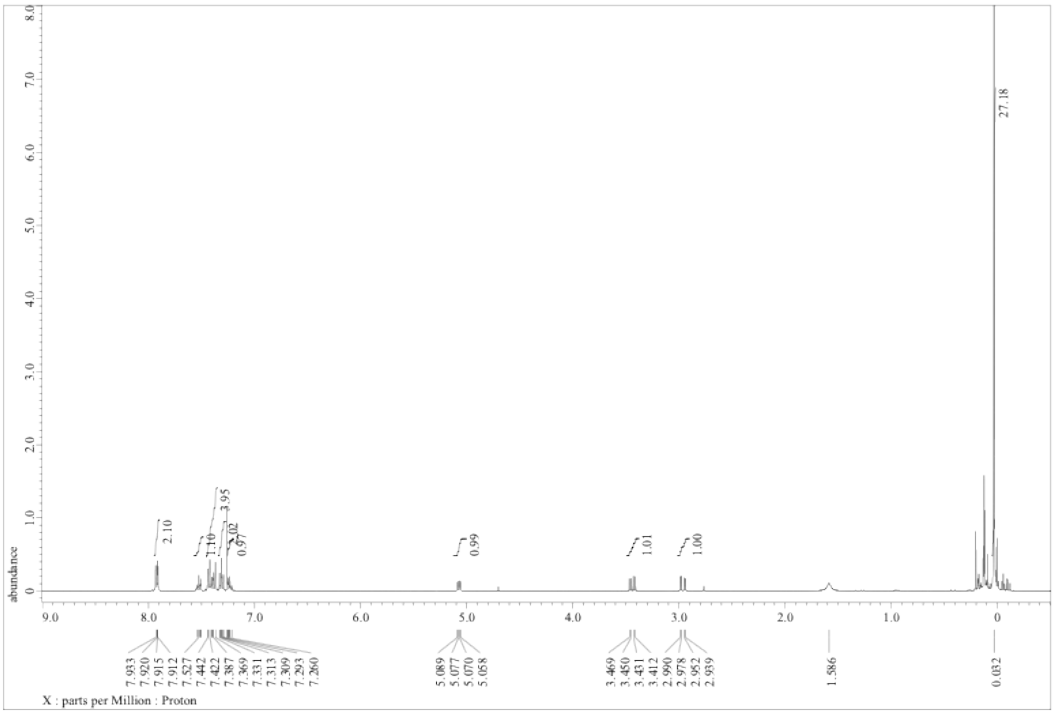

Chart 8. ^{13}C NMR spectrum of **3c** ($CDCl_3$, 100MHz)

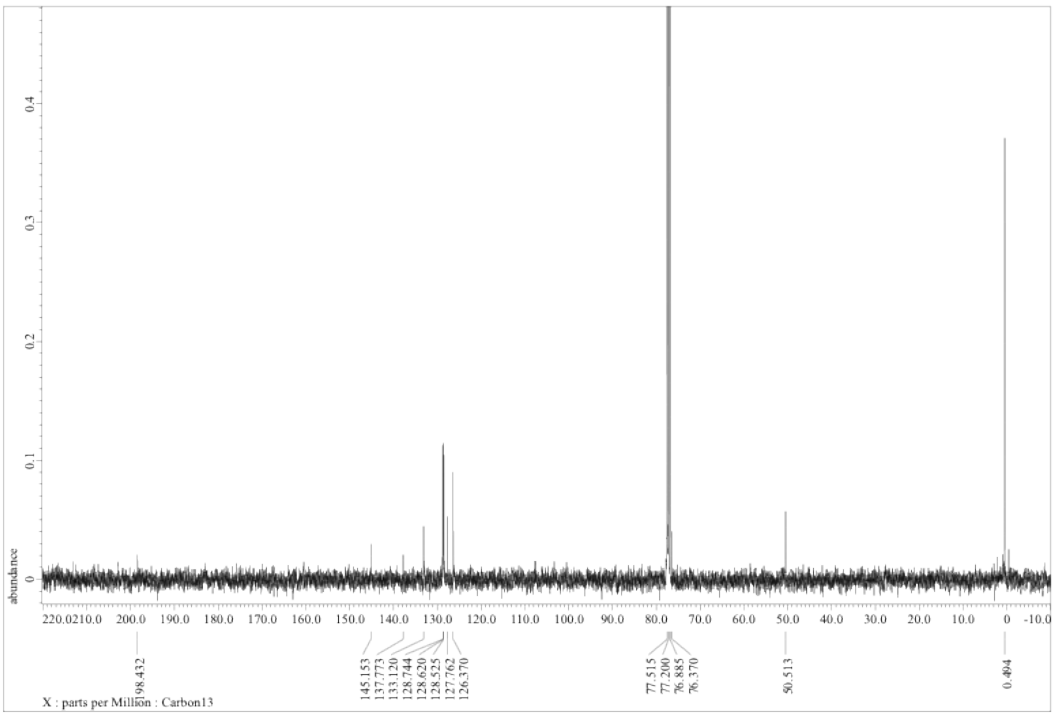

Chart 9. ^{1}H NMR spectrum of **3d** ($CDCl_3$, 400MHz)

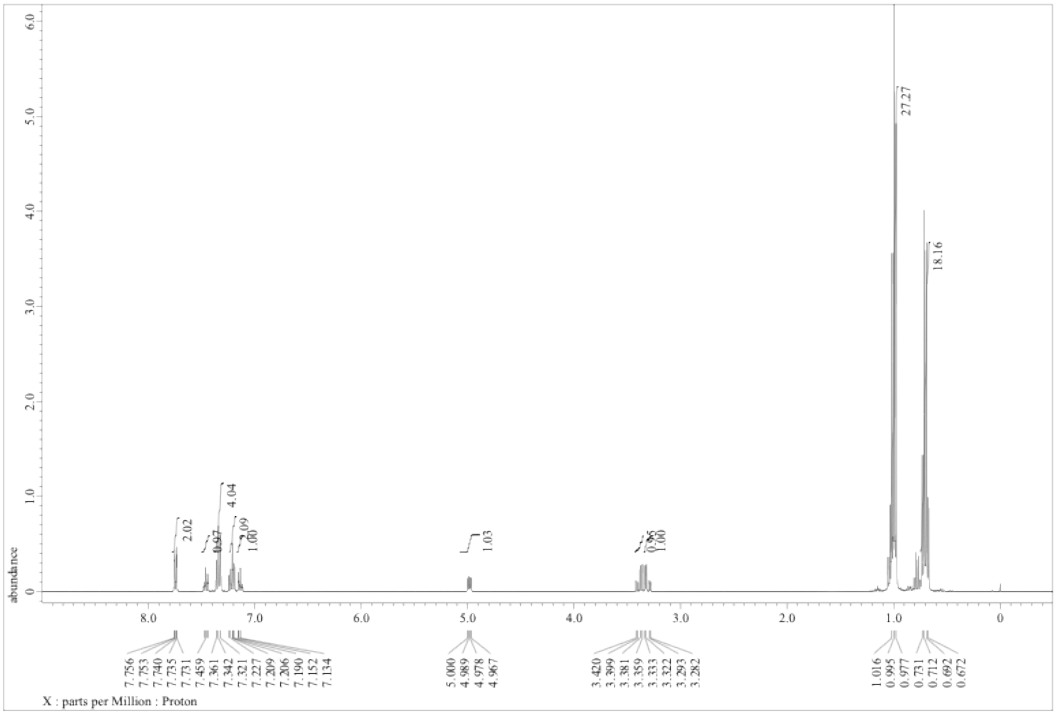

Chart 10. ^{13}C NMR spectrum of **3d** ($CDCl_3$, 100MHz)

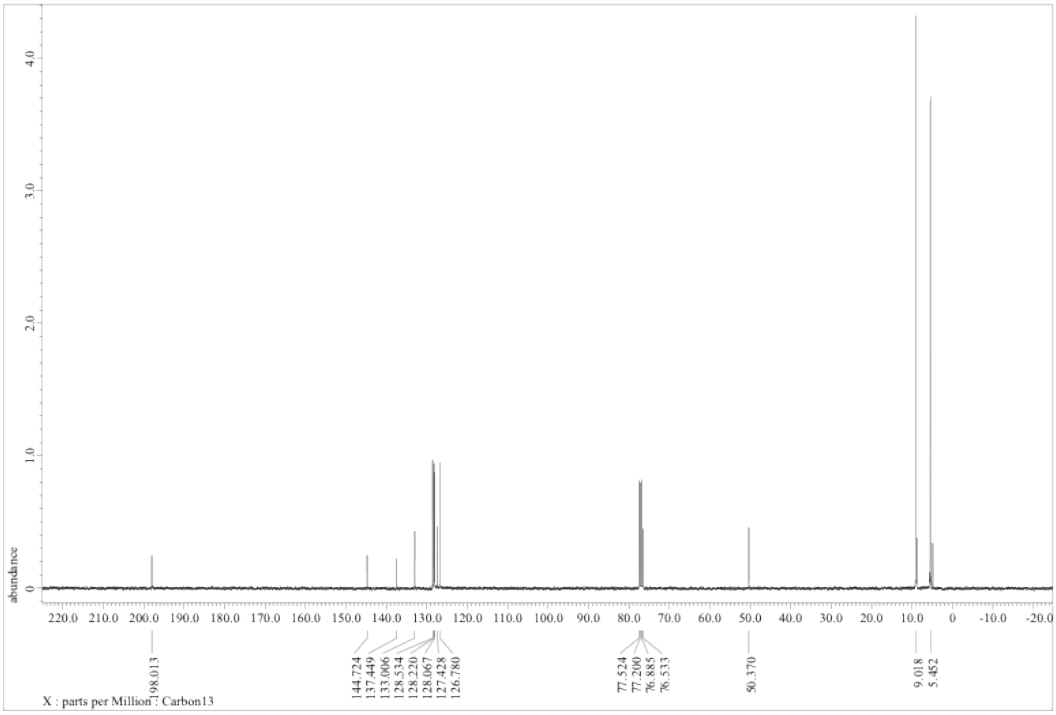

Chart 11. ^{1}H NMR spectrum of **5** ($CDCl_3$, 400MHz)

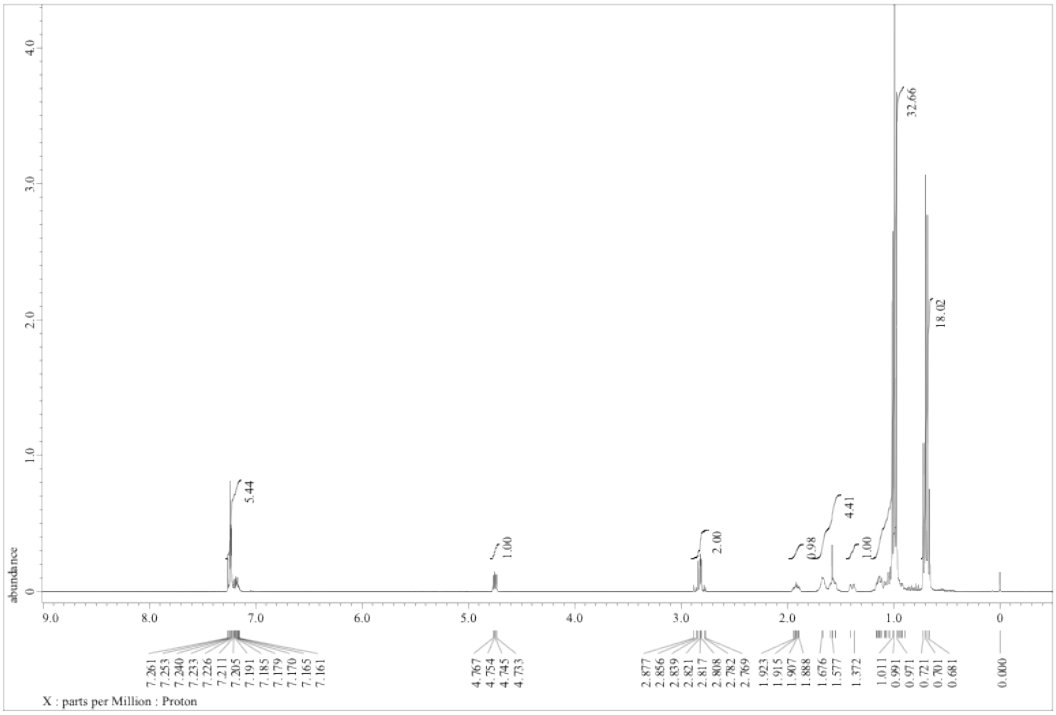

Chart 12. ^{13}C NMR spectrum of **5** ($CDCl_3$, 100MHz)