Diels–Alder *Exo*-Selectivity in Terminal-Substituted Dienes and Dienophiles: Experimental Discoveries and Computational Explanations

Supporting Information

Yu-hong Lam[a], Paul Ha-Yeon Cheong[b], José M. Blasco Mata[a], Steven J. Stanway[c], Véronique Gouverneur[a], K. N. Houk[b]

[a] Chemistry Research Laboratory, University of Oxford, Mansfield Road, Oxford OX1 3TA, UK

[b] Department of Chemistry and Biochemistry, University of California, Los Angeles, CA 90095-1569

[c] Neurology and GI Centre of Excellence for Drug Discovery, GlaxoSmithKline, New Frontiers Science, Third Avenue, Harlow, Essex CM19 5AW, UK

I. Experimental Data

General Information

^{1}H NMR spectra were recorded in deuterated chloroform or benzene using a Bruker AV400, DRX500 or AVII500 spectrometer, calibrated using residual undeuterated solvent as the internal reference. ^{13}C NMR spectra were recorded in deuterated chloroform or benzene using a Bruker AV400, AVII500 with a ^{13}C cryoprobe, or DRX500 spectrometer. Chemical shifts (δ) are quoted in parts per million (ppm). Coupling constants (J) are measured to the nearest 0.5 Hz. The following abbreviations are used to describe multiplicities – s: singlet, d: doublet, t: triplet, q: quartet, m: multiplet, app: apparent. NMR spectra were processed in ACD/SpecManager. High resolution mass spectra (HRMS, m/z) were recorded on a Micromass GCT (NH_3, CI+) instrument. Optical rotations were determined on a Perkin Elmer 241 polarimeter in a 1-decimeter cell. $[\alpha]_D$ values are given in 10^{-1} deg cm^2 g^{-1}. IR spectra were recorded on a Bruker Tensor 27 FT-IR spectrometer. Absorptions are measured in wavenumbers, and only peaks of interest are reported. IUPAC names were obtained using the ACD/I-lab service.

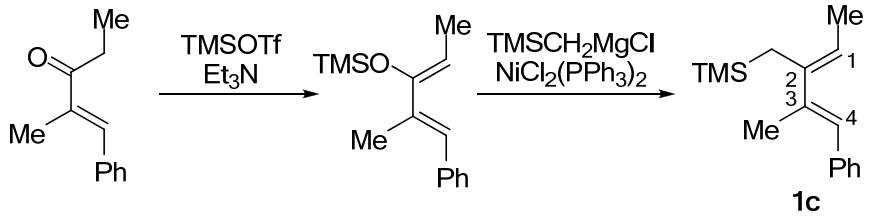
All reactions were conducted in dried glassware under an inert atmosphere of argon or nitrogen. Solvents were dried on an alumina column before use. All reactions were monitored by TLC using Merck Kieselgel 60 F_{254} plates. Visualization of the reaction components was achieved using UV fluorescence (254 nm), and $KMnO_4$ or ceric ammonium molybdate stain. Flash column chromatography was carried out over Merck silica gel C60 (40–60 μm).

A. Synthesis of Starting Materials

The following dienes and dienophiles were prepared by reported procedures: trimethyl[(3*E*)–2-methylene-4-phenylbut-3-en-1-yl]silane (**1a**),[1] trimethyl{(2*Z*)–2-[(*E*)–2-phenylvinyl]but–2-en-1-yl}silane (**1b**),[2] trimethyl({(1*Z*)-1-[(*E*)–2-phenylvinyl]prop-1-en-1-yl}oxy)silane (**2a**),[2] triisopropyl({(1*Z*)-1-[(*E*)–2-phenylvinyl]prop-1-en-1-yl}oxy)silane (**2b**),[3] {[(1*Z*,2*E*)-1-ethylidenebut–2-

en-1-yl]oxy}(trimethyl)silane (**2c**),[4] {[(1*Z*,2*E*)-1-ethylidenebut–2-en-1-yl]oxy}(triisopropyl)silane (**2d**),[5] (4*R*)-4-benzyl-3-[(2*E*)-but–2-enoyl]-1,3-oxazolidin–2-one (**3***),[6] 3-[(2*E*)-but–2-enoyl]-1,3-oxazolidin–2-one (**3**),[7] and 3-acryloyl-1,3-oxazolidin–2-one (**4**).[8]

Trimethyl{(2*Z*)-2-[(*E*)-1-methyl-2-phenylvinyl]but-2-en-1-yl}silane, **1c**



1c

To a solution of (1*E*)–2-methyl-1-phenylpent-1-en-3-one[9] (28.8 mmol, 5.030 g) in THF (72 mL) at 0 °C was added Et_3N (74.9 mmol, 10.4 mL), followed by dropwise addition of TMSOTf (31.4 mmol, 5.6 mL). After the reaction was stirred at 0 °C for 2 h, 40 mL of a pH 7 buffer solution and 80 mL of Et_2O were added. The mixture was allowed to warm to room temperature. The organic phase was washed with the buffer solution (3 × 40 mL), and the combined aqueous layers were extracted with Et_2O (80 mL). The combined organic layers were dried over sodium sulfate, filtered, and evaporated under reduced pressure to yield the silyl enol ether as a pale yellow oil (6.550 g, 92%), which was committed to the next step without purification.

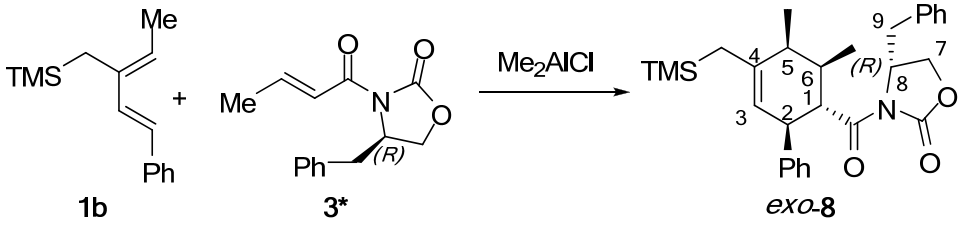
A freshly prepared solution of (trimethylsilyl)methylmagnesium chloride[10] (66.5 mmol, 1 *M* solution in Et_2O) was added to bis(triphenylphosphine)nickel(II) dichloride (880 μmol, 574 mg) in a round-bottomed flask. The solvent was then removed under reduced pressure. To the residue was added the silyl enol ether prepared as above (26.6 mmol, 6.550 g) in toluene (70 mL). The solution was heated to 90 °C for 16 h. The reaction was cooled by an ice-water bath and quenched by cautious addition of saturated aqueous NH_4Cl (80 mL). The mixture was then poured into Et_2O (80 mL) in a separation funnel and the phases separated. The organic phase was further washed with saturated aqueous NH_4Cl (2 × 40 mL) and brine (40 mL). The combined organic phase was dried, filtered through Celite® and evaporated *in vacuo* to yield the crude product, which was purified by column chromatography (hexane/Et_3N 96:4) to afford **1c** as an oil (2.516 g, 38%, (*Z*,*E*)/(*E*,*E*) = 5:1 by ^1H NMR).

***R*f** (hexane/diethyl ether, 9:1)**:** 0.67. Major isomer, (*Z*,*E*)-**1c**. **^{1}H NMR** ($CDCl_3$, 400 MHz,) ***δ*:** 7.36–7.19 (m, 5H, Ph); 6.53 (s, 1H, H4); 5.69 (q, 1H, *J* 7.0, H1); 1.99 (s, 3H, Me^3); 1.90 (s, 2H, CH_2SiMe_3); 1.73 (d, 3H, *J* 7.0, Me^1); 0.05 (s, 9H, $SiMe_3$). **^{13}C NMR** ($CDCl_3$, 101 MHz) ***δ*:** 140.5, 139.3, 139.1 (C2, C3, *ipso*-Ph); 129.2, 128.0, 125.9, 125.5 (Ph, C4); 118.8 (C1); 18.0 (CH_2SiMe_3); 16.2 (Me^3); 14.8 (Me^1); −0.6 ($SiMe_3$); **IR** (ν, cm^{-1})**:** 2955, 1708, 1448, 1249, 850; **HRMS:** required for $C_{16}H_{25}Si$ ($[M+H]^+$) 245.1726, found 245.1722.

B. Synthesis of Diels–Alder Adducts

The characterization data of *endo*-**7** has been reported previously.[2]

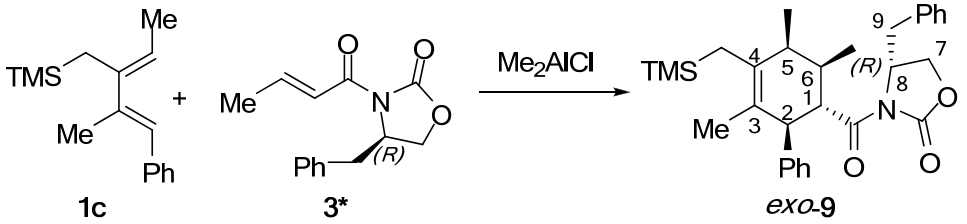
(4*R*)-4-Benzyl-3-({(1*S*,2*S*,5*S*,6*R*)-5,6-dimethyl-2-phenyl-4-[(trimethylsilyl)methyl]cyclohex-3-en-1-yl}carbonyl)-1,3-oxazolidin-2-one, *exo*-**8**



At −40 °C, dimethylaluminum chloride (3.0 mmol, 3.0 mL of a 1 *M* solution in hexanes) was added to a solution of **3*** (2.2 mmol, 532 mg) in CH_2Cl_2 (20 mL). Silylated diene **1b** (2.2 mmol, 500 mg of a 3:1 (*Z*,*E*)/(*E*,*E*) mixture) was added dropwise. The reaction was stirred at −40 °C for 4 h, before being quenched by saturated aqueous NH_4Cl (10 mL) at 0 °C. The phases were separated, and the aqueous phase was extracted with Et_2O (2 × 20 mL). The combined organic phases were dried, filtered and the solvent evaporated to give a crude white solid, which was purified by column chromatography (hexane/diethyl ether, 4:1) to yield *exo*-**8** as a white solid (58%, 601 mg). Crystals suitable for X-ray crystallography were grown by slow evaporation of EtOAc subsequent to chromatographic purification. **mp:** 140–141 °C. ***R*f** (hexane/diethyl ether, 4:1)**:** 0.24. **^{1}H NMR** ($CDCl_3$, 400 MHz) ***δ*:** 7.30–7.19 (m, 8H, Ph); 6.92–6.87 (m, 2H, Ph); 5.12 (d, 1H, *J* 1.0, H3); 4.67 (tt, 1H, *J* 9.0, 3.0, H8); 4.40 (t, 1H, *J* 11.0, H1); 4.03 (t, 1H, *J* 8.5, H7); 3.93 (dd, 1H, *J* 9.0, 3.0, H7′); 3.87 (d, 1H, *J* 11.0, H2); 2.94 (dd, 1H, *J* 13.5,

3.0, H9); 2.29–2.23 (m, 1H, H6); 2.20 (dd, 1H, *J* 13.5, 9.0, H9′); 1.99 (m, 1H, H5); 1.58 (d, 1H, *J* 14.0, CHH′SiMe$_3$); 1.50 (d, 1H, *J* 14.0, CHH′SiMe$_3$); 1.14 (d, 3H, *J* 7.0, Me^5); 0.94 (d, 3H, *J* 7.0, Me^6); 0.03 (s, 9H, SiMe$_3$). **^{13}C NMR** ($CDCl_3$, 126 MHz) ***δ*:** 176.9, 153.0 (C=O); 144.1 (C4); 141.0, 135.2 (*ipso*-Ph); 129.3, 128.8, 128.6, 128.4, 127.1, 126.7 (Ph); 121.3 (C3); 65.2 (C7); 54.8 (C8); 48.4 (C2); 45.3 (C1); 39.5 (C5); 37.5 (C9); 36.7 (C6); 25.1 (CH_2SiMe_3); 16.1 (Me^6); 13.8 (Me^5); −1.2 ($SiMe_3$). **IR** (*ν*, cm^{-1})**:** 1767, 1697. **HRMS:** required for $C_{29}H_{38}NO_3Si$ ([*M*+H]$^+$): 476.2621, found 476.2643. **[α]$^{25}_D$:** +7.7 (*c* = 0.03, CH_2Cl_2).

(4*R*)-4-Benzyl-3-({(1*S*,2*S*,5*S*,6*R*)-3,5,6-trimethyl-2-phenyl-4-[(trimethylsilyl)methyl]cyclohex-3-en-1-yl}carbonyl)-1,3-oxazolidin-2-one, *exo*-**9**

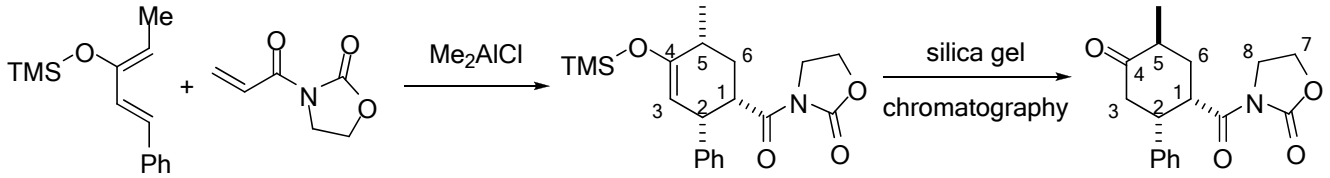


At −40 °C, dimethylaluminum chloride (1.9 mmol, 1.9 mL of a 1 *M* solution in hexanes) was added slowly to a solution of **3*** (1.4 mmol, 355 mg) in CH_2Cl_2 (15 mL). A solution of diene **1c** (1.6 mmol, 424 mg of a 5:1 (*Z*,*E*)/(*E*,*E*) mixture) in CH_2Cl_2 (5 mL) was then added dropwise. The reaction was stirred at −40 °C for 5 h before being quenched by saturated aqueous NH_4Cl (10 mL) at 0 °C. The layers were separated and the aqueous phase was further washed with Et_2O (2 × 30 mL). The combined organic phases were dried, filtered and evaporated *in vacuo*. Column chromatography (hexane/diethyl ether, 4:1) afforded *exo*-**9** (65%, 460 mg) as a white solid.

***R*$_f$** (hexane/diethyl ether, 4:1)**:** 0.21. **^{1}H NMR** (C_6D_6, 500 MHz) ***δ*:** 7.48 (d, 2H, *J* 7.5, Ph); 7.24 (t, 2H, *J* 7.5, Ph); 7.17–7.10 (m, 4H, Ph); 6.74–6.72 (m, 2H, Ph); 5.12 (t, 1H, *J* 11.0, H1); 4.41 (tt, 1H, *J* 8.5, 3.0, H8); 4.25 (d, 1H, *J* 11.0, H2); 3.37 (dd, 1H, *J* 8.5, 3.0, H7); 3.16 (t, 1H, *J* 8.5, H7′); 2.96 (dd, 1H, *J* 13.5, 3.0, H9); 2.59 (m, 1H, *J* 7.0, H5); 2.16 (dd, 1H, *J* 13.5, 8.5, H9′); 2.16 (m, 1H, H6); 1.91 (d, 1H, *J* 14.0, CHH′SiMe$_3$); 1.55 (d, 1H, *J* 14.0, CHH′SiMe$_3$); 1.50 (s, 3H, Me^3); 1.49 (d, 3H, *J* 7.0, Me^5); 1.20 (d, 3H, *J* 7.0, Me^6); 0.16 (s, 9H, $SiMe_3$). **^{13}C NMR** (C_6D_6, 126 MHz) ***δ*:** 176.7, 153.1 (C=O); 144.3 (C4); 136.2,

135.8, 129.6, 129.0, 128.8, 128.7, 127.2, 126.9 (Ph); 123.6 (C3); 64.7 (C7); 54.9 (C8); 53.6 (C2); 47.1 (C1); 41.4 (C5); 37.8 (C9); 36.9 (C6); 22.9 ($\underline{C}H_2SiMe_3$); 18.2 (Me^3); 16.4 (Me^6); 14.5 (Me^5); −0.09 ($SiMe_3$). **IR** (ν, cm^{-1})**:** 1767, 1698. **HRMS:** required for $C_{30}H_{40}NO_3Si$ ($[M + H]^+$): 490.2777, found 490.2776.

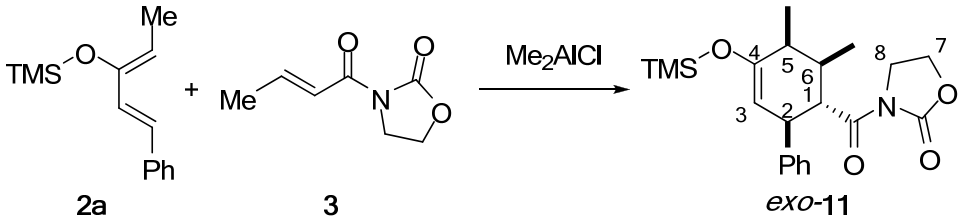
rac-3-{[(1*R*,2*S*,5*R*)-5-Methyl-4-oxo-2-phenylcyclohexyl]carbonyl}-1,3-oxazolidin-2-one, *endo*-**10**



To a solution of **4** (350 μmol, 50 mg) in CH_2Cl_2 (4 mL) at −100 °C was added dimethylaluminum chloride (490 μmol, 490 μL of a 1 *M* solution in hexanes) and the silyl enol ether **2a** (480 μmol, 112 mg). The yellow solution was stirred for 1 h. The reaction was then quenched with saturated $NaHCO_3$ (4 mL). The resultant slurry was diluted with dichloromethane (4 mL), and the layers were separated. The aqueous layer was extracted with dichloromethane (2 × 4 mL), and the combined organic layers were dried and concentrated *in vacuo*. After flash column chromatography over silica gel (40°–60° petroleum spirit/ethyl acetate, 9:1), *endo*-**10** was obtained as a white oil. (78%, 82 mg).

$\boldsymbol{R}_\mathbf{f}$ (hexane/ethyl acetate, 9:1)**:** 0.12. **^{1}H NMR** (C_6D_6, 500 MHz) $\boldsymbol{\delta}$**:** 7.04–6.92 (m, 5H, Ph); 4.32 (dt, 1H, *J* 12.0, 4.5, H1); 3.83 (app q, 1H, *J* 5.0, H2); 3.16–2.97 (m, 4H, H7, H8); 2.74 (dd, 1H, *J* 15.5, 4.0, H3); 2.55 (dd, 1H, *J* 15.5, 6.5, H3′); 2.04 (q, 1H, *J* 13.0, $H6^{ax}$); 1.94 (m, 1H, H5); 1.70 (dt, 1H, *J* 13.5, 4.5, $H6^{eq}$); 1.10 (d, 3H, *J* 6.5, Me^5). **^{13}C NMR** (C_6D_6, 126 MHz) $\boldsymbol{\delta}$**:** 210.5 (C4); 173.0, 153.5 (C=O, C=O); 141.4, 129.0, 128.9, 127.6 (Ph); 61.8 (C7); 45.2 (C1); 45.0 (C3); 43.8 (C2); 43.5 (C5); 42.8 (C8); 31.4 (C6); 15.2 (Me^5). **IR** (ν, cm^{-1})**:** 3057, 2969, 1778, 1706, 1480, 1454, 1388, 1266, 1222, 1105. **HRMS:** required for $C_{17}H_{20}NO_4$($[M+H]^+$) 302.1392, found 302.1388.

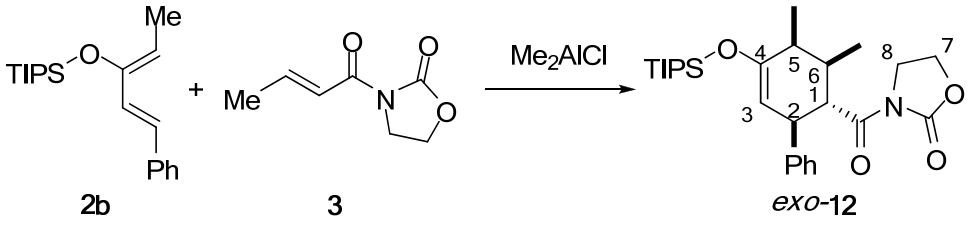
rac-3-({(1*R*,2*R*,5*R*,6*S*)-5,6-Dimethyl-2-phenyl-4-[(trimethylsilyl)oxy]cyclohex-3-en-1-yl}carbonyl)-1,3-oxazolidin-2-one, *exo*-**11**



To a solution of **3** (320 μmol, 50 mg) in CH_2Cl_2 (4 mL) at −40 °C was added dimethylaluminum chloride (450 μmol, 450 μL of a 1 *M* solution in hexanes) and the silyl enol ether **2a** (440 μmol, 102 mg). The brown solution was stirred for 3 h. The reaction was then quenched with saturated $NaHCO_3$ (4 mL). The resultant slurry was diluted with dichloromethane (4 mL), and the layers were separated. The aqueous layer was extracted with dichloromethane (2 × 4 mL), and the combined organic layers were dried and concentrated *in vacuo*. The crude mixture was purified by flash chromatography on silica gel (40°–60° petroleum spirit/ethyl acetate, 19:1) to yield *exo*-**11** (62%, 77 mg) as an oil.

***R*$_f$** (hexane/ethyl acetate, 4:1)**:** 0.21. **^{1}H NMR** (C_6D_6, 500 MHz) ***δ*:** 7.40 (dd, 2H, *J* 7.5, 1.0, Ph); 7.13 (t, 2H, *J* 7.5, Ph); 6.98 (tt, 1H, *J* 7.5, 1.0, Ph); 4.89 (d, 1H, *J* 2.0, H3); 4.68 (t, 1H, *J* 10.5, H1); 4.17 (dm, 1H, *J* 10.5, H2); 3.04 (ddd, 1H, *J* 10.5, 9.5, 8.0, H8); 2.97 (ddd, 1H, *J* 10.5, 9.0, 5.5, H8′); 2.88 (td, 1H, *J* 9.0, 5.5, H7); 2.65 (q, 1H, *J* 9.0, H7′); 2.51 (dq, 1H, *J* 7.0, 5.0, H5); 2.25 (m, 1H, H6); 1.38 (d, 3H, *J* 7.0, Me^6); 0.98 (d, 3H, *J* 7.0, Me^5); 0.14 (s, 9H, $SiMe_3$).**^{13}C NMR** (C_6D_6, 126 MHz) ***δ*:** 176.4, 155.9, 153.5, 145.3 (C=O, C=O, C4, *ipso*-Ph); 129.1, 128.8, 127.5 (Ph); 106.5 (C3); 61.0 (C7); 47.7 (C2); 46.7 (C1); 42.6 (C8); 40.2 (C6); 37.4 (C5); 16.1 (Me^6); 13.7 (Me^5); 0.8 ($SiMe_3$). **IR** (ν, cm^{-1})**:** 3055, 2967, 1780, 1694, 1662, 1454, 1386, 1265, 1184, 1108, 912, 895, 846. **HRMS:** required for $C_{21}H_{30}NO_4Si$ ($[M+H]^+$) 388.1944, found 388.1935.

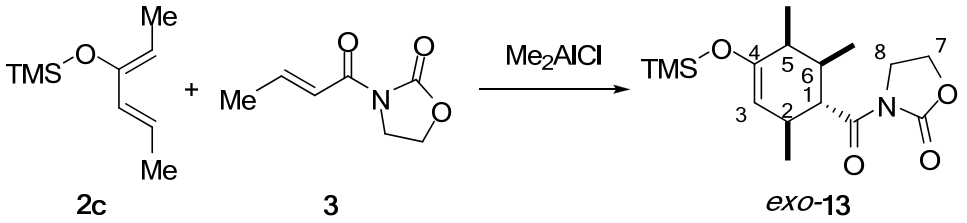
rac-3-({(1*R*,2*R*,5*R*,6*S*)-5,6-Dimethyl-2-phenyl-4-[(triisopropylsilyl)oxy]cyclohex-3-en-1-yl}carbonyl)-1,3-oxazolidin-2-one, *exo*-**12**



To a solution of **3** (320 μmol, 50 mg) in CH_2Cl_2 (4 mL) at −40 °C was added dimethylaluminum chloride (450 μmol, 450 μL of a 1 *M* solution in hexanes) and the silyl enol ether **2b** (360 μmol, 114 mg). The brown solution was stirred for 3.5 h. The reaction was then quenched with saturated $NaHCO_3$ (4 mL). The resultant slurry was diluted with dichloromethane (4 mL), and the layers were separated. The aqueous layer was extracted with dichloromethane (2 × 4 mL), and the combined organic layers were dried and concentrated *in vacuo*. The product was purified by flash chromatography on silica gel (40°–60° petroleum spirit/ethyl acetate, 9:1) to yield *exo*-**12** (89%, 135 mg) as an oil.

***R*f** (hexane/ethyl acetate, 4:1)**:** 0.30. **^{1}H NMR** (C_6D_6, 500 MHz) ***δ*:** 7.42 (d, 2H, *J* 7.5, Ph); 7.12 (t, 2H, *J* 7.5, Ph); 6.98 (t, 1H, *J* 7.5, Ph); 4.89 (d, 1H, *J* 1.5, H3); 4.70 (t, 1H, *J* 10.5, H1); 4.21 (d, 1H, *J* 10.5, H2); 3.08-3.02 (m, 1H, H8); 2.99 (t, 1H, *J* 10.0, 5.5, H8′); 2.88 (td, 1H, *J* 8.5, 5.5, H7); 2.65 (q, 1H, *J* 8.5, H7′); 2.53 (m, 1H, H5); 2.30 (m, 1H, H6); 1.45 (d, 3H, *J* 7.0, Me^6); 1.09 (m, 21H, Si(*i*-Pr)$_3$); 1.01 (d, 3H, *J* 7.0, Me^5). **^{13}C NMR** (C_6D_6, 126 MHz) ***δ*:** 176.4, 156.0, 153.5, 145.3 (C=O, C=O, C4, *ipso*-Ph); 129.1, 128.8, 127.5 (Ph); 105.3 (C3); 61.1 (C7); 47.8 (C2); 46.8 (C1); 42.6 (C8); 40.3 (C6); 37.4 (C5); 18.7 (Si(CHMe$_2$)$_3$); 16.1 (Me^6); 14.1 (Me^5); 13.3 (Si(CHMe$_2$)$_3$). **IR** (*ν*, cm^{-1})**:** 3055, 2946, 2868, 1780, 1694, 1661, 1464, 1385, 1265, 1188, 1108, 1065, 884. **HRMS:** required for $C_{27}H_{42}NO_4Si([M+H]^+)$ 472.2883, found 472.2888.

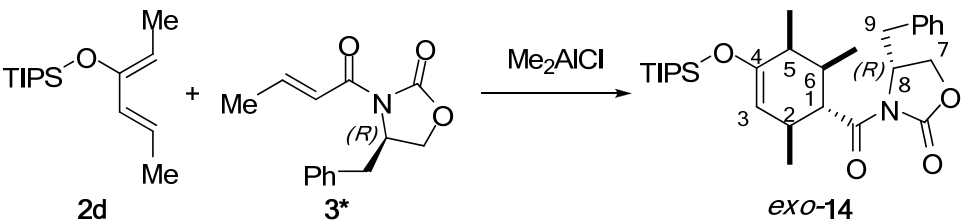
rac-3-({(1*R*,2*S*,5*S*,6*R*)-2,5,6-Trimethyl-4-[(trimethylsilyl)oxy]cyclohex-3-en-1-yl}carbonyl)-1,3-oxazolidin-2-one, *exo*-**13**



To a solution of **3** (320 μmol, 50 mg) in CH_2Cl_2 (4 mL) at −40 °C was added dimethylaluminum chloride (450 μmol, 450 μL of a 1 *M* solution in hexanes) and the silyl enol ether **2c** (440 μmol, 75 mg). The brown solution was stirred for 2 h. The reaction was then quenched with saturated $NaHCO_3$ (4 mL). The resultant slurry was diluted with dichloromethane (4 mL), and the layers were separated. The aqueous layer was extracted with dichloromethane (2 × 4 mL), and the combined organic layers were dried and concentrated *in vacuo*. The product was purified by flash chromatography on silica gel (hexane/ethyl acetate, 4:1) to yield *exo*-**13** (80%, 83 mg) as an oil.

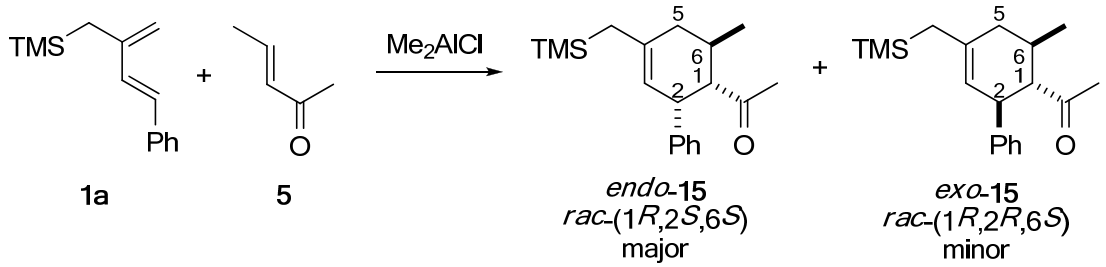
***R*$_f$** (hexane/ethyl acetate, 4:1)**:** 0.24. **^{1}H NMR** (C_6D_6, 400 MHz) ***δ*:** 4.74 (d, 1H, *J* 2.0, H3); 4.17 (t, 1H, *J* 10.5, H1); 3.19 (dd, 1H, *J* 7.5, 1.5, H8); 3.16 (d, 1H, *J* 7.5, H8′); 3.06–2.97 (m, 3H, H2, H7, H7′); 2.38 (m, 1H, H6); 2.15 (m, 1H, H5); 1.25 (d, 3H, *J* 7.0, Me^5); 1.05 (d, 3H, *J* 7.0, Me^2); 0.93 (d, 3H, *J* 7.0, Me^6); 0.20 (s, 9H, $SiMe_3$); **^{13}C NMR** (C_6D_6, 126 MHz) ***δ*:** 177.4, 155.0, 153.8 (C=O, C=O, C4); 108.0 (C3); 61.2 (C7); 46.2 (C1); 42.8 (C8); 40.1 (C5); 37.3 (C6); 35.4 (C2); 21.5 (Me^2); 16.1 (Me^6); 13.7 (Me^5); 0.8 ($SiMe_3$). **IR** (*ν*, cm^{-1})**:** 3055, 2965, 1780, 1694, 1386, 1266, 1192, 1103, 887, 845. **HRMS:** required for $C_{16}H_{28}NO_4Si$ ([*M*+H]$^+$) 326.1788, found 326.1781.

(4*R*)-4-Benzyl-3-({(1*R*,2*S*,5*S*,6*R*)-2,5,6-trimethyl-4-[(triisopropylsilyl)oxy]cyclohex-3-en-1-yl}carbonyl)-1,3-oxazolidin-2-one, *exo*-**14**



To a solution of **3*** (200 μmol, 50 mg) in CH_2Cl_2 (2.5 mL) at −40 °C was added dimethylaluminum chloride (280 μmol, 280 μL of a 1 *M* solution in hexanes) and silyl enol ether **2d** (220 μmol, 61 mg of a 15:1 (*Z,E)/(E,E*) mixture). The yellow solution was stirred for 2 h. The reaction was then quenched with saturated $NaHCO_3$ (3 mL). The resultant slurry was diluted with dichloromethane (3 mL), and the layers were separated. The aqueous layer was extracted with dichloromethane (2 × 3 mL), and the combined organic layers were dried and concentrated *in vacuo*. The product was purified by flash chromatography on silica gel (40°–60° petroleum spirit/ethyl acetate, 4:1) to yield *exo*-**14** (48%, 48 mg) as a yellow oil. ***R*f** (hexane/ethyl acetate, 4:1)**:** 0.45. **^{1}H NMR** (C_6D_6, 400 MHz) ***δ*:** 7.17–7.11 (m, 3H, Ph); 6.99 (m, 2H, Ph); 4.90 (m, 1H, H3); 4.46–4.40 (m, 1H, H8); 4.36 (t, 1H, *J* 10.5, H1); 3.54 (dd, 1H, *J* 9.0, 3.0, H7); 3.31 (dd, 1H, *J* 13.0, 3.0, H9); 3.24 (t, 1H, *J* 8.5, H7′); 3.20–3.10 (m, 1H, H2); 2.58–2.49 (m, 1H, H5); 2.36–2.31 (m, 1H, H6); 2.27 (dd, 1H, *J* 13.0, 10.5, H9′); 1.42 (d, 3H, *J* 7.0, Me^6); 1.29–1.24 (m, 24H, Si(*i*-Pr)$_3$, Me^2); 1.06 (d, 3H, *J* 7.0, Me^5); **^{13}C NMR** (C_6D_6, 126 MHz) ***δ*:** 177.4, 155.1, 153.9 (C=O, C=O, C4); 136.5, 130.0, 129.3, 127.6 (Ph); 107.3 (C3); 65.6 (C7); 56.0 (C8); 46.4 (C1); 40.2 (C5); 38.6 (C9); 37.3 (C6); 35.8 (C2); 21.6 (Me^2); 18.7 (Si(CH$\underline{Me}_2$)$_3$); 16.1 (Me^6); 14.0 (Me^5); 13.4 (Si($\underline{C}$HMe$_2$)$_3$); **IR** (*ν*, cm^{-1})**:** 2962, 2868, 1782, 1694, 1454, 1384, 1262, 1100, 801. **HRMS:** required for $C_{29}H_{46}NO_4Si$ ([*M*+H]$^+$) 500.3196, found 500.3190; **[α]$^{25}_D$**: −9.00 (*c* = 0.20, CH_2Cl_2).

1-(6-Methyl-2-phenyl-4-((trimethylsilyl)methyl)cyclohex-3-enyl)ethanone – [*rac*-(1*R*,2*S*,6*S*): *endo*-**15** (major)] [*rac*-(1*R*,2*R*,6*S*): *exo*-**15** (minor)]



To a solution of (*E*)-pent-3-en–2-one (**5**) at −40 °C (53 mg, 0.63 mmol) in CH_2Cl_2 (6 mL) was added dropwise dimethylaluminum chloride (0.20 mL, 1 *M* solution in hexanes, 0.20 mmol) followed by a solution of **1a** (150 mg, 0.69 mmol) in CH_2Cl_2 (1.5 mL). The reaction mixture was warmed to room

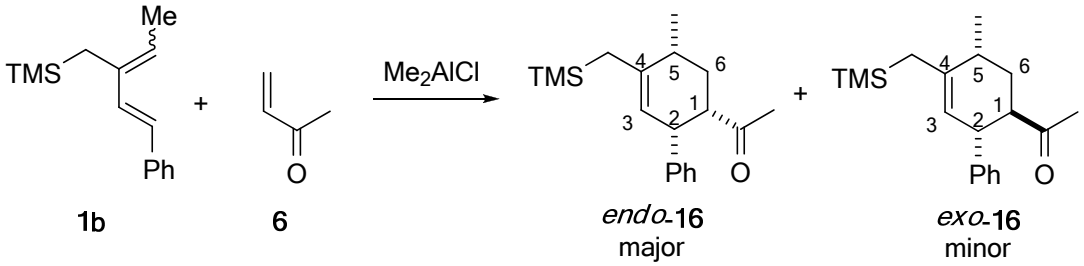
temperature and stirred for 7.5 hours. The reaction was quenched by saturated NH_4Cl(aq) (6 mL), diluted by Et_2O and transferred to a separation funnel. The phases were separated. The aqueous phase was extracted with Et_2O (2 × 7 mL). The combined organic phases were dried over $MgSO_4$, filtered and evaporated under reduced pressure to furnish the crude product, which was purified by column chromatography (40°–60° petroleum spirit / Et_2O, 95:5) to afford the minor isomer, *exo*-**15**, as a colorless oil (28 mg, 15%) and the major isomer, *endo*-**15**, as a colorless oil (118 mg, 62%).

The diastereoselectivity of the cycloaddition was determined by ^{1}H NMR after aqueous workup. Integration of the signal due to H3 of the major isomer (δ_H 5.23) versus that of the minor isomer (δ_H 5.17) gave the crude *endo*/*exo* ratio as 4:1.

Major isomer, *endo*-**15**. $\boldsymbol{R_f}$ (hexane / Et_2O, 94:6)**:** 0.19. **^{1}H NMR** (C_6D_6, 400 MHz) δ: 7.12–7.01 (m, 5H, Ph); 5.23 (dt, 1H, *J* 3.5, 1.0, H3); 3.62 (m, 1H, H2); 2.50 (dd, 1H, *J* 10.5, 6.0, H1); 2.21–2.12 (m, 1H, H6); 2.07 (dd, 1H, *J* 17.5, 5.5, H5^{eq}); 1.56 (ddm, 1H, *J* 17.5, 9.5, H5^{ax}); 1.49 (s, 3H, CO<u>Me</u>); 1.46 (d, 1H, *J* 13.5, C<u>H</u>H′SiMe$_3$); 1.39 (d, 1H, *J* 13.5, CH<u>H′</u>SiMe$_3$); 0.84 (d, 3H, *J* 6.5, Me^6); 0.05 (s, 9H, SiMe$_3$). **^{13}C NMR** (C_6D_6, 126 MHz) **δ:** 208.1 (C=O); 142.1, 135.6 (C4, *ipso*-Ph); 129.7, 128.3, 127.0 (Ph); 120.9 (C3); 59.4 (C1); 44.4 (C2); 39.3 (C5); 29.7 (CO<u>Me</u>), 27.6 (<u>C</u>H$_2$SiMe$_3$), 25.8 (C6), 20.5 (Me^6), −1.0 (SiMe$_3$). **IR** (ν, cm^{-1}): 3490, 2955, 1712. **HRMS:** required for $C_{19}H_{29}OSi$ ([*M*+H]$^+$) 301.1988, found 301.1985.

Minor isomer, *exo*-**15**. $\boldsymbol{R_f}$ (hexane / Et_2O, 94:6)**:** 0.28. **^{1}H NMR** (C_6D_6, 400 MHz) **δ:** 7.17–7.01 (m, 5H, Ph); 5.17 (s, 1H, H3); 3.76 (dm, 1H, *J* 10.5, H2); 2.30 (t, 1H, *J* 10.5, H1); 2.19–2.08 (m, 1H, H6); 1.83 (dd, 1H, *J* 17.5, 5.0, H5^{eq}); 1.73−1.65 (ddm, 1H, *J* 17.5, 11.0, H5^{ax}); 1.51 (s, 3H, CO<u>Me</u>); 1.40 (d, 1H, *J* 13.7, C<u>H</u>H′SiMe$_3$); 1.36 (d, 1H, *J* 13.7, CH<u>H′</u>SiMe$_3$); 0.76 (d, 3H, *J* 6.5, Me^6); 0.02 (s, 9H, SiMe$_3$). **^{13}C NMR** (C_6D_6, 126 MHz) **δ:** 211.6 (C=O); 145.3, 135.3 (C4, *ipso*-Ph); 128.8, 126.8 (Ph); 123.0 (C3); 62.7 (C1); 48.1 (C2); 40.2 (C5); 33.3, 32.7 (CO<u>Me</u>, C6); 27.5 (<u>C</u>H$_2$SiMe$_3$), 19.7 (Me^6), −1.1 (SiMe$_3$). **HRMS:** required for $C_{19}H_{32}NOSi$ ([*M*+NH_4]$^+$) 318.2253, found 318.2269.

1-(5-Methyl-2-phenyl-4-((trimethylsilyl)methyl)cyclohex-3-enyl)ethanone – [*rac*-(1*R*,2*S*,5*S*): *endo*-**16**] [*rac*-(1*R*,2*S*,5*R*): *exo*-**16**]



To a solution of methyl vinyl ketone (**6**) (44 mg, 0.63 mmol) in CH_2Cl_2 (5 mL) cooled at −40 °C was added dimethylaluminum chloride (0.13 mL, 0.13 mmol of a 1 *M* solution in hexanes), followed by dropwise addition of solution of **1b** (207 mg, 0.90 mmol, *Z*/*E* = 3:1) in CH_2Cl_2 (1 mL). The reaction mixture was warmed to room temperature and stirred for 4 hours. The reaction was quenched by saturated NH_4Cl(aq) (6 mL), diluted by Et_2O and transferred to a separation funnel. The phases were separated. The aqueous phase was extracted with Et_2O (2 × 7 mL). The combined organic phases were dried over $MgSO_4$, filtered and evaporated under reduced pressure to furnish the crude product, which was purified by column chromatography (40°–60° petroleum spirit / Et_2O, 9:1) to furnish the minor isomer, *exo*-**16** (7 mg, 4%), and the major isomer, *endo*-**16** (75 mg, 40%), both as a colorless oil.

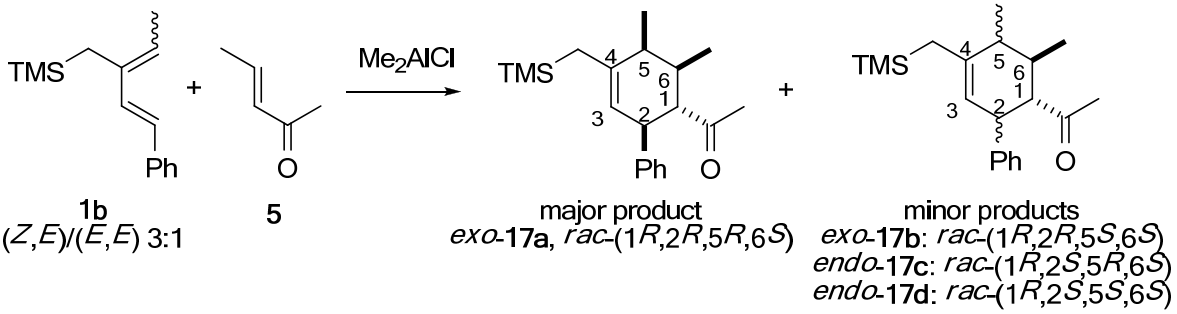
The diastereoselectivity of the cycloaddition was determined by ^{1}H NMR after aqueous workup. Integration of the signal due to H2 of the major isomer (δ_H 3.77) versus that of the minor isomer (δ_H 3.94) gave the crude *endo*/*exo* ratio as 10:1.

Major isomer, *endo*-**16**. R_f (hexane / Et_2O, 9:1)**:** 0.18. **^{1}H NMR** (C_6D_6, 400 MHz) ***δ*:** 7.17 (d, 2H, *J* 7.5, Ph); 7.11 (t, 2H, *J* 7.5, Ph); 7.02 (t, 1H, *J* 7.5, Ph); 5.20 (d, 1H, *J* 5.5, H3); 3.77 (app t, 1H, *J* 5.5, H2); 2.63 (ddd, 1H, *J* 13.0, 5.5, 3.0, H1); 2.01–1.92 (m, 1H, H5); 1.68 (d, 1H, *J* 14.0, C<u>H</u>H′SiMe$_3$); 1.60 (td, 1H, *J* 13.0, 11.0, H6^{ax}); 1.51 (ddd, 1H, *J* 11.0, 6.0, 3.0, H6^{eq}); 1.51 (s, 3H, COMe); 1.39 (d, 1H, *J* 14.0, CH<u>H</u>′SiMe$_3$); 1.02 (d, 3H, *J* 7.0, Me^5); 0.03 (s, 9H, SiMe$_3$). **^{13}C NMR** (C_6D_6, 126 MHz) ***δ*:** 208.5 (C=O); 141.0, 140.1 (C4, *ipso*-Ph); 129.9, 128.3, 127.1 (Ph); 122.3 (C3); 53.2 (C1); 44.4 (C2); 34.1

(C5); 29.6 (C6); 28.4 (CO<u>Me</u>); 24.5 (<u>C</u>H$_2$SiMe$_3$); 20.3 (Me^5); −0.9 (SiMe$_3$). **IR** (ν, cm^{-1})**:** 2954, 1711. **HRMS:** calculated for $C_{19}H_{29}OSi$ ([*M*+H]$^+$) 301.1988, found 301.1982.

<u>Minor isomer, *exo*-**16**</u>. R_f (hexane / Et$_2$O, 9:1)**:** 0.28. **^{1}H NMR** (C_6D_6, 400 MHz) δ**:** 7.27 (d, 2H, *J* 8.0, Ph); 7.15 (t, 2H, *J* 8.0, Ph); 7.05 (t, 1H, *J* 8.0, Ph); 5.17 (m, 1H, H3); 3.94 (d, 1H, *J* 9.0, H2); 2.71 (ddd, 1H, *J* 12.5, 9.0, 3.0, H1); 2.05−1.98 (m, 1H, H5); 1.83 (td, 1H, *J* 12.5, 5.5, H6^{ax}); 1.58 (s, 3H, COMe); 1.47−1.41 (m, 3H, H6^{eq}, C<u>H</u>$_2$SiMe$_3$); 1.06 (d, 3H, *J* 7.0, Me^5); −0.02 (s, 9H, SiMe$_3$). **^{13}C NMR** (C_6D_6, 126 MHz) δ**:** 209.3 (C=O); 145.9, 140.0 (C4, *ipso*-Ph); 128.8, 128.5, 126.7 (Ph); 122.5 (C3); 51.2 (C1); 44.8 (C2); 33.3, 33.2 (C5, C6); 29.5 (CO<u>Me</u>); 25.1 (<u>C</u>H$_2$SiMe$_3$); 19.8 (Me^5); −1.1 (SiMe$_3$). **HRMS:** required for $C_{19}H_{29}OSi$ ([*M*+H]$^+$) 301.1988, found 301.1982.

1-{5,6-Dimethyl-2-phenyl-4-[(trimethylsilyl)methyl]cyclohex-3-en-1-yl}ethanone – [*rac*-(1*R*,2*R*,5*R*,6*S*): *exo*-**17a** (major)], [*rac*-(1*R*,2*R*,5*S*,6*S*): *exo*-**17b** (minor)] [*rac*-(1*R*,2*S*,5*R*,6*S*): *endo*-**17c** (minor)] [*rac*-(1*R*,2*S*,5*S*,6*S*): *endo*-**17d** (minor)]



To a solution of (*E*)-pent-3-en–2-one (**5**) (62 mg, 0.63 mmol) in CH_2Cl_2 (5 mL) cooled at −40 °C was added dimethylaluminum chloride (0.13 mL, 0.13 mmol of a 1 *M* solution in hexanes), followed by a solution of **1b** (207 mg, 0.90 mmol, *Z*/*E* = 3:1) in CH_2Cl_2 (1 mL) added dropwise. The reaction mixture was warmed to room temperature and stirred for 4 hours. The reaction was quenched by saturated NH_4Cl(aq) (6 mL), diluted by Et_2O and transferred to a separation funnel. The phases were separated. The aqueous phase was extracted with Et_2O (2 × 7 mL). The combined organic phases were dried over $MgSO_4$, filtered and evaporated under reduced pressure to furnish the crude product, which was purified by column chromatography (40°–60° petroleum spirit / Et_2O, 9:1). The inseparable C5-epimeric mixture

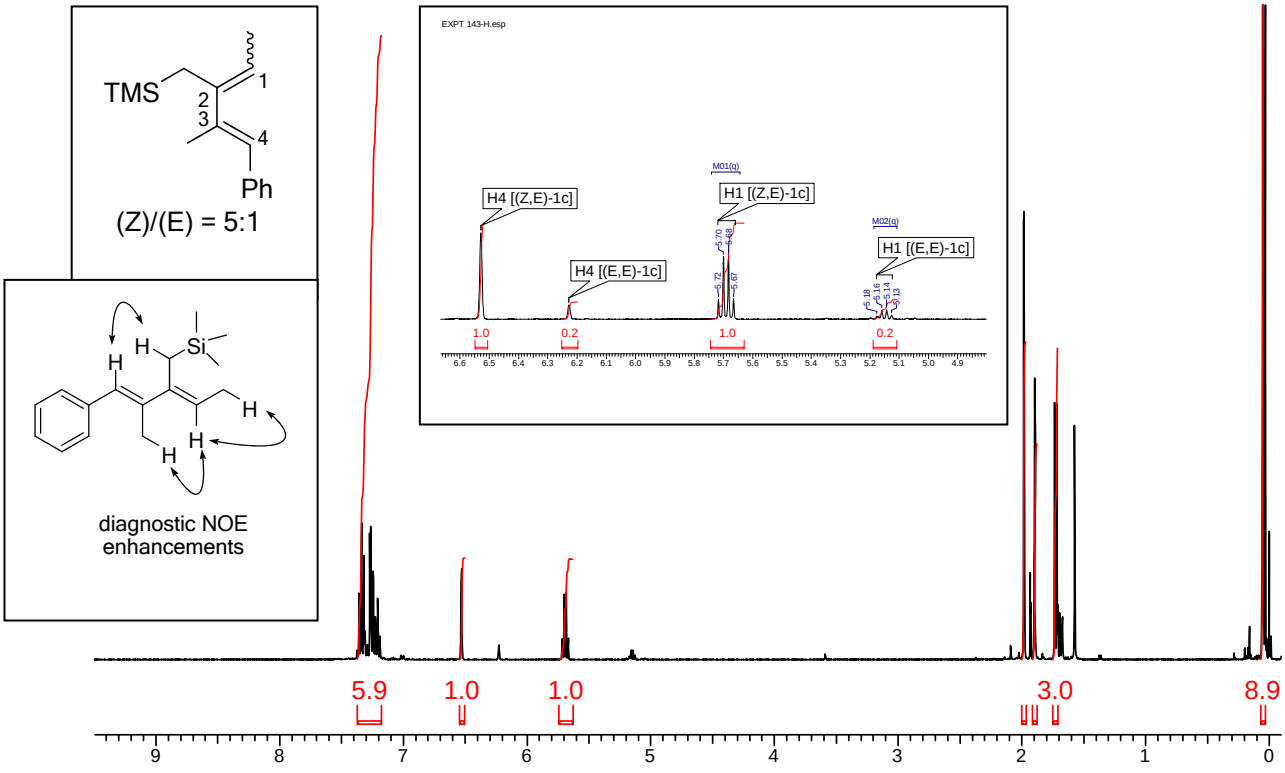
of cycloadducts *exo*-**17a** and *exo*-**17b** was obtained as a colorless oil (154 mg, 78%, **17a** / **17b** = 5:1 by ^{1}H NMR).

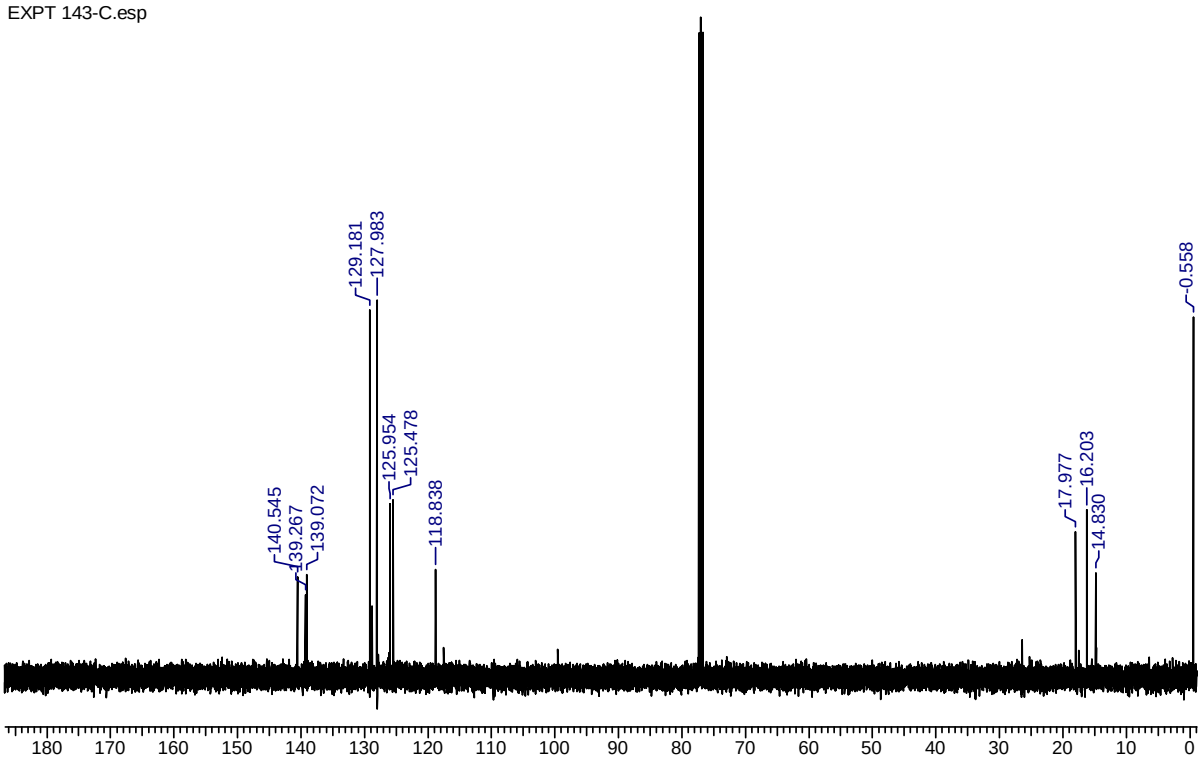
The diastereoselectivity of the cycloaddition was determined by ^{1}H NMR after aqueous workup. Analysis of integration of the signal due to H3 of the major *exo* isomer (**17a**, δ_H 5.13, s), the minor *exo* isomer (**17b**, δ_H 5.23, s), and the *endo* isomers (δ_H 5.30, 5.16, both doublets, tentatively assigned based on NMR coupling constants) gave the d.r. as approximately **17a**:**17b**:(two *endo* isomers) = 11:0.5:(1.8:0.7).

Exo cycloadducts. R_f (hexane / Et_2O, 94:6)**:** 0.27. *Exo*-**17a**. **^{1}H NMR** (400 MHz, C_6D_6) **δ:** 7.20–7.02 (m, 5H, Ph); 5.13 (s, 1H, H3); 3.82 (d, *J* 11.0, 1H, H2); 2.61 (t, *J* 11.0, 1H, H1); 2.32–2.23 (m, 1H, H5); 1.87−1.80 (m, 1H, H6); 1.57 (s, 3H, COMe); 1.48 (d, *J* 14.0, 1H, CHH′SiMe$_3$); 1.38 (d, 1H, *J* 14.0, CHH′SiMe$_3$); 0.96 (d, *J* 7.0, 3H, Me^6); 0.77 (d, *J* 7.0, 3H, Me^5); −0.02 (s, 9H, SiMe$_3$). **^{13}C NMR** (126 MHz, C_6D_6) **δ:** 211.7 (C=O); 145.6 (C4); 141.3, 128.9, 128.3, 126.8 (Ph); 121.8 (C3); 56.3 (C1); 48.1 (C2); 39.7, 35.8 (C5, C6); 33.4 (COMe); 25.3 (CH_2SiMe_3); 16.9 (Me^6); 14.0 (Me^5); −1.1 (SiMe$_3$). *Exo*-**17b**. **^{1}H NMR** (400 MHz, C_6D_6) **δ:** 7.20–7.02 (m, 5H, Ph); 5.23 (s, 1H, H3); 3.66 (d, 1H, *J* 11.0, H2); 2.44 (t, 1H, *J* 11.0, H1); 1.87–1.81 (m, 1H), 1.77–1.69 (m, 1H) (H5, H6); 1.62 (s, 3H, COMe); 1.38 (d, 1H, *J* 12.0, CHH′SiMe$_3$); 1.33 (d, 1H, *J* 12.0, CHH′SiMe$_3$); 0.99 (d, 3H, *J* 6.8), 0.83 (d, 3H, *J* 6.3) (Me^5, Me^6); 0.05 (s, 9H, SiMe$_3$). **^{13}C NMR** (126 MHz, C_6D_6) **δ:** 211.5 (C=O); 145.1 (C4); 139.5, 126.9 (Ph); 124.4 (C3); 62.8 (C1); 47.4 (C2); 41.6, 39.9 (C5, C6); 33.0 (COMe); 24.9 (CH_2SiMe_3); 18.4, 17.9 (Me^5, Me^6); −0.8 (SiMe$_3$). **HRMS:** required for $C_{20}H_{34}NOSi$ ($[M+NH_4]^+$) 332.2410, found 332.2411. Integration of the signal due to H3, H2, H1, Me^5 or Me^6 protons of the two isomers gave the diastereomeric ratio of *exo*-**17a**:*exo*-**17b** = 5:1.

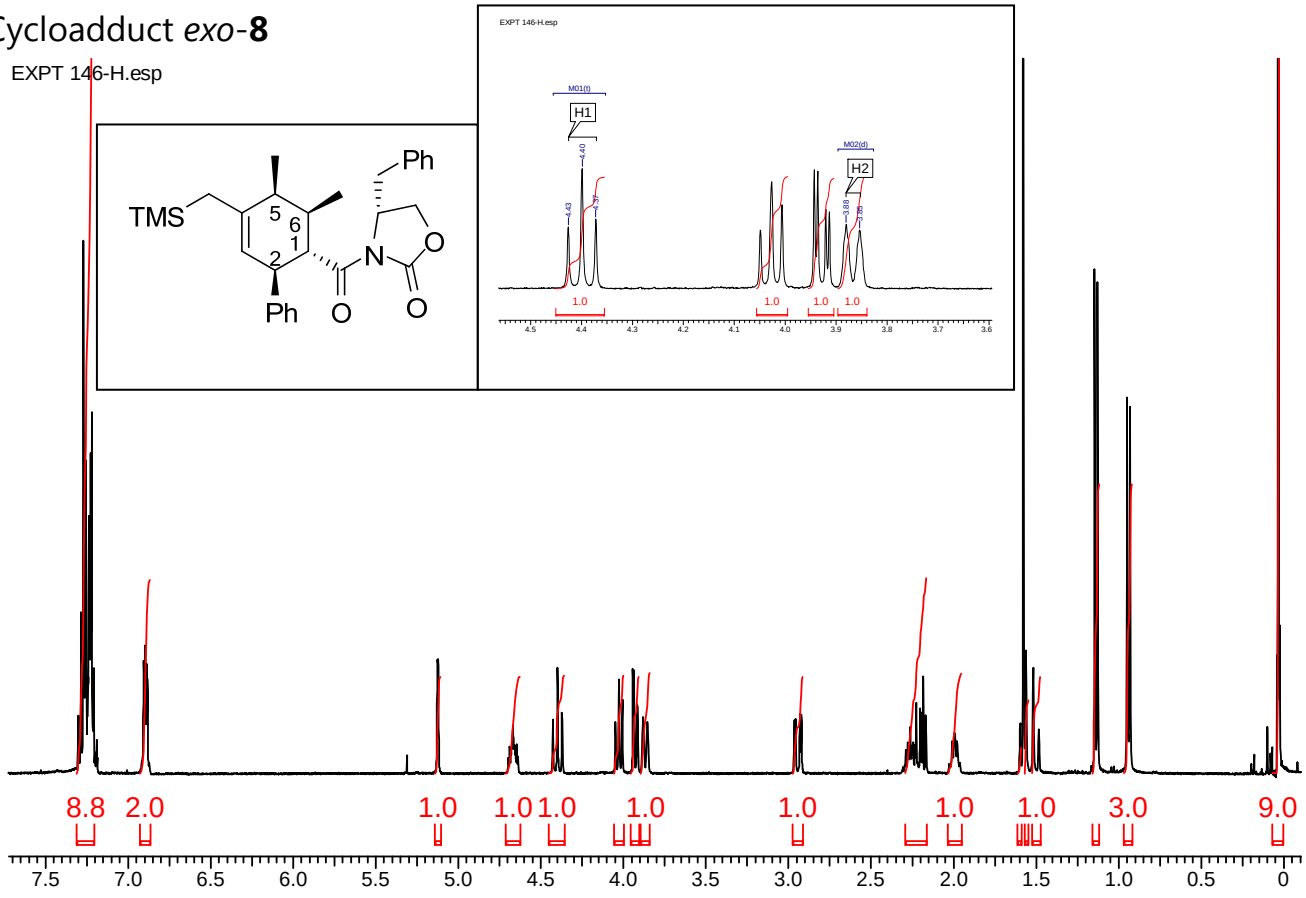
C. NMR Spectra

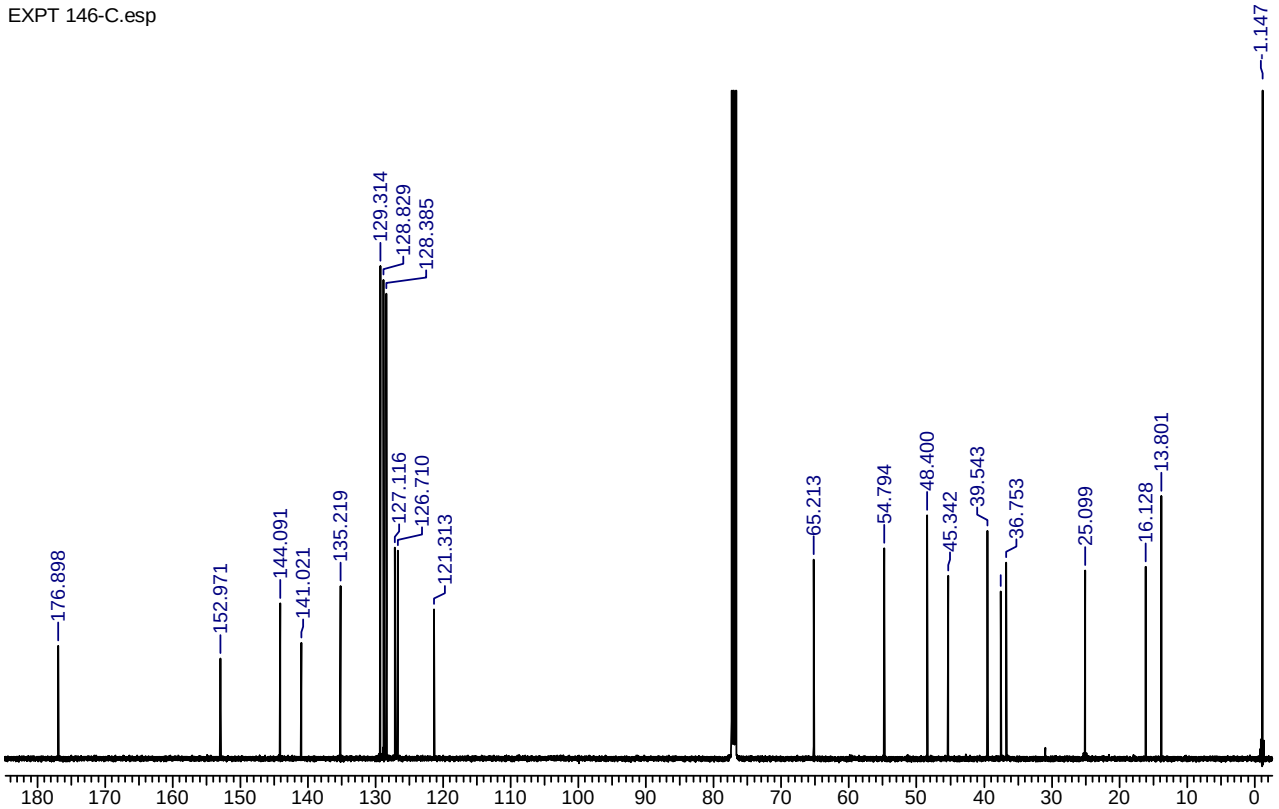
Diene **1c**



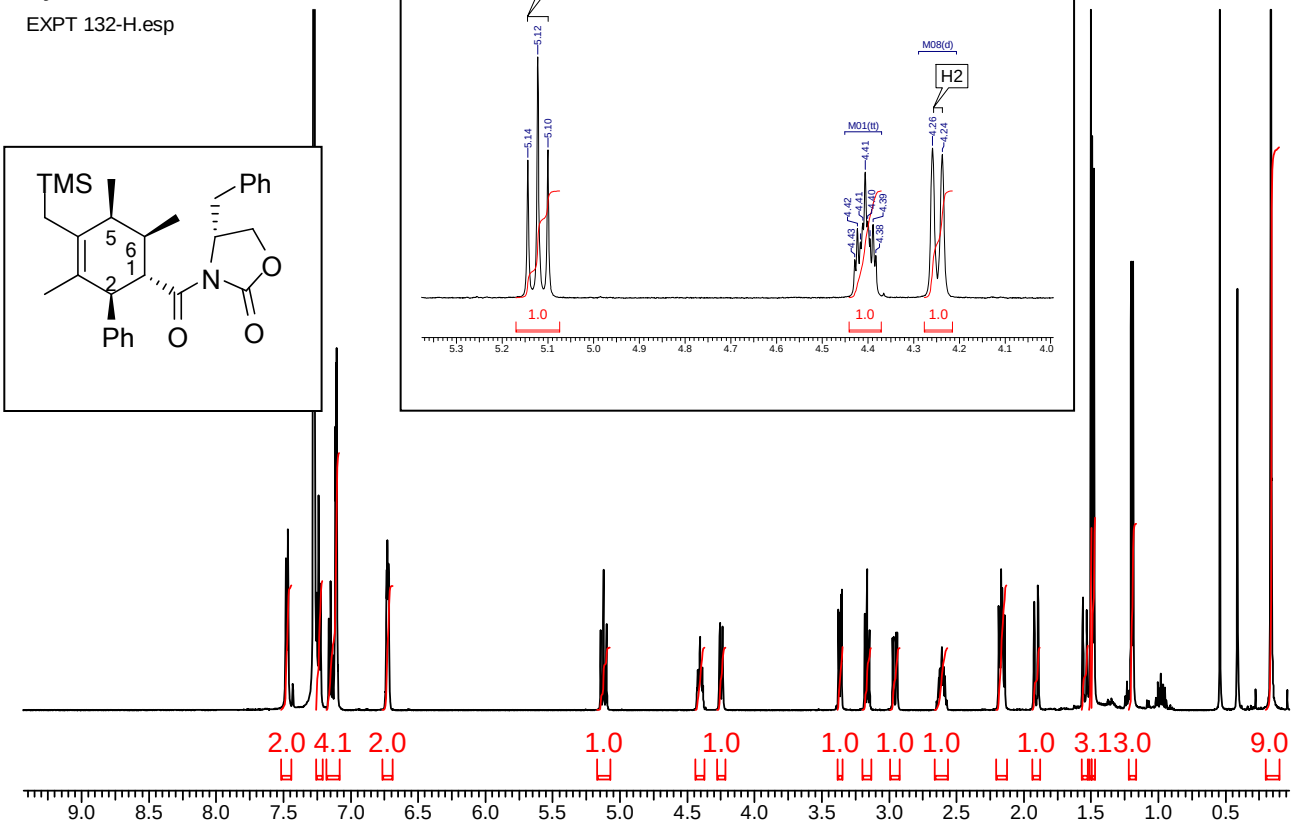


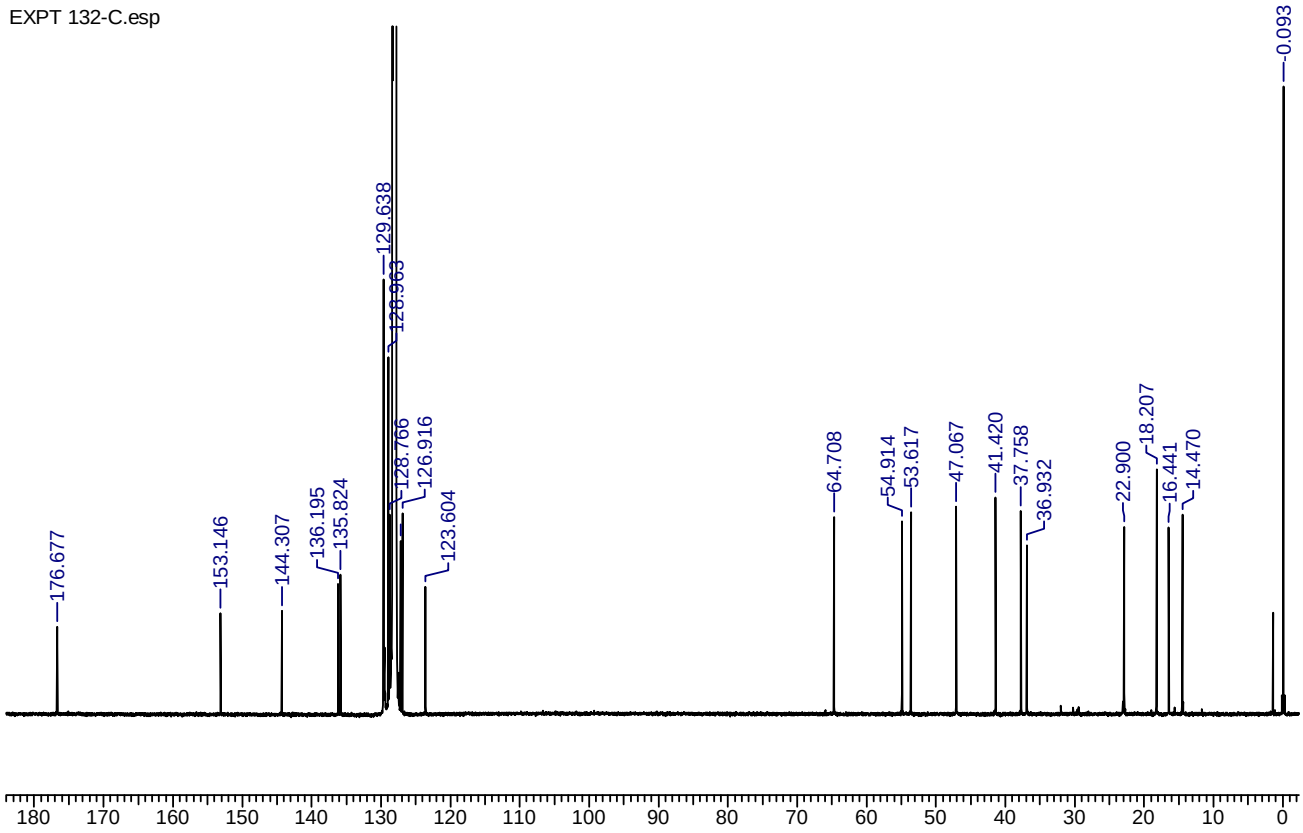
Cycloadduct *exo*-**8**





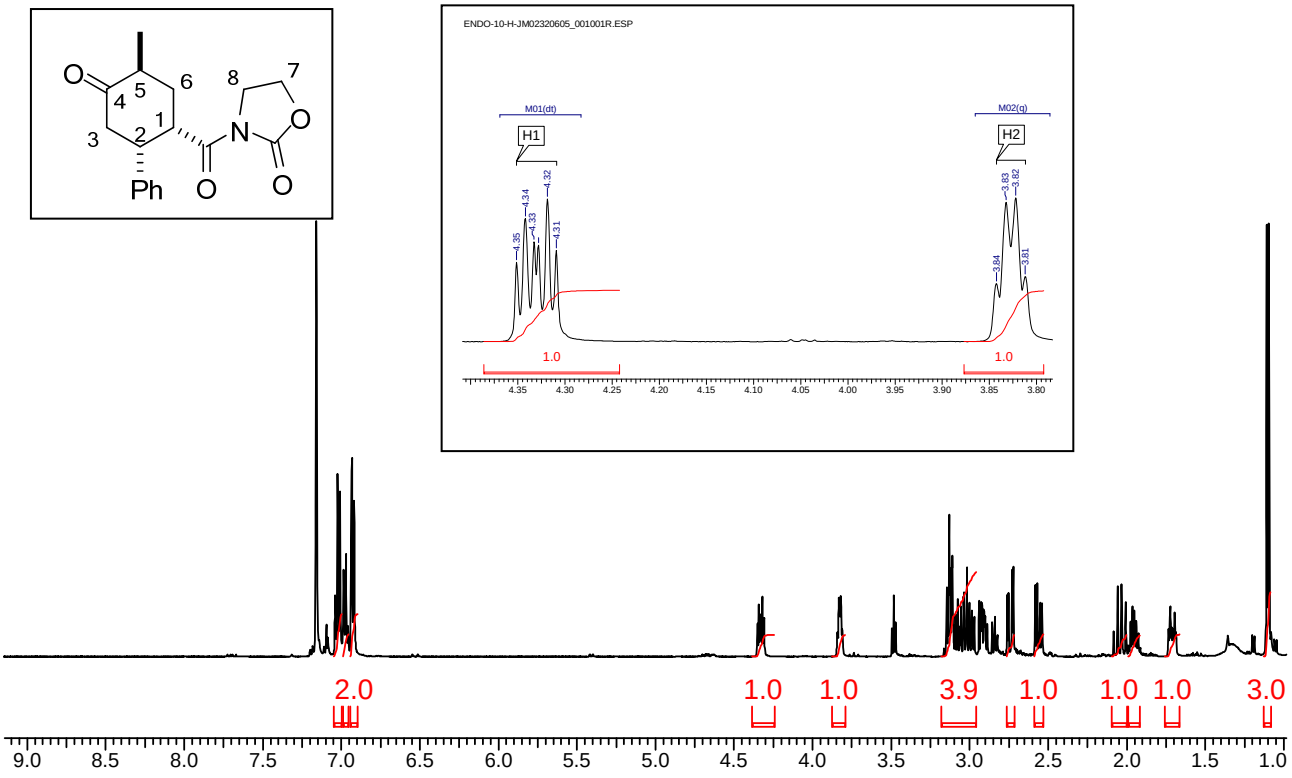
Cycloadduct *exo*-**9**



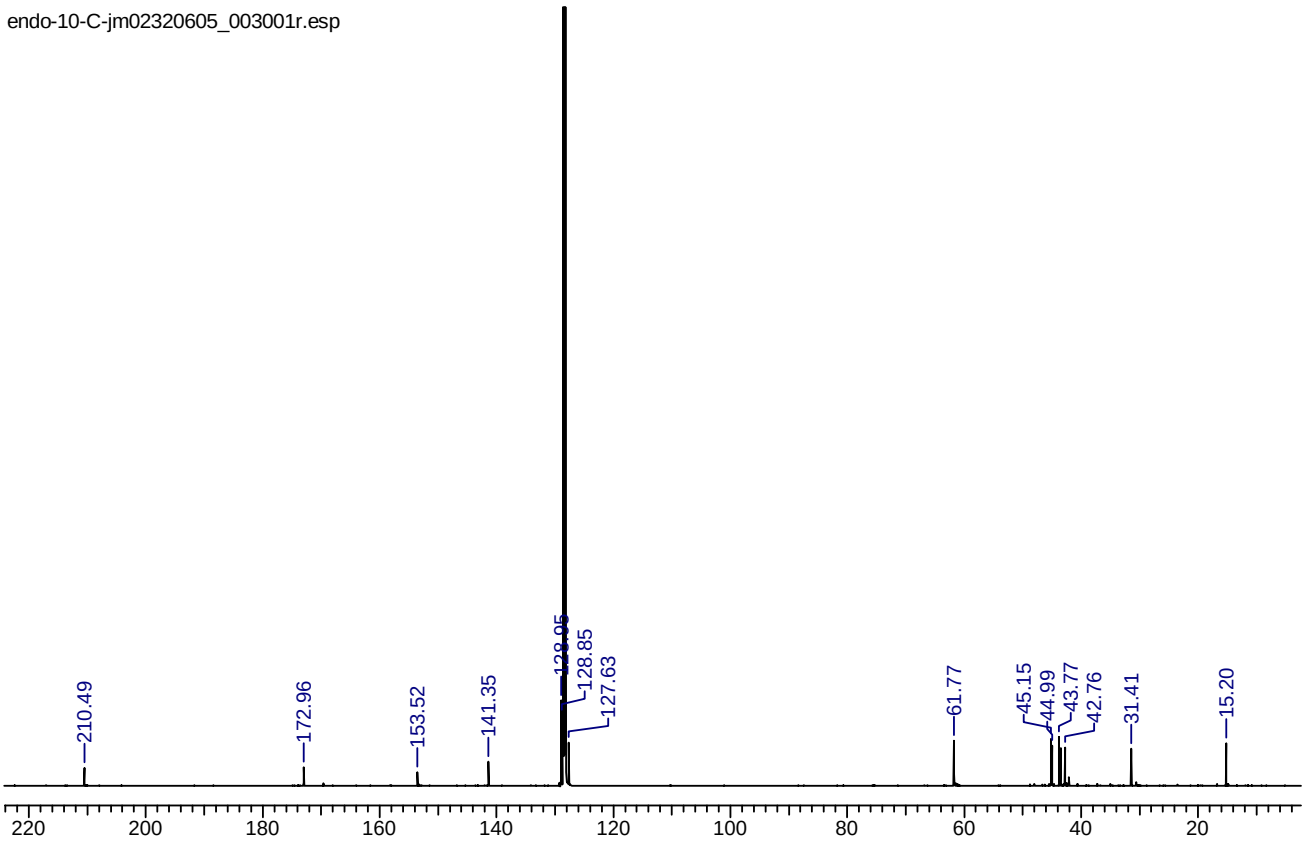


Cycloadduct *endo*-**10**

ENDO-10-H-JM02320605_001001R.ESP

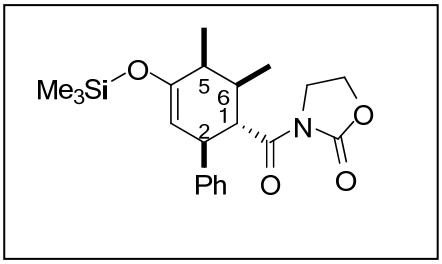


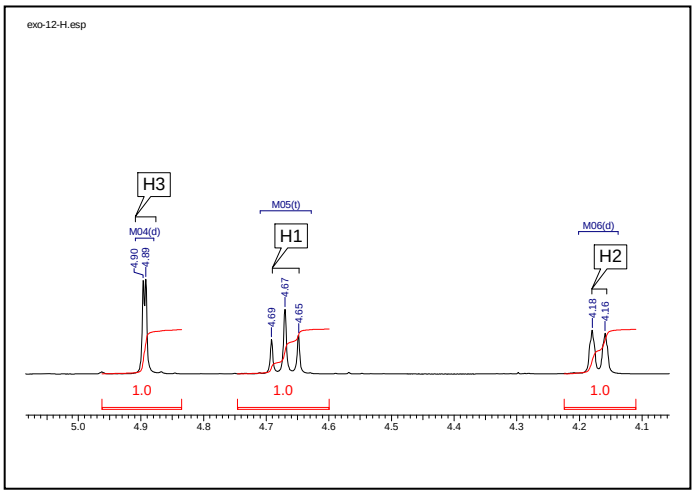
endo-10-C-jm02320605_003001r.esp

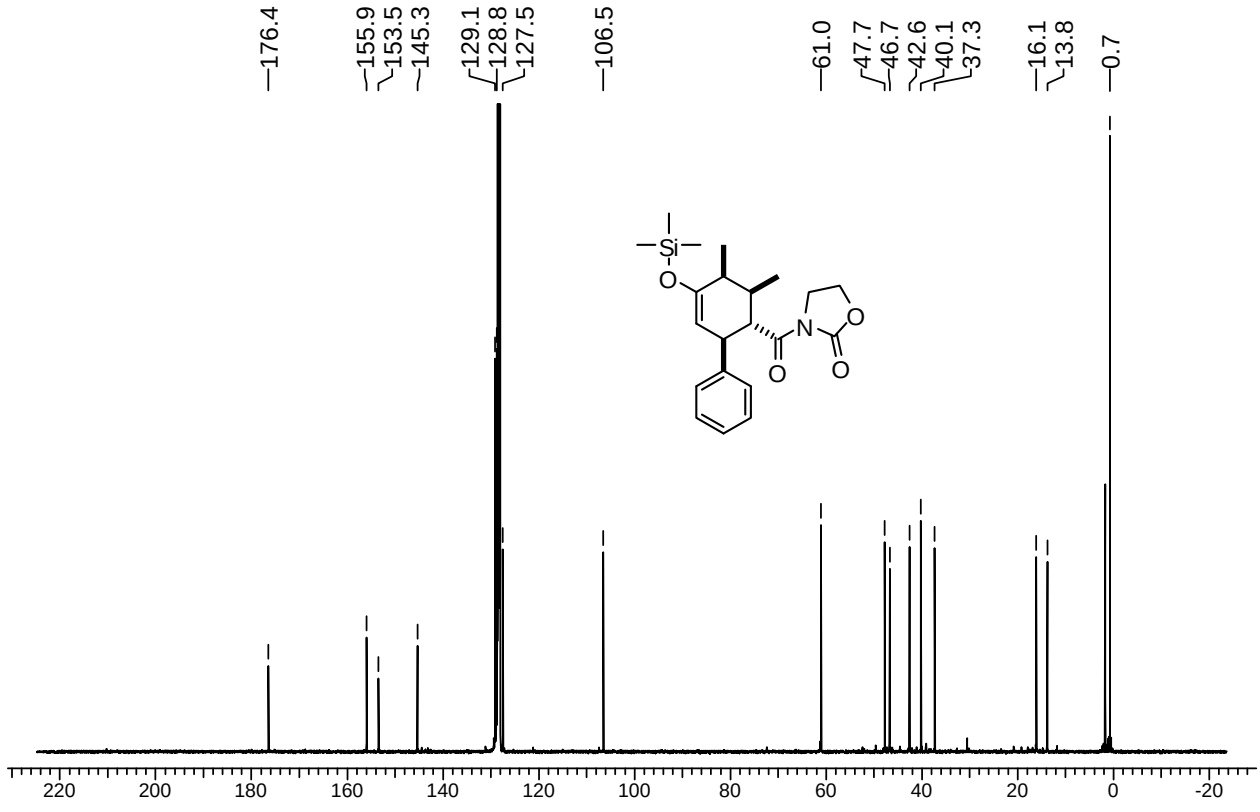


Cycloadduct *exo*-**11**

EXO-11-H.ESP

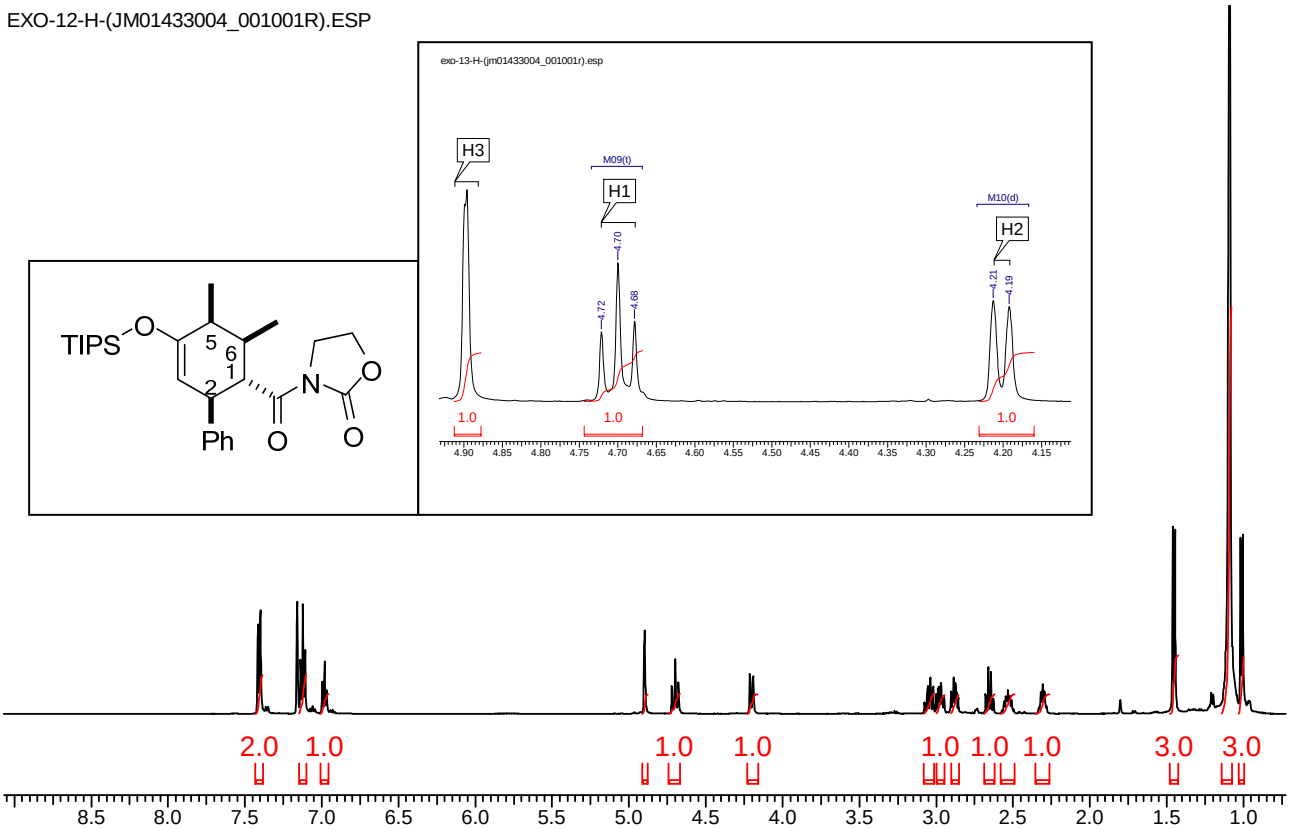


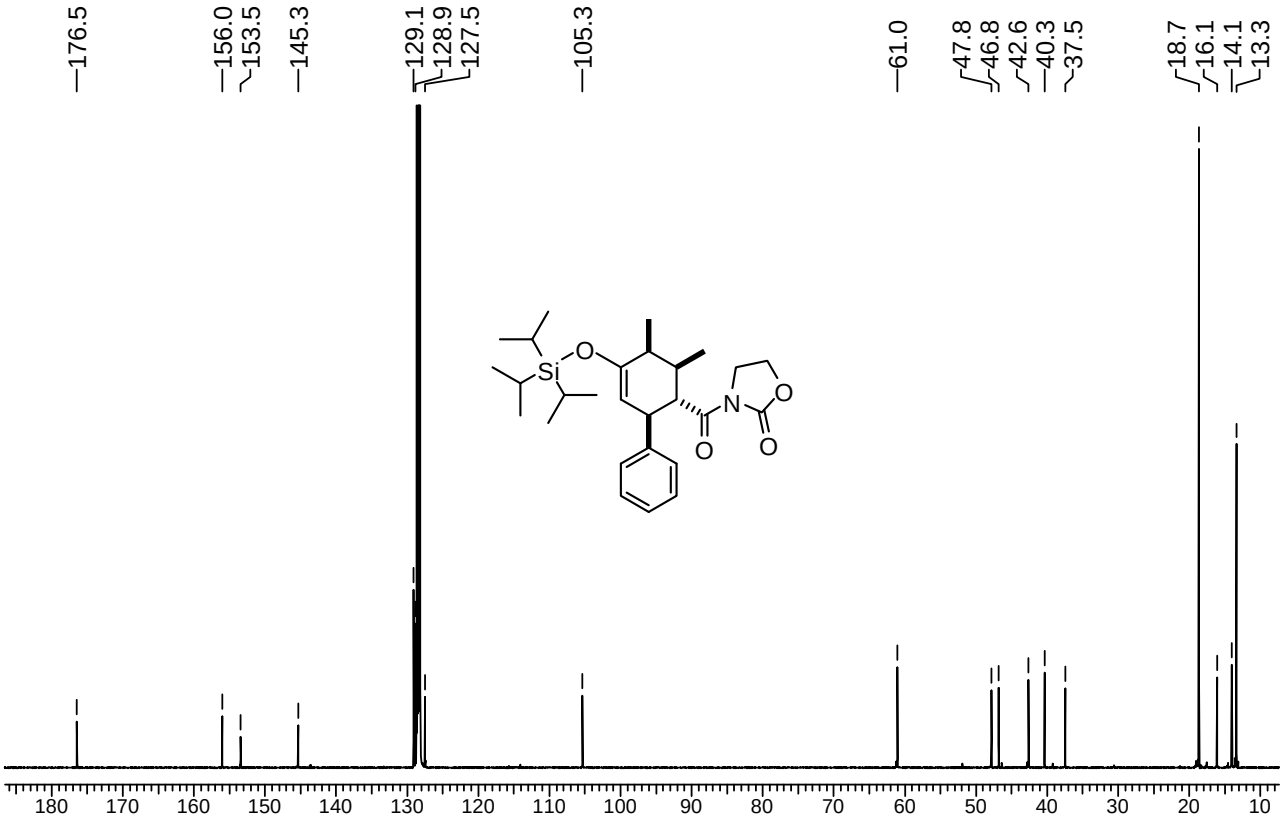




Cycloadduct *exo*-**12**

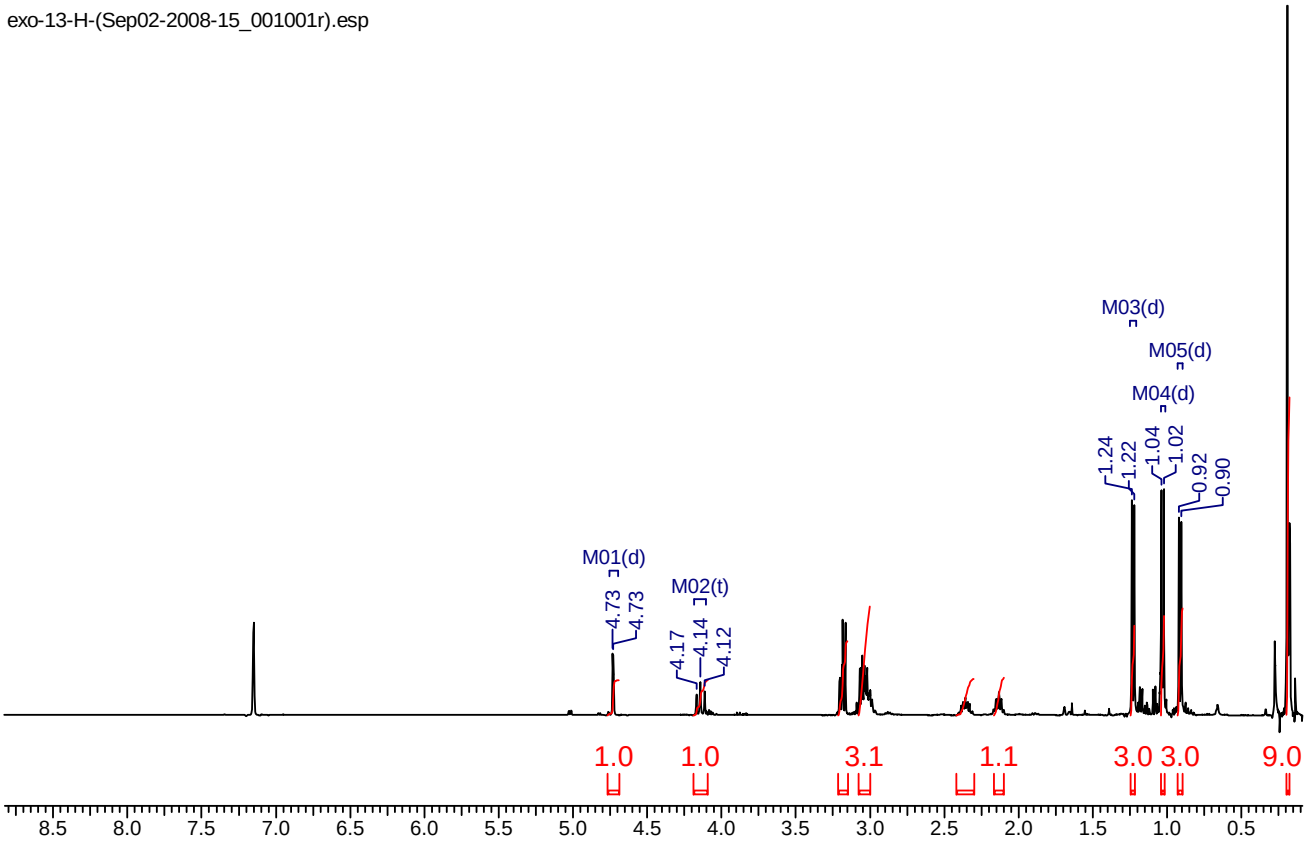
EXO-12-H-(JM01433004_001001R).ESP

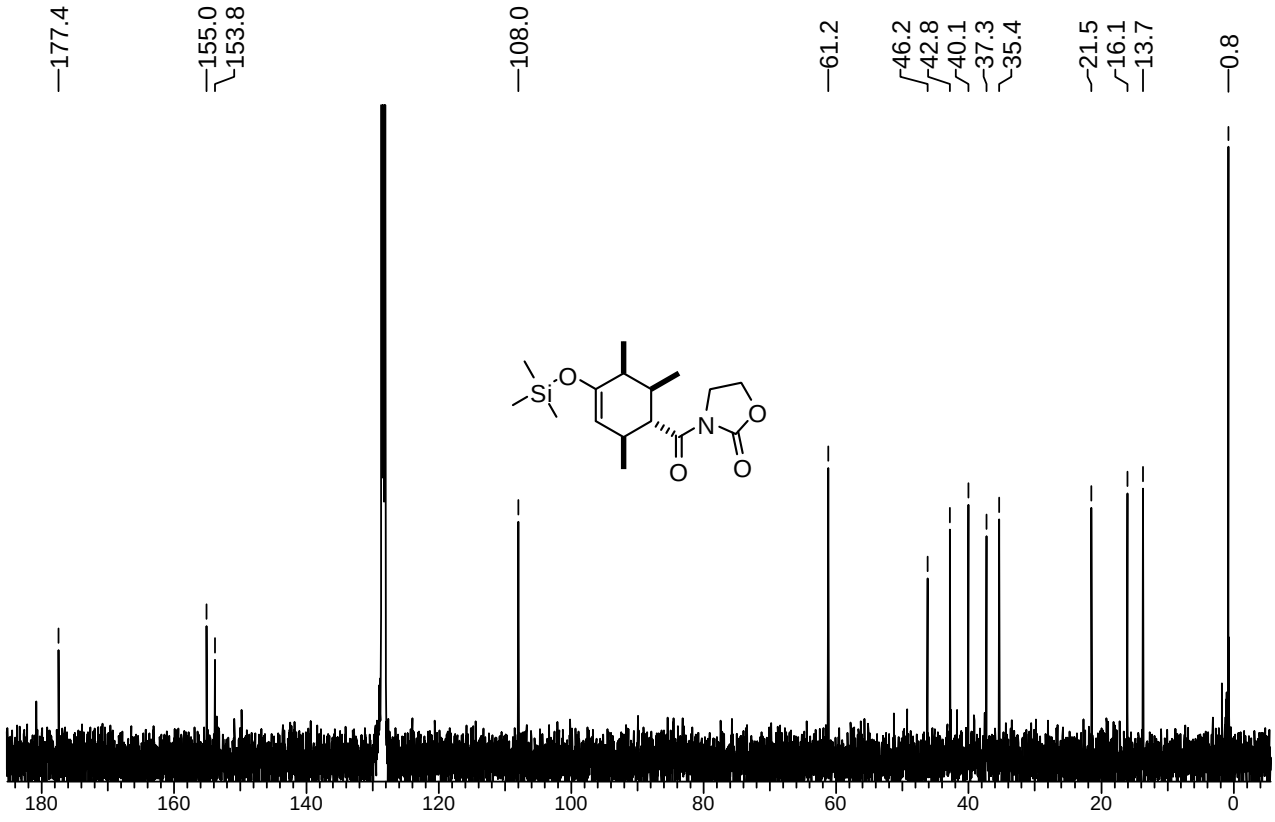




Cycloadduct *exo*-**13**

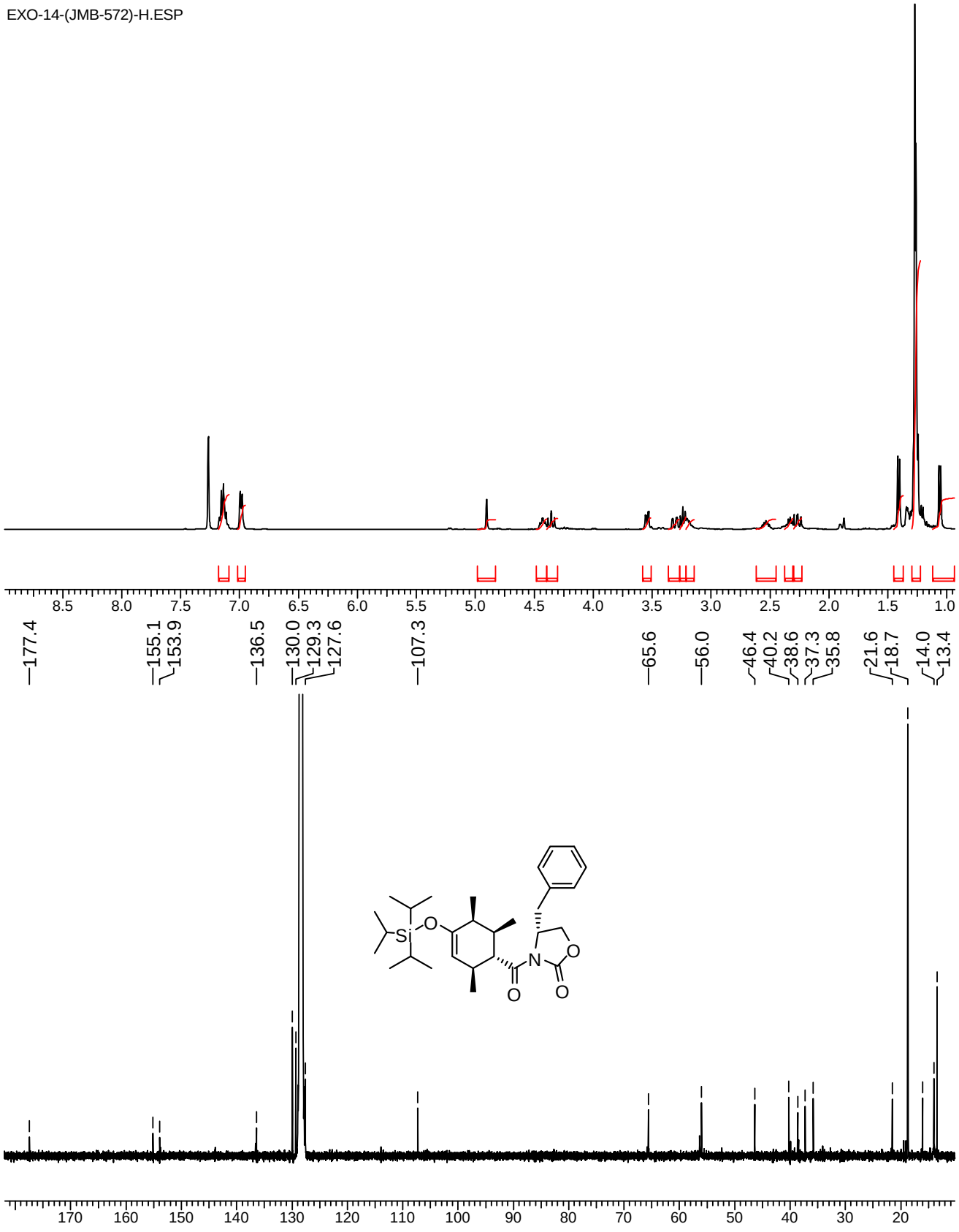
exo-13-H-(Sep02-2008-15_001001r).esp



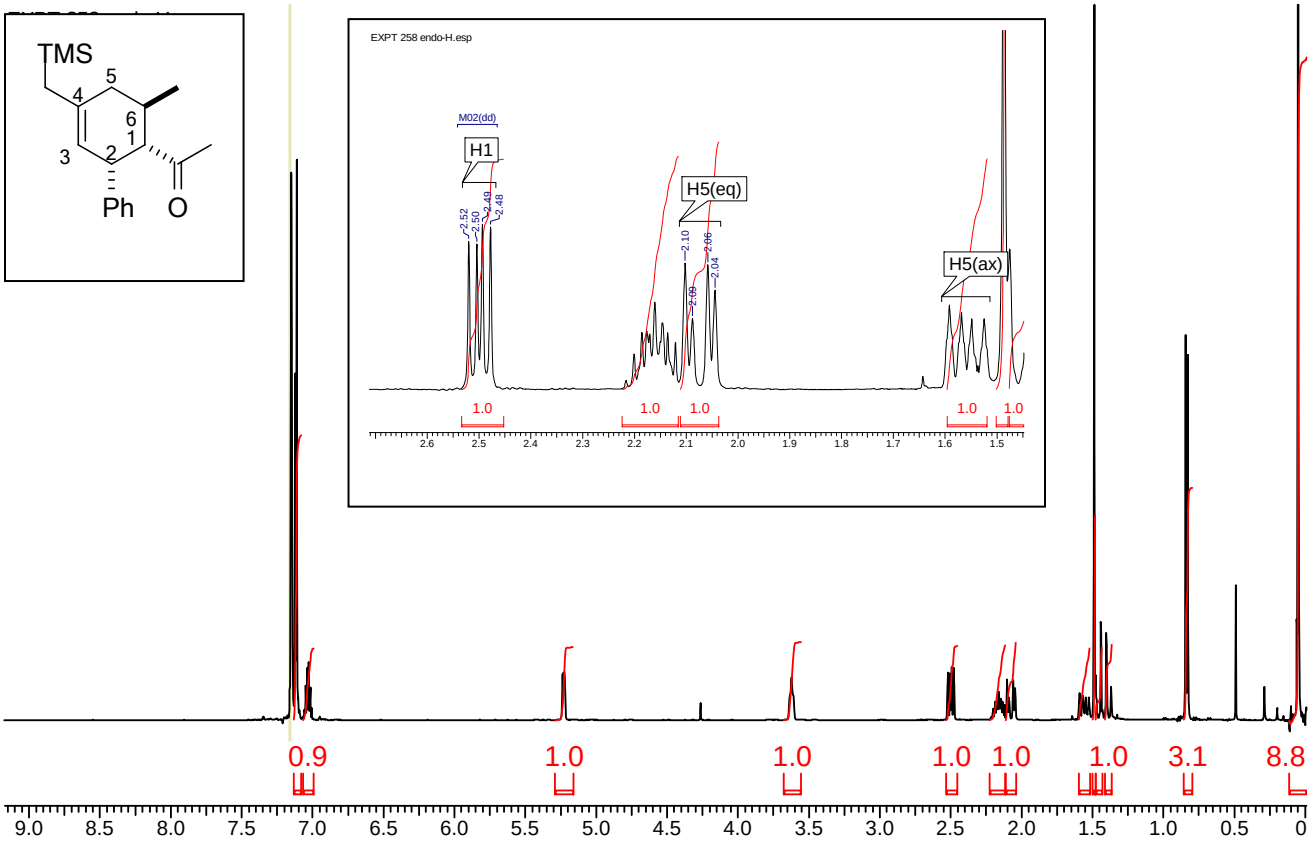


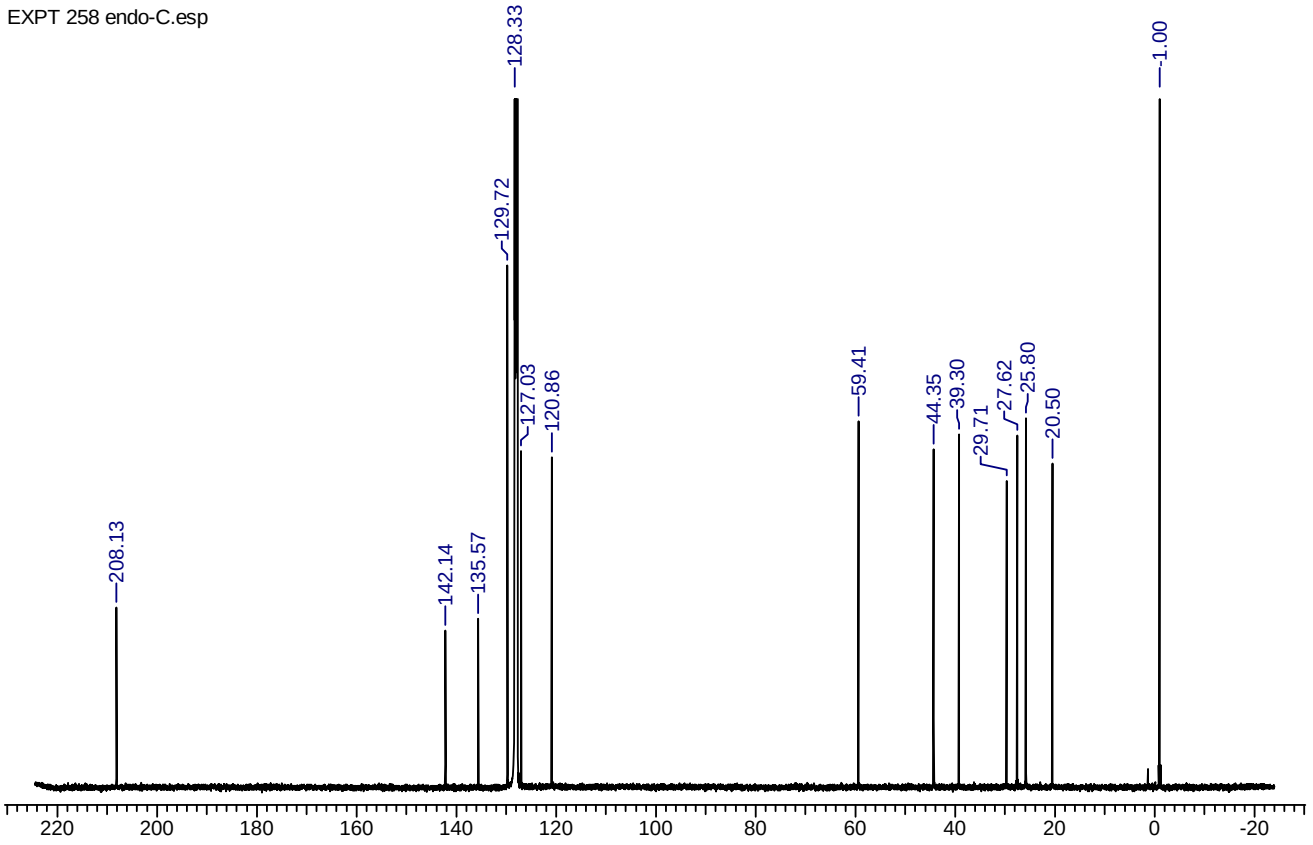
Cycloadduct *exo*-**14**

EXO-14-(JMB-572)-H.ESP

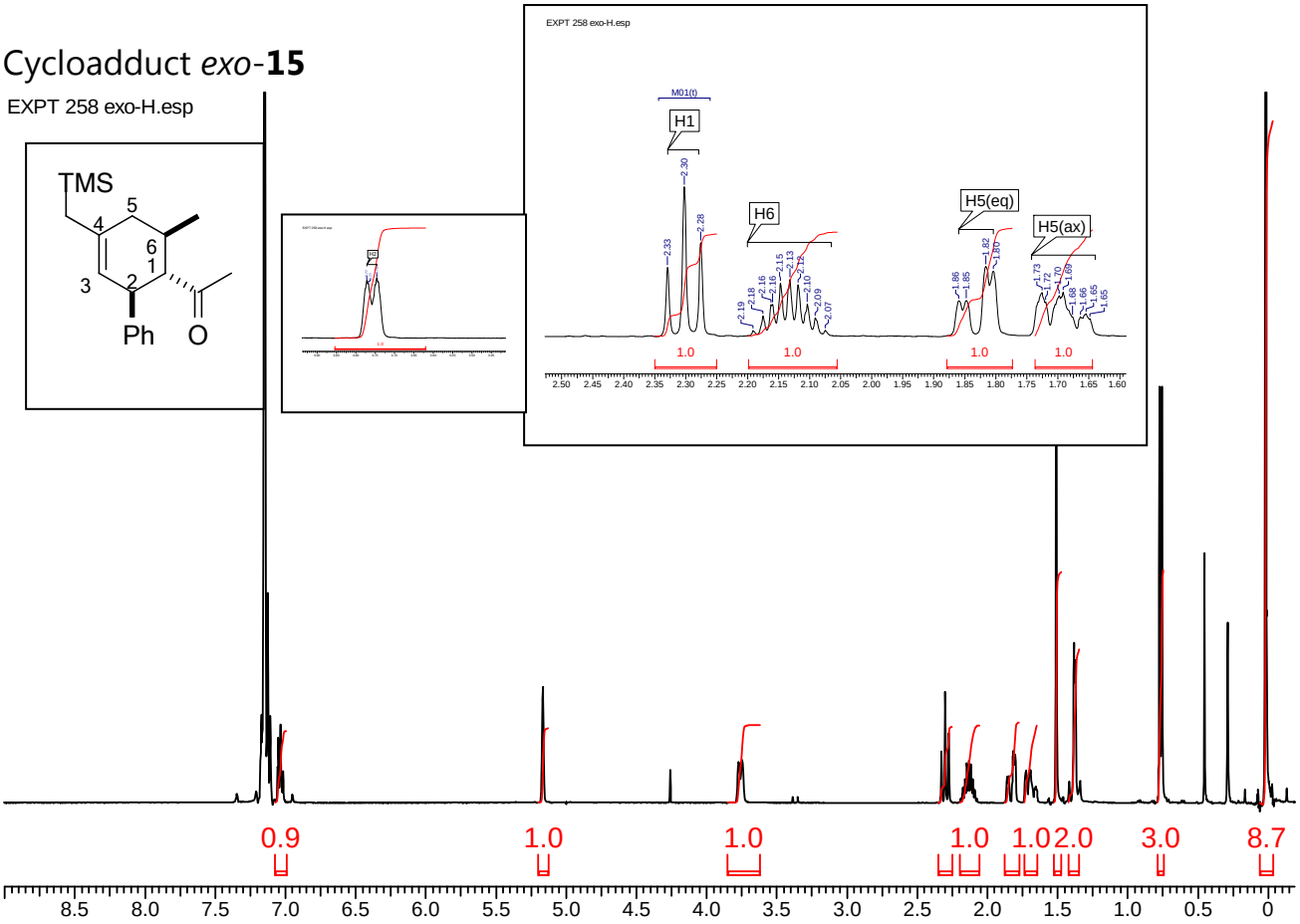


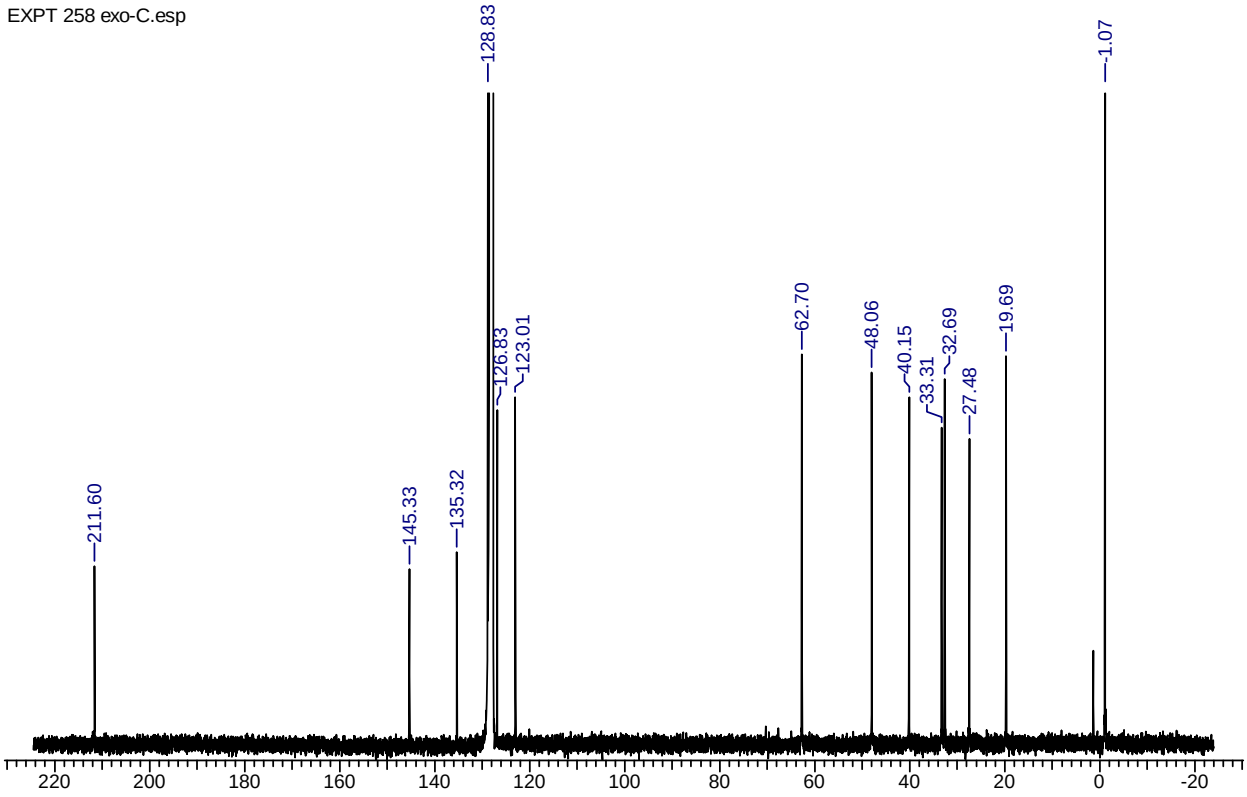
Cycloadduct *endo*-**15**



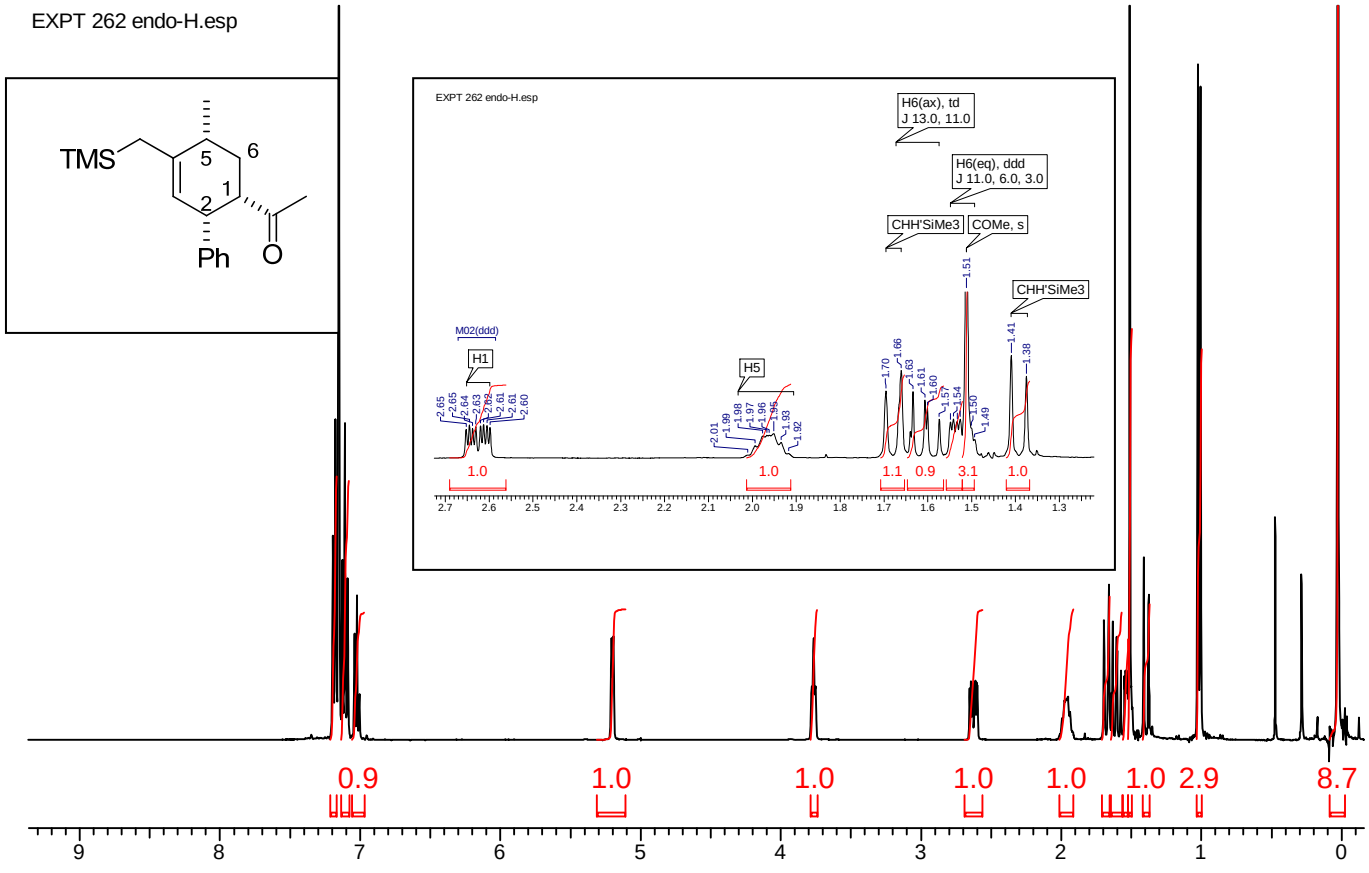


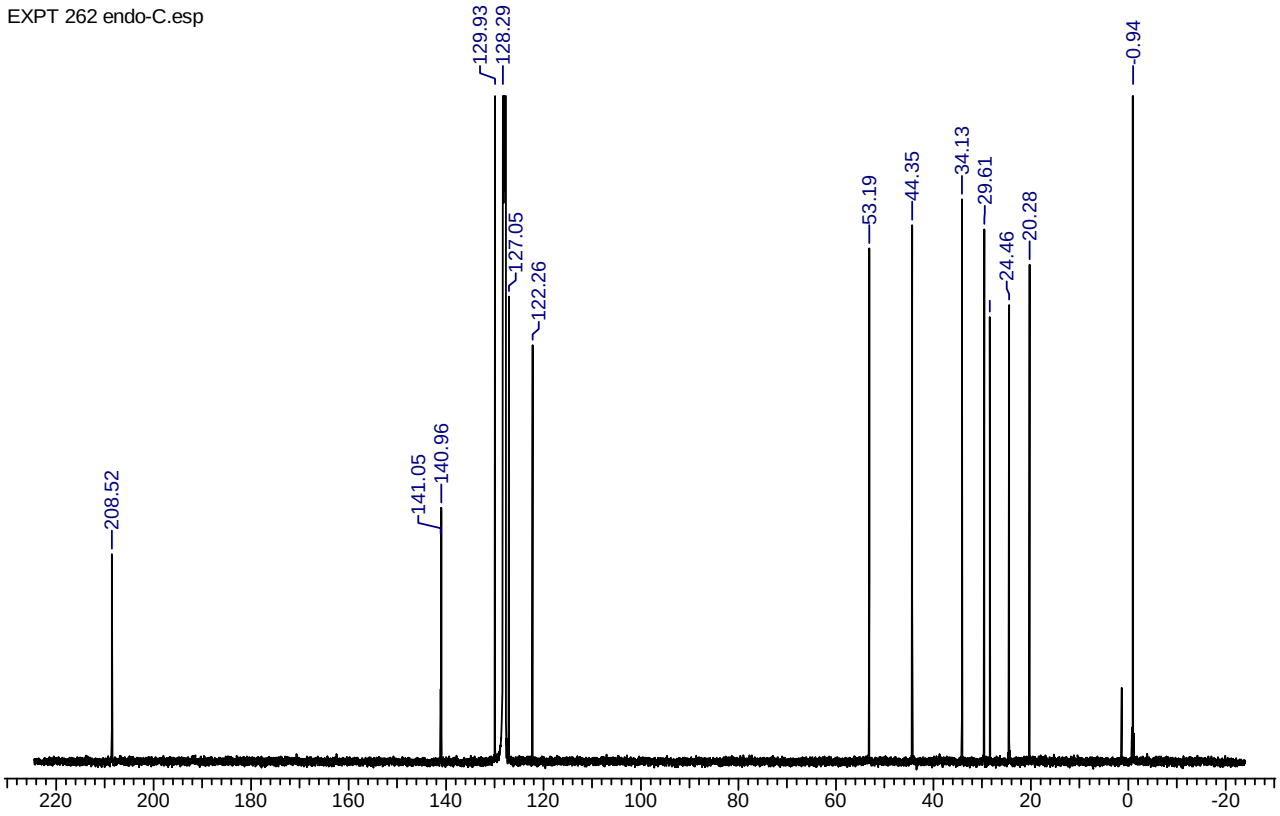
Cycloadduct *exo*-**15**





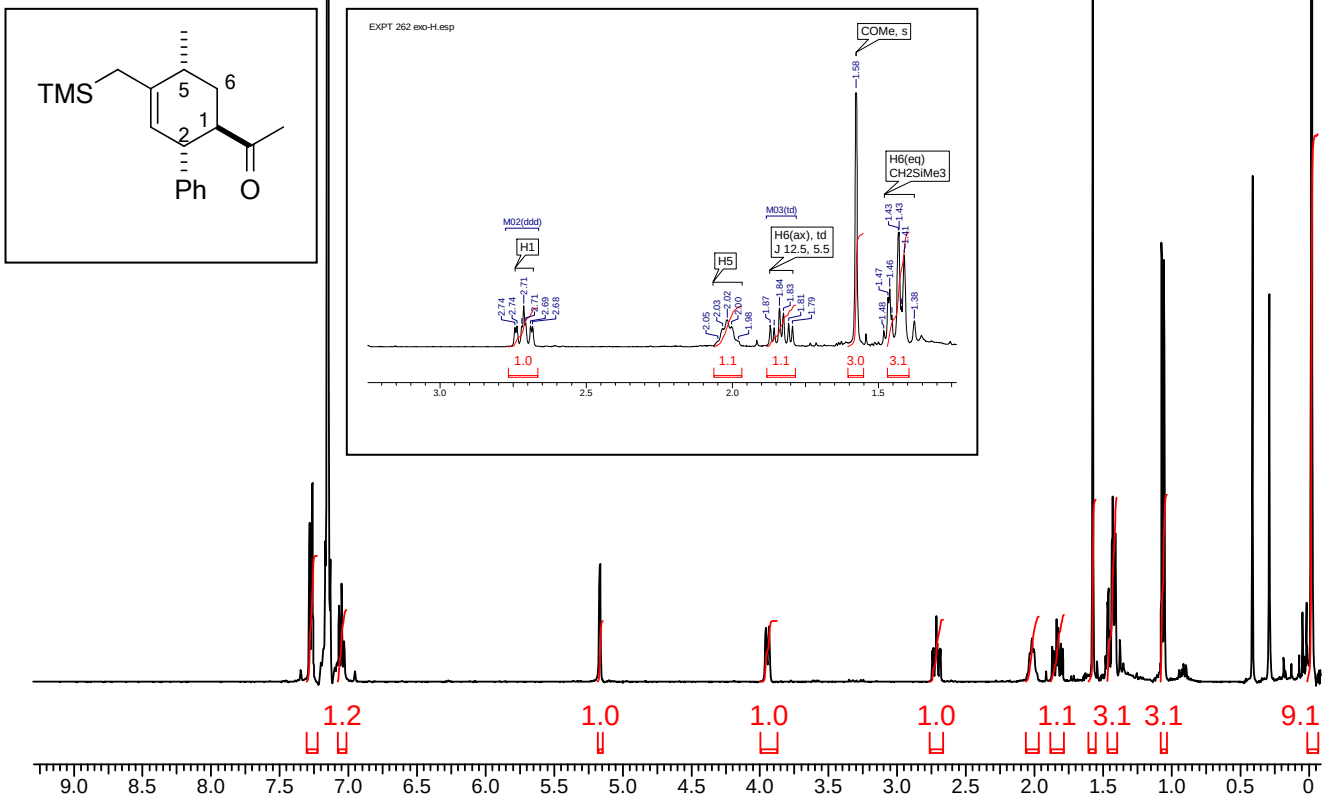
Cycloadduct *endo*-**16**



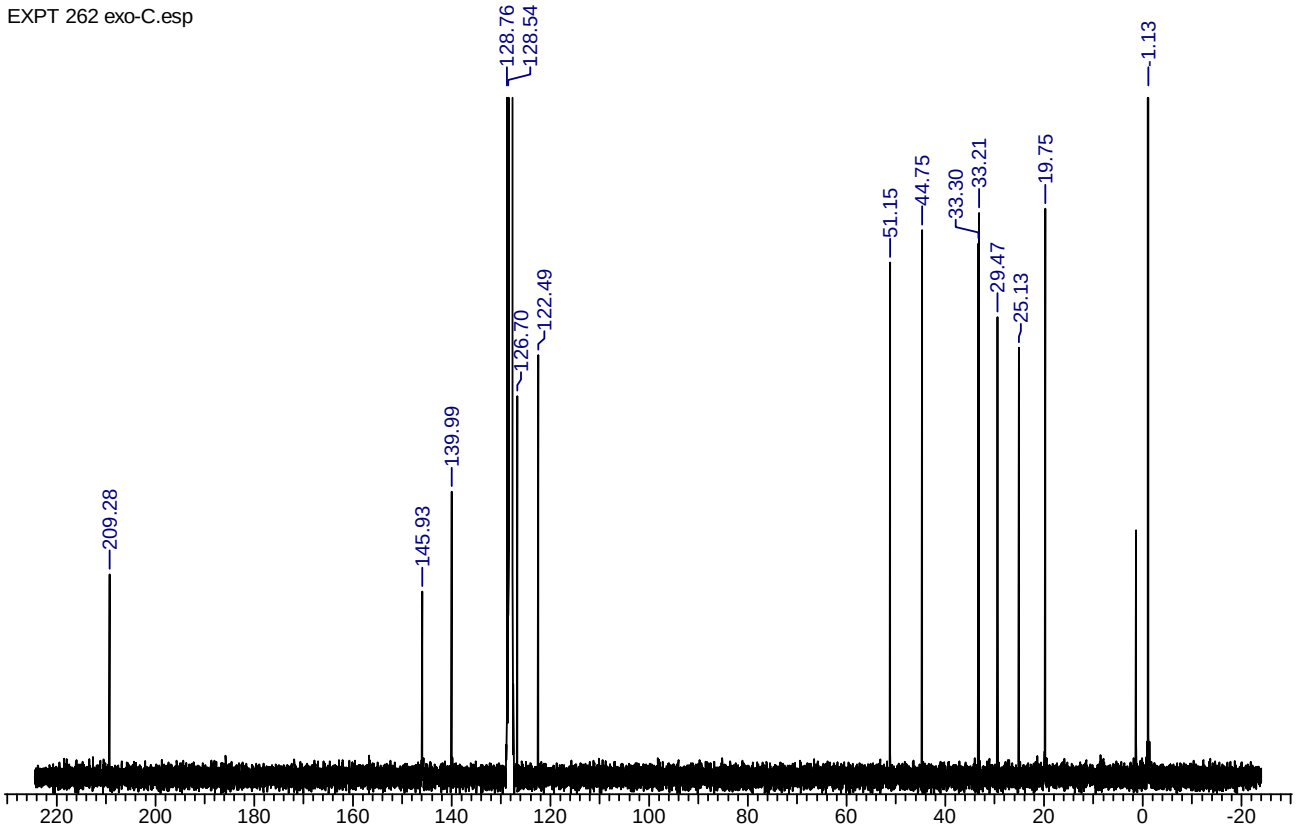


Cycloadduct *exo*-**16**

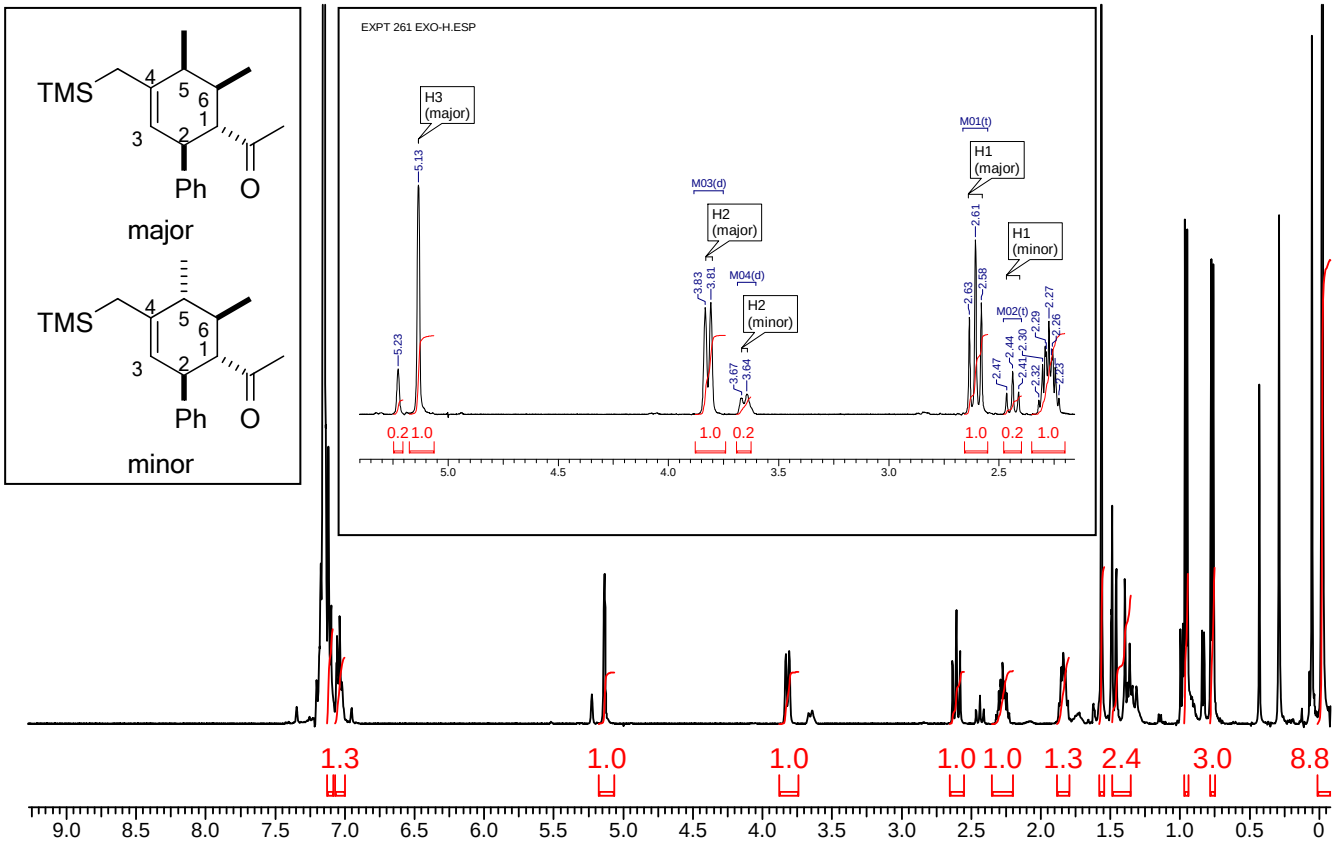
EXPT 262 exo-H.esp

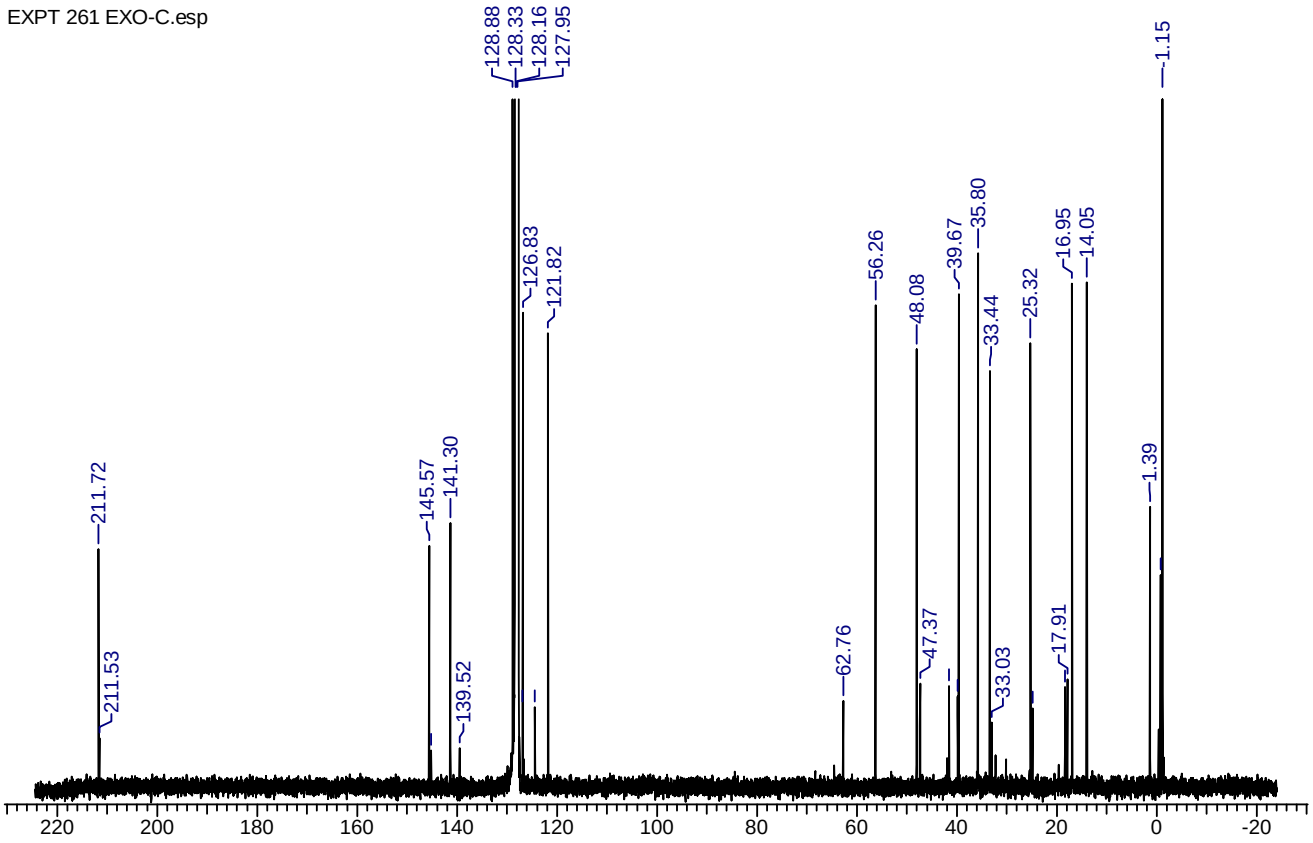


EXPT 262 exo-C.esp



Cycloadducts *exo*-**17a**/*exo*-**17b**





References (Experimental)

(1) Narayanan, B. A.; Bunnelle, W. H. *Tetrahedron Lett.* **1987**, *28*, 6261–6264.

(2) Lam, Y.-h.; Bobbio, C.; Cooper, I. R.; Gouverneur, V. *Angew. Chem. Int. Ed.* **2007**, *46*, 5106–5110.

(3) Yamamoto, Y.; Yamamoto, H. *Angew. Chem. Int. Ed.* **2005**, *44*, 7082–7085.

(4) Kanemasa, S.; Kumegawa, M.; Wada, E.; Nomura, M. *Bull. Chem. Soc. Jpn.* **1991**, *64*, 2990–3004.

(5) Nakashima, D.; Yamamoto, H. *J. Am. Chem. Soc.* **2006**, *128*, 9626–9627.

(6) Evans, D. A.; Chapman, K. T.; Bisaha, J. *J. Am. Chem. Soc.* **1984**, *106*, 4261–4263.

(7) Kanemasa, S.; Kanai, T. *J. Am. Chem. Soc.* **2000**, *122*, 10710–10711.

(8) Thom, C.; Kocienski, P. *Synthesis* **1992**, 582–586.

(9) Gößnitzer, E.; Wendelin, W. *Monatsh. Chem.* **2001**, *132*, 607–624.

(10) Carter, M. J.; Fleming, I.; Percival, A. *J. Chem. Soc. Perkin Trans. 1* **1981**, 2415–2434.

II. Computational Data

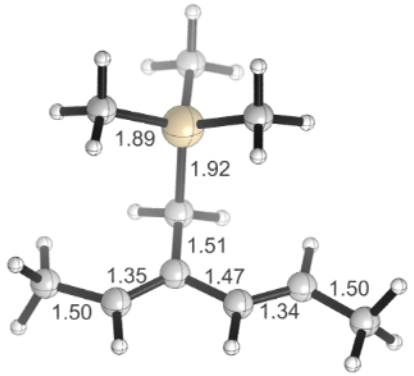
A. Complete ref. 35

Gaussian 03, Revision C.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.

Gaussian 03, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, 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, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.

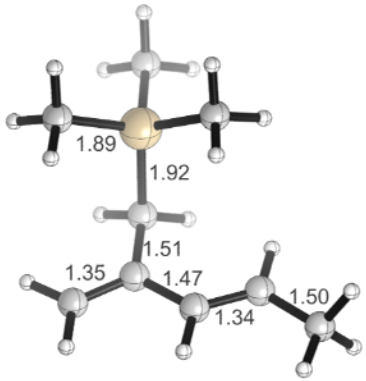
B. Optimized Structure and Energies of Reactants

Diene **1d**



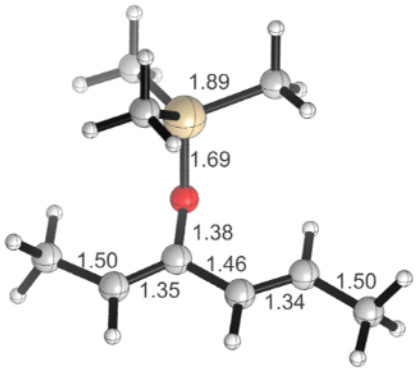

```
 ---------------------------------------------------------------------
 Analyzing Gaussian Output File: 11_t_SM_080426.out
 Using Gaussian 03:  IA64L-G03RevD.01 13-Oct-2005
 [#Processors=4  Memory=4gb  CheckPoint=11_t_SM_080426.chk]
=====================================================================
 #p b3lyp/6-31g(d) geom=check freq=noraman opt=(maxstep=15)
 #P Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq
 ---------------------------------------------------------------------
 Pointgroup=C1   Stoichiometry=C10H20Si   C1[X(C10H20Si)]
 Charge = 0     Multiplicity = 1
 ---------------------------------------------------------------------
 Standard basis: 6-31G(d) (6D, 7F)       #Basis: 209
 SCF Energy= -682.618112308
 Predicted Change= -1.089985D-08
=====================================================================
 Optimization completed on the basis of negligible forces.     {Found 2 times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force     0.000003 || 0.000450   [ YES ]     0.000001 || 0.000300   [ YES ]
 Displ     0.003241 || 0.001800   [ NO ]      0.000599 || 0.001200   [ YES ]
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
   1          6            0       -0.623093    2.379483    0.143788
   2          1            0       -1.437282    2.844719    0.701087
   3          6            0       -0.808021    1.100026   -0.257271
   4          6            0       -2.094470    0.468132    0.073282
   5          1            0       -2.768290    1.092307    0.663295
   6          6            0       -2.530111   -0.752442   -0.279856
   7          1            0       -1.893012   -1.405530   -0.874085
   8          6            0       -3.874015   -1.312913    0.086007
   9         14            0        1.420101   -0.773609    0.032941
  10          6            0        2.547645   -1.701860   -1.179024
  11          1            0        3.120539   -1.011901   -1.810760
  12          1            0        3.268444   -2.333857   -0.645731
  13          1            0        1.967895   -2.353577   -1.844282
  14          6            0        0.501064   -2.028920    1.111240
  15          1            0        1.210458   -2.596782    1.726545
  16          1            0       -0.209723   -1.537304    1.784119
  17          1            0       -0.062619   -2.750166    0.507974
  18          6            0        2.474449    0.341129    1.144963
  19          1            0        1.851245    0.921789    1.834718
  20          1            0        3.169801   -0.256282    1.747387
  21          1            0        3.070631    1.050192    0.558337
  22          1            0       -4.460045   -0.601434    0.677835
  23          1            0       -3.775936   -2.238834    0.670001
  24          1            0       -4.457782   -1.570492   -0.808866
  25          6            0        0.227587    0.301464   -1.017312
  26          1            0        0.867788    0.970494   -1.605413
  27          1            0       -0.262817   -0.350075   -1.751823
  28          6            0        0.561739    3.270186   -0.087701
  29          1            0        0.246254    4.226736   -0.526776
  30          1            0        1.066085    3.515873    0.857868
  31          1            0        1.310318    2.828942   -0.751301
 ---------------------------------------------------------------------
 Statistical Thermodynamic Analysis for 11_t_SM_080426.out
 Temperature=   298.150  Kelvin       Pressure=   1.00000  Atm
=====================================================================
 SCF Energy=                            -682.618112308
 Zero-point correction (ZPE)=           -682.34522        0.272886
 Internal Energy (U)=                   -682.32875        0.289354
 Enthalpy (H)=                          -682.32781        0.290298
 Gibbs Free Energy (G)=                 -682.38882        0.229285
 Entropy (S)=                                             0.00020464
 ---------------------------------------------------------------------
 Frequencies --    21.9970        67.1106        90.5103
 Frequencies --    97.6416       106.5213       139.4847

 ---------------------------------------------------------------------
 Analyzing Gaussian Output File: MP2_11_t_SM_080729.out
 Using Gaussian 03:  AM64L-G03RevC.02 12-Jun-2004
 [#Processors=2  Memory=2gb  CheckPoint=MP2_11_t_SM_080729.chk]
=====================================================================
 #p mp2/6-31+g(d) scf=tight
 ---------------------------------------------------------------------
 Pointgroup=C1   Stoichiometry=C10H20Si   C1[X(C10H20Si)]
 Charge = 0     Multiplicity = 1
 ---------------------------------------------------------------------
 Standard basis: 6-31+G(d) (6D, 7F)      #Basis: 253
 SCF Energy= -679.251562413
 MP2 Energy= -680.65330196918   Correl. Energy= -1.401739556
=====================================================================
 No optimization variables found.
```

Diene **1e**



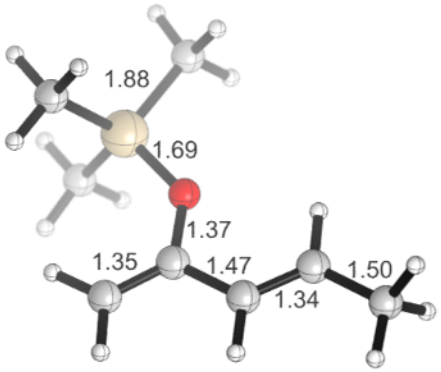

```
 ---------------------------------------------------------------------------
 Analyzing Gaussian Output File: 12_t_SM_080305.out
 Using Gaussian 03:  AM64L-G03RevC.02 12-Jun-2004
 [#Processors=2  Memory=1800MB  CheckPoint=12_t_SM_080305.chk]
 ===========================================================================
 # opt freq=noraman b3lyp/6-31g(d) geom=connectivity
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq
 ---------------------------------------------------------------------------
 Pointgroup=C1   Stoichiometry=C9H18Si   C1[X(C9H18Si)]
 Charge = 0     Multiplicity = 1
 ---------------------------------------------------------------------------
 Standard basis: 6-31G(d) (6D, 7F)       #Basis: 190
 SCF Energy= -643.301526081
 Predicted Change= -2.287246D-07
 ===========================================================================
 Optimization completed.     {Found 1 times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force     0.000011 || 0.000450   [ YES ]     0.000004 || 0.000300   [ YES ]
 Displ     0.016432 || 0.001800   [ NO ]      0.004528 || 0.001200   [ NO ]
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.725370    2.609603    0.042820
    2          1             0       -1.501250    3.131274    0.597289
    3          6             0       -0.860532    1.315742   -0.310659
    4          6             0       -2.101474    0.614651    0.046664
    5          1             0       -2.815497    1.213493    0.614635
    6          6             0       -2.445981   -0.645338   -0.264792
    7          1             0       -1.757929   -1.267252   -0.835490
    8          6             0       -3.746295   -1.290100    0.116719
    9         14             0        1.524179   -0.333174    0.035005
   10          6             0        2.831481   -1.053698   -1.135925
   11          1             0        3.313865   -0.267914   -1.729987
   12          1             0        3.618922   -1.575679   -0.578419
   13          1             0        2.391706   -1.774760   -1.835885
   14          6             0        0.742268   -1.738479    1.036007
   15          1             0        1.494433   -2.223567    1.670758
   16          1             0       -0.061027   -1.373421    1.685025
   17          1             0        0.315770   -2.510639    0.384351
   18          6             0        2.336598    0.906334    1.212422
   19          1             0        1.588917    1.390760    1.850342
   20          1             0        3.067248    0.412887    1.864948
   21          1             0        2.864664    1.696478    0.664542
   22          1             0       -4.384473   -0.605312    0.685425
   23          1             0       -3.582352   -2.188370    0.728097
   24          1             0       -4.305274   -1.616423   -0.771351
   25          6             0        0.238791    0.587867   -1.051839
   26          1             0        0.817264    1.315082   -1.637093
   27          1             0       -0.179815   -0.117181   -1.781494
   28          1             0        0.159414    3.185485   -0.214261
 ---------------------------------------------------------------------------
 Statistical Thermodynamic Analysis for 12_t_SM_080305.out
 Temperature=   298.150  Kelvin       Pressure=   1.00000  Atm
 ===========================================================================
 SCF Energy=                             -643.301526081
 Zero-point correction (ZPE)=             -643.05720        0.244319
 Internal Energy (U)=                     -643.04226        0.259264
 Enthalpy (H)=                            -643.04131        0.260208
 Gibbs Free Energy (G)=                   -643.09875        0.202774
 Entropy (S)=                                               0.00019264
 ---------------------------------------------------------------------------
 Frequencies --     26.4176               60.4555              102.5756
 Frequencies --    124.1166              140.8431              143.0017

 ---------------------------------------------------------------------------
 Analyzing Gaussian Output File: MP2_12_t_SM_080729.out
 Using Gaussian 03:  AM64L-G03RevC.02 12-Jun-2004
 [#Processors=2  Memory=2gB  CheckPoint=MP2_12_t_SM_080729.chk]
 ===========================================================================
 #p mp2/6-31+g(d) scf=(direct,tight)
 ---------------------------------------------------------------------------
 Pointgroup=C1   Stoichiometry=C9H18Si   C1[X(C9H18Si)]
 Charge = 0     Multiplicity = 1
 ---------------------------------------------------------------------------
 Standard basis: 6-31+G(d) (6D, 7F)      #Basis: 230
 SCF Energy= -640.216827348
 MP2 Energy= -641.48272682987   Correl. Energy= -1.265899482
 ===========================================================================
 No optimization variables found.
```

Diene **2c**



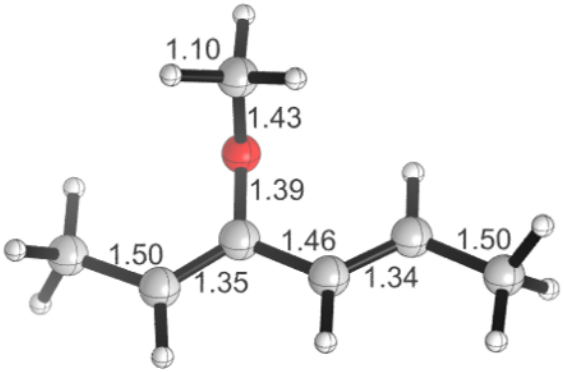

```
 ---------------------------------------------------------------------------
 Analyzing Gaussian Output File: methylmethylOTMS_s-trans.out
 Using Gaussian 03:  AM64L-G03RevC.02 12-Jun-2004
 [#Processors=2  Memory=1800MB  CheckPoint=methylmethylOTMS_s-trans.chk]
 ===========================================================================
 # opt freq=noraman b3lyp/6-31g(d) geom=connectivity
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq
 ---------------------------------------------------------------------------
 Pointgroup=C1   Stoichiometry=C9H18OSi   C1[X(C9H18OSi)]
 Charge = 0     Multiplicity = 1
 ---------------------------------------------------------------------------
 Standard basis: 6-31G(d) (6D, 7F)       #Basis: 205
 SCF Energy= -718.563833146
 Predicted Change= -1.535859D-09
 ===========================================================================
 Optimization completed.     {Found 2 times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force     0.000002 || 0.000450   [ YES ]     0.000001 || 0.000300   [ YES ]
 Displ     0.001219 || 0.001800   [ YES ]     0.000279 || 0.001200   [ YES ]
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        1.110003    2.964661   -0.179049
    2          1             0        1.036235    3.886112   -0.772204
    3          1             0        1.632408    3.234835    0.750467
    4          1             0        1.737677    2.259813   -0.730473
    5          6             0       -0.248605    2.395482    0.093039
    6          1             0       -0.990870    3.069987    0.514870
    7          6             0       -0.653145    1.133709   -0.157725
    8          6             0       -2.030850    0.704527    0.092984
    9          1             0       -2.660036    1.444605    0.587234
   10          6             0       -2.559851   -0.477793   -0.257232
   11          1             0       -1.930747   -1.196706   -0.777713
   12          6             0       -3.981915   -0.884115   -0.006024
   13         14             0        1.259184   -0.857767    0.037695
   14          6             0        2.829765   -0.833780   -1.000995
   15          1             0        3.309399    0.151655   -0.986690
   16          1             0        3.559214   -1.566430   -0.634000
   17          1             0        2.608739   -1.079693   -2.046221
   18          6             0        0.531462   -2.598119    0.034056
   19          1             0        1.255200   -3.321680    0.430619
   20          1             0       -0.372827   -2.659755    0.649571
   21          1             0        0.268089   -2.917729   -0.981300
   22          6             0        1.587582   -0.298711    1.807887
   23          1             0        0.662821   -0.265254    2.395143
   24          1             0        2.272391   -0.996687    2.305618
   25          1             0        2.040759    0.697900    1.845077
   26          1             0       -4.542131   -0.100690    0.515845
   27          1             0       -4.035709   -1.799576    0.599747
   28          1             0       -4.504639   -1.105059   -0.947118
   29          8             0        0.189847    0.204740   -0.725979
 ---------------------------------------------------------------------
 Statistical Thermodynamic Analysis for methylmethylOTMS_s-trans.out
 Temperature=   298.150  Kelvin       Pressure=   1.00000  Atm
 ===========================================================================
 SCF Energy=                            -718.563833146
 Zero-point correction (ZPE)=            -718.31491        0.248917
 Internal Energy (U)=                    -718.29858        0.265251
 Enthalpy (H)=                           -718.29763        0.266195
 Gibbs Free Energy (G)=                  -718.35908        0.204746
 Entropy (S)=                                              0.0002061
 ---------------------------------------------------------------------------
 Frequencies --    11.9490               53.0701               93.9444
 Frequencies --   100.9179              127.2964              134.9863

 ---------------------------------------------------------------------------
 Analyzing Gaussian Output File: SP_MP2_1_t_SM_080430.out
 Using Gaussian 03:  IA64L-G03RevD.01 13-Oct-2005
 [#Processors=4  Memory=4gb  CheckPoint=SP_MP2_1_t_SM_080430.chk]
 ===========================================================================
 #p mp2/6-31+g(d) scf=(direct,tight) geom=check guess=read
 ---------------------------------------------------------------------------
 Pointgroup=C1   Stoichiometry=C9H18OSi   C1[X(C9H18OSi)]
 Charge = 0     Multiplicity = 1
 ---------------------------------------------------------------------------
 Standard basis: 6-31+G(d) (6D, 7F)      #Basis: 249
 SCF Energy= -715.122649994
 MP2 Energy= -716.56719997436   Correl. Energy= -1.444549981
 ===========================================================================
 No optimization variables found.
```

Diene **2e**



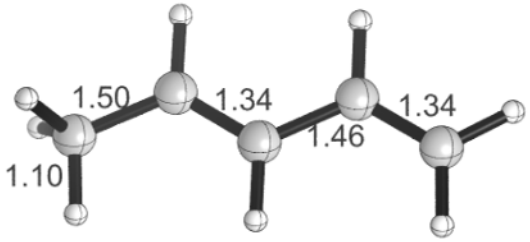

```
-----------------------------------------------------------------------------
 Analyzing Gaussian Output File: 2_s-trans_SMopt_050208.out
 Using Gaussian 03:  AM64L-G03RevC.02 12-Jun-2004
 [#Processors=2  Memory=1800MB  CheckPoint=2_s-trans_SMopt_050208.chk]
=============================================================================
 # opt freq b3lyp/6-31g(d) geom=connectivity
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq
-----------------------------------------------------------------------------
 Pointgroup=C1   Stoichiometry=C8H16OSi   C1[X(C8H16OSi)]
 Charge = 0     Multiplicity = 1
-----------------------------------------------------------------------------
 Standard basis: 6-31G(d) (6D, 7F)       #Basis: 186
 SCF Energy= -679.248096564
 Predicted Change= -1.316370D-08
=============================================================================
 Optimization completed.     {Found 1 times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force     0.000013 || 0.000450   [ YES ]     0.000003 || 0.000300   [ YES ]
 Displ     0.003187 || 0.001800   [ NO ]      0.000699 || 0.001200   [ YES ]
-----------------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
-----------------------------------------------------------------------------
    1          6             0       -0.420268    2.242054   -0.000133
    2          1             0       -1.134704    3.057107   -0.000109
    3          6             0       -0.858204    0.968448   -0.000196
    4          6             0       -2.289036    0.647478   -0.000193
    5          1             0       -2.955023    1.509075   -0.000293
    6          6             0       -2.800458   -0.591413   -0.000022
    7          1             0       -2.112622   -1.434603    0.000163
    8          6             0       -4.265674   -0.909548    0.000070
    9         14             0        1.636041   -0.302567    0.000082
   10          6             0        1.883877   -2.166041   -0.000666
   11          1             0        1.428656   -2.624767   -0.885770
   12          1             0        2.950130   -2.423508   -0.001199
   13          1             0        1.429371   -2.625448    0.884456
   14          6             0        2.374572    0.459765    1.559146
   15          1             0        3.459967    0.301315    1.588805
   16          1             0        2.193292    1.537618    1.625578
   17          1             0        1.947003   -0.002678    2.456440
   18          6             0        2.375590    0.460680   -1.558057
   19          1             0        2.195441    1.538748   -1.623774
   20          1             0        3.460832    0.301127   -1.587376
   21          1             0        1.948005   -0.000704   -2.455904
   22          1             0       -4.879420   -0.002282   -0.000574
   23          1             0       -4.542254   -1.506677    0.880165
   24          1             0       -4.542089   -1.507854   -0.879266
   25          8             0       -0.047967   -0.132030   -0.000259
   26          1             0        0.630180    2.507185   -0.000114
-----------------------------------------------------------------------------
 Statistical Thermodynamic Analysis for 2_s-trans_SMopt_050208.out
 Temperature=   298.150  Kelvin       Pressure=   1.00000  Atm
=============================================================================
 SCF Energy=                              -679.248096564
 Zero-point correction (ZPE)=              -679.02748        0.220608
 Internal Energy (U)=                      -679.01267        0.235423
 Enthalpy (H)=                             -679.01172        0.236367
 Gibbs Free Energy (G)=                    -679.06958        0.178513
 Entropy (S)=                                                0.00019404
-----------------------------------------------------------------------------
 Frequencies --    19.2573               65.9063               81.7709
 Frequencies --   109.9346              122.7910              134.6027

-----------------------------------------------------------------------------
 Analyzing Gaussian Output File: SP_MP2_2_s-trans_SM_080507.out
 Using Gaussian 03:  IA64L-G03RevD.01 13-Oct-2005
 [#Processors=4  Memory=3gb  CheckPoint=SP_MP2_2_s-trans_SM_080507.chk]
=============================================================================
 #p mp2/6-31+g(d) geom=check guess=read scf=tight
-----------------------------------------------------------------------------
 Pointgroup=C1   Stoichiometry=C8H16OSi   C1[X(C8H16OSi)]
 Charge = 0     Multiplicity = 1
-----------------------------------------------------------------------------
 Standard basis: 6-31+G(d) (6D, 7F)      #Basis: 226
 SCF Energy= -676.088467501
 MP2 Energy= -677.39563741851   Correl. Energy= -1.307169918
=============================================================================
 No optimization variables found.
```

Diene **2f**



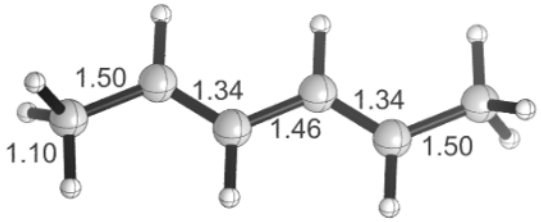

```
 Analyzing Gaussian Output File: 3_s-trans_SMopt_050208.out
 Using Gaussian 03:  AM64L-G03RevC.02 12-Jun-2004
 [#Processors=2  Memory=1800MB  CheckPoint=3_s-trans_SMopt_050208.chk]
 # opt freq b3lyp/6-31g(d) geom=connectivity
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq
 Pointgroup=C1   Stoichiometry=C7H12O   C1[X(C7H12O)]
 Charge = 0     Multiplicity = 1
 Standard basis: 6-31G(d) (6D, 7F)       #Basis: 144
 SCF Energy= -349.149642609
 Predicted Change= -1.317494D-08
 Optimization completed.     {Found 2 times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force     0.000023 || 0.000450   [ YES ]     0.000005 || 0.000300   [ YES ]
 Displ     0.001368 || 0.001800   [ YES ]     0.000360 || 0.001200   [ YES ]
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
    1          6            0       -1.505790   -1.132814    0.160926
    2          1            0       -1.277357   -2.132821    0.525949
    3          6            0       -0.464401   -0.307969   -0.056462
    4          6            0        0.927876   -0.699125    0.172174
    5          1            0        1.068986   -1.660843    0.665751
    6          6            0        2.001373    0.015083   -0.200016
    7          1            0        1.841217    0.960399   -0.716338
    8          6            0        3.424753   -0.402165    0.020884
    9          1            0        3.489396   -1.369248    0.531300
   10          1            0        3.966994   -0.483804   -0.931362
   11          1            0        3.969596    0.336991    0.624803
   12          6            0       -2.946334   -0.805492   -0.087809
   13          1            0       -3.397806   -1.526039   -0.783483
   14          1            0       -3.535803   -0.856212    0.838538
   15          1            0       -3.055308    0.193823   -0.515931
   16          8            0       -0.676139    0.962046   -0.578435
   17          6            0       -0.695411    1.999182    0.400641
   18          1            0       -0.806487    2.939469   -0.145506
   19          1            0       -1.541829    1.877937    1.090079
   20          1            0        0.235127    2.023773    0.981655
 Statistical Thermodynamic Analysis for 3_s-trans_SMopt_050208.out
 Temperature=   298.150  Kelvin       Pressure=   1.00000  Atm
 SCF Energy=                              -349.149642609
 Zero-point correction (ZPE)=              -348.97453        0.175110
 Internal Energy (U)=                      -348.96442        0.185219
 Enthalpy (H)=                             -348.96348        0.186163
 Gibbs Free Energy (G)=                    -349.00955        0.140089
 Entropy (S)=                                                0.00015453
 Frequencies --     75.6347              107.7878              136.6928
 Analyzing Gaussian Output File: SP_MP2_3_t_SM_080502.out
 Using Gaussian 03:  IA64L-G03RevD.01 13-Oct-2005
 [#Processors=2  Memory=1800MB  CheckPoint=SP_MP2_3_t_SM_080502.chk]
 #p mp2/6-31+g(d) scf=tight
 Pointgroup=C1   Stoichiometry=C7H12O   C1[X(C7H12O)]
 Charge = 0     Multiplicity = 1
 Standard basis: 6-31+G(d) (6D, 7F)      #Basis: 176
 SCF Energy= -346.880910491
 MP2 Energy= -347.97091763217   Correl. Energy= -1.090007141
 No optimization variables found.
```

Diene **18**



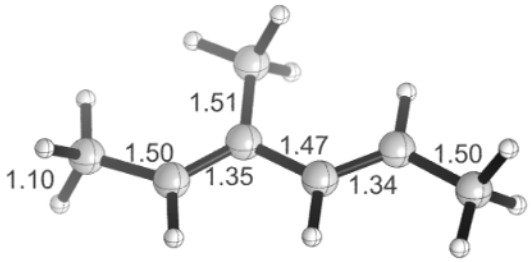

```
--------------------------------------------------------------------------------
Analyzing Gaussian Output File: 8_t_SM_080428.out
 Using Gaussian 03:  IA64L-G03RevD.01 13-Oct-2005
 [#Processors=4  Memory=4gB  CheckPoint=8_t_SM_080428.chk]
================================================================================
 #p opt=calcfc freq=noraman b3lyp/6-31g(d)
 #P Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq
--------------------------------------------------------------------------------
 Pointgroup=C1   Stoichiometry=C5H8   C1[X(C5H8)]
 Charge = 0     Multiplicity = 1
--------------------------------------------------------------------------------
 Standard basis: 6-31G(d) (6D, 7F)       #Basis: 91
 SCF Energy= -195.312252467
 Predicted Change= -3.384823D-08
================================================================================
 Optimization completed.     {Found 2 times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force     0.000125 || 0.000450   [ YES ]     0.000020 || 0.000300   [ YES ]
 Displ     0.000580 || 0.001800   [ YES ]     0.000179 || 0.001200   [ YES ]
--------------------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
--------------------------------------------------------------------------------
    1          6             0       -1.114486    0.419354   -0.000095
    2          1             0       -1.092781    1.510683   -0.000069
    3          6             0        0.053058   -0.244841   -0.000093
    4          1             0        0.044956   -1.336206   -0.000207
    5          6             0        1.360621    0.395569    0.000009
    6          6             0        2.530449   -0.260230    0.000046
    7          1             0        2.574139   -1.347274   -0.000029
    8          1             0        3.480692    0.265069    0.000155
    9          1             0        1.362202    1.486338    0.000082
   10          6             0       -2.471971   -0.217134    0.000050
   11          1             0       -3.055442    0.087552   -0.879883
   12          1             0       -2.404640   -1.310280    0.000310
   13          1             0       -3.055150    0.087807    0.880142
--------------------------------------------------------------------------------
 Statistical Thermodynamic Analysis for 8_t_SM_080428.out
 Temperature=   298.150  Kelvin       Pressure=   1.00000  Atm
================================================================================
 SCF Energy=                            -195.312252467
 Zero-point correction (ZPE)=            -195.19843        0.113819
 Internal Energy (U)=                    -195.19234        0.119911
 Enthalpy (H)=                           -195.19139        0.120856
 Gibbs Free Energy (G)=                  -195.22722        0.085029
 Entropy (S)=                                              0.00012016
--------------------------------------------------------------------------------
 Frequencies --   140.2539              196.7805              215.0693
--------------------------------------------------------------------------------
 Analyzing Gaussian Output File: MP2_8_t_SM_080428.out
 Using Gaussian 03:  IA64L-G03RevD.01 13-Oct-2005
 [#Processors=4  Memory=4gB  CheckPoint=MP2_8_t_SM_080428.chk]
================================================================================
 #p mp2/6-31+g(d) scf=tight
--------------------------------------------------------------------------------
 Pointgroup=C1   Stoichiometry=C5H8   C1[X(C5H8)]
 Charge = 0     Multiplicity = 1
--------------------------------------------------------------------------------
 Standard basis: 6-31+G(d) (6D, 7F)      #Basis: 111
 SCF Energy= -193.964081686
 MP2 Energy= -194.60582583013   Correl. Energy= -0.6417441443
================================================================================
 No optimization variables found.
```

Diene **19**



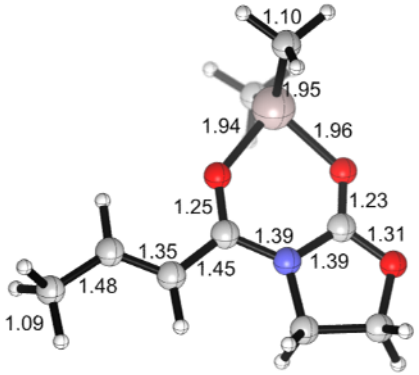

```
 ---------------------------------------------------------------------------
Analyzing Gaussian Output File: 6_s-trans_SMopt_050208.out
 Using Gaussian 03:  AM64L-G03RevC.02 12-Jun-2004
 [#Processors=2  Memory=1800MB  CheckPoint=6_s-trans_SMopt_050208.chk]
 ===========================================================================
 # opt freq b3lyp/6-31g(d) geom=connectivity
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq
 ---------------------------------------------------------------------------
 Pointgroup=C1   Stoichiometry=C6H10   C1[X(C6H10)]
 Charge = 0     Multiplicity = 1
 ---------------------------------------------------------------------------
 Standard basis: 6-31G(d) (6D, 7F)       #Basis: 110
 SCF Energy= -234.632032487
 Predicted Change= -2.534289D-07
 ===========================================================================
 Optimization completed.     {Found 2 times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force     0.000130 || 0.000450   [ YES ]     0.000041 || 0.000300   [ YES ]
 Displ     0.001664 || 0.001800   [ YES ]     0.000664 || 0.001200   [ YES ]
 ---------------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -1.804907    0.433447    0.000022
    2          1             0       -1.733425    1.522619    0.000028
    3          6             0       -0.669443   -0.284641    0.000005
    4          1             0       -0.733032   -1.374520   -0.000007
    5          6             0        0.669244    0.285470   -0.000014
    6          6             0        1.804698   -0.432876   -0.000032
    7          1             0        1.732582   -1.522142   -0.000042
    8          6             0        3.190543    0.139668   -0.000011
    9          1             0        3.173848    1.234943   -0.000057
   10          1             0        3.760092   -0.190531    0.880041
   11          1             0        3.760149   -0.190609   -0.879994
   12          6             0       -3.190362   -0.140618    0.000022
   13          1             0       -3.172208   -1.235823   -0.000018
   14          1             0       -3.760303    0.188914    0.880070
   15          1             0       -3.760341    0.188983   -0.879975
   16          1             0        0.733998    1.375466    0.000004
 ---------------------------------------------------------------------------
 Statistical Thermodynamic Analysis for 6_s-trans_SMopt_050208.out
 Temperature=   298.150  Kelvin       Pressure=   1.00000  Atm
 ===========================================================================
 SCF Energy=                          -234.632032487
 Zero-point correction (ZPE)=          -234.48994        0.142084
 Internal Energy (U)=                  -234.48234        0.149686
 Enthalpy (H)=                         -234.48140        0.150631
 Gibbs Free Energy (G)=                -234.52104        0.110986
 Entropy (S)=                                            0.00013297
 ---------------------------------------------------------------------------
 Frequencies --   105.6851              138.5189              168.7471

 ---------------------------------------------------------------------------
 Analyzing Gaussian Output File: MP2_6_t_SM_080430.out
 Using Gaussian 03:  IA64L-G03RevD.01 13-Oct-2005
 [#Processors=2  Memory=2gB  CheckPoint=MP2_6_t_SM_080430.chk]
 ===========================================================================
 #p mp2/6-31+g(d) scf=tight
 ---------------------------------------------------------------------------
 Pointgroup=C1   Stoichiometry=C6H10   C1[X(C6H10)]
 Charge = 0     Multiplicity = 1
 ---------------------------------------------------------------------------
 Standard basis: 6-31+G(d) (6D, 7F)      #Basis: 134
 SCF Energy= -233.002624344
 MP2 Energy= -233.77772529114   Correl. Energy= -0.7751009474
 ===========================================================================
 No optimization variables found.
```

Diene **20**



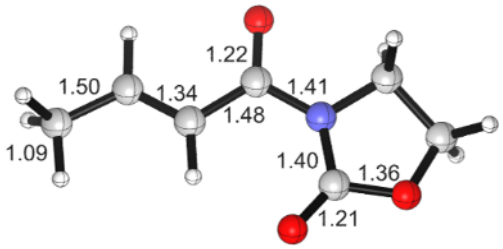

```
 ---------------------------------------------------------------------------
 Analyzing Gaussian Output File: 9_t_SM+PCM_080731.out
 Using Gaussian 03:  AM64L-G03RevC.02 12-Jun-2004
 [#Processors=2  Memory=2gB  CheckPoint=9_t_SM+PCM_080731.chk]
 ===========================================================================
 #p opt freq=noraman b3lyp/6-31g(d)
 #P Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq
 ---------------------------------------------------------------------------
 Pointgroup=C1   Stoichiometry=C7H12   C1[X(C7H12)]
 Charge = 0     Multiplicity = 1
 ---------------------------------------------------------------------------
 Standard basis: 6-31G(d) (6D, 7F)       #Basis: 129
 SCF Energy= --273.946855938
 Predicted Change= -6.992295D-08
 ===========================================================================
 Optimization completed.     {Found 1 times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force     0.000026 || 0.000450   [ YES ]     0.000007 || 0.000300   [ YES ]
 Displ     0.005242 || 0.001800   [ NO ]      0.001126 || 0.001200   [ YES ]
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        1.938654    0.228322    0.000511
    2          1             0        1.912739    1.317481    0.001786
    3          6             0        0.787371   -0.463493   -0.000834
    4          1             0        0.844629   -1.553563   -0.002131
    5          6             0       -0.572231    0.090797   -0.000513
    6          6             0       -1.615738   -0.766379    0.000018
    7          1             0       -1.376290   -1.831070   -0.000101
    8          6             0       -3.085233   -0.464991    0.000551
    9          1             0       -3.310526    0.604445    0.003037
   10          1             0       -3.573424   -0.906484   -0.879738
   11          1             0       -3.573428   -0.910410    0.878830
   12          6             0        3.304784   -0.393575    0.000317
   13          1             0        3.249213   -1.487609   -0.000919
   14          1             0        3.886322   -0.083251   -0.879181
   15          1             0        3.885665   -0.085201    0.880931
   16          6             0       -0.713578    1.594579   -0.000330
   17          1             0       -0.227465    2.032101    0.881095
   18          1             0       -0.226010    2.032345   -0.880743
   19          1             0       -1.755596    1.919653   -0.001185
 ---------------------------------------------------------------------------
 Statistical Thermodynamic Analysis for 9_t_SM+PCM_080731.out
 Temperature=   298.150  Kelvin       Pressure=   1.00000  Atm
 ===========================================================================
 SCF Energy=                             -273.946855938
 Zero-point correction (ZPE)=             -273.77623        0.170622
 Internal Energy (U)=                     -273.76723        0.179622
 Enthalpy (H)=                            -273.76629        0.180566
 Gibbs Free Energy (G)=                   -273.80938        0.137470
 Entropy (S)=                                               0.00014455
 ---------------------------------------------------------------------------
 Frequencies --    99.7759              117.1021              163.0502

 ---------------------------------------------------------------------------
 Analyzing Gaussian Output File: 9_t_MP2_080805.out
 Using Gaussian 03:  AM64L-G03RevC.02 12-Jun-2004
 [#Processors=2  Memory=2gb  CheckPoint=9_t_MP2_080805.chk]
 ===========================================================================
 #p mp2/6-31+g(d) scf=(direct,tight) geom=check guess=read
 ---------------------------------------------------------------------------
 Pointgroup=C1   Stoichiometry=C7H12   C1[X(C7H12)]
 Charge = 0     Multiplicity = 1
 ---------------------------------------------------------------------------
 Standard basis: 6-31+G(d) (6D, 7F)      #Basis: 157
 SCF Energy= -272.035585191
 MP2 Energy= -272.94687811226   Correl. Energy= -0.9112929209
 ===========================================================================
 No optimization variables found.
```

Dienophile $\mathbf{A_2}$




```
================================================================================
Analyzing Gaussian Output File: Medienophileachiral_s-cis_AlMe2.out
 Using Gaussian 03:  AM64L-G03RevC.02 12-Jun-2004
 [#Processors=2  Memory=1800Mb  CheckPoint=Medienophileachiral_s-cis_AlMe2.chk]
================================================================================
 # opt freq=noraman rb3lyp/6-31g(d) geom=connectivity
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq
--------------------------------------------------------------------------------
 Pointgroup=C1   Stoichiometry=C9H15AlNO3(1+)   C1[X(C9H15AlNO3)]
 Charge = 1     Multiplicity = 1
--------------------------------------------------------------------------------
 Standard basis: 6-31G(d) (6D, 7F)       #Basis: 244
 SCF Energy= -874.734526729
 Predicted Change= -2.536120D-08
================================================================================
 Optimization completed on the basis of negligible forces.     {Found 2 times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force     0.000003 || 0.000450   [ YES ]     0.000001 || 0.000300   [ YES ]
 Displ     0.008272 || 0.001800   [ NO ]      0.001451 || 0.001200   [ NO ]
--------------------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
--------------------------------------------------------------------------------
    1          6           0        5.084653   -1.674563   -0.121645
    2          1           0        5.405680   -2.250118    0.757460
    3          1           0        5.332666   -2.298191   -0.991579
    4          1           0        5.658583   -0.746096   -0.171213
    5          6           0        3.618443   -1.449579   -0.066948
    6          1           0        2.983737   -2.333186   -0.016066
    7          6           0        3.017477   -0.236582   -0.075888
    8          1           0        3.610829    0.669154   -0.126565
    9          6           0        1.575691   -0.130396   -0.024920
   10          8           0        0.830099   -1.137516    0.025270
   11          6           0        1.743951    2.425353   -0.123150
   12          6           0        0.595257    3.447307    0.015072
   13          1           0        2.255944    2.499599   -1.086171
   14          1           0        2.470094    2.515645    0.686697
   15          1           0        0.568089    4.185429   -0.785548
   16          1           0        0.575827    3.945597    0.985461
   17          7           0        1.012463    1.143498   -0.032015
   18          6           0       -0.359426    1.374194   -0.052702
   19          8           0       -1.251100    0.523347   -0.049152
   20          8           0       -0.625013    2.657649   -0.084056
   21         13           0       -1.084571   -1.423035    0.043636
   22          6           0       -1.591556   -2.137689   -1.696188
   23          1           0       -2.676202   -2.067170   -1.848680
   24          1           0       -1.115206   -1.618907   -2.537481
   25          1           0       -1.332840   -3.200631   -1.783755
   26          6           0       -1.586164   -1.963624    1.846959
   27          1           0       -1.114597   -1.360954    2.633296
   28          1           0       -2.671442   -1.887502    1.991955
   29          1           0       -1.318703   -3.010539    2.039375
--------------------------------------------------------------------------------
 Statistical Thermodynamic Analysis for Medienophileachiral_s-cis_AlMe2.out
 Temperature=   298.150  Kelvin       Pressure=   1.00000  Atm
================================================================================
 SCF Energy=                              -874.734526729
 Zero-point correction (ZPE)=              -874.50026        0.234257
 Internal Energy (U)=                      -874.48316        0.251366
 Enthalpy (H)=                             -874.48221        0.252310
 Gibbs Free Energy (G)=                    -874.54652        0.187998
 Entropy (S)=                                                0.0002157
--------------------------------------------------------------------------------
 Frequencies --    34.7071               43.4105               62.7412
 Frequencies --    63.7295               71.3681               94.6161

--------------------------------------------------------------------------------
 Analyzing Gaussian Output File: MP2_a2_SM_080427.out
 Using Gaussian 03:  IA64L-G03RevD.01 13-Oct-2005
 [#Processors=4  Memory=4gb  CheckPoint=MP2_a2_SM_080427.chk]
================================================================================
 #p mp2/6-31+g(d) scf=tight
--------------------------------------------------------------------------------
 Pointgroup=C1   Stoichiometry=C9H15AlNO3(1+)   C1[X(C9H15AlNO3)]
 Charge = 1     Multiplicity = 1
--------------------------------------------------------------------------------
 Standard basis: 6-31+G(d) (6D, 7F)      #Basis: 300
 SCF Energy= -870.414167194
 MP2 Energy= -872.30738476521   Correl. Energy= -1.893217571
================================================================================
 No optimization variables found.
```

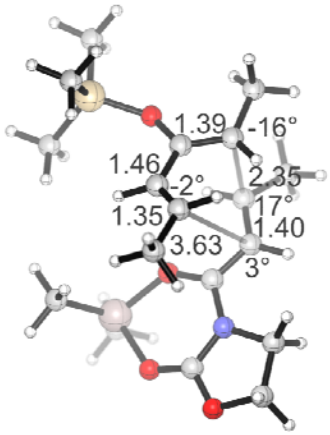
Dienophile **3**




```
-------------------------------------------------------------------------------
Analyzing Gaussian Output File: a0_s-cis_0711xx.out
 Using Gaussian 03:  AM64L-G03RevC.02 12-Jun-2004
 [#Processors=2  Memory=1800Mb  CheckPoint=methyldienophileachiral_s-cis.chk]
===============================================================================
 # opt freq b3lyp/6-31g(d) geom=connectivity
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq
-------------------------------------------------------------------------------
 Pointgroup=C1   Stoichiometry=C7H9NO3   C1[X(C7H9NO3)]
 Charge = 0     Multiplicity = 1
-------------------------------------------------------------------------------
 Standard basis: 6-31G(d) (6D, 7F)       #Basis: 183
 SCF Energy= -552.598793369
 Predicted Change= -2.332558D-08
===============================================================================
 Optimization completed.     {Found 1 times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force     0.000012 || 0.000450   [ YES ]     0.000003 || 0.000300   [ YES ]
 Displ     0.002214 || 0.001800   [ NO ]      0.000578 || 0.001200   [ YES ]
-------------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
-------------------------------------------------------------------------
    1          6             0       -4.099745   -0.846027    0.804148
    2          1             0       -3.958189    0.241914    0.750462
    3          1             0       -5.054455   -1.057592    0.303711
    4          1             0       -4.188025   -1.132913    1.856273
    5          6             0       -2.976395   -1.557436    0.120293
    6          1             0       -2.809569   -1.333471   -0.932695
    7          6             0       -2.162365   -2.447003    0.707636
    8          1             0       -2.258682   -2.716332    1.752213
    9          6             0       -1.087482   -3.079895   -0.085496
   10          8             0       -0.878240   -2.853270   -1.270439
   11          6             0        0.823450   -4.644166   -0.215910
   12          6             0        1.302851   -5.719543    0.767333
   13          1             0        1.597047   -3.904711   -0.451820
   14          1             0        0.446361   -5.050785   -1.155732
   15          1             0        2.389107   -5.810104    0.820780
   16          1             0        0.868229   -6.701802    0.552628
   17          7             0       -0.255661   -4.024451    0.551938
   18          6             0       -0.166188   -4.365282    1.909257
   19          8             0       -0.813431   -3.951353    2.838065
   20          8             0        0.825543   -5.285694    2.054688
-------------------------------------------------------------------------------
 Statistical Thermodynamic Analysis for a0_s-cis_0711xx.out
 Temperature=   298.150  Kelvin       Pressure=   1.00000  Atm
===============================================================================
 SCF Energy=                             -552.598793369
 Zero-point correction (ZPE)=             -552.43950        0.159291
 Internal Energy (U)=                     -552.42887        0.169915
 Enthalpy (H)=                            -552.42793        0.170859
 Gibbs Free Energy (G)=                   -552.47663        0.122157
 Entropy (S)=                                               0.00016335
-------------------------------------------------------------------------------
 Frequencies --    48.7979               79.1381               111.7337

-------------------------------------------------------------------------------
 Analyzing Gaussian Output File: SP_MP2_a0sc_SM_080502.out
 Using Gaussian 03:  IA64L-G03RevD.01 13-Oct-2005
 [#Processors=2  Memory=1800Mb  CheckPoint=SP_MP2_a0sc_SM_080502.chk]
===============================================================================
 #p mp2/6-31+g(d) scf=tight
-------------------------------------------------------------------------------
 Pointgroup=C1   Stoichiometry=C7H9NO3   C1[X(C7H9NO3)]
 Charge = 0     Multiplicity = 1
-------------------------------------------------------------------------------
 Standard basis: 6-31+G(d) (6D, 7F)      #Basis: 227
 SCF Energy= -549.386819685
 MP2 Energy= -550.97928084211   Correl. Energy= -1.592461157
===============================================================================
 No optimization variables found.
```

C. Optimized Structure and Energies of Diels–Alder Transition Structures

2c+$\mathbf{A_2}$, *endo* TS

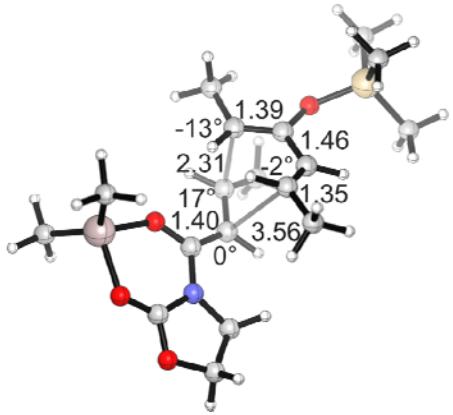



```
-----------------------------------------------------------------------------
Analyzing Gaussian Output File: MeMeOTMS_MeOxazolAlMe2_endo_s-cis.out
 Using Gaussian 03:  AM64L-G03RevC.02 12-Jun-2004
 [#Processors=2  Memory=1800MB  CheckPoint=MeMeOTMS_MeOxazolAlMe2_endo_s-cis.chk]
=============================================================================
 # opt=modredundant b3lyp/6-31g(d) geom=connectivity
 Modredundant Input:  B    1    6 F
 # b3lyp/6-31g* opt=(calcfc,ts,noeigentest,nofreeze) geom=check guess=read
 freq=noraman
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq
-----------------------------------------------------------------------------
 Pointgroup=C1   Stoichiometry=C18H33AlNO4Si(1+)   C1[X(C18H33AlNO4Si)]
 Charge = 1     Multiplicity = 1
-----------------------------------------------------------------------------
 Standard basis: 6-31G(d) (6D, 7F)       #Basis: 449
 SCF Energy= -1593.29850982
 Predicted Change= -7.943272D-09
=============================================================================
 Optimization completed.     {Found 2 times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force     0.000006 || 0.000450   [ YES ]     0.000001 || 0.000300   [ YES ]
 Displ     0.002102 || 0.001800   [ NO ]      0.000458 || 0.001200   [ YES ]
---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
```

Number	Number	Type	X	Y	Z
1	6	0	-1.823899	2.375843	0.097226
2	6	0	-2.018724	1.039584	0.425314
3	6	0	-1.173073	0.300349	1.357215
4	6	0	-0.416027	0.853354	2.326070
5	6	0	1.042686	1.884351	-0.838962
6	6	0	-0.179730	1.940906	-1.525153
7	1	0	-1.186643	-0.782375	1.255799
8	1	0	-0.616776	0.992668	-1.823551
9	1	0	1.560814	2.812123	-0.624547
10	1	0	-0.441717	1.931940	2.474198
11	1	0	-1.083233	2.911084	0.680729
12	6	0	1.661543	0.671392	-0.527025
13	8	0	1.165303	-0.478478	-0.788630
14	7	0	2.948229	0.711255	0.073175
15	13	0	1.875065	-2.216599	-0.865808
16	6	0	3.690919	1.938096	0.408098
17	6	0	3.753860	-0.384188	0.247069
18	8	0	3.497942	-1.563797	-0.034560
19	6	0	1.001133	-3.371957	0.452222
20	6	0	2.294572	-2.674591	-2.719785
21	6	0	4.931971	1.358777	1.112602
22	1	0	3.103548	2.580865	1.066798
23	1	0	3.941157	2.488994	-0.503942
24	8	0	4.919122	-0.055002	0.776748
25	1	0	1.631712	-4.240984	0.682488
26	1	0	0.795974	-2.870676	1.407370
27	1	0	0.049096	-3.772798	0.081411
28	1	0	2.830721	-1.878877	-3.253036
29	1	0	2.920375	-3.574787	-2.776021
30	1	0	1.386489	-2.890000	-3.298240
31	1	0	4.881955	1.435657	2.200866
32	1	0	5.873925	1.772652	0.754484
33	6	0	-2.920936	3.192556	-0.531934
34	1	0	-3.695188	3.413136	0.216474
35	1	0	-2.551337	4.152256	-0.901104
36	1	0	-3.412186	2.659230	-1.350292
37	6	0	0.428980	0.079153	3.288686
38	1	0	0.414140	-0.994572	3.080499
39	1	0	1.472047	0.423522	3.263732
40	1	0	0.082969	0.236918	4.318762
41	6	0	-0.485179	3.114235	-2.410996
42	1	0	0.112107	2.998871	-3.327521
43	1	0	-1.530857	3.153787	-2.716750
44	1	0	-0.203150	4.069114	-1.955995
45	8	0	-3.000017	0.389657	-0.199224
46	14	0	-3.979677	-1.006942	0.117943
47	6	0	-5.459664	-0.724250	-0.991824
48	1	0	-6.168679	-1.556814	-0.910078
49	1	0	-5.993157	0.193606	-0.721595
50	1	0	-5.163136	-0.645122	-2.043713
51	6	0	-4.440048	-1.008068	1.938867
52	1	0	-3.572034	-1.114704	2.598134
53	1	0	-4.965645	-0.087779	2.218031

```
   54          1             0       -5.115545   -1.846542    2.148941
   55          6             0       -3.023207   -2.542960   -0.388130
   56          1             0       -3.680703   -3.420055   -0.340616
   57          1             0       -2.661935   -2.462856   -1.420006
   58          1             0       -2.162955   -2.747819    0.258340
---------------------------------------------------------------------------
 Statistical Thermodynamic Analysis for MeMeOTMS_MeOxazolAlMe2_endo_s-cis.out
 Temperature=   298.150  Kelvin       Pressure=   1.00000  Atm
===========================================================================
 SCF Energy=                            -1593.29850982
 Zero-point correction (ZPE)=           -1592.81354        0.484968
 Internal Energy (U)=                   -1592.77972        0.518784
 Enthalpy (H)=                          -1592.77878        0.519729
 Gibbs Free Energy (G)=                 -1592.88153        0.416973
 Entropy (S)=                                              0.00034464
---------------------------------------------------------------------------
 Frequencies --  -193.8705               14.5054               16.5448
 Frequencies --    24.9405               38.4371               39.4197

---------------------------------------------------------------------------
 Analyzing Gaussian Output File: SP_MP2_1+a2_n_080427.log
 Using Gaussian 03:  IA64L-G03RevD.01 13-Oct-2005
 [#Processors=4  Memory=4gB  CheckPoint=SP_MP2_1+a2_n_080427.chk]
===========================================================================
 #p mp2/6-31+g(d) scf=tight
---------------------------------------------------------------------------
 Pointgroup=C1   Stoichiometry=C18H33AlNO4Si(1+)   C1[X(C18H33AlNO4Si)]
 Charge = 1     Multiplicity = 1
---------------------------------------------------------------------------
 Standard basis: 6-31+G(d) (6D, 7F)      #Basis: 549
 SCF Energy= -1585.51058517
 MP2 Energy= -1588.8926871845   Correl. Energy= -3.382102017
===========================================================================
 No optimization variables found.
```

2c+$\mathbf{A_2}$, *exo* TS




```
---------------------------------------------------------------------------
 Analyzing Gaussian Output File: MeMeOTMS_MeOxazolAlMe2_exo_s-cis.out
 Using Gaussian 03:  AM64L-G03RevC.02 12-Jun-2004
 [#Processors=2  Memory=1800MB  CheckPoint=MeMeOTMS_MeOxazolAlMe2_exo_s-cis.chk]
===========================================================================
 # opt=modredundant b3lyp/6-31g(d) geom=connectivity
 Modredundant Input:  B    1    6 F
 # b3lyp/6-31g* opt=(calcfc,ts,noeigentest,nofreeze) geom=check guess=read
 freq=noraman
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq
---------------------------------------------------------------------------
 Pointgroup=C1   Stoichiometry=C18H33AlNO4Si(1+)   C1[X(C18H33AlNO4Si)]
 Charge = 1     Multiplicity = 1
---------------------------------------------------------------------------
 Standard basis: 6-31G(d) (6D, 7F)       #Basis: 449
 SCF Energy= -1593.30320185
 Predicted Change= -8.919766D-09
===========================================================================
 Optimization completed.     {Found 2 times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force     0.000006 || 0.000450   [ YES ]     0.000001 || 0.000300   [ YES ]
 Displ     0.002566 || 0.001800   [ NO ]      0.000434 || 0.001200   [ YES ]
---------------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
    1          6             0        1.290351   -1.443957    0.158963
    2          6             0        2.176322   -0.387754    0.295678
    3          6             0        1.817221    0.900940    0.883185
    4          6             0        0.793305    1.121062    1.731009
    5          6             0       -0.638654    0.337631   -1.434184
    6          6             0        0.244461   -0.700146   -1.758380
    7          1             0        2.457134    1.737841    0.609005
    8          1             0        0.182904    0.281756    2.061725
    9          1             0        0.337440   -1.353328    0.668535
   10          6             0        1.735592   -2.835579   -0.198153
```

11	1	0	2.075886	-3.367392	0.700989
12	1	0	0.913604	-3.422887	-0.621168
13	1	0	2.568638	-2.831607	-0.905240
14	6	0	0.456706	2.451288	2.329628
15	1	0	1.091806	3.252934	1.940903
16	1	0	-0.593338	2.714310	2.142750
17	1	0	0.569778	2.420848	3.421435
18	8	0	3.399931	-0.524812	-0.224024
19	14	0	4.959288	0.160103	0.097205
20	6	0	6.115891	-1.051962	-0.736140
21	1	0	7.159088	-0.735507	-0.617508
22	1	0	6.022330	-2.054971	-0.305674
23	1	0	5.913846	-1.126051	-1.810606
24	6	0	5.197170	0.226892	1.958804
25	1	0	4.477200	0.887896	2.453585
26	1	0	5.104192	-0.768858	2.406899
27	1	0	6.201363	0.599950	2.194799
28	6	0	5.068524	1.860156	-0.702666
29	1	0	6.105168	2.217236	-0.658812
30	1	0	4.783943	1.824616	-1.760680
31	1	0	4.448882	2.616678	-0.208230
32	1	0	-0.153212	-1.708441	-1.701301
33	6	0	1.363121	-0.478158	-2.731199
34	1	0	2.166830	-1.207954	-2.611802
35	1	0	0.968368	-0.593324	-3.751043
36	1	0	1.786910	0.527452	-2.649153
37	1	0	-0.384254	1.354519	-1.706937
38	6	0	-1.840200	0.081289	-0.766999
39	8	0	-2.155052	-1.068155	-0.304797
40	7	0	-2.763827	1.141851	-0.593474
41	13	0	-3.647272	-1.761847	0.615056
42	6	0	-2.620066	2.485572	-1.177259
43	6	0	-4.007502	0.998089	-0.032737
44	8	0	-4.490716	-0.020399	0.481200
45	6	0	-4.626979	-2.993636	-0.541481
46	6	0	-3.154929	-2.019485	2.492401
47	6	0	-3.894236	3.185379	-0.660393
48	1	0	-2.582794	2.419626	-2.268628
49	1	0	-1.710168	2.969591	-0.815875
50	8	0	-4.701374	2.120415	-0.089702
51	1	0	-5.618742	-3.222243	-0.130213
52	1	0	-4.782660	-2.603104	-1.555216
53	1	0	-4.103659	-3.953268	-0.644534
54	1	0	-2.640649	-1.154334	2.932078
55	1	0	-4.040172	-2.209643	3.112994
56	1	0	-2.493930	-2.886637	2.622430
57	1	0	-4.483564	3.657274	-1.446171
58	1	0	-3.695785	3.904527	0.136509

Statistical Thermodynamic Analysis for MeMeOTMS_MeOxazolAlMe2_exo_s-cis.out
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy=	-1593.30320185	
Zero-point correction (ZPE)=	-1592.81872	0.484478
Internal Energy (U)=	-1592.78447	0.518731
Enthalpy (H)=	-1592.78352	0.519676
Gibbs Free Energy (G)=	-1592.88855	0.414648
Entropy (S)=		0.00035226

Frequencies --	-172.6185	13.2429	16.3670
Frequencies --	23.0545	25.0315	35.6782

Analyzing Gaussian Output File: SP_MP2_1+a2_x_080427.out
Using Gaussian 03: IA64L-G03RevD.01 13-Oct-2005
[#Processors=4 Memory=4gB CheckPoint=SP_MP2_1+a2_x_080427.chk]

==========

#p mp2/6-31+g(d) scf=tight

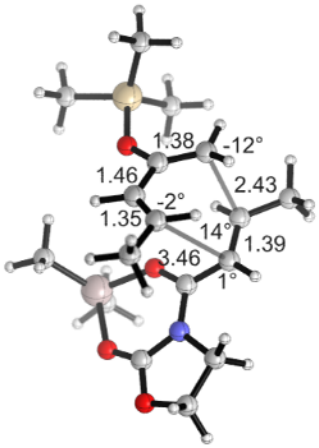
Pointgroup=C1 Stoichiometry=C18H33AlNO4Si(1+) C1[X(C18H33AlNO4Si)]
Charge = 1 Multiplicity = 1

Standard basis: 6-31+G(d) (6D, 7F) #Basis: 549
SCF Energy= -1585.51703867
MP2 Energy= -1588.8961179741 Correl. Energy= -3.3790793

==========

No optimization variables found.

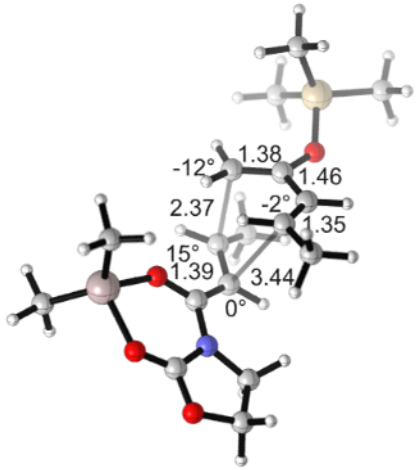
2e+$\mathbf{A_2}$, *endo* TS




```
 ---------------------------------------------------------------------------
 Analyzing Gaussian Output File: 2+a_endo_sp_0711xx.out
 Using Gaussian 03:  AM64L-G03RevC.02 12-Jun-2004
 [#Processors=2  Memory=1800MB  CheckPoint=MeHOTMS_MeOxazolAlMe2_endo_s-cis.chk]
 ===========================================================================
 # opt=modredundant b3lyp/6-31g(d) geom=connectivity
 Modredundant Input:  B    1    6 F
 # b3lyp/6-31g* opt=(calcfc,ts,noeigentest,nofreeze) geom=check guess=read
 freq=noraman
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq
 ---------------------------------------------------------------------------
 Pointgroup=C1   Stoichiometry=C17H31AlNO4Si(1+)   C1[X(C17H31AlNO4Si)]
 Charge = 1     Multiplicity = 1
 ---------------------------------------------------------------------------
 Standard basis: 6-31G(d) (6D, 7F)       #Basis: 430
 SCF Energy= -1553.98587047
 Predicted Change= -5.207152D-10
 ===========================================================================
 Optimization completed.     {Found 3 times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force     0.000005 || 0.000450   [ YES ]     0.000001 || 0.000300   [ YES ]
 Displ     0.000935 || 0.001800   [ YES ]     0.000128 || 0.001200   [ YES ]
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6           0       1.949786   -2.114624   -0.148369
    2          6           0       1.760496   -1.074760    0.731128
    3          6           0       0.723885   -1.050032    1.761738
    4          6           0      -0.161178   -2.029201    2.030648
    5          6           0      -0.954387   -1.639493   -1.313957
    6          6           0       0.310777   -1.663349   -1.881628
    7          1           0       0.701528   -0.132169    2.344861
    8          1           0       0.820235   -0.713528   -2.004742
    9          1           0      -1.556133   -2.540937   -1.313753
   10          1           0      -0.126920   -2.959614    1.465329
   11          1           0       1.487417   -3.074456    0.040759
   12          6           0      -1.488832   -0.447928   -0.781836
   13          8           0      -0.830274    0.635626   -0.707311
   14          7           0      -2.833100   -0.446176   -0.348897
   15         13           0      -1.228239    2.402034   -0.158116
   16          6           0      -3.766162   -1.580514   -0.463394
   17          6           0      -3.501899    0.676829    0.078652
   18          8           0      -3.044413    1.818824    0.213794
   19          6           0      -0.362340    2.748874    1.560969
   20          6           0      -1.286872    3.556530   -1.732842
   21          6           0      -5.033699   -1.005413    0.201370
   22          1           0      -3.383470   -2.453265    0.069451
   23          1           0      -3.919706   -1.838186   -1.515393
   24          8           0      -4.766083    0.415592    0.349721
   25          1           0      -0.452294    3.802337    1.853964
   26          1           0      -0.786413    2.154075    2.380559
   27          1           0       0.710440    2.519371    1.517594
   28          1           0      -1.837725    3.115441   -2.573346
   29          1           0      -1.767282    4.516543   -1.503476
   30          1           0      -0.279166    3.792842   -2.099159
   31          1           0      -5.214677   -1.406740    1.200260
   32          1           0      -5.931651   -1.106930   -0.407311
   33          6           0      -1.178080   -1.965286    3.128860
   34          1           0      -1.171108   -0.996754    3.637375
   35          1           0      -2.192401   -2.152722    2.749703
   36          1           0      -0.986031   -2.745994    3.876948
   37          6           0       0.741779   -2.797387   -2.764765
   38          1           0       0.339849   -2.619079   -3.773155
   39          1           0       1.826942   -2.865889   -2.861928
   40          1           0       0.352341   -3.761217   -2.422599
   41          8           0       2.466906    0.061116    0.693275
   42         14           0       4.028531    0.474664    0.073051
   43          6           0       3.962724    0.505574   -1.809125
   44          1           0       4.891808    0.936762   -2.202384
   45          1           0       3.858556   -0.489515   -2.256251
   46          1           0       3.138954    1.132416   -2.170833
   47          6           0       5.274400   -0.772228    0.721977
   48          1           0       5.282008   -0.788042    1.817682
   49          1           0       5.082432   -1.792534    0.373124
   50          1           0       6.283489   -0.497692    0.390828
   51          6           0       4.299919    2.189477    0.770608
   52          1           0       5.269066    2.591315    0.451681
   53          1           0       3.525122    2.886919    0.432666
   54          1           0       4.288511    2.179770    1.866009
   55          1           0       2.794656   -2.112701   -0.825411
 ---------------------------------------------------------------------------
 Statistical Thermodynamic Analysis for 2+a_endo_sp_0711xx.out
 Temperature=   298.150  Kelvin       Pressure=   1.00000  Atm
 ===========================================================================
 SCF Energy=                            -1553.98587047
 Zero-point correction (ZPE)=           -1553.52988         0.455991
 Internal Energy (U)=                   -1553.49729         0.488581
 Enthalpy (H)=                          -1553.49634         0.489525
 Gibbs Free Energy (G)=                 -1553.59639         0.389472
 Entropy (S)=                                               0.00033558
 ---------------------------------------------------------------------------
 Frequencies --  -150.2332               17.7074               23.7090
 Frequencies --    28.2696               33.0103               41.5075
 ---------------------------------------------------------------------------
 Analyzing Gaussian Output File: SP_MP2_syn2+a2_n_080506.out
 Using Gaussian 03:  AM64L-G03RevC.02 12-Jun-2004
 [#Processors=2  Memory=1800mb  CheckPoint=SP_MP2_syn2+a2_n_080506.chk]
 ===========================================================================
 #p mp2/6-31+g(d) scf=(direct,tight) geom=check guess=read
 ---------------------------------------------------------------------------
 Pointgroup=C1   Stoichiometry=C17H31AlNO4Si(1+)   C1[X(C17H31AlNO4Si)]
```

```
 Charge = 1     Multiplicity = 1
-------------------------------------------------------------------------------
 Standard basis: 6-31+G(d) (6D, 7F)      #Basis: 526
 SCF Energy= -1546.48459853
 MP2 Energy= -1549.7238797036   Correl. Energy= -3.239281172
===============================================================================
 No optimization variables found.
```

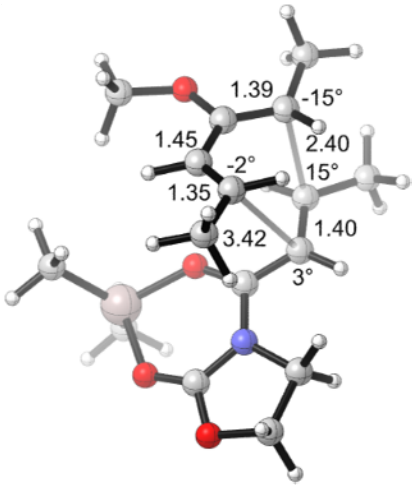
2e+$\mathbf{A_2}$, *exo* TS




```
-------------------------------------------------------------------------------
 Analyzing Gaussian Output File: 2+a_exo_sp_040208.out
 Using Gaussian 03:  AM64L-G03RevC.02 12-Jun-2004
 [#Processors=2  Memory=1800MB  CheckPoint=2+a_exo_040208.chk]
===============================================================================
 # opt=(modredundant,gdiis) b3lyp/6-31g(d)
 Modredundant Input:  B    1    6 F
 # b3lyp/6-31g* opt=(calcfc,ts,noeigentest,nofreeze,gdiis) geom=check
 guess=read freq=noraman
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq
-------------------------------------------------------------------------------
 Pointgroup=C1   Stoichiometry=C17H31AlNO4Si(1+)   C1[X(C17H31AlNO4Si)]
 Charge = 1     Multiplicity = 1
-------------------------------------------------------------------------------
 Standard basis: 6-31G(d) (6D, 7F)       #Basis: 430
 SCF Energy= -1553.98590590
 Predicted Change= -6.234866D-13
===============================================================================
 Optimization completed.     {Found 3 times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force     0.000000 || 0.000450   [ YES ]     0.000000 || 0.000300   [ YES ]
 Displ     0.000019 || 0.001800   [ YES ]     0.000004 || 0.001200   [ YES ]
-------------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
-------------------------------------------------------------------------
    1          6           0       -1.710355    0.984926    0.185317
    2          6           0       -2.263752   -0.238285    0.486864
    3          6           0       -1.559693   -1.308154    1.190561
    4          6           0       -0.362716   -1.205900    1.800501
    5          6           0        0.511414   -0.469582   -1.442778
    6          6           0       -0.490025    0.437643   -1.775021
    7          1           0       -2.098421   -2.253283    1.218829
    8          1           0        0.154359   -0.247309    1.814917
```

```
    9          1             0       -0.797480    1.305220    0.670708
   10          6             0        0.300873   -2.318852    2.550880
   11          1             0       -0.252679   -3.258756    2.468509
   12          1             0        1.327368   -2.483322    2.194311
   13          1             0        0.389312   -2.064664    3.615589
   14          8             0       -3.480610   -0.607642    0.066779
   15         14             0       -5.011230    0.206055    0.054924
   16          6             0       -6.229220   -1.208012   -0.080625
   17          1             0       -7.258673   -0.831615   -0.112268
   18          1             0       -6.063759   -1.795080   -0.991037
   19          1             0       -6.149173   -1.885966    0.776088
   20          6             0       -5.126562    1.349555   -1.434882
   21          1             0       -4.432344    2.196390   -1.386079
   22          1             0       -4.950243    0.812549   -2.373891
   23          1             0       -6.138438    1.770598   -1.490765
   24          6             0       -5.157217    1.149116    1.671908
   25          1             0       -6.117168    1.677692    1.715257
   26          1             0       -5.113983    0.473361    2.533518
   27          1             0       -4.365896    1.897406    1.790547
   28          1             0       -0.243730    1.491987   -1.698059
   29          6             0       -1.602303    0.059973   -2.705150
   30          1             0       -2.437152    0.760411   -2.650310
   31          1             0       -1.221015    0.085347   -3.736572
   32          1             0       -1.975974   -0.950299   -2.512688
   33          1             0        0.379381   -1.517235   -1.683997
   34          6             0        1.686289   -0.052223   -0.796544
   35          8             0        1.864131    1.135072   -0.368718
   36          7             0        2.727129   -0.990701   -0.613328
   37         13             0        3.290697    2.040348    0.483553
   38          6             0        2.728996   -2.365753   -1.142577
   39          6             0        3.958419   -0.683873   -0.084774
   40          8             0        4.329236    0.403550    0.376663
   41          6             0        4.080232    3.330503   -0.750731
   42          6             0        2.815793    2.300505    2.363676
   43          6             0        4.077633   -2.896571   -0.614897
   44          1             0        2.677353   -2.348624   -2.235123
   45          1             0        1.882231   -2.932587   -0.750202
   46          8             0        4.772253   -1.721557   -0.113988
   47          1             0        5.052577    3.685672   -0.385521
   48          1             0        4.245157    2.922395   -1.756021
   49          1             0        3.446768    4.219750   -0.865449
   50          1             0        2.431286    1.393239    2.848478
   51          1             0        3.684002    2.627910    2.950164
   52          1             0        2.050360    3.078595    2.483579
   53          1             0        4.704911   -3.342515   -1.386102
   54          1             0        3.968772   -3.588981    0.221949
   55          1             0       -2.316380    1.761839   -0.266444
--------------------------------------------------------------------------------
 Statistical Thermodynamic Analysis for 2+a_exo_sp_040208.out
 Temperature=   298.150  Kelvin       Pressure=   1.00000  Atm
================================================================================
 SCF Energy=                          -1553.98590590
 Zero-point correction (ZPE)=         -1553.52952        0.456378
 Internal Energy (U)=                 -1553.49702        0.488885
 Enthalpy (H)=                        -1553.49607        0.489830
 Gibbs Free Energy (G)=               -1553.59650        0.389403
 Entropy (S)=                                            0.00033683
--------------------------------------------------------------------------------
 Frequencies --  -157.9776               18.7232               21.0271
 Frequencies --    26.5028               27.8129               38.0269

--------------------------------------------------------------------------------
 Analyzing Gaussian Output File: SP_MP2_syn2+a2_x_080506.out
 Using Gaussian 03:  AM64L-G03RevC.02 12-Jun-2004
 [#Processors=2  Memory=1800mb  CheckPoint=SP_MP2_syn2+a2_x_080506.chk]
================================================================================
 #p mp2/6-31+g(d) scf=(direct,tight) geom=check guess=read
--------------------------------------------------------------------------------
 Pointgroup=C1   Stoichiometry=C17H31AlNO4Si(1+)   C1[X(C17H31AlNO4Si)]
 Charge = 1     Multiplicity = 1
--------------------------------------------------------------------------------
 Standard basis: 6-31+G(d) (6D, 7F)      #Basis: 526
 SCF Energy= -1546.48393233
 MP2 Energy= -1549.7212560658   Correl. Energy= -3.237323738
================================================================================
 No optimization variables found.
```

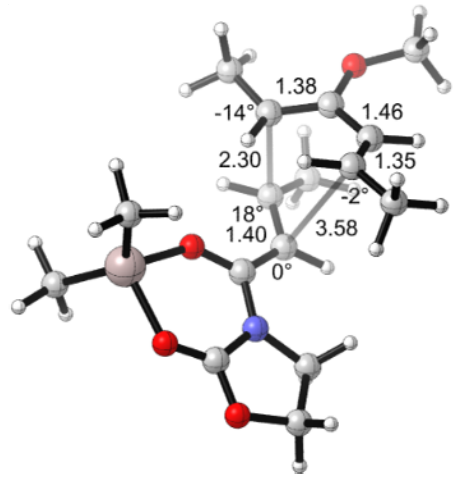
2f+$\mathbf{A_2}$, *endo* TS




```
 ---------------------------------------------------------------------------
 Analyzing Gaussian Output File: 3+a_ap_endo_0711xx.out
 Using Gaussian 03:  AM64L-G03RevC.02 12-Jun-2004
 [#Processors=2  Memory=1800MB  CheckPoint=MeMeOMe_MeOxazolAlMe2_endo_s-cis.chk]
 ===========================================================================
 # opt=modredundant b3lyp/6-31g(d) geom=connectivity
 Modredundant Input:  B    1    6 F
 # b3lyp/6-31g* opt=(calcfc,ts,noeigentest,nofreeze) geom=check guess=read
 freq=noraman
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq
 ---------------------------------------------------------------------------
 Pointgroup=C1   Stoichiometry=C16H27AlNO4(1+)   C1[X(C16H27AlNO4)]
 Charge = 1     Multiplicity = 1
 ---------------------------------------------------------------------------
 Standard basis: 6-31G(d) (6D, 7F)       #Basis: 388
 SCF Energy= -1223.88357865
 Predicted Change= -5.962382D-09
 ===========================================================================
 Optimization completed.     {Found 2 times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force     0.000006 || 0.000450   [ YES ]     0.000001 || 0.000300   [ YES ]
 Displ     0.002079 || 0.001800   [ NO ]      0.000384 || 0.001200   [ YES ]
 ---------------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        3.283821   -0.904210   -0.027953
    2          6             0        2.743668    0.162878    0.672282
    3          6             0        1.691192    0.061683    1.670645
    4          6             0        1.231753   -1.085526    2.213918
    5          6             0        0.386692   -1.514880   -1.072530
    6          6             0        1.569878   -1.106139   -1.690568
    7          1             0        1.240786    0.991838    2.003445
    8          1             0        1.682164   -0.046982   -1.901809
    9          1             0        0.178615   -2.575514   -0.991238
   10          1             0        1.688530   -2.035308    1.941730
   11          1             0        3.017623   -1.898131    0.311396
   12          6             0       -0.583265   -0.593797   -0.653066
   13          8             0       -0.429561    0.672738   -0.711693
   14          7             0       -1.824007   -1.091343   -0.182413
   15         13             0       -1.605237    2.139846   -0.566601
   16          6             0       -2.197482   -2.514860   -0.114735
   17          6             0       -2.916928   -0.307401    0.088495
   18          8             0       -2.993696    0.927864    0.023915
   19          6             0       -1.133793    3.237166    0.986178
   20          6             0       -2.074259    2.778778   -2.352179
   21          6             0       -3.589691   -2.433676    0.540884
   22          1             0       -1.486412   -3.075113    0.495605
   23          1             0       -2.227359   -2.945058   -1.120488
   24          8             0       -3.961266   -1.031536    0.445623
   25          1             0       -1.995349    3.844451    1.294925
   26          1             0       -0.831565    2.655431    1.867090
   27          1             0       -0.326607    3.948529    0.767448
   28          1             0       -2.344255    1.971792   -3.045447
   29          1             0       -2.927537    3.468480   -2.316240
   30          1             0       -1.245826    3.331980   -2.813895
   31          1             0       -3.581029   -2.696173    1.600765
   32          1             0       -4.353978   -3.010917    0.021779
   33          6             0        4.572643   -0.745221   -0.793268
   34          1             0        5.370699   -0.397487   -0.124335
   35          1             0        4.896652   -1.693109   -1.227769
   36          1             0        4.494125    0.001749   -1.590854
   37          6             0        0.160090   -1.149823    3.257286
   38          1             0       -0.262142   -0.164734    3.477236
   39          1             0       -0.656094   -1.818987    2.951815
   40          1             0        0.559094   -1.568484    4.190837
   41          6             0        2.311005   -2.060548   -2.582318
   42          1             0        1.767115   -2.120194   -3.536671
   43          1             0        3.321051   -1.725160   -2.816387
   44          1             0        2.352033   -3.072920   -2.167191
   45          8             0        3.256683    1.363730    0.346301
   46          6             0        2.869812    2.566644    1.023745
   47          1             0        3.038204    2.483661    2.102089
   48          1             0        3.515669    3.342596    0.612886
   49          1             0        1.823824    2.816391    0.821904
 ---------------------------------------------------------------------------
 Statistical Thermodynamic Analysis for 3+a_ap_endo_0711xx.out
 Temperature=   298.150  Kelvin       Pressure=   1.00000  Atm
 ===========================================================================
 SCF Energy=                            -1223.88357865
 Zero-point correction (ZPE)=           -1223.47219        0.411381
 Internal Energy (U)=                   -1223.44468        0.438890
 Enthalpy (H)=                          -1223.44374        0.439834
 Gibbs Free Energy (G)=                 -1223.53183        0.351740
 Entropy (S)=                                              0.00029547
 ---------------------------------------------------------------------------
 Frequencies --  -157.7583               15.0259               26.1153
 Frequencies --    37.0582               44.3551               47.5156

 ---------------------------------------------------------------------------
 Analyzing Gaussian Output File: SP_MP2_3a+a2_n_080501.out
 Using Gaussian 03:  IA64L-G03RevD.01 13-Oct-2005
 [#Processors=4  Memory=4gb  CheckPoint=SP_MP2_3a+a2_n_080501.chk]
 ===========================================================================
 #p mp2/6-31+g(d) scf=(direct,tight) geom=check guess=read
 ---------------------------------------------------------------------------
 Pointgroup=C1   Stoichiometry=C16H27AlNO4(1+)   C1[X(C16H27AlNO4)]
 Charge = 1     Multiplicity = 1
```

```
--------------------------------------------------------------------------------
 Standard basis: 6-31+G(d) (6D, 7F)      #Basis: 476
 SCF Energy= -1217.26739887
 MP2 Energy= -1220.2958120964   Correl. Energy= -3.028413223
================================================================================
 No optimization variables found.
```

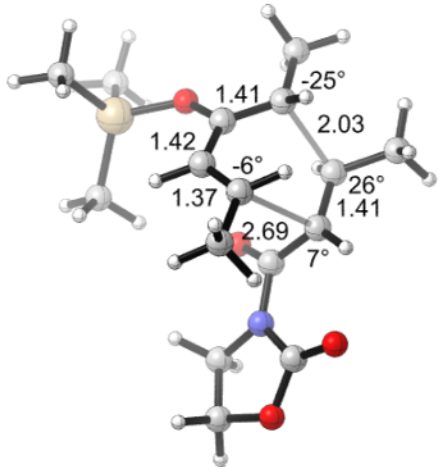
2f+$\mathbf{A_2}$, *exo* TS




```
--------------------------------------------------------------------------------
 Analyzing Gaussian Output File: 3+a_ap_exo_0711xx.out
 Using Gaussian 03:  AM64L-G03RevC.02 12-Jun-2004
 [#Processors=2  Memory=1800MB  CheckPoint=MeMeOMe2_MeOxazolAlMe2_exo_s-cis.chk]
================================================================================
 # opt=modredundant rb3lyp/6-31g(d) geom=connectivity
 Modredundant Input:  B    1    6 F
 # b3lyp/6-31g* opt=(calcfc,ts,noeigentest,nofreeze) geom=check guess=read
 freq=noraman
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq
--------------------------------------------------------------------------------
 Pointgroup=C1   Stoichiometry=C16H27AlNO4(1+)   C1[X(C16H27AlNO4)]
 Charge = 1     Multiplicity = 1
--------------------------------------------------------------------------------
 Standard basis: 6-31G(d) (6D, 7F)       #Basis: 388
 SCF Energy= -1223.88681897
 Predicted Change= -5.265475D-09
================================================================================
 Optimization completed.     {Found 2 times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force     0.000005 || 0.000450   [ YES ]     0.000001 || 0.000300   [ YES ]
 Displ     0.002359 || 0.001800   [ NO ]      0.000488 || 0.001200   [ YES ]
--------------------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
--------------------------------------------------------------------------------
    1          6           0       -2.339450    1.265579    0.221025
    2          6           0       -3.194911    0.193846    0.414221
    3          6           0       -2.798188   -1.073225    1.014324
    4          6           0       -1.744577   -1.239532    1.839520
    5          6           0       -0.376154   -0.457723   -1.377855
```

```
     6          6             0       -1.323522    0.520674   -1.705386
     7          1             0       -3.408575   -1.942820    0.782735
     8          1             0       -1.160290   -0.371853    2.142261
     9          1             0       -1.371948    1.209081    0.705960
    10          6             0       -2.832123    2.638726   -0.149847
    11          1             0       -3.240574    3.147992    0.733376
    12          1             0       -2.016225    3.260807   -0.531443
    13          1             0       -3.630216    2.607081   -0.896122
    14          6             0       -1.343773   -2.545424    2.449830
    15          1             0       -1.954825   -3.377667    2.088128
    16          1             0       -0.288344   -2.769434    2.244378
    17          1             0       -1.434797   -2.500163    3.543246
    18          8             0       -4.443510    0.351149   -0.065468
    19          1             0       -0.978697    1.549836   -1.694478
    20          6             0       -2.457202    0.208272   -2.636149
    21          1             0       -3.316655    0.864626   -2.480359
    22          1             0       -2.116125    0.363740   -3.669689
    23          1             0       -2.787040   -0.831637   -2.548164
    24          1             0       -0.578665   -1.494255   -1.618448
    25          6             0        0.827973   -0.114670   -0.753767
    26          8             0        1.082524    1.061655   -0.323963
    27          7             0        1.821209   -1.111217   -0.590936
    28         13             0        2.540838    1.857050    0.571119
    29          6             0        1.753186   -2.467049   -1.161130
    30          6             0        3.069595   -0.877510   -0.070382
    31          8             0        3.496884    0.176338    0.420821
    32          6             0        3.415912    3.152078   -0.599292
    33          6             0        2.058505    2.076582    2.456050
    34          6             0        3.086485   -3.073597   -0.676517
    35          1             0        1.680480   -2.413116   -2.251359
    36          1             0        0.889770   -3.009847   -0.770434
    37          8             0        3.836238   -1.950112   -0.140926
    38          1             0        4.399536    3.440867   -0.206717
    39          1             0        3.575379    2.774721   -1.617374
    40          1             0        2.832101    4.077580   -0.687935
    41          1             0        1.625480    1.172392    2.904814
    42          1             0        2.934446    2.341071    3.062402
    43          1             0        1.329813    2.886046    2.596147
    44          1             0        3.682854   -3.513861   -1.475204
    45          1             0        2.960911   -3.794872    0.133134
    46          6             0       -5.463803   -0.633954    0.153284
    47          1             0       -5.542425   -0.890029    1.214027
    48          1             0       -6.388781   -0.164507   -0.181325
    49          1             0       -5.280752   -1.535591   -0.440830
--------------------------------------------------------------------------------
 Statistical Thermodynamic Analysis for 3+a_ap_exo_0711xx.out
 Temperature=   298.150  Kelvin       Pressure=   1.00000  Atm
================================================================================
 SCF Energy=                            -1223.88681897
 Zero-point correction (ZPE)=           -1223.47565        0.411168
 Internal Energy (U)=                   -1223.44782        0.438992
 Enthalpy (H)=                          -1223.44688        0.439937
 Gibbs Free Energy (G)=                 -1223.53673        0.350082
 Entropy (S)=                                              0.00030137
--------------------------------------------------------------------------------
 Frequencies --  -164.1526               15.7262               20.5998
 Frequencies --    29.3669               35.0578               49.8706

--------------------------------------------------------------------------------
 Analyzing Gaussian Output File: SP_MP2_3a+a2_x_080501.out
 Using Gaussian 03:  IA64L-G03RevD.01 13-Oct-2005
 [#Processors=4  Memory=4gb  CheckPoint=SP_MP2_3a+a2_x_080501.chk]
================================================================================
 #p mp2/6-31+g(d) scf=(direct,tight) geom=check guess=read
--------------------------------------------------------------------------------
 Pointgroup=C1   Stoichiometry=C16H27AlNO4(1+)   C1[X(C16H27AlNO4)]
 Charge = 1     Multiplicity = 1
--------------------------------------------------------------------------------
 Standard basis: 6-31+G(d) (6D, 7F)      #Basis: 476
 SCF Energy= -1217.27182283
 MP2 Energy= -1220.2964101443   Correl. Energy= -3.024587318
================================================================================
 No optimization variables found.
```

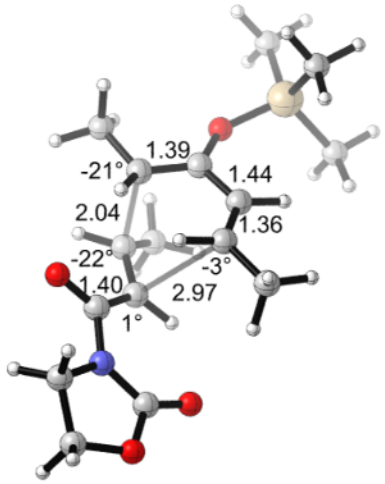
2c+**3**, *endo* TS




```
 ---------------------------------------------------------------------------
 Analyzing Gaussian Output File: 1+a0ac_n_080217.out
 Using Gaussian 03:  AM64L-G03RevC.02 12-Jun-2004
 [#Processors=2  Memory=1800MB  CheckPoint=1+a0ac_n_080217.chk]
 ===========================================================================
 # opt=(gdiis,modredundant) b3lyp/6-31g(d) geom=connectivity
 Modredundant Input:  B    1    6 F
 # b3lyp/6-31g* opt=(calcfc,ts,noeigentest,nofreeze,gdiis) geom=check
 guess=read freq=noraman
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq
 ---------------------------------------------------------------------------
 Pointgroup=C1   Stoichiometry=C16H27NO4Si   C1[X(C16H27NO4Si)]
 Charge = 0     Multiplicity = 1
 ---------------------------------------------------------------------------
 Standard basis: 6-31G(d) (6D, 7F)       #Basis: 388
 SCF Energy= -1271.12918213
 Predicted Change= -2.758604D-09
 ===========================================================================
 Optimization completed.     {Found 2 times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force     0.000010 || 0.000450   [ YES ]     0.000002 || 0.000300   [ YES ]
 Displ     0.002304 || 0.001800   [ NO ]      0.000293 || 0.001200   [ YES ]
 ---------------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -1.434181    2.237679    0.259332
    2          6             0       -1.620533    0.883892    0.622689
    3          6             0       -0.731435    0.197208    1.489710
    4          6             0        0.395323    0.763241    2.019442
    5          6             0        1.317366    1.530037   -0.386512
    6          6             0        0.259524    2.337297   -0.864161
    7          1             0       -0.878304   -0.872732    1.614771
    8          1             0       -0.253524    1.939932   -1.738113
    9          1             0        2.166219    1.966358    0.121700
   10          1             0        0.512217    1.840663    2.007303
   11          1             0       -1.010084    2.854329    1.047607
   12          6             0        1.377031    0.161018   -0.806099
   13          8             0        0.464412   -0.423740   -1.407412
   14          7             0        2.548109   -0.615150   -0.535203
   15          6             0        2.655795   -1.949052   -1.120059
   16          6             0        3.753197   -0.211905    0.023876
   17          8             0        4.044277    0.849356    0.526546
   18          6             0        3.976112   -2.436843   -0.506362
   19          1             0        2.689473   -1.887546   -2.214111
   20          1             0        1.800945   -2.569288   -0.845254
   21          8             0        4.643492   -1.246249   -0.054498
   22          1             0        4.627378   -2.945186   -1.220273
   23          1             0        3.814065   -3.090170    0.358623
   24          6             0       -2.537046    2.899168   -0.543833
   25          1             0       -3.499745    2.818366   -0.023775
   26          1             0       -2.337566    3.961190   -0.705341
   27          1             0       -2.661955    2.417609   -1.519185
   28          6             0        1.401363    0.015989    2.841195
   29          1             0        1.266707   -1.068171    2.765577
   30          1             0        2.420317    0.267722    2.527712
   31          1             0        1.318874    0.295115    3.901950
   32          6             0        0.532929    3.833354   -0.893573
   33          1             0        1.261358    4.057119   -1.682955
   34          1             0       -0.358445    4.431426   -1.097056
   35          1             0        0.967650    4.175996    0.052942
   36          8             0       -2.632822    0.235188    0.013851
   37         14             0       -3.196588   -1.369807   -0.081819
   38          6             0       -4.347785   -1.315626   -1.565013
   39          1             0       -4.865027   -2.273694   -1.698861
   40          1             0       -5.109199   -0.536243   -1.449369
   41          1             0       -3.789269   -1.105262   -2.484116
   42          6             0       -4.145567   -1.742469    1.504353
   43          1             0       -3.500181   -1.674656    2.388055
   44          1             0       -4.978211   -1.043988    1.646115
   45          1             0       -4.561779   -2.757486    1.477013
   46          6             0       -1.804739   -2.607852   -0.357973
   47          1             0       -2.189488   -3.476437   -0.907399
   48          1             0       -0.998701   -2.152325   -0.943602
   49          1             0       -1.377255   -2.976538    0.581963
 ---------------------------------------------------------------------------
 Statistical Thermodynamic Analysis for 1+a0ac_n_080217.out
 Temperature=   298.150  Kelvin       Pressure=   1.00000  Atm
 ===========================================================================
 SCF Energy=                             -1271.12918213
 Zero-point correction (ZPE)=            -1270.71847        0.410713
 Internal Energy (U)=                    -1270.69167        0.437511
 Enthalpy (H)=                           -1270.69072        0.438455
 Gibbs Free Energy (G)=                  -1270.77549        0.353687
 Entropy (S)=                                               0.00028431
 ---------------------------------------------------------------------------
 Frequencies --  -405.5773               28.1412               29.3065
 Frequencies --    41.4262               53.8699               62.3325

 ---------------------------------------------------------------------------
Analyzing Gaussian Output File: SP_MP2_1+a0ac_n_080502.out
 Using Gaussian 03:  IA64L-G03RevD.01 13-Oct-2005
 [#Processors=4  Memory=4gb  CheckPoint=SP_MP2_1+a0ac_n_080502.chk]
 ===========================================================================
 #p mp2/6-31+g(d) scf=(direct,tight) geom=check guess=read
 ---------------------------------------------------------------------------
 Pointgroup=C1   Stoichiometry=C16H27NO4Si   C1[X(C16H27NO4Si)]
 Charge = 0     Multiplicity = 1
```

```
--------------------------------------------------------------------------------
 Standard basis: 6-31+G(d) (6D, 7F)      #Basis: 476
 SCF Energy= -1264.43584646
 MP2 Energy= -1267.5392379172   Correl. Energy= -3.103391455
================================================================================
 No optimization variables found.
```

2c+**3**, *exo* TS

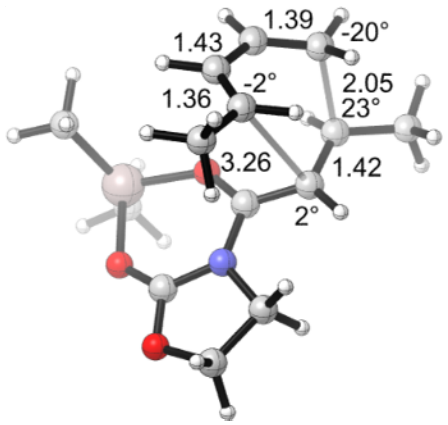



```
--------------------------------------------------------------------------------
 Analyzing Gaussian Output File: 1+a0ac_x_080217.out
 Using Gaussian 03:  AM64L-G03RevC.02 12-Jun-2004
 [#Processors=2  Memory=1800MB  CheckPoint=1+a0ac_x_080217.chk]
================================================================================
 # b3lyp/6-31g* opt=(calcfc,ts,noeigentest,nofreeze,gdiis) geom=check
 guess=read freq=noraman
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq
--------------------------------------------------------------------------------
 Pointgroup=C1   Stoichiometry=C16H27NO4Si   C1[X(C16H27NO4Si)]
 Charge = 0     Multiplicity = 1
--------------------------------------------------------------------------------
 Standard basis: 6-31G(d) (6D, 7F)       #Basis: 388
 SCF Energy= -1271.13038165
 Predicted Change= -9.469143D-10
================================================================================
 Optimization completed.     {Found 2 times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force     0.000007 || 0.000450   [ YES ]     0.000001 || 0.000300   [ YES ]
 Displ     0.000474 || 0.001800   [ YES ]     0.000085 || 0.001200   [ YES ]
--------------------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
--------------------------------------------------------------------------------
    1          6            0        0.903994    1.538391   -0.663847
    2          6            0        1.662936    0.356113   -0.528721
    3          6            0        1.073099   -0.934011   -0.604867
    4          6            0       -0.216230   -1.173551   -0.994271
    5          6            0       -1.330884    0.640389    0.792384
    6          6            0       -0.263158    1.566272    0.912111
    7          1            0        1.650952   -1.771314   -0.218234
```

```
     8          1             0       -0.766707   -0.407521   -1.528146
     9          1             0        0.057196    1.474558   -1.342566
    10          6             0        1.618334    2.872718   -0.727600
    11          1             0        2.215881    2.949516   -1.644926
    12          1             0        0.893374    3.692914   -0.734294
    13          1             0        2.301805    3.016270    0.114089
    14          6             0       -0.852388   -2.529606   -0.925001
    15          1             0       -0.164766   -3.277387   -0.515819
    16          1             0       -1.741856   -2.509883   -0.285159
    17          1             0       -1.174320   -2.864684   -1.920720
    18          8             0        2.948041    0.498179   -0.118841
    19         14             0        4.276452   -0.552075    0.037047
    20          6             0        5.710055    0.618134    0.356095
    21          1             0        6.650262    0.066429    0.477204
    22          1             0        5.838168    1.321014   -0.474609
    23          1             0        5.547442    1.204667    1.267382
    24          6             0        4.525734   -1.508233   -1.567408
    25          1             0        3.666052   -2.139150   -1.817342
    26          1             0        4.692307   -0.824923   -2.408224
    27          1             0        5.405134   -2.159929   -1.490831
    28          6             0        4.037733   -1.709757    1.506212
    29          1             0        4.967392   -2.256343    1.709873
    30          1             0        3.782604   -1.144920    2.410352
    31          1             0        3.249418   -2.452932    1.345176
    32          1             0       -0.543458    2.589425    0.660506
    33          6             0        0.622053    1.445477    2.138521
    34          1             0        1.522325    2.062930    2.064545
    35          1             0        0.069767    1.767695    3.030407
    36          1             0        0.930909    0.407216    2.302692
    37          1             0       -1.419111   -0.207683    1.456288
    38          6             0       -2.397512    0.950150   -0.113640
    39          8             0       -2.343612    1.831317   -0.985478
    40          7             0       -3.622675    0.215370   -0.044848
    41          6             0       -4.709529    0.557816   -0.958060
    42          6             0       -3.946580   -0.894376    0.722590
    43          8             0       -3.248598   -1.530963    1.478786
    44          6             0       -5.875131   -0.208588   -0.320217
    45          1             0       -4.483930    0.217428   -1.976046
    46          1             0       -4.863277    1.637339   -0.991307
    47          8             0       -5.251254   -1.226410    0.484175
    48          1             0       -6.527570   -0.699029   -1.045272
    49          1             0       -6.479374    0.428754    0.335439
---------------------------------------------------------------------------
 Statistical Thermodynamic Analysis for 1+a0ac_x_080217.out
 Temperature=   298.150  Kelvin       Pressure=   1.00000  Atm
===========================================================================
 SCF Energy=                            -1271.13038165
 Zero-point correction (ZPE)=           -1270.71994        0.410434
 Internal Energy (U)=                   -1270.69293        0.437452
 Enthalpy (H)=                          -1270.69198        0.438396
 Gibbs Free Energy (G)=                 -1270.77804        0.352342
 Entropy (S)=                                              0.00028863
---------------------------------------------------------------------------
 Frequencies --  -398.8900               18.4804               31.6915
 Frequencies --    35.1604               47.6626               51.9330

---------------------------------------------------------------------------
 Analyzing Gaussian Output File: SP_MP2_1+a0ac_x_080502.out
 Using Gaussian 03:  IA64L-G03RevD.01 13-Oct-2005
 [#Processors=4  Memory=4gb  CheckPoint=SP_MP2_1+a0ac_x_080502.chk]
===========================================================================
 #p mp2/6-31+g(d) scf=(direct,tight) geom=check guess=read
---------------------------------------------------------------------------
 Pointgroup=C1   Stoichiometry=C16H27NO4Si   C1[X(C16H27NO4Si)]
 Charge = 0     Multiplicity = 1
---------------------------------------------------------------------------
 Standard basis: 6-31+G(d) (6D, 7F)      #Basis: 476
```

```
 SCF Energy= -1264.43838854
 MP2 Energy= -1267.5375614304   Correl. Energy= -3.099172891
===========================================================================
 No optimization variables found.
```

18+$\mathbf{A_2}$, *endo* TS




```
 Analyzing Gaussian Output File: 8+a2_n_080226.out
 Using Gaussian 03:  AM64L-G03RevC.02 12-Jun-2004
 [#Processors=2  Memory=1800MB  CheckPoint=8+a2_n_080226.chk]
```

```
 # opt=(modredundant,gdiis) b3lyp/6-31g(d) geom=connectivity
 Modredundant Input:  B    1    6 F
 # b3lyp/6-31g* opt=(calcfc,ts,noeigentest,nofreeze,gdiis) geom=check
 guess=read freq=noraman
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq
```

```
 Pointgroup=C1   Stoichiometry=C14H23AlNO3(1+)   C1[X(C14H23AlNO3)]
 Charge = 1     Multiplicity = 1
```

```
 Standard basis: 6-31G(d) (6D, 7F)       #Basis: 335
 SCF Energy= -1070.03581270
 Predicted Change= -2.805976D-09
```

```
 Optimization completed on the basis of negligible forces.     {Found 3 times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force     0.000001 || 0.000450   [ YES ]     0.000000 || 0.000300   [ YES ]
 Displ     0.002475 || 0.001800   [ NO ]      0.000308 || 0.001200   [ YES ]
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.550537	0.724661	-0.047853
2	6	0	2.734088	1.226102	0.958854
3	6	0	2.001441	0.453980	1.908586
4	6	0	2.011964	-0.906502	1.977081
5	6	0	1.347026	-0.703703	-1.209037
6	6	0	2.335137	0.219556	-1.625810
7	1	0	1.355378	1.002332	2.590589
8	1	0	1.978825	1.234241	-1.778729
9	1	0	1.523390	-1.765979	-1.330489
10	1	0	2.687240	-1.468237	1.334714
11	1	0	3.982812	-0.266160	0.056773
12	6	0	0.123954	-0.247465	-0.707090
13	8	0	-0.107043	0.989141	-0.483044
14	7	0	-0.915585	-1.179183	-0.466140
15	13	0	-1.634263	1.968828	0.047977
16	6	0	-0.860082	-2.609508	-0.811833
17	6	0	-2.192025	-0.830678	-0.102422
18	8	0	-2.617419	0.302582	0.161496
19	6	0	-1.383357	2.612392	1.879848
20	6	0	-2.319895	2.971268	-1.481464
21	6	0	-2.237074	-3.097160	-0.317728
22	1	0	-0.037773	-3.105366	-0.291610
23	1	0	-0.727633	-2.731642	-1.891214
24	8	0	-2.989193	-1.881651	-0.054252
25	1	0	-2.306085	3.064758	2.265682
26	1	0	-1.103410	1.819699	2.586096
27	1	0	-0.611619	3.391479	1.940222
28	1	0	-2.368647	2.376677	-2.402639
29	1	0	-3.333196	3.346587	-1.288438
30	1	0	-1.698897	3.849966	-1.699673
31	1	0	-2.184392	-3.655772	0.618793
32	1	0	-2.791164	-3.670453	-1.060275
33	6	0	1.212958	-1.705985	2.952257
34	1	0	0.551761	-1.080753	3.558511
35	1	0	0.607978	-2.468442	2.442680
36	1	0	1.883078	-2.257661	3.626346
37	6	0	3.389220	-0.249671	-2.606193
38	1	0	2.921347	-0.349083	-3.594261
39	1	0	4.212443	0.461290	-2.706257
40	1	0	3.800103	-1.226827	-2.332916
41	1	0	4.174787	1.433883	-0.583171
42	1	0	2.564068	2.300684	0.981772

```
 Statistical Thermodynamic Analysis for 8+a2_n_080226.out
 Temperature=   298.150  Kelvin       Pressure=   1.00000  Atm
```

SCF Energy=	-1070.03581270	
Zero-point correction (ZPE)=	-1069.68512	0.350687
Internal Energy (U)=	-1069.66200	0.373804
Enthalpy (H)=	-1069.66106	0.374748
Gibbs Free Energy (G)=	-1069.73865	0.297163
Entropy (S)=		0.00026022

```
 Frequencies --  -315.9695               26.8364               35.2505
 Frequencies --    43.7652               47.5763               70.1779
```

```
 Analyzing Gaussian Output File: SP_MP2_8+a2_n_080427.out
 Using Gaussian 03:  IA64L-G03RevD.01 13-Oct-2005
 [#Processors=4  Memory=4gb  CheckPoint=SP_MP2_8+a2_n_080427.chk]
```

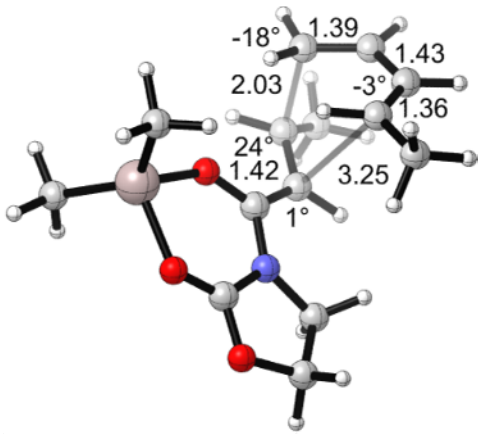
```
 #p mp2/6-31+g(d) geom=connectivity scf=tight
```

```
 Pointgroup=C1   Stoichiometry=C14H23AlNO3(1+)   C1[X(C14H23AlNO3)]
 Charge = 1     Multiplicity = 1
```

```
 Standard basis: 6-31+G(d) (6D, 7F)      #Basis: 411
 SCF Energy= -1064.33854444
 MP2 Energy= -1066.9192893048   Correl. Energy= -2.580744865
```

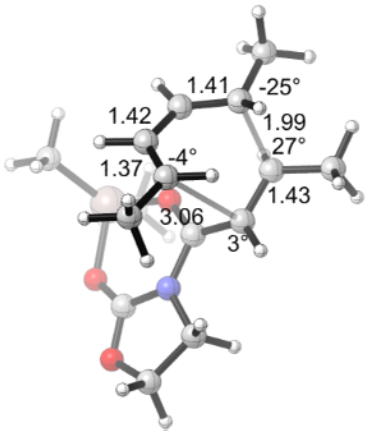
```
 No optimization variables found.
```

18+$\mathbf{A_2}$, *exo* TS




```
------------------------------------------------------------------------------
 Analyzing Gaussian Output File: 8+a2_x_080226.out
 Using Gaussian 03:  AM64L-G03RevC.02 12-Jun-2004
 [#Processors=2  Memory=1800MB  CheckPoint=8+a2_x_080226.chk]
==============================================================================
 # opt=(gdiis,modredundant) b3lyp/6-31g(d) geom=connectivity
 Modredundant Input:  B    1    6 F
 # b3lyp/6-31g* opt=(calcfc,ts,noeigentest,nofreeze,gdiis) geom=check
 guess=read freq=noraman
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq
------------------------------------------------------------------------------
 Pointgroup=C1   Stoichiometry=C14H23AlNO3(1+)   C1[X(C14H23AlNO3)]
 Charge = 1     Multiplicity = 1
------------------------------------------------------------------------------
 Standard basis: 6-31G(d) (6D, 7F)       #Basis: 335
 SCF Energy= -1070.03515580
 Predicted Change= -3.295011D-10
==============================================================================
 Optimization completed.     {Found 3 times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force     0.000000 || 0.000450   [ YES ]     0.000000 || 0.000300   [ YES ]
 Displ     0.000461 || 0.001800   [ YES ]     0.000103 || 0.001200   [ YES ]
------------------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
------------------------------------------------------------------------------
    1          6           0        2.962061   -1.591164    0.052385
    2          6           0        3.783567   -0.593408    0.562866
    3          6           0        3.360874    0.507931    1.363818
    4          6           0        2.100994    0.661365    1.861843
    5          6           0        1.247794    0.284678   -1.253065
    6          6           0        2.104915   -0.787630   -1.608357
    7          1           0        4.096678    1.284182    1.565856
    8          1           0        1.380772   -0.144883    1.739033
    9          1           0        2.013996   -1.812905    0.533836
   10          6           0        1.650917    1.826942    2.676825
   11          1           0        2.399658    2.622587    2.718114
   12          1           0        0.710353    2.241687    2.289604
   13          1           0        1.431864    1.502804    3.704238
   14          1           0        1.598358   -1.741326   -1.745844
   15          6           0        3.234306   -0.522132   -2.577738
   16          1           0        3.950026   -1.347486   -2.609150
   17          1           0        2.815055   -0.414396   -3.586575
   18          1           0        3.771775    0.400911   -2.340356
   19          1           0        1.570943    1.301574   -1.438771
   20          6           0       -0.016674    0.051072   -0.707576
   21          8           0       -0.413292   -1.108084   -0.340563
   22          7           0       -0.908855    1.141098   -0.554495
   23         13           0       -2.014591   -1.786659    0.402276
   24          6           0       -0.673676    2.498076   -1.077727
   25          6           0       -2.209250    1.017759   -0.128798
   26          8           0       -2.772104   -0.003946    0.286976
   27          6           0       -2.923672   -2.911050   -0.909114
   28          6           0       -1.700567   -2.153875    2.298920
   29          6           0       -1.960047    3.224626   -0.635369
   30          1           0       -0.554185    2.466148   -2.164847
   31          1           0        0.220388    2.938598   -0.631376
   32          8           0       -2.856853    2.165007   -0.204383
   33          1           0       -3.955560   -3.124957   -0.602013
   34          1           0       -2.974094   -2.456238   -1.906606
   35          1           0       -2.425095   -3.882367   -1.023968
   36          1           0       -1.189457   -1.337088    2.826232
   37          1           0       -2.646070   -2.326951    2.829083
   38          1           0       -1.095783   -3.058821    2.443617
   39          1           0       -2.456325    3.766136   -1.440088
   40          1           0       -1.807097    3.887134    0.218752
   41          1           0        3.441230   -2.446624   -0.416034
   42          1           0        4.822986   -0.581794    0.239402
------------------------------------------------------------------------------
 Statistical Thermodynamic Analysis for 8+a2_x_080226.out
 Temperature=   298.150  Kelvin       Pressure=   1.00000  Atm
==============================================================================
 SCF Energy=                              -1070.03515580
 Zero-point correction (ZPE)=             -1069.68434        0.350810
 Internal Energy (U)=                     -1069.66121        0.373945
 Enthalpy (H)=                            -1069.66026        0.374889
 Gibbs Free Energy (G)=                   -1069.73848        0.296675
 Entropy (S)=                                                0.00026233
------------------------------------------------------------------------------
 Frequencies --  -304.7981                20.1768               29.5001
 Frequencies --    39.8743                45.2366               62.1674

------------------------------------------------------------------------------
 Analyzing Gaussian Output File: SP_MP2_8+a2_x_080427.out
 Using Gaussian 03:  IA64L-G03RevD.01 13-Oct-2005
 [#Processors=4  Memory=4gB  CheckPoint=SP_MP2_8+a2_x_080427.chk]
==============================================================================
 #p mp2/6-31+g(d) scf=tight
------------------------------------------------------------------------------
 Pointgroup=C1   Stoichiometry=C14H23AlNO3(1+)   C1[X(C14H23AlNO3)]
 Charge = 1     Multiplicity = 1
------------------------------------------------------------------------------
 Standard basis: 6-31+G(d) (6D, 7F)      #Basis: 411
 SCF Energy= -1064.33811981
 MP2 Energy= -1066.9165930452   Correl. Energy= -2.578473238
==============================================================================
 No optimization variables found.
```

19+$\mathbf{A_2}$, *endo* TS

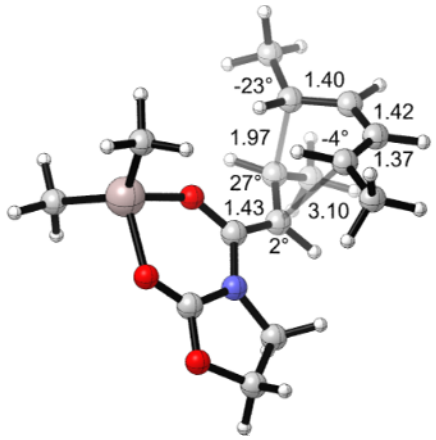



```
 Analyzing Gaussian Output File: 6+a_endo_080211.out
 Using Gaussian 03:  AM64L-G03RevC.02 12-Jun-2004
 [#Processors=2  Memory=1800MB  CheckPoint=6+a_endo_080211.chk]
 # opt=(gdiis,modredundant) b3lyp/6-31g(d) geom=connectivity
 Modredundant Input:  B    1    6 F
 # opt=(gdiis,ts,noeigentest,nofreeze,calcfc) b3lyp/6-31g(d) geom=check
 guess=read freq=noraman
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq
 Pointgroup=C1   Stoichiometry=C15H25AlNO3(1+)   C1[X(C15H25AlNO3)]
 Charge = 1     Multiplicity = 1
 Standard basis: 6-31G(d) (6D, 7F)       #Basis: 354
 SCF Energy= -1109.34959787
 Predicted Change= -2.151210D-09
 Optimization completed.     {Found 3 times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force     0.000001 || 0.000450   [ YES ]     0.000000 || 0.000300   [ YES ]
 Displ     0.001512 || 0.001800   [ YES ]     0.000228 || 0.001200   [ YES ]
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.287879	0.283898	0.112762
2	6	0	2.403135	0.622284	1.153788
3	6	0	1.637578	-0.271500	1.942485
4	6	0	1.621718	-1.627701	1.780125
5	6	0	0.995059	-0.952192	-1.133149
6	6	0	2.173383	-0.214080	-1.461114
7	1	0	0.973575	0.170871	2.682281
8	1	0	1.989605	0.825173	-1.725862
9	1	0	0.966561	-2.019025	-1.319438
10	1	0	2.319182	-2.087626	1.084082
11	1	0	3.743997	-0.703267	0.184897
12	6	0	-0.138056	-0.292729	-0.664833
13	8	0	-0.116490	0.950450	-0.357314
14	7	0	-1.358645	-0.999273	-0.519821
15	13	0	-1.437844	2.188152	0.185699
16	6	0	-1.582495	-2.383931	-0.965563
17	6	0	-2.547649	-0.418492	-0.166543
18	8	0	-2.742299	0.759784	0.167523
19	6	0	-1.125181	2.676241	2.056345
20	6	0	-1.844398	3.395951	-1.295075
21	6	0	-3.050419	-2.605789	-0.547951
22	1	0	-0.902529	-3.071554	-0.458167
23	1	0	-1.429681	-2.461359	-2.046445
24	8	0	-3.546626	-1.280792	-0.215259
25	1	0	-1.952163	3.284243	2.445447
26	1	0	-1.029585	1.812320	2.727317
27	1	0	-0.217740	3.283626	2.175925
28	1	0	-1.981675	2.878889	-2.253382
29	1	0	-2.764716	3.962608	-1.102685
30	1	0	-1.048058	4.137291	-1.442644
31	1	0	-3.153818	-3.224992	0.345212
32	1	0	-3.678497	-2.999570	-1.346424
33	6	0	4.222243	1.381432	-0.371852
34	1	0	5.051869	1.502676	0.334232
35	1	0	4.663095	1.163280	-1.346877
36	1	0	3.700907	2.342000	-0.441918
37	6	0	0.788843	-2.562761	2.591453
38	1	0	0.062035	-2.037567	3.217331
39	1	0	0.261607	-3.287503	1.957938
40	1	0	1.437786	-3.161031	3.247647
41	6	0	3.158656	-0.942968	-2.358762
42	1	0	2.739395	-0.997411	-3.371087
43	1	0	4.122329	-0.438291	-2.438610
44	1	0	3.332681	-1.968544	-2.015498
45	1	0	2.237879	1.682182	1.339082

```
 Statistical Thermodynamic Analysis for 6+a_endo_080211.out
 Temperature=   298.150  Kelvin       Pressure=   1.00000  Atm
 SCF Energy=                          -1109.34959787
 Zero-point correction (ZPE)=         -1108.97064        0.378956
 Internal Energy (U)=                 -1108.94611        0.403483
 Enthalpy (H)=                        -1108.94517        0.404427
 Gibbs Free Energy (G)=               -1109.02554        0.324052
 Entropy (S)=                                            0.00026958
 Frequencies --  -336.8374               25.4899               31.2109
 Frequencies --    43.1423               48.1478               71.2578

 Analyzing Gaussian Output File: SP_MP2_6+a2_n_080429.out
 Using Gaussian 03:  IA64L-G03RevD.01 13-Oct-2005
 [#Processors=4  Memory=4gb  CheckPoint=SP_MP2_6+a2_n_080429.chk]
 #p mp2/6-31+g(d) geom=check guess=read scf=tight
 Pointgroup=C1   Stoichiometry=C15H25AlNO3(1+)   C1[X(C15H25AlNO3)]
 Charge = 1     Multiplicity = 1
 Standard basis: 6-31+G(d) (6D, 7F)      #Basis: 434
 SCF Energy= -1103.36832154
 MP2 Energy= -1106.0918341154   Correl. Energy= -2.723512571
 No optimization variables found.
```

19+$\mathbf{A_2}$, *exo* TS

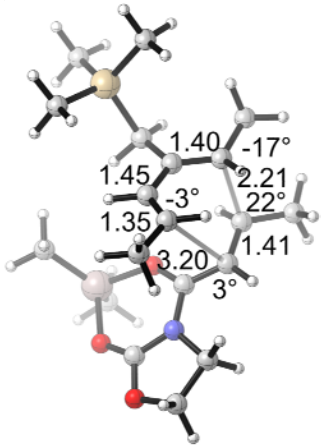



```
 Analyzing Gaussian Output File: 6+a_exo_050208.out
 Using Gaussian 03:  AM64L-G03RevC.02 12-Jun-2004
 [#Processors=2  Memory=1800MB  CheckPoint=6+a_exo_050208.chk]
 # opt=modredundant b3lyp/6-31g(d) geom=connectivity
 Modredundant Input:  B    1    6 F
 # opt=(ts,calcfc,noeigentest,nofreeze,gdiis) b3lyp/6-31g(d) geom=check
 guess=read freq=noraman
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq
 Pointgroup=C1   Stoichiometry=C15H25AlNO3(1+)   C1[X(C15H25AlNO3)]
 Charge = 1     Multiplicity = 1
 Standard basis: 6-31G(d) (6D, 7F)       #Basis: 354
 SCF Energy= -1109.35212796
 Predicted Change= -2.379263D-09
 Optimization completed.     {Found 3 times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force     0.000006 || 0.000450   [ YES ]     0.000001 || 0.000300   [ YES ]
 Displ     0.001661 || 0.001800   [ YES ]     0.000249 || 0.001200   [ YES ]
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.973244	0.911252	0.145595
2	6	0	-3.595301	-0.237176	0.658125
3	6	0	-2.962706	-1.282122	1.378302
4	6	0	-1.677330	-1.233300	1.841297
5	6	0	-0.996875	-0.665621	-1.125302
6	6	0	-2.078866	0.206126	-1.461057
7	1	0	-3.538410	-2.191054	1.544262
8	1	0	-1.128772	-0.296232	1.785902
9	1	0	-2.037351	1.211426	0.614123
10	6	0	-3.829415	2.077987	-0.308413
11	1	0	-4.096001	2.695124	0.557590
12	1	0	-3.296028	2.723627	-1.013462
13	1	0	-4.761701	1.748255	-0.777457
14	6	0	-0.999203	-2.349375	2.561879
15	1	0	-1.574142	-3.278850	2.532174
16	1	0	0.002760	-2.533897	2.152249
17	1	0	-0.842481	-2.072002	3.614336
18	1	0	-1.757540	1.222388	-1.687488
19	6	0	-3.128743	-0.335270	-2.410903
20	1	0	-3.999214	0.321188	-2.482924
21	1	0	-2.694528	-0.408897	-3.415756
22	1	0	-3.465605	-1.335466	-2.121138
23	1	0	-1.100890	-1.727532	-1.310149
24	6	0	0.212866	-0.168103	-0.647417
25	8	0	0.377226	1.054029	-0.298887
26	7	0	1.324681	-1.044953	-0.543322
27	13	0	1.818343	2.040674	0.415638
28	6	0	1.365191	-2.410523	-1.093685
29	6	0	2.585744	-0.647781	-0.175209
30	8	0	2.934987	0.465980	0.240235
31	6	0	2.427063	3.362123	-0.886543
32	6	0	1.493854	2.304437	2.328781
33	6	0	2.798161	-2.846991	-0.727404
34	1	0	1.189027	-2.385136	-2.173348
35	1	0	0.610941	-3.044552	-0.622998
36	8	0	3.463628	-1.624917	-0.308282
37	1	0	3.404601	3.775532	-0.606468
38	1	0	2.530330	2.954185	-1.900079
39	1	0	1.736586	4.213184	-0.952120
40	1	0	1.210727	1.384807	2.858653
41	1	0	2.389051	2.693060	2.831344
42	1	0	0.696733	3.038047	2.508502
43	1	0	3.360288	-3.254564	-1.567098
44	1	0	2.833825	-3.541180	0.114517
45	1	0	-4.637326	-0.400276	0.383982

```
 Statistical Thermodynamic Analysis for 6+a_exo_050208.out
 Temperature=   298.150  Kelvin       Pressure=   1.00000  Atm
 SCF Energy=                            -1109.35212796
 Zero-point correction (ZPE)=           -1108.97314        0.378985
 Internal Energy (U)=                   -1108.94850        0.403622
 Enthalpy (H)=                          -1108.94756        0.404566
 Gibbs Free Energy (G)=                 -1109.02899        0.323137
 Entropy (S)=                                              0.00027311
 Frequencies --  -298.1387               19.6919              31.1023
 Frequencies --    37.6115               42.9941              61.4837

 Analyzing Gaussian Output File: SP_MP2_6+a2_x_080429.out
 Using Gaussian 03:  IA64L-G03RevD.01 13-Oct-2005
 [#Processors=4  Memory=4gb  CheckPoint=SP_MP2_6+a2_x_080429.chk]
 #p mp2/6-31+g(d) geom=check guess=read scf=tight
 Pointgroup=C1   Stoichiometry=C15H25AlNO3(1+)   C1[X(C15H25AlNO3)]
 Charge = 1     Multiplicity = 1
 Standard basis: 6-31+G(d) (6D, 7F)      #Basis: 434
 SCF Energy= -1103.37295098
 MP2 Energy= -1106.092289129    Correl. Energy= -2.719338144
 No optimization variables found.
```

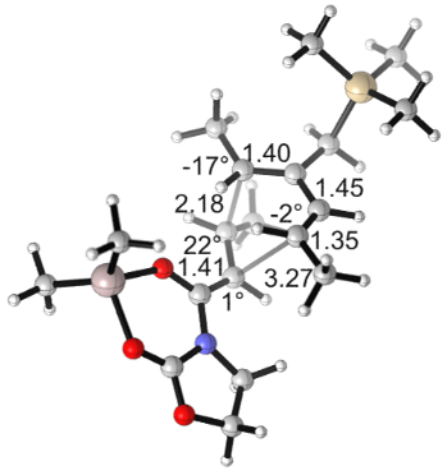
1d+$\mathbf{A_2}$, *endo* TS




```
 ---------------------------------------------------------------------------
 Analyzing Gaussian Output File: 11+a2_n_080303.out
 Using Gaussian 03:  AM64L-G03RevC.02 12-Jun-2004
 [#Processors=2  Memory=1800MB  CheckPoint=11+a2_n_080303.chk]
 ===========================================================================
 # opt=(gdiis,modredundant) b3lyp/6-31g(d) geom=connectivity
 Modredundant Input:  B    1    6 F
 # opt=(gdiis,ts,calcfc,nofreeze,noeigentest) freq=noraman b3lyp/6-31g(d)
 guess=read geom=check
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq
 ---------------------------------------------------------------------------
 Pointgroup=C1   Stoichiometry=C19H35AlNO3Si(1+)   C1[X(C19H35AlNO3Si)]
 Charge = 1     Multiplicity = 1
 ---------------------------------------------------------------------------
 Standard basis: 6-31G(d) (6D, 7F)       #Basis: 453
 SCF Energy= -1557.34952477
 Predicted Change= -2.510335D-09
 ===========================================================================
 Optimization completed.     {Found 3 times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force     0.000003 || 0.000450   [ YES ]     0.000001 || 0.000300   [ YES ]
 Displ     0.001139 || 0.001800   [ YES ]     0.000309 || 0.001200   [ YES ]
 ---------------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------------
    1          6             0       -1.747224    2.129877   -0.411061
    2          6             0       -1.720282    0.822899    0.092771
    3          6             0       -0.925138    0.465927    1.252614
    4          6             0       -0.218057    1.302218    2.048262
    5          6             0        1.244687    1.929653   -0.731308
    6          6             0        0.133126    2.150653   -1.571145
    7          1             0       -0.894392   -0.596038    1.488385
    8          1             0       -0.186688    1.303923   -2.171724
    9          1             0        1.761543    2.784805   -0.311559
   10          1             0       -0.252977    2.376427    1.878070
   11          1             0       -1.372518    2.911444    0.244188
   12          6             0        1.746525    0.647263   -0.512468
   13          8             0        1.180663   -0.414174   -0.950215
   14          7             0        2.967909    0.501634    0.196849
   15         13             0        1.668793   -2.226083   -1.022023
   16          6             0        3.812853    1.614272    0.660446
   17          6             0        3.615610   -0.690519    0.382266
   18          8             0        3.239794   -1.819001    0.030508
   19          6             0        0.466173   -3.283657    0.108443
   20          6             0        2.260594   -2.688797   -2.826806
   21          6             0        4.934164    0.859292    1.401692
   22          1             0        3.254642    2.276171    1.325580
   23          1             0        4.179793    2.190326   -0.194532
   24          8             0        4.765073   -0.530748    1.014101
   25          1             0        0.872977   -4.290926    0.268689
   26          1             0        0.299010   -2.850544    1.103332
   27          1             0       -0.518844   -3.424615   -0.357096
   28          1             0        2.968345   -1.965268   -3.251545
   29          1             0        2.756173   -3.668234   -2.843385
   30          1             0        1.415727   -2.755645   -3.525001
   31          1             0        4.838016    0.907797    2.488270
   32          1             0        5.937701    1.162603    1.104968
   33          6             0       -2.809836    2.581332   -1.391341
   34          1             0       -3.810507    2.382139   -0.991739
   35          1             0       -2.746582    3.656023   -1.572948
   36          1             0       -2.743900    2.070007   -2.359144
   37          6             0        0.566048    0.857461    3.243260
   38          1             0        0.576083   -0.231493    3.347378
   39          1             0        1.604312    1.213988    3.198022
   40          1             0        0.141764    1.286663    4.161100
   41          6             0        0.009139    3.508588   -2.219615
   42          1             0        0.823301    3.609737   -2.950364
   43          1             0       -0.924489    3.637238   -2.765993
   44          1             0        0.116264    4.324622   -1.496957
   45         14             0       -4.106864   -0.858428    0.387585
   46          6             0       -4.924971   -2.090913   -0.783527
   47          1             0       -5.834671   -2.503065   -0.330666
   48          1             0       -5.214295   -1.621776   -1.731142
   49          1             0       -4.263525   -2.933930   -1.015080
   50          6             0       -5.249464    0.604285    0.737323
   51          1             0       -4.754766    1.386942    1.324442
   52          1             0       -5.635713    1.058923   -0.182008
   53          1             0       -6.116326    0.264617    1.317275
   54          6             0       -3.617953   -1.700166    2.006298
   55          1             0       -4.506607   -2.134163    2.480606
   56          1             0       -2.904512   -2.517035    1.844705
   57          1             0       -3.177418   -1.000255    2.725081
   58          6             0       -2.487355   -0.276447   -0.546429
   59          1             0       -1.878942   -1.188685   -0.595275
   60          1             0       -2.797618   -0.025011   -1.564957
 ---------------------------------------------------------------------------
 Statistical Thermodynamic Analysis for 11+a2_n_080303.out
 Temperature=   298.150  Kelvin       Pressure=   1.00000  Atm
 ===========================================================================
 SCF Energy=                            -1557.34952477
 Zero-point correction (ZPE)=           -1556.84023        0.509294
 Internal Energy (U)=                   -1556.80661        0.542910
 Enthalpy (H)=                          -1556.80567        0.543855
 Gibbs Free Energy (G)=                 -1556.90640        0.443119
 Entropy (S)=                                              0.00033787
 ---------------------------------------------------------------------------
 Frequencies --  -259.8220               19.9396               25.2098
```

```
 Frequencies --    30.4932               34.0021               41.4079

---------------------------------------------------------------------------
 Analyzing Gaussian Output File: SP_MP2_11+a2_n_080501.out
 Using Gaussian 03:  IA64L-G03RevD.01 13-Oct-2005
 [#Processors=4  Memory=4gb  CheckPoint=SP_MP2_11+a2_n_080501.chk]
===========================================================================
 #p mp2/6-31+g(d) scf=(direct,tight) guess=read geom=check
---------------------------------------------------------------------------
 Pointgroup=C1   Stoichiometry=C19H35AlNO3Si(1+)   C1[X(C19H35AlNO3Si)]
 Charge = 1     Multiplicity = 1
---------------------------------------------------------------------------
 Standard basis: 6-31+G(d) (6D, 7F)      #Basis: 553
 SCF Energy= -1549.63445469
 MP2 Energy= -1552.9843096348   Correl. Energy= -3.349854948
===========================================================================
 No optimization variables found.
```

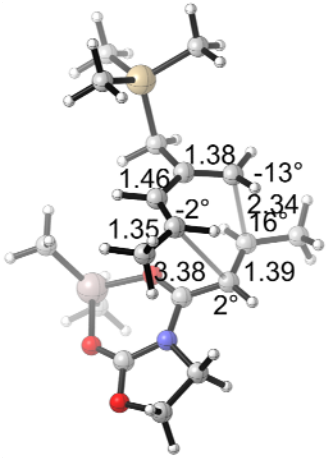
1d+$\mathbf{A_2}$, *exo* TS




```
---------------------------------------------------------------------------
 Analyzing Gaussian Output File: 11+a2_x_080303.out
 Using Gaussian 03:  AM64L-G03RevC.02 12-Jun-2004
 [#Processors=2  Memory=1800MB  CheckPoint=11+a2_x_080303.chk]
===========================================================================
 # opt=(gdiis,modredundant) b3lyp/6-31g(d) geom=connectivity
 Modredundant Input:  B    1    6 F
 # opt=(gdiis,ts,calcfc,noeigentest,nofreeze) b3lyp/6-31g(d) guess=read
 geom=check freq=noraman
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq
---------------------------------------------------------------------------
 Pointgroup=C1   Stoichiometry=C19H35AlNO3Si(1+)   C1[X(C19H35AlNO3Si)]
 Charge = 1     Multiplicity = 1
---------------------------------------------------------------------------
 Standard basis: 6-31G(d) (6D, 7F)       #Basis: 453
 SCF Energy= -1557.35282565
 Predicted Change= -9.419317D-10
===========================================================================
 Optimization completed.     {Found 3 times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force     0.000002 || 0.000450   [ YES ]     0.000000 || 0.000300   [ YES ]
 Displ     0.001306 || 0.001800   [ YES ]     0.000171 || 0.001200   [ YES ]
---------------------------------------------------------------------------
 Center     Atomic     Atomic             Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
---------------------------------------------------------------------------
    1          6           0        1.441324    1.069388    0.400411
    2          6           0        2.193728   -0.098879    0.243748
    3          6           0        1.660732   -1.242186   -0.480786
    4          6           0        0.575037   -1.259746   -1.287782
    5          6           0       -0.822138   -0.478332    1.564302
```

```
     6          6           0        0.118559    0.469316    2.020131
     7          1           0        2.212442   -2.174173   -0.360053
     8          1           0        0.038850   -0.335910   -1.496188
     9          1           0        0.575130    1.181072   -0.245868
    10          6           0        2.009303    2.384794    0.877193
    11          1           0        2.569441    2.870630    0.068846
    12          1           0        1.209135    3.073125    1.168181
    13          1           0        2.691959    2.283376    1.726060
    14          6           0        0.087873   -2.471407   -2.018797
    15          1           0        0.643277   -3.372932   -1.743914
    16          1           0       -0.980683   -2.644959   -1.830564
    17          1           0        0.180522   -2.327049   -3.103782
    18         14           0        5.046746   -0.059588   -0.399445
    19          6           0        6.588130   -0.213828    0.677308
    20          1           0        7.493172   -0.116888    0.065730
    21          1           0        6.627791    0.566438    1.446317
    22          1           0        6.637053   -1.185561    1.182426
    23          6           0        4.967493    1.631151   -1.234989
    24          1           0        4.044267    1.762811   -1.811448
    25          1           0        5.039543    2.452108   -0.512663
    26          1           0        5.804925    1.740927   -1.934670
    27          6           0        4.992849   -1.433781   -1.694059
    28          1           0        5.865080   -1.354118   -2.354260
    29          1           0        5.022748   -2.430702   -1.238256
    30          1           0        4.099947   -1.376241   -2.326631
    31          1           0       -0.204304    1.505638    1.970923
    32          6           0        1.006071    0.118371    3.183777
    33          1           0        1.840639    0.813987    3.296321
    34          1           0        0.414010    0.177521    4.107533
    35          1           0        1.401520   -0.899331    3.109079
    36          1           0       -0.710950   -1.514888    1.857442
    37          6           0       -1.900530   -0.101044    0.766111
    38          8           0       -2.041582    1.077573    0.284728
    39          7           0       -2.903303   -1.061030    0.470861
    40         13           0       -3.364484    1.933964   -0.744637
    41          6           0       -2.969518   -2.411289    1.054127
    42          6           0       -4.062250   -0.782673   -0.207140
    43          8           0       -4.385044    0.285691   -0.745850
    44          6           0       -4.326545    3.232261    0.353882
    45          6           0       -2.678461    2.190739   -2.560576
    46          6           0       -4.230782   -2.977940    0.372250
    47          1           0       -3.064902   -2.346573    2.142334
    48          1           0       -2.075124   -2.986490    0.806025
    49          8           0       -4.870654   -1.827244   -0.241974
    50          1           0       -5.235989    3.584440   -0.150006
    51          1           0       -4.635346    2.830602    1.327480
    52          1           0       -3.716756    4.123141    0.553927
    53          1           0       -2.203067    1.294550   -2.981322
    54          1           0       -3.483200    2.474525   -3.251199
    55          1           0       -1.935879    2.998617   -2.603317
    56          1           0       -4.945125   -3.418003    1.067408
    57          1           0       -4.004167   -3.688005   -0.425684
    58          6           0        3.543784   -0.270793    0.835916
    59          1           0        3.666081   -1.287453    1.233581
    60          1           0        3.735227    0.432793    1.651298
--------------------------------------------------------------------------------
 Statistical Thermodynamic Analysis for 11+a2_x_080303.out
 Temperature=   298.150  Kelvin       Pressure=   1.00000  Atm
================================================================================
 SCF Energy=                          -1557.35282565
 Zero-point correction (ZPE)=         -1556.84369        0.509130
 Internal Energy (U)=                 -1556.80983        0.542990
 Enthalpy (H)=                        -1556.80889        0.543934
 Gibbs Free Energy (G)=               -1556.91133        0.441494
 Entropy (S)=                                            0.00034359
--------------------------------------------------------------------------------
 Frequencies --  -236.7640               16.4313               20.8758
 Frequencies --    23.3930               30.0799               39.6320

--------------------------------------------------------------------------------
 Analyzing Gaussian Output File: SP_MP2_11+a2_x_080501.out
 Using Gaussian 03:  IA64L-G03RevD.01 13-Oct-2005
 [#Processors=4  Memory=4gb  CheckPoint=SP_MP2_11+a2_x_080501.chk]
================================================================================
 #p mp2/6-31+g(d) scf=(direct,tight) guess=read geom=check
--------------------------------------------------------------------------------
 Pointgroup=C1   Stoichiometry=C19H35AlNO3Si(1+)   C1[X(C19H35AlNO3Si)]
 Charge = 1     Multiplicity = 1
--------------------------------------------------------------------------------
 Standard basis: 6-31+G(d) (6D, 7F)      #Basis: 553
 SCF Energy= -1549.63903947
 MP2 Energy= -1552.9831835728   Correl. Energy= -3.344144107
================================================================================
 No optimization variables found.
```

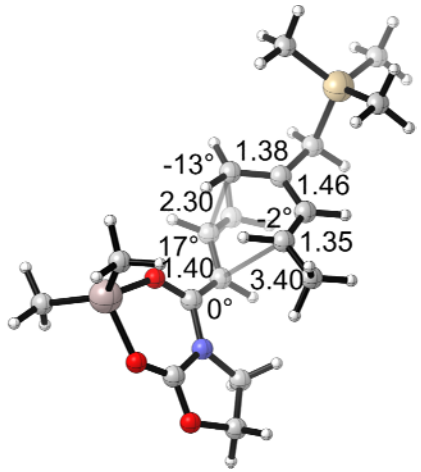
1e+$\mathbf{A_2}$, *endo* TS




```
 ---------------------------------------------------------------------
 Analyzing Gaussian Output File: 12+a2_n_080418.out
 Using Gaussian 03:  AM64L-G03RevC.02 12-Jun-2004
 [#Processors=2  Memory=1800MB  CheckPoint=12+a2_n_080418.chk]
 =====================================================================
 # opt=(gdiis,modredundant) b3lyp/6-31g(d) geom=connectivity
 Modredundant Input:  B    1    6 F
 # b3lyp/6-31g* opt=(calcfc,ts,noeigentest,nofreeze,gdiis) geom=check
 guess=read freq=noraman
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq
 ---------------------------------------------------------------------
 Pointgroup=C1   Stoichiometry=C18H33AlNO3Si(1+)   C1[X(C18H33AlNO3Si)]
 Charge = 1     Multiplicity = 1
 ---------------------------------------------------------------------
 Standard basis: 6-31G(d) (6D, 7F)       #Basis: 434
 SCF Energy= -1518.03820981
 Predicted Change= -4.955717D-09
 =====================================================================
 Optimization completed.     {Found 3 times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force     0.000026 || 0.000450   [ YES ]     0.000003 || 0.000300   [ YES ]
 Displ     0.001542 || 0.001800   [ YES ]     0.000267 || 0.001200   [ YES ]
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        1.802595   -2.000515   -0.817846
    2          6             0        1.819026   -0.858300   -0.046128
    3          6             0        1.083653   -0.758440    1.209932
    4          6             0        0.322439   -1.718472    1.779407
    5          6             0       -1.243015   -1.756254   -1.215634
    6          6             0       -0.153611   -1.786585   -2.082335
    7          1             0        1.148415    0.203748    1.715783
    8          1             0        0.217373   -0.831940   -2.440878
    9          1             0       -1.754063   -2.680467   -0.972436
   10          1             0        0.255131   -2.700522    1.313973
   11          1             0        1.458209   -2.949348   -0.421912
   12          6             0       -1.723404   -0.540455   -0.697071
   13          8             0       -1.155463    0.579440   -0.906477
   14          7             0       -2.919091   -0.552399    0.057517
   15         13             0       -1.619834    2.380207   -0.573554
   16          6             0       -3.751881   -1.740359    0.312501
   17          6             0       -3.559876    0.577804    0.503599
   18          8             0       -3.191749    1.753141    0.373416
   19          6             0       -0.408906    3.139074    0.763606
   20          6             0       -2.215343    3.209581   -2.239132
   21          6             0       -4.846388   -1.155995    1.227918
   22          1             0       -3.173278   -2.520786    0.810463
   23          1             0       -4.150134   -2.130989   -0.628726
   24          8             0       -4.686936    0.285382    1.124181
   25          1             0       -0.808275    4.081901    1.159871
   26          1             0       -0.240246    2.479705    1.624755
   27          1             0        0.574587    3.378135    0.337490
   28          1             0       -2.920345    2.588669   -2.806702
   29          1             0       -2.714717    4.168568   -2.049383
   30          1             0       -1.370624    3.425194   -2.906525
   31          1             0       -4.714436   -1.421991    2.278560
   32          1             0       -5.859795   -1.396506    0.908479
   33          6             0       -0.404169   -1.558006    3.078940
   34          1             0       -0.303897   -0.546567    3.483742
   35          1             0       -1.474545   -1.784517    2.973380
   36          1             0       -0.018824   -2.265745    3.825213
   37          6             0        0.099338   -2.987528   -2.950307
   38          1             0       -0.579887   -2.934882   -3.813620
   39          1             0        1.116801   -3.014637   -3.344883
   40          1             0       -0.105577   -3.927444   -2.428448
   41         14             0        4.382709    0.467724    0.268975
   42          6             0        5.118445    2.058750   -0.431115
   43          1             0        6.142992    2.201765   -0.067291
   44          1             0        5.159839    2.040053   -1.526509
   45          1             0        4.539065    2.940374   -0.132687
   46          6             0        5.371924   -1.039418   -0.291191
   47          1             0        4.936351   -1.977604    0.071270
   48          1             0        5.438749   -1.098934   -1.384229
   49          1             0        6.397308   -0.985386    0.093710
   50          6             0        4.288532    0.546000    2.154077
   51          1             0        5.295879    0.644950    2.576234
   52          1             0        3.706989    1.409483    2.498755
   53          1             0        3.842340   -0.357113    2.586003
   54          6             0        2.587327    0.342355   -0.478946
   55          1             0        2.068356    1.267896   -0.201339
   56          1             0        2.728426    0.348828   -1.566819
   57          1             0        2.448441   -2.061071   -1.687967
 ---------------------------------------------------------------------
 Statistical Thermodynamic Analysis for 12+a2_n_080418.out
 Temperature=   298.150  Kelvin       Pressure=   1.00000  Atm
 =====================================================================
 SCF Energy=                            -1518.03820981
 Zero-point correction (ZPE)=           -1517.55810        0.480101
 Internal Energy (U)=                   -1517.52552        0.512689
 Enthalpy (H)=                          -1517.52457        0.513633
 Gibbs Free Energy (G)=                 -1517.62442        0.413789
 Entropy (S)=                                              0.00033488
 ---------------------------------------------------------------------
 Frequencies --  -175.3272               16.9412               20.7381
 Frequencies --    22.5467               37.9569               40.8774

 ---------------------------------------------------------------------
 Analyzing Gaussian Output File: MP2_12+a2_n_080904.out
 Using Gaussian 03:  IA64L-G03RevD.01 13-Oct-2005
```

```
 [#Processors=2  Memory=1800MB  CheckPoint=MP2_12+a2_n_080904.chk]
================================================================================
 #p mp2/6-31+g(d) scf=tight
--------------------------------------------------------------------------------
 Pointgroup=C1   Stoichiometry=C18H33AlNO3Si(1+)   C1[X(C18H33AlNO3Si)]
 Charge = 1     Multiplicity = 1
--------------------------------------------------------------------------------
 Standard basis: 6-31+G(d) (6D, 7F)      #Basis: 530
 SCF Energy= -1510.61065661
 MP2 Energy= -1513.8106356191   Correl. Energy= -3.199979011
================================================================================
 No optimization variables found.
```

1e+$\mathbf{A_2}$, *exo* TS




```
--------------------------------------------------------------------------------
 Analyzing Gaussian Output File: 12+a2_x_080305.out
 Using Gaussian 03:  AM64L-G03RevC.02 12-Jun-2004
 [#Processors=2  Memory=1800MB  CheckPoint=12+a2_x_080305.chk]
================================================================================
 # opt=(gdiis,modredundant) b3lyp/6-31g(d) geom=connectivity
 Modredundant Input:  B    1    6 F
 # opt=(gdiis,ts,calcfc,noeigentest,nofreeze) freq=noraman b3lyp/6-31g(d)
 geom=check guess=read
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq
--------------------------------------------------------------------------------
 Pointgroup=C1   Stoichiometry=C18H33AlNO3Si(1+)   C1[X(C18H33AlNO3Si)]
 Charge = 1     Multiplicity = 1
--------------------------------------------------------------------------------
 Standard basis: 6-31G(d) (6D, 7F)       #Basis: 434
 SCF Energy= -1518.03819023
 Predicted Change= -9.160034D-10
================================================================================
 Optimization completed.     {Found 3 times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force     0.000003 || 0.000450   [ YES ]     0.000000 || 0.000300   [ YES ]
 Displ     0.001034 || 0.001800   [ YES ]     0.000233 || 0.001200   [ YES ]
--------------------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
--------------------------------------------------------------------------------
    1          6           0        1.590815    1.104319    0.545294
    2          6           0        2.274639   -0.048933    0.217241
    3          6           0        1.727411   -1.037145   -0.706051
    4          6           0        0.605620   -0.912808   -1.448697
    5          6           0       -0.749515   -0.512316    1.643761
```

6	6	0	0.142219	0.414043	2.188668
7	1	0	2.293981	-1.963547	-0.794839
8	1	0	0.042993	0.019001	-1.423875
9	1	0	0.751488	1.452409	-0.046276
10	6	0	0.099695	-1.955914	-2.395584
11	1	0	0.688033	-2.877029	-2.348397
12	1	0	-0.952613	-2.201411	-2.194832
13	1	0	0.128271	-1.582531	-3.428178
14	14	0	5.125325	0.152969	-0.293544
15	6	0	6.656668	-0.350203	0.687356
16	1	0	7.567809	-0.097356	0.132027
17	1	0	6.709036	0.164778	1.653702
18	1	0	6.679944	-1.429121	0.880467
19	6	0	5.072557	2.019310	-0.567706
20	1	0	4.162902	2.333458	-1.092289
21	1	0	5.124545	2.572483	0.377745
22	1	0	5.927102	2.337676	-1.176787
23	6	0	5.048354	-0.770453	-1.939098
24	1	0	5.923695	-0.519140	-2.550310
25	1	0	5.053161	-1.858289	-1.800421
26	1	0	4.158283	-0.507075	-2.521565
27	1	0	-0.157181	1.456963	2.146066
28	6	0	1.068604	0.026925	3.303887
29	1	0	1.883018	0.743539	3.431696
30	1	0	0.497934	0.017279	4.243836
31	1	0	1.492399	-0.971918	3.163611
32	1	0	-0.607665	-1.567094	1.845314
33	6	0	-1.825024	-0.101428	0.843433
34	8	0	-1.994224	1.105128	0.464731
35	7	0	-2.778320	-1.066081	0.440689
36	13	0	-3.318382	2.008549	-0.537674
37	6	0	-2.791582	-2.473165	0.876002
38	6	0	-3.926005	-0.772846	-0.255020
39	8	0	-4.274248	0.327486	-0.703817
40	6	0	-4.356456	3.171096	0.638444
41	6	0	-2.579274	2.431106	-2.299622
42	6	0	-4.022061	-3.018198	0.121575
43	1	0	-2.899757	-2.530469	1.963052
44	1	0	-1.870023	-2.977970	0.578640
45	8	0	-4.683488	-1.841107	-0.416744
46	1	0	-5.275092	3.515475	0.145953
47	1	0	-4.658317	2.683009	1.573873
48	1	0	-3.794003	4.072729	0.913975
49	1	0	-2.067654	1.585003	-2.777443
50	1	0	-3.367501	2.754789	-2.991675
51	1	0	-1.856336	3.255918	-2.247090
52	1	0	-4.738068	-3.529894	0.764058
53	1	0	-3.759421	-3.657045	-0.723687
54	6	0	3.601076	-0.352610	0.818115
55	1	0	3.714414	-1.426283	1.017762
56	1	0	3.745783	0.185136	1.762292
57	1	0	2.080718	1.859670	1.152793

Statistical Thermodynamic Analysis for 12+a2_x_080305.out
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy=	-1518.03819023	
Zero-point correction (ZPE)=	-1517.55811	0.480073
Internal Energy (U)=	-1517.52540	0.512788
Enthalpy (H)=	-1517.52445	0.513733
Gibbs Free Energy (G)=	-1517.62554	0.412643
Entropy (S)=		0.00033906

Frequencies --	-185.6009	15.6794	18.0714
Frequencies --	23.8168	26.0880	37.4570

Analyzing Gaussian Output File: MP2_12+a2_x_080729.out
Using Gaussian 03: AM64L-G03RevC.02 12-Jun-2004
[#Processors=2 Memory=2gB CheckPoint=MP2_12+a2_x_080729.chk]

---

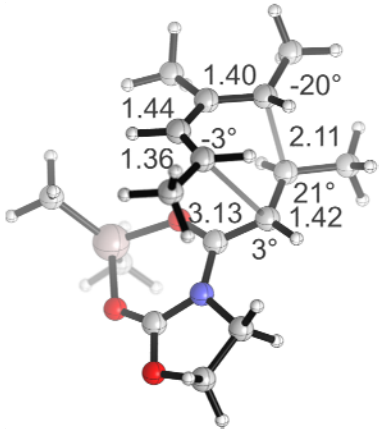
mp2/6-31+g(d) scf=(direct,tight)

Pointgroup=C1 Stoichiometry=C18H33AlNO3Si(1+) C1[X(C18H33AlNO3Si)]
Charge = 1 Multiplicity = 1

Standard basis: 6-31+G(d) (6D, 7F) #Basis: 530
SCF Energy= -1510.60983890
MP2 Energy= -1513.8079453513 Correl. Energy= -3.198106453

No optimization variables found.

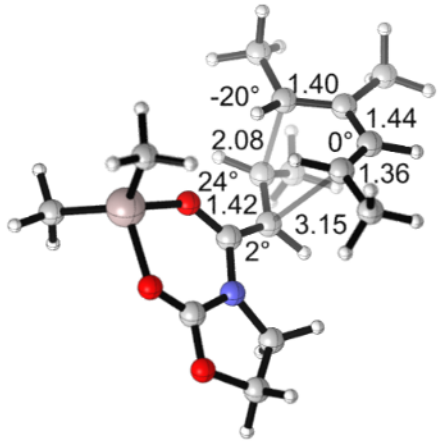
20+$\mathbf{A_2}$, *endo* TS




```
 ---------------------------------------------------------------------------
 Analyzing Gaussian Output File: 9+a2_n_080731.out
 Using Gaussian 03:  AM64L-G03RevC.02 12-Jun-2004
 [#Processors=2  Memory=2gB  CheckPoint=9+a2_n_080731.chk]
 ===========================================================================
 #p opt=(modredundant,gdiis) b3lyp/6-31g(d)
 Modredundant Input:  B    1    6 F
 #p opt=(calcfc,ts,noeigentest,nofreeze,gdiis) b3lyp/6-31g(d) freq=noraman
 geom=check guess=read
 #P Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq
 ---------------------------------------------------------------------------
 Pointgroup=C1   Stoichiometry=C16H27AlNO3(1+)   C1[X(C16H27AlNO3)]
 Charge = 1     Multiplicity = 1
 ---------------------------------------------------------------------------
 Standard basis: 6-31G(d) (6D, 7F)       #Basis: 373
 SCF Energy= -1148.67056846
 Predicted Change= -2.877597D-09
 ===========================================================================
 Optimization completed on the basis of negligible forces.     {Found 3 times}
 Item      Max Val.     Criteria    Pass?      RMS Val.     Criteria    Pass?
 Force     0.000003 || 0.000450   [ YES ]     0.000001 || 0.000300   [ YES ]
 Displ     0.002511 || 0.001800   [ NO ]      0.000371 || 0.001200   [ YES ]
 ---------------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        3.329145   -0.371377    0.038321
    2          6             0        2.611185    0.465474    0.907250
    3          6             0        1.633518   -0.030004    1.834185
    4          6             0        1.294659   -1.332140    2.030545
    5          6             0        0.736871   -1.250056   -1.045496
    6          6             0        1.940433   -0.676628   -1.525523
    7          1             0        1.096336    0.722377    2.408442
    8          1             0        1.886381    0.381548   -1.769149
    9          1             0        0.616699   -2.326342   -1.085486
   10          1             0        1.842475   -2.119726    1.518135
   11          1             0        3.347113   -1.428110    0.292450
   12          6             0       -0.331042   -0.450660   -0.638054
   13          8             0       -0.247649    0.821998   -0.530912
   14          7             0       -1.582928   -1.062073   -0.365683
   15         13             0       -1.492608    2.195412   -0.189703
   16          6             0       -1.888913   -2.485826   -0.582829
   17          6             0       -2.734243   -0.371246   -0.091072
   18          8             0       -2.865138    0.853475    0.049721
   19          6             0       -1.150475    2.982909    1.570932
   20          6             0       -1.875013    3.158451   -1.846683
   21          6             0       -3.348925   -2.562365   -0.094077
   22          1             0       -1.225476   -3.122850    0.005594
   23          1             0       -1.780352   -2.736782   -1.642559
   24          8             0       -3.774626   -1.177550    0.018005
   25          1             0       -2.000195    3.601949    1.887909
   26          1             0       -0.990935    2.241125    2.364574
   27          1             0       -0.276273    3.647554    1.563792
   28          1             0       -2.038309    2.495260   -2.705877
   29          1             0       -2.775191    3.778683   -1.745896
   30          1             0       -1.057864    3.839320   -2.119140
   31          1             0       -3.446839   -3.013825    0.895287
   32          1             0       -4.021028   -3.056349   -0.794969
   33          6             0        0.261971   -1.786384    3.011011
   34          1             0       -0.272466   -0.948468    3.467455
   35          1             0       -0.469744   -2.457672    2.541646
   36          1             0        0.733558   -2.372208    3.812352
   37          6             0        2.765258   -1.519661   -2.474954
   38          1             0        2.193610   -1.644257   -3.403940
   39          1             0        3.711967   -1.052439   -2.744275
   40          1             0        2.962500   -2.519766   -2.074189
   41          6             0        2.833405    1.951750    0.855897
   42          1             0        2.111571    2.495803    1.467906
   43          1             0        3.842040    2.201234    1.213004
   44          1             0        2.770152    2.329849   -0.171914
   45          6             0        4.592600    0.137410   -0.629389
   46          1             0        5.109814   -0.660051   -1.165247
   47          1             0        4.401958    0.956669   -1.331769
   48          1             0        5.289594    0.520362    0.126882
 ---------------------------------------------------------------------------
 Statistical Thermodynamic Analysis for 9+a2_n_080731.out
 Temperature=   298.150  Kelvin       Pressure=   1.00000  Atm
 ===========================================================================
 SCF Energy=                            -1148.67056846
 Zero-point correction (ZPE)=           -1148.26385        0.406716
 Internal Energy (U)=                   -1148.23765        0.432917
 Enthalpy (H)=                          -1148.23670        0.433862
 Gibbs Free Energy (G)=                 -1148.32088        0.349688
 Entropy (S)=                                              0.00028232
 ---------------------------------------------------------------------------
 Frequencies --  -291.3732               19.5708               29.8911
 Frequencies --    41.6013               47.9738               70.3425

 ---------------------------------------------------------------------------
 Analyzing Gaussian Output File: MP2_9+a2_n_080801.out
 Using Gaussian 03:  AM64L-G03RevC.02 12-Jun-2004
 [#Processors=2  Memory=2gB  CheckPoint=MP2_9+a2_n_080801.chk]
 ===========================================================================
 #p mp2/6-31+g(d) scf=(direct,tight)
 ---------------------------------------------------------------------------
 Pointgroup=C1   Stoichiometry=C16H27AlNO3(1+)   C1[X(C16H27AlNO3)]
 Charge = 1     Multiplicity = 1
 ---------------------------------------------------------------------------
```

```
 Standard basis: 6-31+G(d) (6D, 7F)      #Basis: 457
 SCF Energy= -1142.41030825
 MP2 Energy= -1145.2699068846   Correl. Energy= -2.859598631
================================================================================
 No optimization variables found.
```

20+$\mathbf{A_2}$, *exo* TS




```
--------------------------------------------------------------------------------
 Analyzing Gaussian Output File: 9+a2_x_080731.out
 Using Gaussian 03:  AM64L-G03RevC.02 12-Jun-2004
 [#Processors=2  Memory=2gB  CheckPoint=9+a2_x_080731.chk]
================================================================================
 #p opt=(gdiis,modredundant) b3lyp/6-31g(d)
 Modredundant Input:  B    1    6 F
 #p opt=(gdiis,calcfc,ts,noeigentest,nofreeze) b3lyp/6-31g(d) freq=noraman
 guess=read geom=check
 #P Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/6-31G(d) Freq
--------------------------------------------------------------------------------
 Pointgroup=C1   Stoichiometry=C16H27AlNO3(1+)   C1[X(C16H27AlNO3)]
 Charge = 1     Multiplicity = 1
--------------------------------------------------------------------------------
 Standard basis: 6-31G(d) (6D, 7F)       #Basis: 373
 SCF Energy= -1148.67264317
 Predicted Change= -1.445285D-09
================================================================================
 Optimization completed.     {Found 3 times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force     0.000002 || 0.000450   [ YES ]     0.000000 || 0.000300   [ YES ]
 Displ     0.001520 || 0.001800   [ YES ]     0.000227 || 0.001200   [ YES ]
--------------------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
--------------------------------------------------------------------------------
    1          6           0       -2.748072    0.987820    0.149277
    2          6           0       -3.407377   -0.165040    0.600259
    3          6           0       -2.717110   -1.217316    1.295296
    4          6           0       -1.451051   -1.159044    1.788363
    5          6           0       -0.735765   -0.588745   -1.225545
```

```
     6          6             0       -1.774189    0.319090   -1.558856
     7          1             0       -3.270127   -2.145554    1.433992
     8          1             0       -0.903218   -0.220068    1.760475
     9          1             0       -1.789829    1.208484    0.612853
    10          6             0       -3.504687    2.224045   -0.283858
    11          1             0       -3.921728    2.731359    0.595852
    12          1             0       -2.841621    2.938224   -0.781633
    13          1             0       -4.338990    2.006890   -0.956487
    14          6             0       -0.776030   -2.284528    2.502393
    15          1             0       -1.353839   -3.212092    2.460746
    16          1             0        0.224885   -2.470143    2.089514
    17          1             0       -0.618664   -2.021893    3.557831
    18          1             0       -1.448209    1.349627   -1.682317
    19          6             0       -2.826974   -0.134759   -2.540854
    20          1             0       -3.679364    0.547367   -2.584452
    21          1             0       -2.385088   -0.153944   -3.545920
    22          1             0       -3.189401   -1.143854   -2.320889
    23          1             0       -0.869216   -1.642168   -1.438230
    24          6             0        0.469156   -0.144132   -0.685423
    25          8             0        0.661716    1.062939   -0.301545
    26          7             0        1.544252   -1.061767   -0.556565
    27         13             0        2.124133    1.997593    0.436418
    28          6             0        1.551623   -2.425861   -1.111599
    29          6             0        2.803285   -0.719071   -0.132219
    30          8             0        3.181025    0.377985    0.302525
    31          6             0        2.819031    3.275903   -0.866610
    32          6             0        1.767734    2.300210    2.337590
    33          6             0        2.944130   -2.925188   -0.677686
    34          1             0        1.430199   -2.389459   -2.198504
    35          1             0        0.748158   -3.027009   -0.681096
    36          8             0        3.644499   -1.732265   -0.232045
    37          1             0        3.804756    3.654317   -0.566414
    38          1             0        2.932251    2.849932   -1.871733
    39          1             0        2.165120    4.152664   -0.962085
    40          1             0        1.436323    1.399197    2.871194
    41          1             0        2.665566    2.660490    2.856273
    42          1             0        0.995653    3.066282    2.489005
    43          1             0        3.525684   -3.362877   -1.488433
    44          1             0        2.908150   -3.615209    0.167745
    45          6             0       -4.872470   -0.368171    0.322762
    46          1             0       -5.469255    0.317542    0.940292
    47          1             0       -5.132280   -0.148220   -0.718329
    48          1             0       -5.194731   -1.386784    0.552042
---------------------------------------------------------------------------
 Statistical Thermodynamic Analysis for 9+a2_x_080731.out
 Temperature=   298.150  Kelvin       Pressure=   1.00000  Atm
===========================================================================
 SCF Energy=                            -1148.67264317
 Zero-point correction (ZPE)=           -1148.26612        0.406522
 Internal Energy (U)=                   -1148.23972        0.432916
 Enthalpy (H)=                          -1148.23878        0.433861
 Gibbs Free Energy (G)=                 -1148.32417        0.348468
 Entropy (S)=                                              0.00028641
---------------------------------------------------------------------------
 Frequencies --  -283.3083               18.8924               28.3043
 Frequencies --    32.9051               42.2947               60.3825

---------------------------------------------------------------------------
 Analyzing Gaussian Output File: MP2_9+a2_x_080801.out
 Using Gaussian 03:  AM64L-G03RevC.02 12-Jun-2004
 [#Processors=2  Memory=2gB  CheckPoint=MP2_9+a2_x_080801.chk]
===========================================================================
 #p mp2/6-31+g(d) scf=(direct,tight)
---------------------------------------------------------------------------
 Pointgroup=C1   Stoichiometry=C16H27AlNO3(1+)   C1[X(C16H27AlNO3)]
 Charge = 1     Multiplicity = 1
---------------------------------------------------------------------------
 Standard basis: 6-31+G(d) (6D, 7F)      #Basis: 457
 SCF Energy= -1142.41296580
 MP2 Energy= -1145.2692547061   Correl. Energy= -2.856288908
===========================================================================
 No optimization variables found.
```