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Electronic supplementary information

Synthetic and Computational Studies of Acyl Radical Cyclizations with β-Alkoxyacrylates : Formal Synthesis of (±)-Longianone

Heather M. Aitken,[a,b] Carl H. Schiesser*[a,b] and Christopher D. Donner*[a,b]

[a] School of Chemistry, The University of Melbourne, Victoria 3010, Australia
[b] Bio21 Molecular Science and Biotechnology Institute, The University of Melbourne, Victoria 3010, Australia

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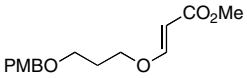
1.1 GENERAL EXPERIMENTAL DETAILS

^{1}H and ^{13}C NMR spectra were recorded using a Varian-500 spectrometer operating at 500 MHz and 125 MHz, respectively. Chemical shifts are given using residual $CHCl_3$ (δ=7.26 for ^{1}H and 77.0 for ^{13}C) as internal standard. Infrared (IR) spectra were recorded on a Perkin-Elmer Spectrum One FT-IR spectrometer. Gas chromatography-mass spectrometry (GCMS) spectra were recorded on an Agilent 7890A GC system using a HP-5MS column (30 m, i.d. 0.25 mm, film thickness 0.25 μm) and 5975C MS system (EI, 70 eV). GC heat programs - Method 1: $100_5 \rightarrow 250_5$, heating rate 5 °C min^{-1}, Method 2: $100_5 \rightarrow 250_{30}$, heating rate 10 °C min^{-1}. The retention time (R_t) and selected fragment ions as their mass/charge ratio (*m/z*) are reported. High resolution ESI mass spectra (HRMS) were recorded on a Thermo-Finnigan LTQ-FT ICR hybrid mass spectrometer. All moisture sensitive reactions were performed under a dry nitrogen or argon atmosphere in oven-dried or flame-dried glassware. Anhydrous dichloromethane was pre-dried over activated alumina under argon. Thin layer chromatography was performed on pre-coated silica plates (Merck $60GF_{254}$) and compounds were visualised at 254 nm and 365 nm or stained with either phosphomolybdic acid or potassium permanganate solutions. Flash column chromatography was performed on silica gel (Kieselgel 60, 230-400 mesh) using the indicated solvent system.

1.2 EXPERIMENTAL PROCEDURES

1.2.1 : Monosubstituted β-alkoxyacrylate :

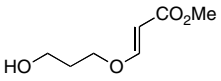
(*E*)-Methyl 3-(3-(4-methoxybenzyloxy)propoxy)acrylate (11)



To a solution of alcohol **10**[S1] (1.00 g, 5.1 mmol) and trimethylphosphine (1 M in THF, 1.02 mL) in dichloromethane (25 mL) at 0 °C was added methyl propiolate (0.47 g, 5.6 mmol) dropwise over 15 min and stirring was continued for a further 30 min. Saturated NH_4Cl (20 mL) was added and the mixture extracted with ethyl acetate (3×15 mL) and the combined organic layers were washed with brine (2×15 mL), dried ($MgSO_4$) and concentrated *in vacuo*. Flash column chromatography (ethyl acetate:petrol 1:2) gave the (*E*)-acrylate **11** (1.40 mg, 98%) as a colourless oil.
HRMS (ESI) found 281.1384, $C_{15}H_{21}O_5$ $[M+H]^+$ requires 281.1384; ^{1}H NMR ($CDCl_3$, 500 MHz) δ 1.97 (2H, m), 3.53 (2H, t, *J* 6.0 Hz), 3.70 (3H, s), 3.80 (3H, s), 3.95 (2H, t, *J* 6.2 Hz), 4.43 (2H, s), 5.22 (1H, d, *J* 12.7 Hz), 6.88 (2H, d, *J* 8.5 Hz), 7.24 (2H, d, *J* 8.5 Hz), 7.58 (1H, d, *J* 12.7 Hz); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 29.3 (CH_2), 51.0, 55.2 (CH_3), 65.7, 68.1, 72.7 (CH_2), 96.1, 113.8, 129.2 (CH), 130.3, 159.2 (C), 162.6 (CH), 168.2 (C); ν_{max}/cm^{-1} 2951, 1708, 1623, 1512, 1244, 1136, 1096, 1032; GCMS (Method 1, R_t = 29.80 min) *m/z* 280.1 ($[M]^+$, 1%), 177.1 (25), 121.1 (100).

[S1] T. Ueno, M. Oikawa, H. Oikawa, A. Ichihara, *Biosci. Biotech. Biochem*. **1995**, *59*, 2104.

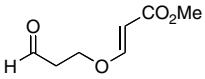
(*E*)-Methyl 3-(3-hydroxypropoxy)acrylate (12)



To a solution of PMB ether **11** (1.40 g, 4.99 mmol) in a mixture of dichloromethane:water (20:1, 31.5 mL) cooled to 0 °C was added DDQ (1.47 g, 6.49 mmol) and the solution was stirred rapidly for 3 h. Saturated $NaHCO_3$ (30 mL) was added and the mixture was extracted with chloroform (3×10 mL). The combined organic layers were washed with saturated $NaHCO_3$ (15 mL), dried ($MgSO_4$) and concentrated *in vacuo*. Flash column chromatography (ethyl acetate:petrol 1:1) gave the alcohol **12** (0.60 g, 75%) as a colourless oil.

HRMS (ESI) found 161.0808, $C_7H_{13}O_4$ $[M+H]^+$ requires 161.0808; ^{1}H NMR ($CDCl_3$, 500 MHz) δ 1.93 (2H, m), 2.13 (1H, brs), 3.67 (3H, s), 3.74 (2H, t, *J* 6.0 Hz), 3.97 (2H, t, *J* 6.1 Hz), 5.20 (1H, d, *J* 12.6 Hz), 7.57 (1H, d, *J* 12.6 Hz); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 31.6 (CH_2), 51.1 (CH_3), 59.0, 68.0 (CH_2), 96.2, 162.5 (CH), 168.3 (C); ν_{max}/cm^{-1} 3424, 2953, 1693, 1620, 1134, 1045; GCMS (Method 1, R_t = 12.00 min) *m/z* 160.1 ($[M]^+$, 5%), 129.1 (28), 102.0 (31), 87.0 (28), 71.0 (100), 59.1 (32).

(*E*)-Methyl 3-(3-oxopropoxy)acrylate (13)

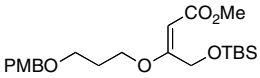


To a solution of alcohol **12** (575 mg, 3.59 mmol) in CH_2Cl_2 (5 mL) was added $PhI(OAc)_2$ (1.39 g, 4.31 mmol) and TEMPO (56 mg, 0.36 mmol) and the mixture was stirred at ambient temperature for 4 h. After removal of the solvent *in vacuo* the remaining residue was purified by flash column chromatography (ethyl acetate:petrol 1:2) to give aldehyde **13** (407 mg, 72%) as a colourless oil.

HRMS (ESI) found 159.0656, $C_7H_{11}O_4$ $[M+H]^+$ requires 159.0652; ^{1}H NMR ($CDCl_3$, 500 MHz) δ 2.87 (2H, td, *J* 6.1 and 1.2 Hz), 3.71 (3H, s), 4.17 (2H, t, *J* 6.1 Hz), 5.24 (1H, d, *J* 12.7 Hz), 7.57 (1H, d, *J* 12.7 Hz), 9.81 (1H, t, *J* 1.2 Hz); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 42.5 (CH_2), 51.1 (CH_3), 64.0 (CH_2), 96.7, 161.8 (CH), 167.8 (C), 198.7 (CH); ν_{max}/cm^{-1} 2953, 1704, 1621, 1133, 1044; GCMS (Method 1, R_t = 9.99 min) *m/z* 158.1 ($[M]^+$, 2%), 127.0 (37), 102.0 (64), 71.0 (100), 57.0 (21).

1.2.2 : Disubstituted β-alkoxyacrylates :

(*E*)-Methyl 4-(*tert*-butyldimethylsilyloxy)-3-(3-(4-methoxybenzyloxy)propoxy)but-2-enoate (16)



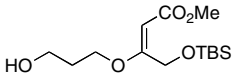
To a solution of alcohol **10**[S1] (2.33 g, 11.9 mmol) and trimethylphosphine (1 M in THF, 3.6 mL) in dichloromethane (60 mL) at 0 °C was added acetylene **15**[S2] (3.25 g, 14.2 mmol) in dichloromethane (20 mL) dropwise over 20 min. The solution was allowed to warm to ambient temperature over 30 min and stirred for a further 1 h. Saturated NH_4Cl (75 mL) was added and the mixture extracted with ethyl acetate (3×50 mL) and the combined organic layers were washed with brine (50 mL), dried ($MgSO_4$) and concentrated *in vacuo*. Flash column chromatography (ethyl acetate:petrol 1:9) gave the (*E*)-acrylate **16** (4.57 g, 91%) as a colourless oil.

[S1] T. Ueno, M. Oikawa, H. Oikawa, A. Ichihara, *Biosci. Biotech. Biochem.* **1995**, *59*, 2104.

[S2] A. T. Koppisch, B. S. J. Blagg, C. D. Poulter, *Org. Lett.* **2000**, *2*, 215.

HRMS (ESI) found 425.2349, $C_{22}H_{37}O_6Si$ $[M+H]^+$ requires 425.2354; ^1H NMR ($CDCl_3$, 500 MHz) δ 0.07 (6H, s), 0.90 (9H, s), 2.03 (2H, m), 3.58 (2H, t, *J* 6.1 Hz), 3.67 (3H, s), 3.80 (3H, s), 3.89 (2H, t, *J* 6.3 Hz), 4.42 (2H, s), 4.80 (2H, s), 5.01 (1H, s), 6.87 (2H, d, *J* 8.8 Hz), 7.24 (2H, d, *J* 8.8 Hz); ^{13}C NMR ($CDCl_3$, 125 MHz) δ –5.3 (CH_3), 18.4 (C), 25.8 (CH_3), 29.1 (CH_2), 50.8, 55.2 (CH_3), 60.5, 65.5, 66.1, 72.7 (CH_2), 91.0, 113.8, 129.2 (CH), 130.3, 159.2, 167.5, 172.3 (C); ν_{max}/cm^{-1} 2930, 1713, 1627, 1613, 1513, 1247, 1142, 1092, 1048; GCMS (Method 1, R_t = 38.25 min) *m/z* 424.3 ($[M]^+$, 1%), 367.2 (16), 121.1 (100).

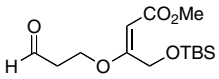
(*E*)-Methyl 4-(*tert*-butyldimethylsilyloxy)-3-(3-hydroxypropoxy)but-2-enoate (17)



To a solution of PMB ether **16** (4.30 g, 10.1 mmol) in a mixture of dichloromethane:water (20:1, 105 mL) cooled to 0 °C was added DDQ (3.00 g, 13.2 mmol) and the solution was stirred rapidly for 3 h. Saturated $NaHCO_3$ (100 mL) was added and the mixture was extracted with chloroform (3×20 mL). The combined organic layers were washed with saturated $NaHCO_3$ (30 mL), dried ($MgSO_4$) and concentrated *in vacuo*. Flash column chromatography (ethyl acetate:petrol 1:4) gave the alcohol **17** (3.01 g, 98%) as a colourless oil.

HRMS (ESI) found 305.1779, $C_{14}H_{29}O_5Si$ $[M+H]^+$ requires 305.1779; ^1H NMR ($CDCl_3$, 500 MHz) δ 0.10 (6H, s), 0.91 (9H, s), 2.01 (2H, m), 3.67 (3H, s), 3.82 (2H, t, *J* 5.6 Hz), 3.97 (2H, t, *J* 5.9 Hz), 4.83 (2H, s), 5.04 (1H, s); ^{13}C NMR ($CDCl_3$, 125 MHz) δ –5.4 (CH_3), 18.4 (C), 25.9 (CH_3), 31.2 (CH_2), 50.9 (CH_3), 60.5, 60.6, 67.1 (CH_2), 91.1 (CH), 167.4, 171.9 (C); ν_{max}/cm^{-1} 3459, 2930, 1714, 1626, 1143, 1048; GCMS (Method 1, R_t = 24.12 min) *m/z* 304.1 ($[M]^+$, 1%), 247.1 (93), 215.1 (39), 189.1 (61), 157.0 (100), 129.0 (37), 89.1 (23), 75.1 (48), 73.1 (29).

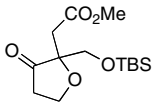
(*E*)-Methyl 4-(*tert*-butyldimethylsilyloxy)-3-(3-oxopropoxy)but-2-enoate (18)



To a solution of alcohol **17** (550 mg, 1.81 mmol) in CH_2Cl_2 (4 mL) was added $PhI(OAc)_2$ (698 mg, 2.17 mmol) and TEMPO (28 mg, 0.18 mmol) and the mixture was stirred at ambient temperature for 4 h. After removal of the solvent *in vacuo* the remaining residue was purified by flash column chromatography (ethyl acetate:petrol 1:4) to give aldehyde **18** (380 mg, 70%) as a colourless oil.

HRMS (ESI) found: 303.1622, $C_{14}H_{27}O_5Si$ $[M+H]^+$ requires 303.1622; ^1H NMR ($CDCl_3$, 500 MHz) δ 0.06 (6H, s), 0.89 (9H, s), 2.90 (2H, td, *J* 6.1 and 1.2 Hz), 3.68 (3H, s), 4.13 (2H, t, *J* 6.1 Hz), 4.80 (2H, s), 5.06 (1H, s), 9.82 (1H, t, *J* 1.2 Hz); ^{13}C NMR ($CDCl_3$, 125 MHz) δ –5.3 (CH_3), 18.3 (C), 25.8 (CH_3), 42.4 (CH_2), 51.0 (CH_3), 60.3, 61.9 (CH_2), 91.8 (CH), 167.1, 171.7 (C), 198.9 (CH); ν_{max}/cm^{-1} 2930, 1714, 1628, 1142, 1104, 1049; GCMS (Method 1, R_t = 22.88 min) *m/z* 302.1 ($[M]^+$, 1%), 245.1 (63), 189.1 (50), 157.0 (38), 129.0 (100), 89.1 (42), 75.1 (28), 73.1 (36).

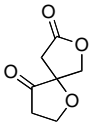
Methyl 2-(2-((*tert*-butyldimethylsilyloxy)methyl)-3-oxo-tetrahydrofuran-2-yl)acetate (19)



A solution of aldehyde **18** (750 mg, 2.48 mmol), *tert*-dodecanethiol (175 μL, 0.74 mmol) and 1,1'-azobis(cyclohexanecarbonitrile) (182 mg, 0.74 mmol) in toluene (5 mL) was flushed with argon for 30 min. The solution was then heated at reflux for

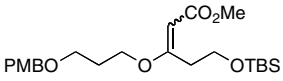
15 h. After removal of the solvent *in vacuo* flash column chromatography (ethyl acetate:petrol 1:4) gave tetrahydrofuranone **19** (210 mg, 28%) as a colourless oil.
HRMS (ESI) found 303.1621, $C_{14}H_{27}O_5Si$ $[M+H]^+$ requires 303.1622; ^{1}H NMR ($CDCl_3$, 500 MHz) δ 0.02 (3H, s), 0.04 (3H, s), 0.86 (9H, s), 2.50 (1H, ddd, *J* 18.1, 8.7 and 5.6 Hz), 2.57 (1H, d, *J* 16.5 Hz), 2.71 (1H, d, *J* 16.5 Hz), 2.79 (1H, ddd, *J* 18.1, 9.2 and 7.0 Hz), 3.58 (1H, d, *J* 10.1 Hz), 3.65 (3H, s), 3.70 (1H, d, *J* 10.1 Hz), 4.31 (1H, m), 4.34 (1H, m); ^{13}C NMR ($CDCl_3$, 125 MHz) δ –5.8, –5.6 (CH_3), 18.1 (C), 25.7 (CH_3), 36.6, 38.5 (CH_2), 51.9 (CH_3), 65.1, 68.0 (CH_2), 82.3, 170.2, 216.1 (C); ν_{max}/cm^{-1} 2930, 1741, 1254, 1135, 1078; GCMS (Method 1, R_t = 20.49 min) *m/z* 287.1 ($[M–15]^+$, 1%), 271.1 (30), 245.1 (81), 227.1 (31), 215.1 (34), 171.0 (100), 153.0 (31), 129.0 (66), 89.0 (69), 73.1 (56), 59.0 (23).

1,7-dioxaspiro[4,4]nonane-4,8-dione (dihydrolongianone) (20)



To the TBS ether **19** (200 mg, 0.69 mmol) in chloroform (5 mL) and methanol (3 mL) was added 10-CSA (113 mg, 0.49 mmol) and the mixture was stirred at ambient temperature for 24 h. After removal of the solvent *in vacuo*, the remaining residue was resuspended in chloroform (5 mL) and stirring was continued for 21 h. Saturated $NaHCO_3$ (10 mL) was added and the mixture was extracted with chloroform (3×5 mL), the combined organic layers dried ($MgSO_4$) and concentrated *in vacuo*. Flash column chromatography (ethyl acetate:petrol 1:1) gave dihydrolongianone **20** (63 mg, 61%) as a colourless oil.
HRMS (ESI) found 157.0495, $C_7H_9O_4$ $[M+H]^+$ requires 157.0495; ^{1}H NMR ($CDCl_3$, 500 MHz) δ 2.63 (1H, dd, *J* 17.9 and 0.9 Hz), 2.64 (2H, m), 2.79 (1H, d, *J* 17.9 Hz), 4.22 (1H, m), 4.27 (1H, m), 4.31 (1H, d, *J* 10.1 Hz), 4.34 (1H, dd, *J* 10.1 and 0.9 Hz); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 35.8, 37.6, 63.2, 74.2 (CH_2), 84.2, 173.1, 211.9 (C); ν_{max}/cm^{-1} 2927, 1777, 1754, 1158, 1029, 1012; GCMS (Method 1, R_t = 12.35 min) *m/z* 156.1 ($[M]^+$, 7%), 126.0 (84), 100.0 (26), 98.0 (100).

(*E*)-Methyl 5-(*tert*-butyldimethylsilyloxy)-3-(3-(4-methoxybenzyloxy)propoxy)pent-2-enoate (22) and (*Z*)-methyl 5-(*tert*-butyldimethylsilyloxy)-3-(3-(4-methoxybenzyloxy)propoxy)pent-2-enoate



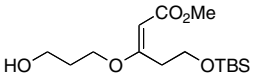
To a solution of alcohol **10**[S1] (0.88 g, 4.47 mmol) and trimethylphosphine (1 M in THF, 1.34 mL) in dichloromethane (25 mL) at 0 °C was added acetylene **21**[S3] (1.30 g, 5.37 mmol) in dichloromethane (5 mL) dropwise over 10 min. The solution was allowed to warm to ambient temperature over 30 min and stirred for a further 2.5 h. Saturated NH_4Cl (30 mL) was added and the mixture extracted with ethyl acetate (3×15 mL) and the combined organic layers were washed with brine (25 mL), dried ($MgSO_4$) and concentrated *in vacuo*. Flash column chromatography (gradient elution, ethyl acetate:petrol 1:9 to 1:2) gave the (*E*)-acrylate **22** (1.65 g, 84%) as a colourless oil and the (*Z*)-acrylate (110 mg, 6%) as a colourless oil.

[S1] T. Ueno, M. Oikawa, H. Oikawa, A. Ichihara, *Biosci. Biotech. Biochem.* **1995**, *59*, 2104.

[S3] Acetylene **21** was prepared from the corresponding terminal acetylene (*n*-BuLi, THF, -78 °C, $ClCO_2Me$). The spectroscopic data was in accord with material prepared by TBS protection of methyl 5-hydroxy-2-pentynoate (E. Piers, J. M. Chong, H. E. Morton, *Tetrahedron* **1989**, *45*, 363).

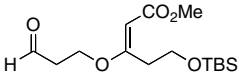
*Data for (*E*)-isomer:*
Found: $[M+H]^+$ 439.2510, $C_{23}H_{39}O_6Si$ requires $[M+H]^+$ 439.2510; ^{1}H NMR ($CDCl_3$, 500 MHz) δ 0.04 (6H, s), 0.87 (9H, s), 1.98 (2H, m), 2.97 (2H, t, *J* 6.9 Hz), 3.54 (2H, t, *J* 6.2 Hz), 3.66 (3H, s), 3.79 (2H, t, *J* 6.9 Hz), 3.80 (3H, s), 3.83 (2H, t, *J* 6.2 Hz), 4.42 (2H, s), 5.03 (1H, s), 6.87 (2H, d, *J* 8.8 Hz), 7.24 (2H, d, *J* 8.8 Hz); ^{13}C NMR ($CDCl_3$, 125 MHz) δ –5.4 (CH_3), 18.2 (C), 25.9 (CH_3), 29.1, 35.9 (CH_2), 50.7, 55.2 (CH_3), 61.0, 65.1, 66.2, 72.7 (CH_2), 91.8, 113.8, 129.2 (CH), 130.3, 159.2, 167.9, 172.8 (C); ν_{max}/cm^{-1} 2951, 1714, 1615, 1513, 1247, 1140, 1094, 1054, 1037; GCMS (Method 2, R_t = 29.16 min) *m/z* 381.2 ($[M–57]^+$, 41%), 121.1 (100).
*Data for (*Z*)-isomer:*
^{1}H NMR ($CDCl_3$, 500 MHz) δ 0.05 (6H, s), 0.88 (9H, s), 1.98 (2H, m), 2.44 (2H, t, *J* 6.8 Hz), 3.62 (2H, t, *J* 6.2 Hz), 3.64 (3H, s), 3.76 (2H, t, *J* 6.8 Hz), 3.80 (3H, s), 4.16 (2H, t, *J* 6.2 Hz), 4.44 (2H, s), 4.96 (1H, s), 6.87 (2H, d, *J* 8.8 Hz), 7.24 (2H, d, *J* 8.8 Hz); ^{13}C NMR ($CDCl_3$, 125 MHz) δ –5.4, 18.2, 25.8, 30.2, 37.2, 50.6, 55.2, 60.9, 66.2, 67.2, 72.7, 97.0, 113.8, 129.2, 130.6, 159.2, 165.7, 168.4; ν_{max}/cm^{-1} 2952, 1716, 1615, 1513, 1247, 1198, 1094, 1057, 1035; GCMS (Method 2, R_t = 29.04 min) *m/z* 381.1 ($[M–57]^+$, 32%), 316.1 (42), 284.1 (20), 121.1 (100).

(*E*)-Methyl 5-(*tert*-butyldimethylsilyloxy)-3-(3-hydroxypropoxy)pent-2-enoate (23)



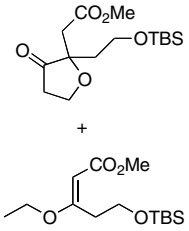
To a solution of PMB ether **22** (1.50 g, 3.42 mmol) in a mixture of dichloromethane:water (20:1, 31.5 mL) cooled to 0 °C was added DDQ (1.01 g, 4.45 mmol) and the solution was stirred rapidly for 2 h. Saturated $NaHCO_3$ (40 mL) was added and the mixture was extracted with chloroform (3×20 mL). The combined organic layers were washed with saturated $NaHCO_3$ (20 mL), dried ($MgSO_4$) and concentrated *in vacuo*. Flash column chromatography (ethyl acetate:petrol 1:4) gave the alcohol **23** (1.04 g, 95%) as a colourless oil.
Found: $[M+H]^+$ 319.1934, $C_{15}H_{31}O_5Si$ requires $[M+H]^+$ 319.1935; ^{1}H NMR ($CDCl_3$, 500 MHz) δ 0.05 (6H, s), 0.87 (9H, s), 1.97 (2H, m), 3.00 (2H, t, *J* 6.7 Hz), 3.66 (3H, s), 3.79 (2H, m), 3.83 (2H, t, *J* 6.7 Hz), 3.90 (2H, t, *J* 6.0 Hz), 5.07 (1H, s); ^{13}C NMR ($CDCl_3$, 125 MHz) δ –5.4 (CH_3), 18.2 (C), 25.8 (CH_3), 31.4, 35.7 (CH_2), 50.7 (CH_3), 59.7, 61.0, 65.6 (CH_2), 92.0 (CH), 167.8, 172.9 (C); ν_{max}/cm^{-1} 3444, 2952, 1715, 1616, 1140, 1098, 1074, 1051; GCMS (Method 1, R_t = 25.98 min) *m/z* 303.1 ($[M–15]^+$, 2%), 261.1 (100), 229.1 (20), 170.9 (88), 75.0 (21).

(*E*)-Methyl 5-(*tert*-butyldimethylsilyloxy)-3-(3-oxopropoxy)pent-2-enoate (24)



To a solution of alcohol **23** (1.00 g, 3.14 mmol) in CH_2Cl_2 (6 mL) was added $PhI(OAc)_2$ (1.21 g, 3.76 mmol) and TEMPO (50 mg, 0.31 mmol) and the mixture was stirred at ambient temperature for 2 h. After removal of the solvent *in vacuo* the remaining residue was purified by flash column chromatography (ethyl acetate:petrol 1:4) to give aldehyde **24** (0.76 g, 77%) as a colourless oil.
Found: $[M+H]^+$ 317.1778, $C_{15}H_{29}O_5Si$ requires $[M+H]^+$ 317.1778; ^{1}H NMR ($CDCl_3$, 500 MHz) δ 0.03 (6H, s), 0.87 (9H, s), 2.85 (2H, td, *J* 6.1 and 1.4 Hz), 2.97 (2H, t, *J* 6.8 Hz), 3.67 (3H, s), 3.78 (2H, t, *J* 6.8 Hz), 4.08 (2H, t, *J* 6.1 Hz), 5.08 (1H, s), 9.80 (1H, t, *J* 1.4 Hz); ^{13}C NMR ($CDCl_3$, 125 MHz) δ –5.4 (CH_3), 18.2 (C), 25.8 (CH_3), 35.6, 42.5 (CH_2), 50.8 (CH_3), 60.8, 61.5 (CH_2), 92.5 (CH), 167.5, 172.4 (C), 199.0 (CH); ν_{max}/cm^{-1} 2952, 1715, 1620, 1139, 1096, 1078, 1054; GCMS (Method 1, R_t = 24.66 min) *m/z* 301.1 ($[M–15]^+$, 1%), 259.1 (100), 229.1 (31), 203.1 (49), 173.1 (66), 171.1 (78), 143.0 (64), 89.0 (68), 75.0 (57).

Methyl 2-(2-(2-(*tert*-butyldimethylsilyloxy)ethyl)-3-oxo-tetrahydrofuran-2-yl)acetate (26) and (*E*)-Methyl 5-(*tert*-butyldimethylsilyloxy)-3-ethoxypent-2-enoate (25)



A solution of aldehyde **24** (50 mg, 0.16 mmol), *tert*-dodecanethiol (11 μL, 0.05 mmol) and 1,1'-azobis(cyclohexanecarbonitrile) (12 mg, 0.05 mmol) in toluene (1 mL) was flushed with argon for 30 min. The solution was then heated at reflux for 21 h with a further portion of initiator (12 mg) added after 6 h. After removal of the solvent *in vacuo* flash column chromatography (ethyl acetate:petrol 1:9) gave tetrahydrofuranone **26** (18 mg, 36%) as a colourless oil and the enol-ether **25** (19 mg, 42%) as a colourless oil.

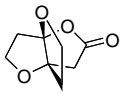
Furan data:

Found: $[M+H]^+$ 317.1777, $C_{15}H_{29}O_5Si$ requires $[M+H]^+$ 317.1779; ^{1}H NMR ($CDCl_3$, 500 MHz) δ 0.03 (3H, s), 0.04 (3H, s), 0.87 (9H, s), 1.70 (1H, dt, *J* 14.2 and 4.4 Hz), 1.91 (1H, ddd, *J* 14.2, 9.1 and 5.5 Hz), 2.63 (1H, ddd, *J* 17.9, 8.6 and 5.7 Hz), 2.72 (1H, d, *J* 16.4 Hz), 2.77 (1H, ddd, *J* 17.9, 9.2 and 7.1 Hz), 2.82 (1H, d, *J* 16.4 Hz), 3.65 (3H, s), 3.67 (1H, ddd, *J* 10.6, 5.5 and 4.4 Hz), 3.79 (1H, ddd, *J* 10.6, 9.1 and 4.4 Hz), 4.21 (1H, m), 4.28 (1H, m); ^{13}C NMR ($CDCl_3$, 125 MHz) δ –5.6, –5.5 (CH_3), 18.3 (C), 25.8 (CH_3), 35.7, 39.9, 42.7 (CH_2), 51.7 (CH_3), 58.1, 64.2 (CH_2), 79.7, 170.5, 216.0 (C); ν_{max}/cm^{-1} 2929, 1742, 1253, 1130, 1088; GCMS (Method 1, R_t = 23.13 min) *m/z* 301.1 ($[M-15]^+$, 1%), 285.1 (20), 259.1 (47), 185.0 (100), 167.1 (21), 89.0 (43), 75.0 (23).

Enol-ether data:

Spectroscopic and physical data (^{1}H and ^{13}C NMR, GCMS) were identical to authentic material prepared directly from acetylene **21**.

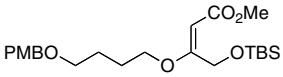
propellane (29)



To the TBS ether **26** (58 mg, 0.18 mmol) in chloroform (3 mL) and methanol (2 mL) was added 10-CSA (30 mg, 0.13 mmol) and the mixture was stirred at ambient temperature for 4 h. After removal of the solvent *in vacuo*, the remaining residue was resuspended in chloroform (3 mL) and stirring was continued for 16 h. Removal of the solvent *in vacuo* and flash column chromatography (ethyl acetate:petrol 1:1) gave the propellane **29** (22 mg, 71%) as a colourless oil.

HRMS (ESI) found 171.0653, $C_8H_{11}O_4$ $[M+H]^+$ requires 171.0652; ^{1}H NMR ($CDCl_3$, 500 MHz) δ 2.14 (1H, ddd, *J* 12.9, 5.1 and 1.7 Hz), 2.18-2.30 (2H, m), 2.41 (1H, ddd, *J* 13.2, 5.9 and 3.6 Hz), 2.89 (1H, dd, *J* 19.1 and 0.4 Hz), 3.07 (1H, dd, *J* 19.1 and 1.4 Hz), 3.94-4.02 (2H, m), 4.13 (1H, ddd, *J* 9.6, 7.6 and 3.6 Hz), 4.23 (1H, ddd, *J* 9.7, 8.1 and 1.7 Hz); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 37.3, 37.8, 42.2, 68.2, 70.0 (CH_2), 92.5, 124.1, 173.6 (C); ν_{max}/cm^{-1} 2933, 1785, 1106, 1093, 988, 960; GCMS (Method 1, R_t = 12.15 min) *m/z* 142.0 ($[M-28]^+$, 100%), 112.0 (55), 96.0 (38), 55.0 (30).

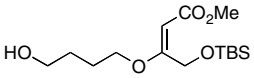
(*E*)-Methyl 4-(*tert*-butyldimethylsilyloxy)-3-(4-(4-methoxybenzyloxy)butoxy)but-2-enoate (30)



To a solution of 4-(4-methoxybenzyloxy)butan-1-ol[S4] (0.88 g, 4.18 mmol) and trimethylphosphine (1 M in THF, 1.26 mL) in dichloromethane (25 mL) at 0 °C was added acetylene **15**[S2] (1.15 g, 5.02 mmol) in dichloromethane (5 mL) dropwise over 15 min. The solution was allowed to warm to ambient temperature over 30 min and stirred for a further 30 min. Saturated NH_4Cl (50 mL) was added and the mixture extracted with ethyl acetate (3×20 mL) and the combined organic layers were washed with brine (50 mL), dried ($MgSO_4$) and concentrated *in vacuo*. Flash column chromatography (ethyl acetate:petrol 1:9) gave the (*E*)-acrylate **30** (1.60 g, 87%) as a colourless oil.

HRMS (ESI) found 461.2329, $C_{23}H_{38}O_6SiNa$ $[M+Na]^+$ requires 461.2330; ^1H NMR ($CDCl_3$, 500 MHz) δ 0.08 (6H, s), 0.90 (9H, s), 1.73 (2H, m), 1.85 (2H, m), 3.48 (2H, t, *J* 6.3 Hz), 3.67 (3H, s), 3.79 (2H, t, *J* 6.5 Hz), 3.80 (3H, s), 4.43 (2H, s), 4.81 (2H, s), 4.98 (1H, s), 6.88 (2H, d, *J* 8.4 Hz), 7.25 (2H, d, *J* 8.4 Hz); ^{13}C NMR ($CDCl_3$, 125 MHz) δ –5.3 (CH_3), 18.4 (C), 25.5 (CH_2), 25.8 (CH_3), 26.1 (CH_2), 50.9, 55.2 (CH_3), 60.6, 68.2, 69.3, 72.5 (CH_2), 90.9, 113.8, 129.2 (CH), 130.6, 159.1, 167.5, 172.5 (C); ν_{max}/cm^{-1} 2930, 1713, 1615, 1513, 1246, 1142, 1094, 1048; GCMS (Method 1, R_t = 29.26 min) *m/z* 381.1 ($[M-57]^+$, 2%), 121.1 (100).

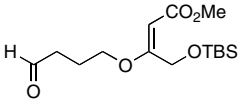
(*E*)-Methyl 4-(*tert*-butyldimethylsilyloxy)-3-(4-hydroxybutoxy)but-2-enoate (31)



To a solution of PMB ether **30** (1.50 g, 3.42 mmol) in a mixture of dichloromethane:water (20:1, 31.5 mL) cooled to 0 °C was added DDQ (1.01 g, 4.45 mmol) and the solution was stirred rapidly for 2 h. Saturated $NaHCO_3$ (40 mL) was added and the mixture was extracted with chloroform (3×20 mL). The combined organic layers were washed with saturated $NaHCO_3$ (20 mL), dried ($MgSO_4$) and concentrated *in vacuo*. Flash column chromatography (ethyl acetate:petrol 1:4) gave the alcohol **31** (1.05 g, 96%) as a colourless oil.

HRMS (ESI) found 319.1935, $C_{15}H_{31}O_5Si$ $[M+H]^+$ requires 319.1935; ^1H NMR ($CDCl_3$, 500 MHz) δ 0.09 (6H, s), 0.91 (9H, s), 1.63 (1H, brm), 1.71 (2H, m), 1.87 (2H, m), 3.67 (3H, s), 3.69 (2H, m), 3.84 (2H, t, *J* 6.1 Hz), 4.82 (2H, s), 5.00 (1H, s); ^{13}C NMR ($CDCl_3$, 125 MHz) δ –5.3 (CH_3), 18.4 (C), 25.0 (CH_2), 25.8 (CH_3), 29.3 (CH_2), 50.9 (CH_3), 60.6, 62.0, 68.4 (CH_2), 91.0 (CH), 167.5, 172.2 (C); ν_{max}/cm^{-1} 3441, 2930, 1713, 1624, 1141, 1100, 1048; GCMS (Method 1, R_t = 26.07 min) *m/z* 318.1 ($[M]^+$, 1%), 261.1 (20), 189.0 (100), 157.0 (65), 129.0 (22), 75.0 (20).

(*E*)-Methyl 4-(*tert*-butyldimethylsilyloxy)-3-(4-oxobutoxy)but-2-enoate (32)



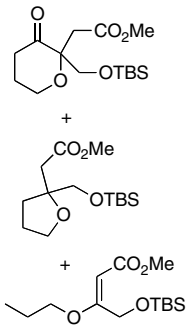
To a solution of alcohol **31** (1.00 g, 3.14 mmol) in CH_2Cl_2 (6 mL) was added $PhI(OAc)_2$ (1.21 g, 3.77 mmol) and TEMPO (50 mg, 0.31 mmol) and the mixture was stirred at ambient temperature for 3 h. After removal of the solvent *in vacuo* the remaining residue was purified by flash column chromatography (ethyl acetate:petrol 1:4) to give aldehyde **32** (0.96 g, 97%) as a colourless oil.

[S4] T. Zheng, R. S. Narayan, J. M. Schomaker, B. Borhan, *J. Am. Chem. Soc*. **2005**, *127*, 6946.

[S2] A. T. Koppisch, B. S. J. Blagg, C. D. Poulter, *Org. Lett*. **2000**, *2*, 215.

HRMS (ESI) found: 317.1779, $C_{15}H_{29}O_5Si$ $[M+H]^+$ requires 317.1779; ^1H NMR ($CDCl_3$, 500 MHz) δ 0.08 (6H, s), 0.90 (9H, s), 2.08 (2H, m), 2.64 (2H, td, *J* 7.0 and 1.0 Hz), 3.66 (3H, s), 3.82 (2H, t, *J* 6.1 Hz), 4.79 (2H, s), 4.99 (1H, s), 9.81 (1H, t, *J* 1.0 Hz); ^{13}C NMR ($CDCl_3$, 125 MHz) δ –5.3 (CH_3), 18.4 (C), 21.2 (CH_2), 25.8 (CH_3), 40.3 (CH_2), 51.0 (CH_3), 60.4, 67.1 (CH_2), 91.4 (CH), 167.3, 172.0 (C), 201.1 (CH); ν_{max}/cm^{-1} 2952, 1714, 1626, 1141, 1103, 1049; GCMS (Method 1, R_t = 24.72 min) *m/z* 316.1 ($[M]^+$, 1%), 259.1 (15), 189.0 (100), 157.0 (25), 71.1 (35).

Methyl 2-(2-((*tert*-butyldimethylsilyloxy)methyl)-3-oxo-tetrahydro-2*H*-pyran-2-yl)acetate (33), methyl 2-(2-((*tert*-butyldimethylsilyloxy)methyl)-tetrahydrofuran-2-yl)acetate (35) and (*E*)-methyl 4-(*tert*-butyldimethylsilyloxy)-3-propoxybut-2-enoate (34)



A solution of aldehyde **32** (100 mg, 0.32 mmol), *tert*-dodecanethiol (22 μL, 0.09 mmol) and 1,1'-azobis(cyclohexanecarbonitrile) (23 mg, 0.09 mmol) in toluene (2 mL) was flushed with argon for 30 min. The solution was then heated at reflux for 42 h with further portions of initiator (20 mg) added after 18 h and 26 h. After removal of the solvent *in vacuo* flash column chromatography (ethyl acetate:petrol 1:9) gave tetrahydropyranone **33** (32 mg, 32%) as a colourless oil, the tetrahydrofuran **35** (17 mg, 19%) as a colourless oil and the enol-ether **34** (24 mg, 26%) as a colourless oil.

Pyran data:

HRMS (ESI) found 317.1779, $C_{15}H_{29}O_5Si$ $[M+H]^+$ requires 317.1779; ^1H NMR ($CDCl_3$, 500 MHz) δ 0.02 (3H, s), 0.05 (3H, s), 0.87 (9H, s), 1.96 (1H, m), 2.25 (1H, m), 2.40 (1H, m), 2.46 (1H, d, *J* 16.1 Hz), 2.72 (1H, m), 2.97 (1H, d, *J* 16.1 Hz), 3.64 (1H, d, *J* 10.1 Hz), 3.65 (3H, s), 3.84 (1H, d, *J* 10.1 Hz), 3.93 (1H, m), 4.25 (1H, m); ^{13}C NMR ($CDCl_3$, 125 MHz) δ –5.7, –5.6 (CH_3), 18.2 (C), 23.8 (CH_2), 25.8 (CH_3), 38.1, 40.7 (CH_2), 51.7 (CH_3), 63.8, 69.9 (CH_2), 84.1, 170.7, 210.5 (C); ν_{max}/cm^{-1} 2930, 1742, 1718, 1137; GCMS (Method 1, R_t = 22.66 min) *m/z* 316.1 ($[M]^+$, 1%), 285.1 (29), 259.1 (100), 241.1 (30), 229.1 (54), 185.1 (63), 173.0 (30), 143.1 (61), 129.0 (31), 89.0 (96), 73.1 (59).

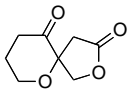
Furan data:

HRMS (ESI) found 289.1829, $C_{14}H_{29}O_4Si$ $[M+H]^+$ requires 289.1830; ^1H NMR ($CDCl_3$, 500 MHz) δ 0.04 (3H, s), 0.05 (3H, s), 0.89 (9H, s), 1.93 (4H, m), 2.57 (1H, d, *J* 14.5 Hz), 2.62 (1H, d, *J* 14.5 Hz), 3.49 (1H, d, *J* 9.9 Hz), 3.58 (1H, d, *J* 9.9 Hz), 3.66 (3H, s), 3.83 (2H, m); ^{13}C NMR ($CDCl_3$, 125 MHz) δ –5.5 (2 x CH_3), 18.2 (C), 25.9 (CH_3), 32.4, 41.0 (CH_2), 51.4 (CH_3), 67.6, 68.6 (CH_2), 83.5, 171.6 (C), one signal obscured; ν_{max}/cm^{-1} 2929, 1739, 1252, 1097; GCMS (Method 1, R_t = 17.94 min) *m/z* 273.1 ($[M–15]^+$, 1%), 257.1 (15), 231.1 (67), 199.1 (40), 171.1 (39), 157.1 (30), 143.1 (100), 101.1 (44), 75.0 (34).

Enol-ether data:

Spectroscopic and physical data (^1H and ^{13}C NMR, GCMS) were identical to authentic material prepared directly from acetylene **15**.

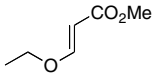
1,8-dioxaspiro[5,4]decane-5,9-dione (36)



To the TBS ether **33** (25 mg, 0.079 mmol) in chloroform (1 mL) and methanol (0.5 mL) was added 10-CSA (9 mg, 0.039 mmol) and the mixture was stirred at ambient temperature for 40 h. After removal of the solvent *in vacuo*, the remaining residue was resuspended in chloroform (1 mL) and stirring was continued for 16 h. Removal of the solvent *in vacuo* and flash column chromatography (ethyl acetate:petrol 3:1) gave the dioxaspirodecane **36** (10 mg, 75%) as a colourless oil.
HRMS (ESI) found 171.0656, $C_8H_{11}O_4$ $[M+H]^+$ requires 171.0652; ^{1}H NMR ($CDCl_3$, 500 MHz) δ 2.15 (2H, m), 2.59 (2H, m), 2.75 (1H, dd, *J* 17.6 and 0.7 Hz), 2.95 (1H, d, *J* 17.6 Hz), 3.93 (2H, m), 4.39 (1H, dd, *J* 10.0 and 0.7 Hz), 4.49 (1H, d, *J* 10.0 Hz); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 24.9, 36.6, 37.6, 62.0, 73.4 (CH_2), 86.2, 173.3, 205.6 (C); ν_{max}/cm^{-1} 2936, 1778, 1717, 1168, 1092, 1023; GCMS (Method 1, R_t = 16.02 min) *m/z* 170.0 ($[M]^+$, 17%), 140.0 (100), 112.0 (82), 84.0 (45).

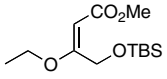
1.2.3 : Decarbonylation standards :

(*E*)-Methyl 3-ethoxyacrylate (38)



To a solution of dry ethanol (200 uL) and trimethylphosphine (1 M in THF, 360 uL) in dichloromethane (4 mL) at 0 °C was added methyl propiolate **37** (150 mg, 1.78 mmol) dropwise over 5 min and stirring was continued for a further 1 h. Saturated NH_4Cl (10 mL) was added, the mixture extracted with dichloromethane (3×5 mL) and the combined organic layers were dried ($MgSO_4$) and concentrated *in vacuo* to give the (*E*)-acrylate **38** (217 mg, 94%) as a colourless oil.
HRMS (ESI) found 131.0703, $C_6H_{11}O_3$ $[M+H]^+$ requires 131.0703; ^{1}H NMR ($CDCl_3$, 500 MHz) δ 1.33 (3H, t, *J* 7.1 Hz), 3.69 (3H, s), 3.90 (2H, q, *J* 7.1 Hz), 5.19 (1H, d, *J* 12.5 Hz), 7.58 (1H, d, *J* 12.5 Hz); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 14.4, 51.0 (CH_3), 66.7 (CH_2), 96.1, 162.4 (CH), 168.3 (C); ν_{max}/cm^{-1} 2986, 1710, 1623, 1205, 1123; GCMS (Method 1, R_t = 3.05 min) *m/z* 130.0 ($[M]^+$, 11%), 115.0 (29), 99.0 (39), 87.0 (29), 71.0 (100).

(*E*)-Methyl 4-(*tert*-butyldimethylsilyloxy)-3-ethoxybut-2-enoate (39)

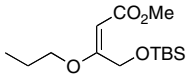


To a solution of ethanol (200 uL) and trimethylphosphine (1 M in THF, 438 uL) in dichloromethane (5 mL) at 0 °C was added acetylene **15**[S2] (200 mg, 0.88 mmol) in dichloromethane (0.5 mL) dropwise over 5 min. The solution was allowed to warm to ambient temperature over 30 min and stirred for a further 1 h. Saturated NH_4Cl (5 mL) was added and the mixture extracted with chloroform (3×5 mL) and the combined organic layers were dried ($MgSO_4$) and concentrated *in vacuo*. Flash column chromatography (ethyl acetate:petrol 1:20) gave the (*E*)-acrylate **39** (198 mg, 83%) as a colourless oil.
HRMS (ESI) found 275.1673, $C_{13}H_{27}O_4Si$ $[M+H]^+$ requires 275.1673; ^{1}H NMR ($CDCl_3$, 500 MHz) δ 0.08 (6H, s), 0.90 (9H, s), 1.38 (3H, t, *J* 7.0 Hz), 3.66 (3H, s), 3.85 (2H, q, *J* 7.0 Hz), 4.82 (2H, s), 4.98 (1H, s); ^{13}C NMR ($CDCl_3$, 125 MHz) δ –5.3, 14.1 (CH_3), 18.4 (C), 25.8, 50.9 (CH_3), 60.7, 64.2 (CH_2), 90.7 (CH), 167.6, 172.5 (C); ν_{max}/cm^{-1} 2931, 1714, 1624, 1141, 1111,

[S2] A. T. Koppisch, B. S. J. Blagg, C. D. Poulter, *Org. Lett.* **2000**, *2*, 215.

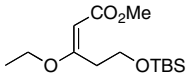
1049; GCMS (Method 1, R_t = 16.77 min) *m/z* 274.1 ($[M]^+$, 1%), 217.1 (100), 157.0 (30), 129.0 (20), 89.0 (20), 75.0 (23).

(*E*)-Methyl 4-(*tert*-butyldimethylsilyloxy)-3-propoxybut-2-enoate (34)



To a solution of 1-propanol (200 uL) and trimethylphosphine (1 M in THF, 438 uL) in dichloromethane (5 mL) at 0 °C was added acetylene **15**[S2] (200 mg, 0.88 mmol) in dichloromethane (0.5 mL) dropwise over 5 min. The solution was allowed to warm to ambient temperature over 30 min and stirred for a further 1 h. Saturated NH_4Cl (5 mL) was added and the mixture extracted with chloroform (3×5 mL) and the combined organic layers were dried ($MgSO_4$) and concentrated *in vacuo*. Flash column chromatography (ethyl acetate:petrol 1:20) gave the (*E*)-acrylate **34** (212 mg, 84%) as a colourless oil.
HRMS (ESI) found 289.1830, $C_{14}H_{29}O_4Si$ $[M+H]^+$ requires 289.1830; ^{1}H NMR ($CDCl_3$, 500 MHz) δ 0.08 (6H, s), 0.90 (9H, s), 1.00 (3H, t, *J* 7.5 Hz), 1.78 (2H, m), 3.66 (3H, s), 3.74 (2H, t, *J* 6.5 Hz), 4.82 (2H, s), 4.99 (1H, s); ^{13}C NMR ($CDCl_3$, 125 MHz) δ –5.3, 10.4 (CH_3), 18.4 (C), 21.9 (CH_2), 25.8, 50.9 (CH_3), 60.6, 70.1 (CH_2), 90.7 (CH), 167.6, 172.6 (C); ν_{max}/cm^{-1} 2930, 1714, 1626, 1137, 1100, 1049; GCMS (Method 1, R_t = 18.64 min) *m/z* 288.1 ($[M]^+$, 1%), 231.1 (100), 189.0 (79), 157.0 (80), 129.0 (29), 89.0 (21), 75.0 (36).

(*E*)-Methyl 5-(*tert*-butyldimethylsilyloxy)-3-ethoxypent-2-enoate (25)

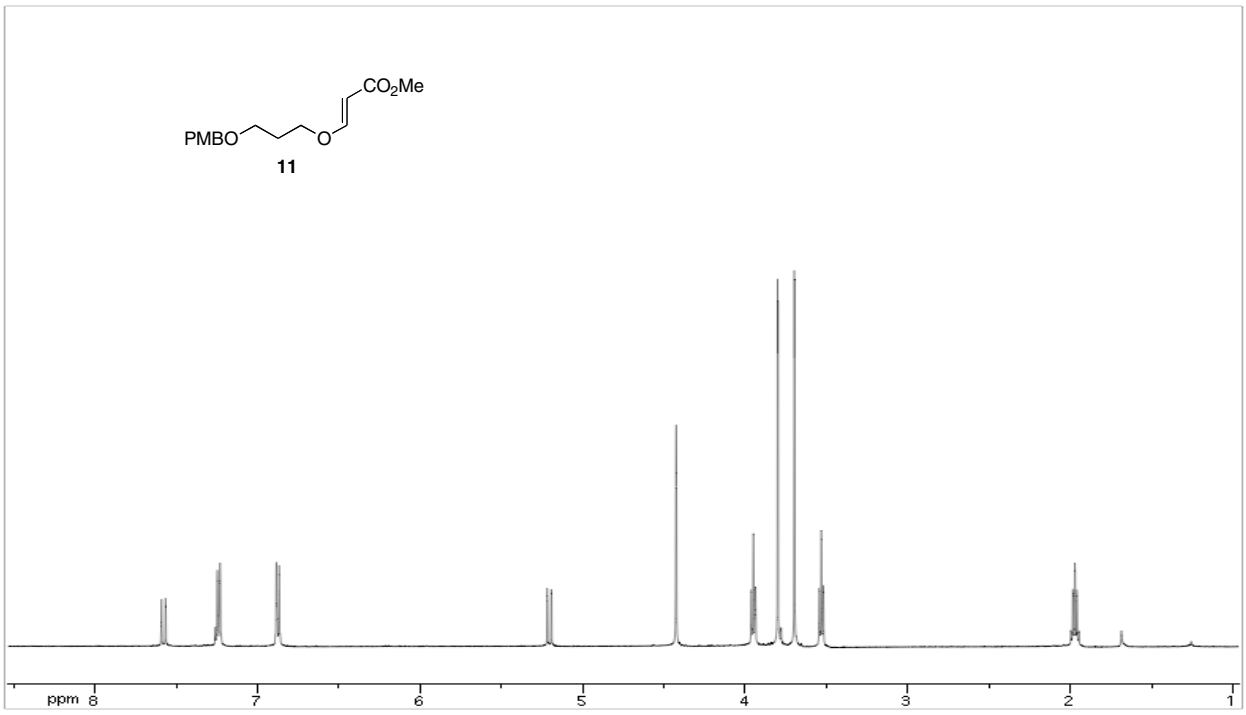


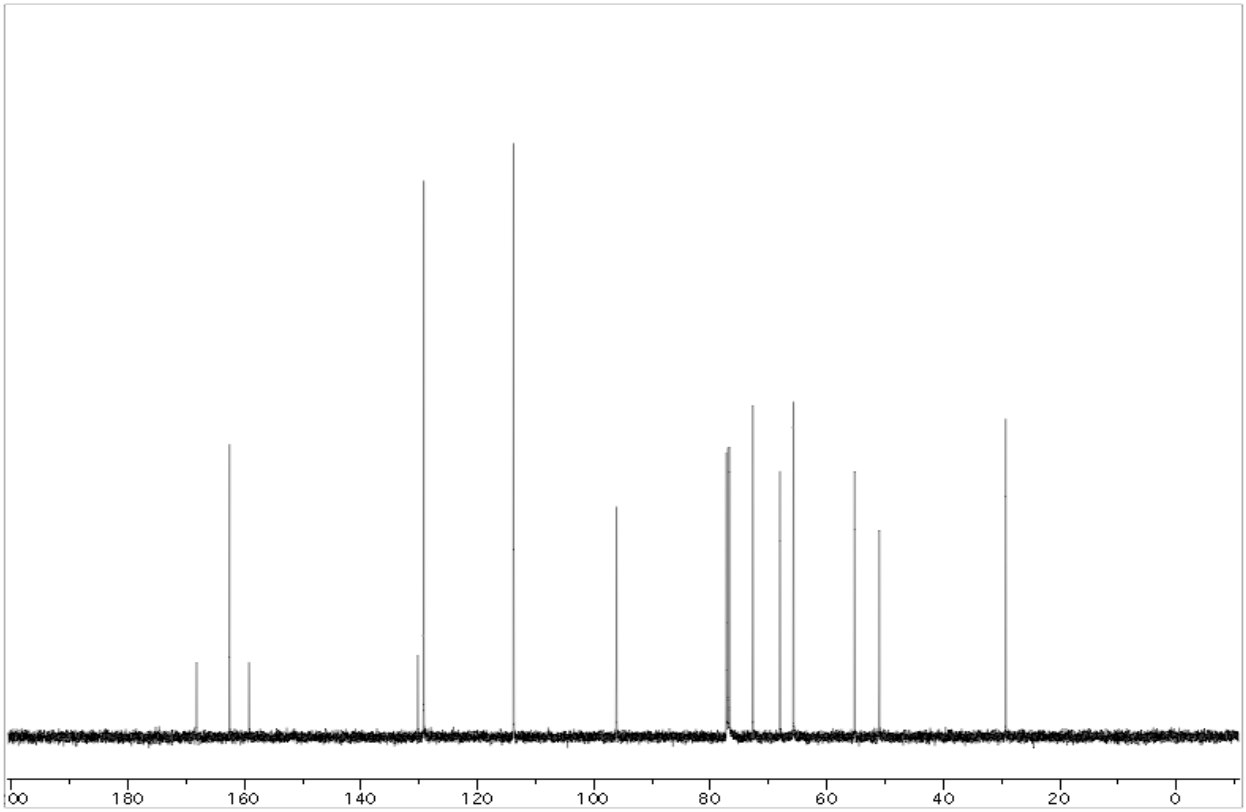
To a solution of ethanol (200 uL) and trimethylphosphine (1 M in THF, 580 uL) in dichloromethane (5 mL) at 0 °C was added acetylene **21**[S3] (200 mg, 0.83 mmol) in dichloromethane (1 mL) dropwise over 5 min. The solution was allowed to warm to ambient temperature over 30 min and stirred for a further 5 h. Saturated NH_4Cl (5 mL) was added and the mixture extracted with chloroform (3×5 mL) and the combined organic layers were dried ($MgSO_4$) and concentrated *in vacuo*. Flash column chromatography (ethyl acetate:petrol 1:20) gave the (*E*)-acrylate **25** (205 mg, 86%) as a colourless oil.
HRMS (ESI) found 289.1830, $C_{14}H_{29}O_4Si$ $[M+H]^+$ requires 289.1830; ^{1}H NMR ($CDCl_3$, 500 MHz) δ 0.03 (6H, s), 0.87 (9H, s), 1.33 (3H, t, *J* 7.0 Hz), 2.98 (2H, t, *J* 6.8 Hz), 3.66 (3H, s), 3.79 (2H, q, *J* 7.0 Hz), 3.82 (2H, t, *J* 6.8 Hz), 5.00 (1H, s); ^{13}C NMR ($CDCl_3$, 125 MHz) δ –5.4, 14.1 (CH_3), 18.2 (C), 25.9 (CH_3), 35.9 (CH_2), 50.7 (CH_3), 61.0, 63.7 (CH_2), 91.6 (CH), 167.9, 173.1 (C); ν_{max}/cm^{-1} 2930, 1716, 1618, 1140, 1099, 1076, 1054; GCMS (Method 1, R_t = 18.70 min) *m/z* 273.1 ($[M-15]^+$, 3%), 231.1 (100), 171.0 (57), 89.1 (23).

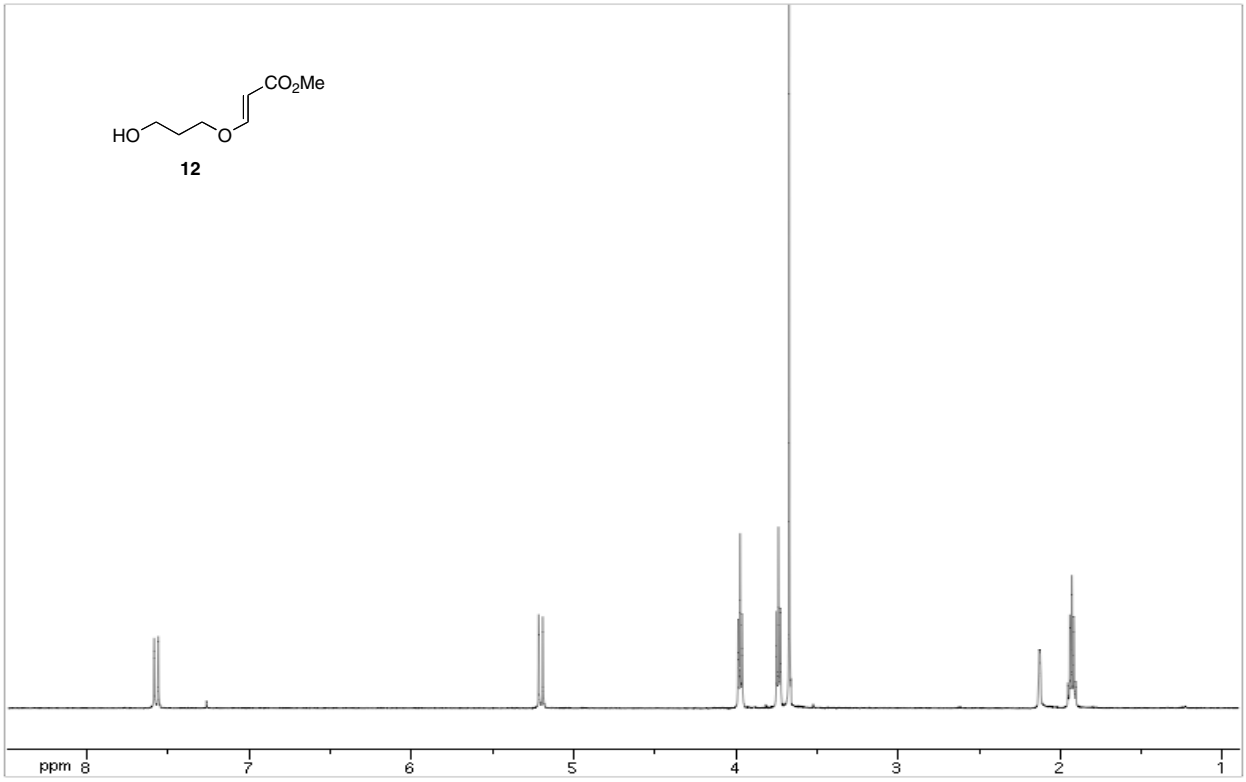
[S2] A. T. Koppisch, B. S. J. Blagg, C. D. Poulter, *Org. Lett.* **2000**, *2*, 215.

[S3] Acetylene **21** was prepared from the corresponding terminal acetylene (*n*-BuLi, THF, -78 °C, $ClCO_2Me$). The spectroscopic data was in accord with material prepared by TBS protection of methyl 5-hydroxy-2-pentynoate (E. Piers, J. M. Chong, H. E. Morton, *Tetrahedron* **1989**, *45*, 363).

1.3 NMR SPECTRA FOR COMPOUNDS 11-13, 16-20, 22-26, 29-36 and 38-39



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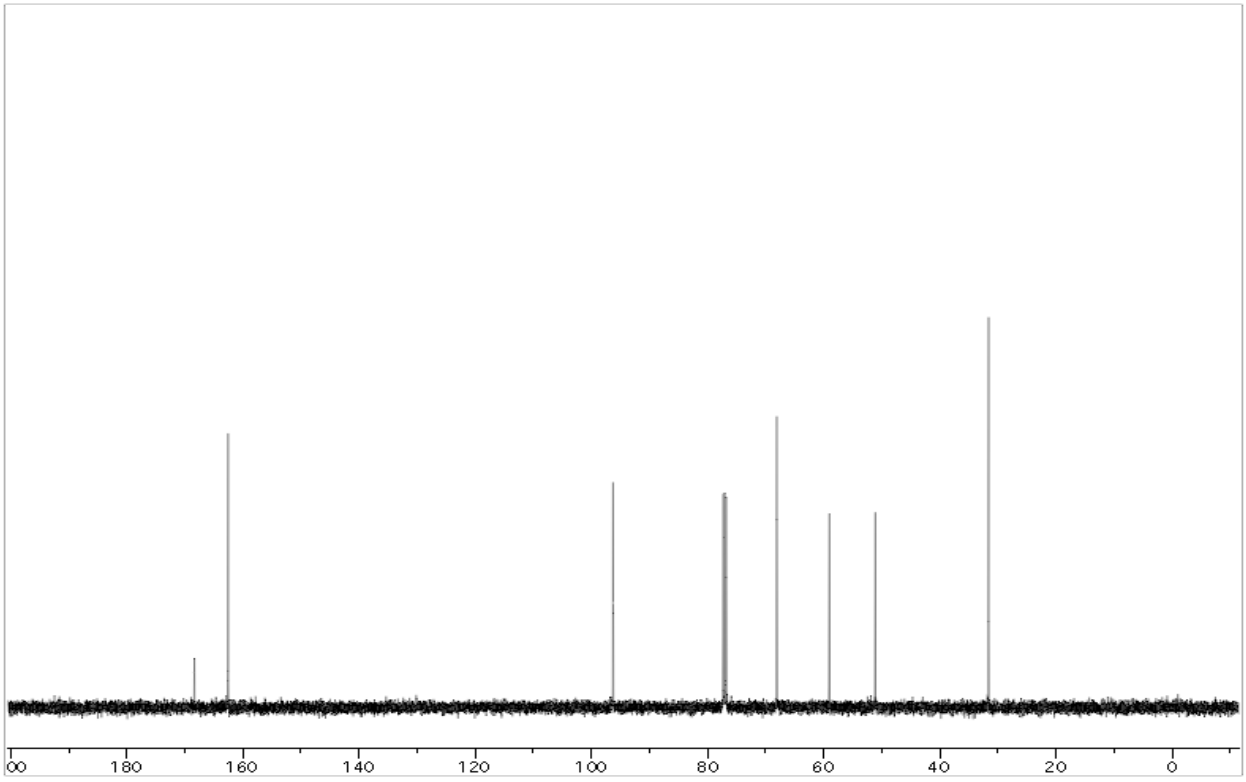
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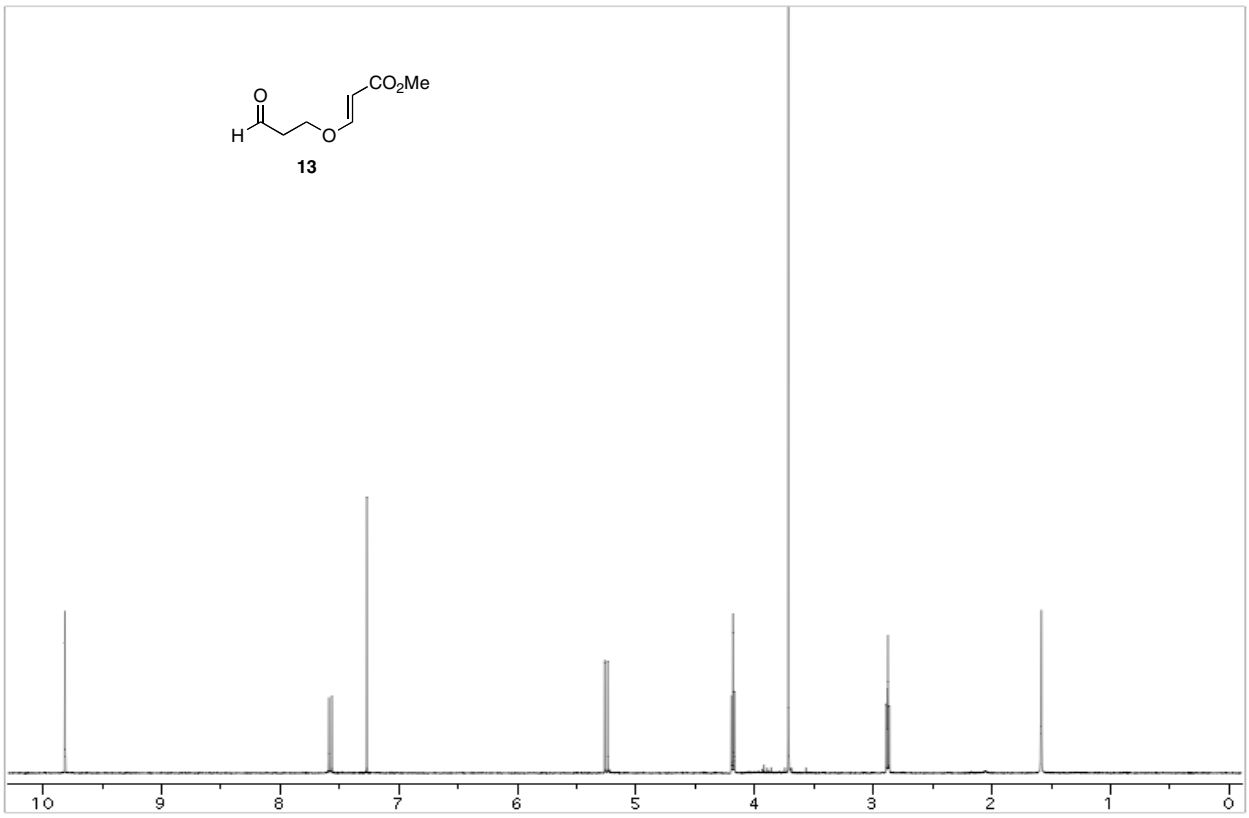
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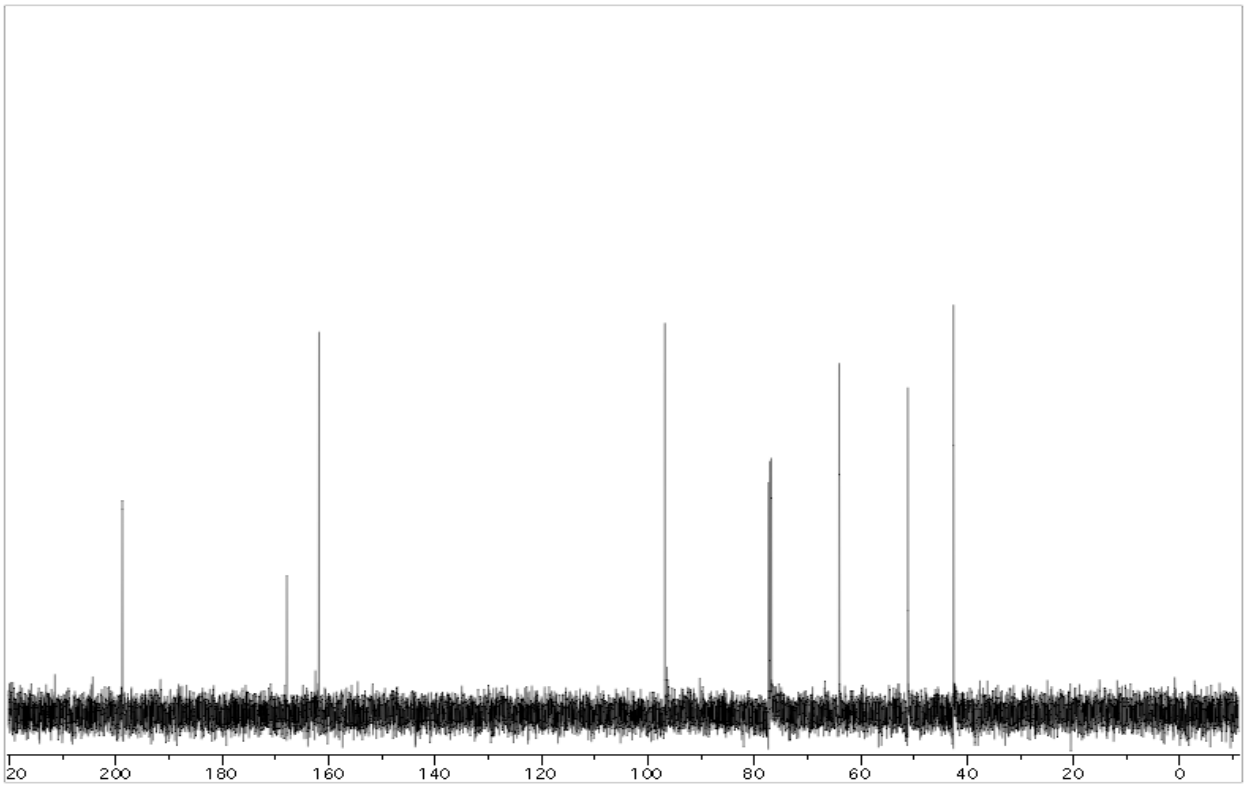
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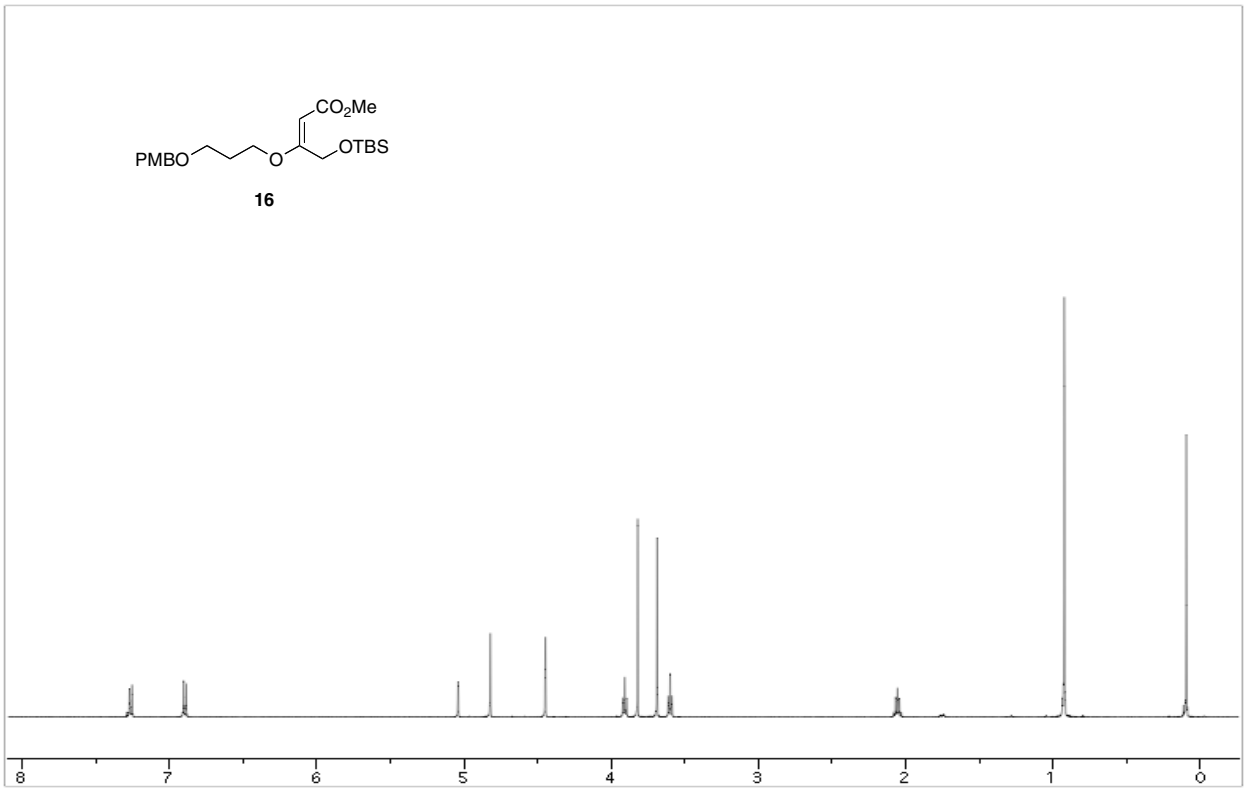
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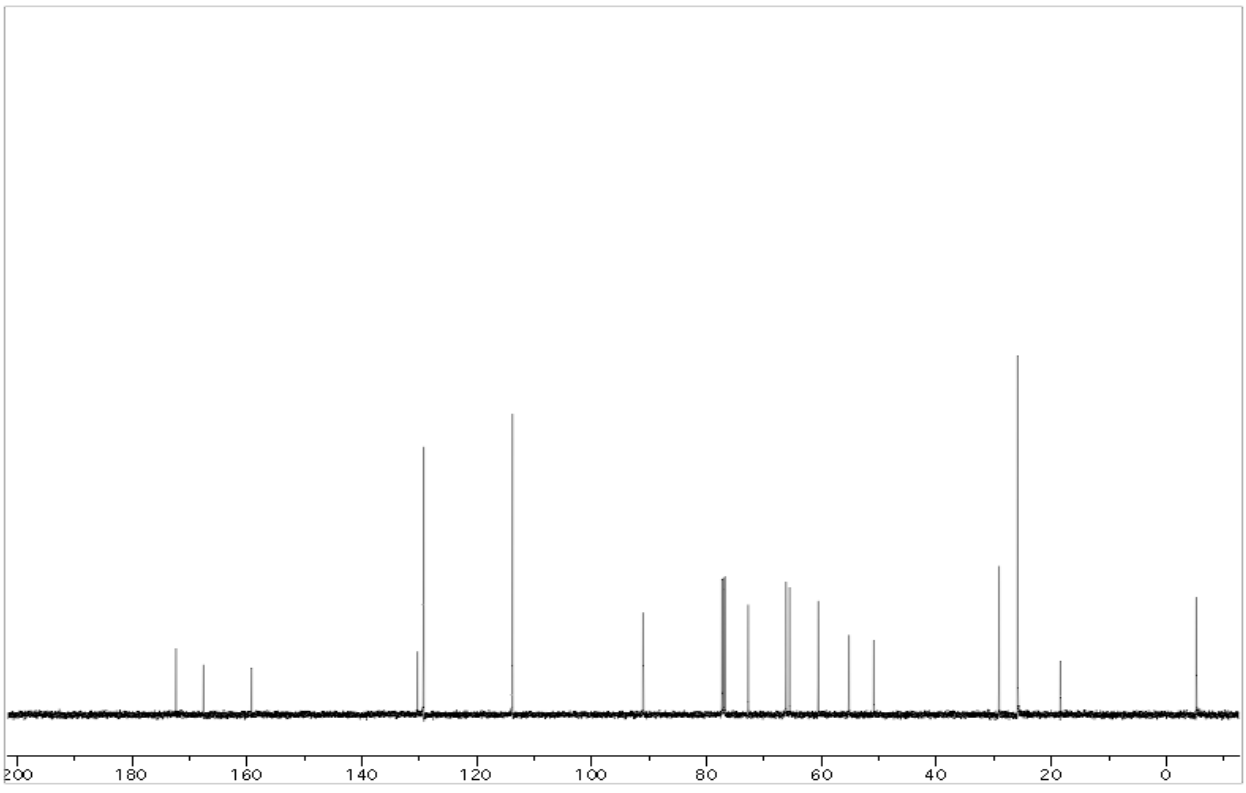
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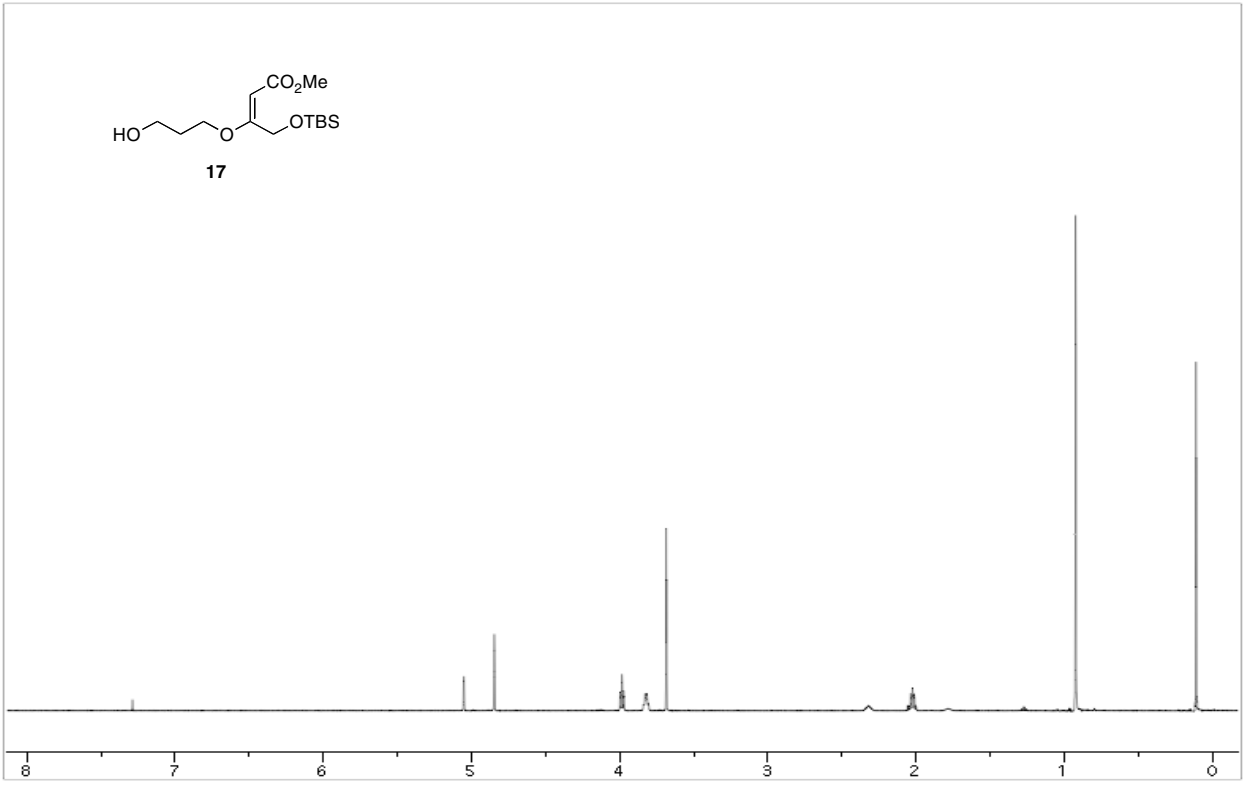
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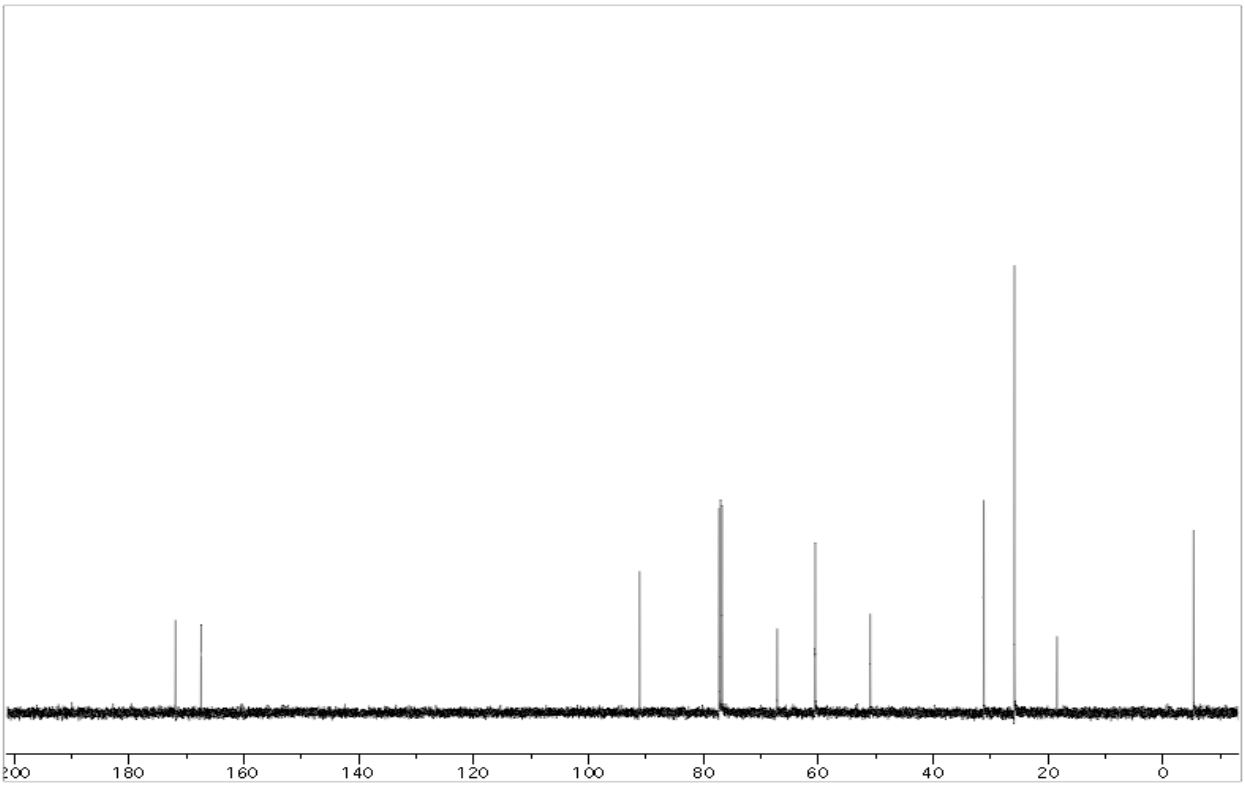
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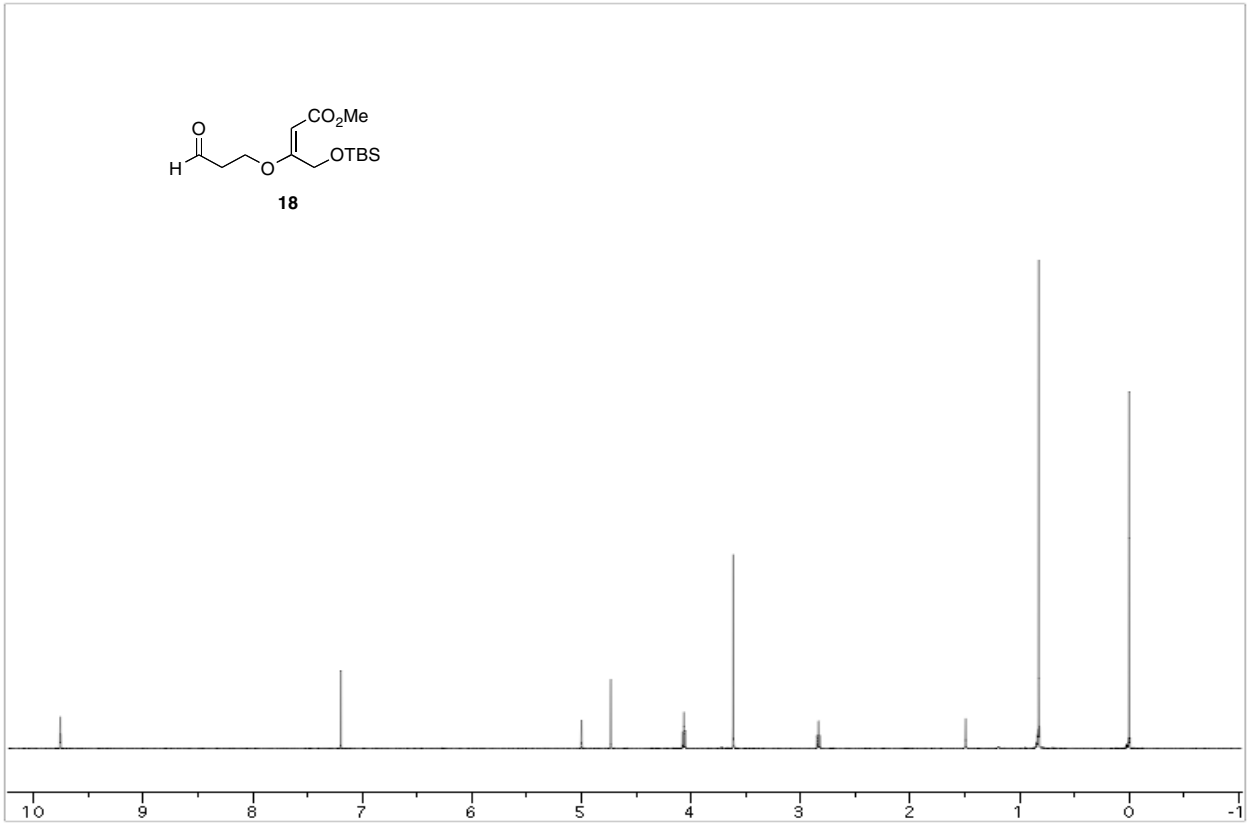
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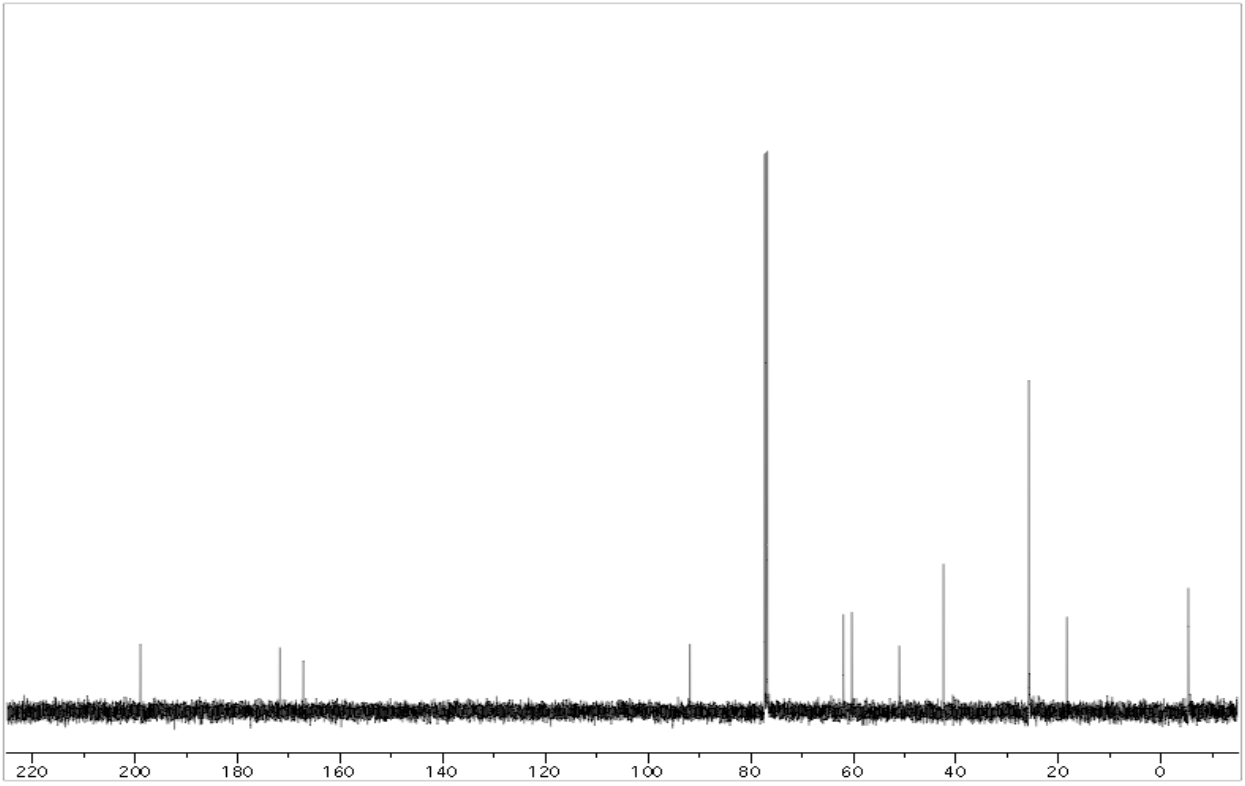
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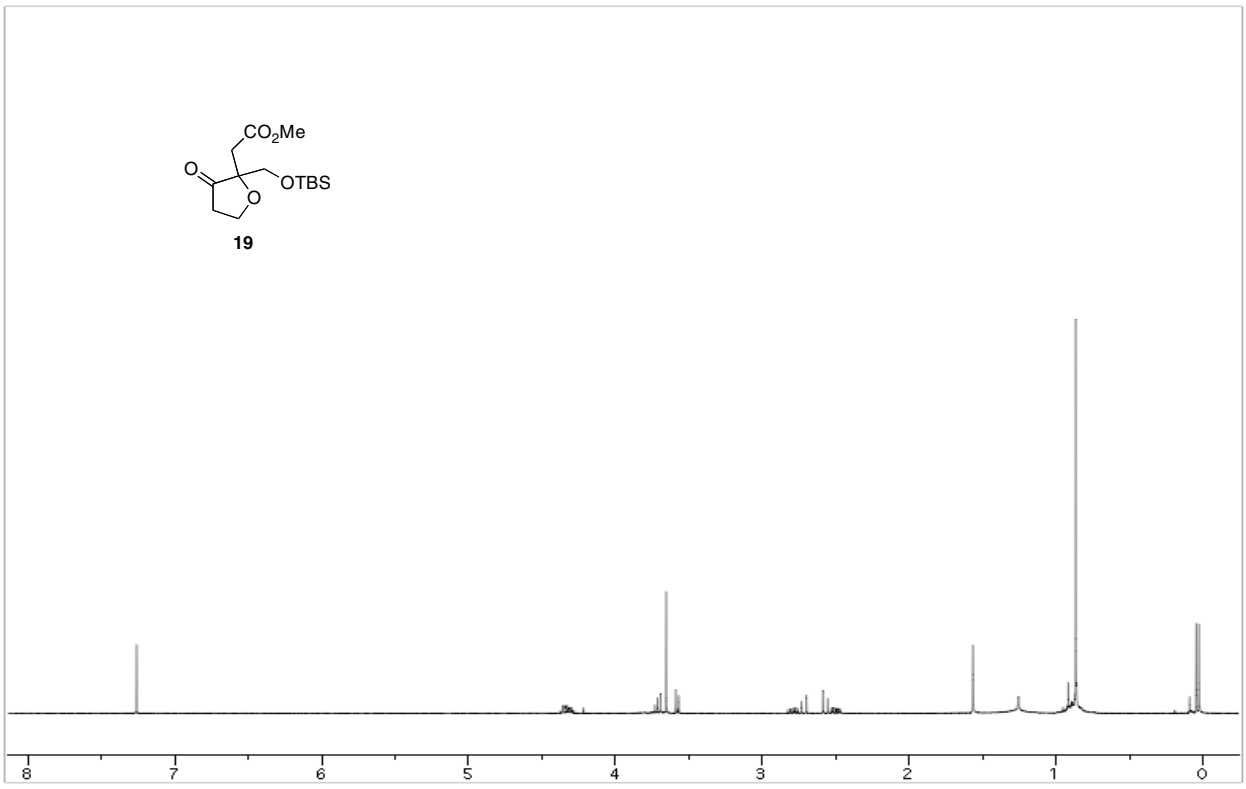
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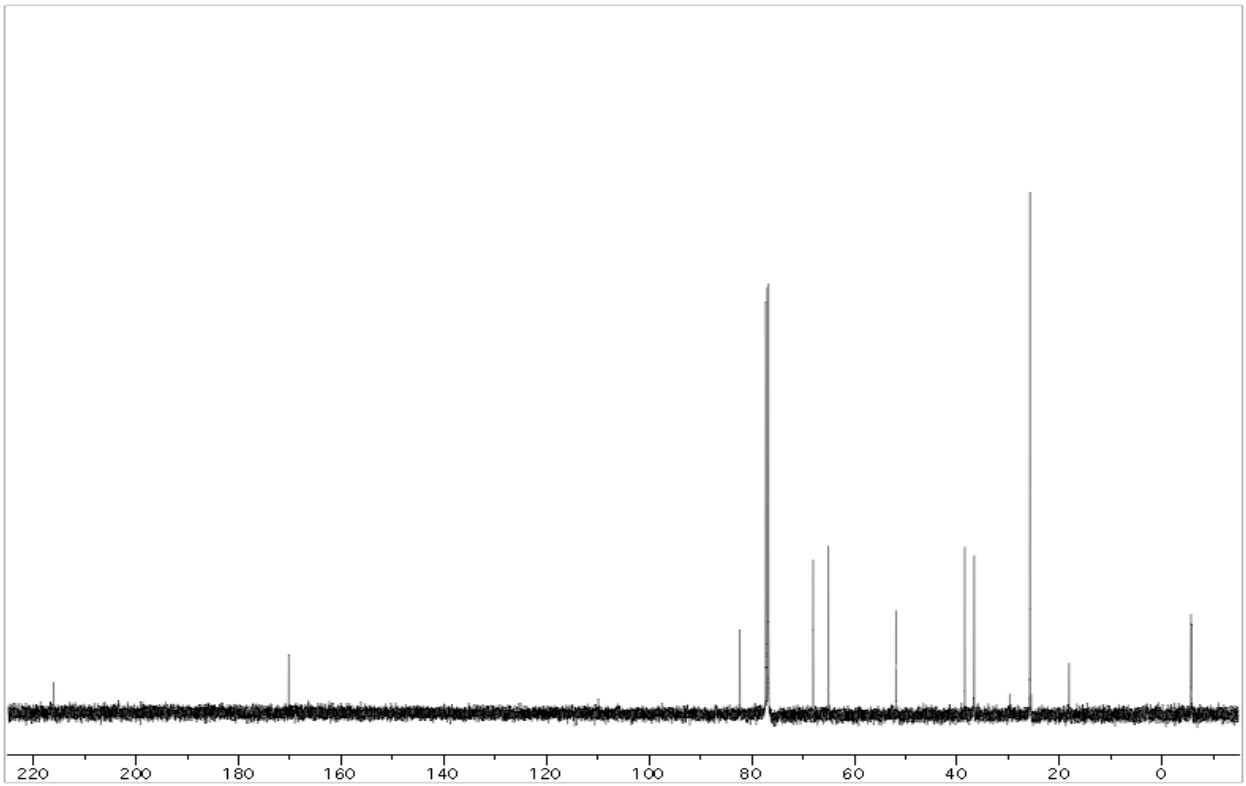
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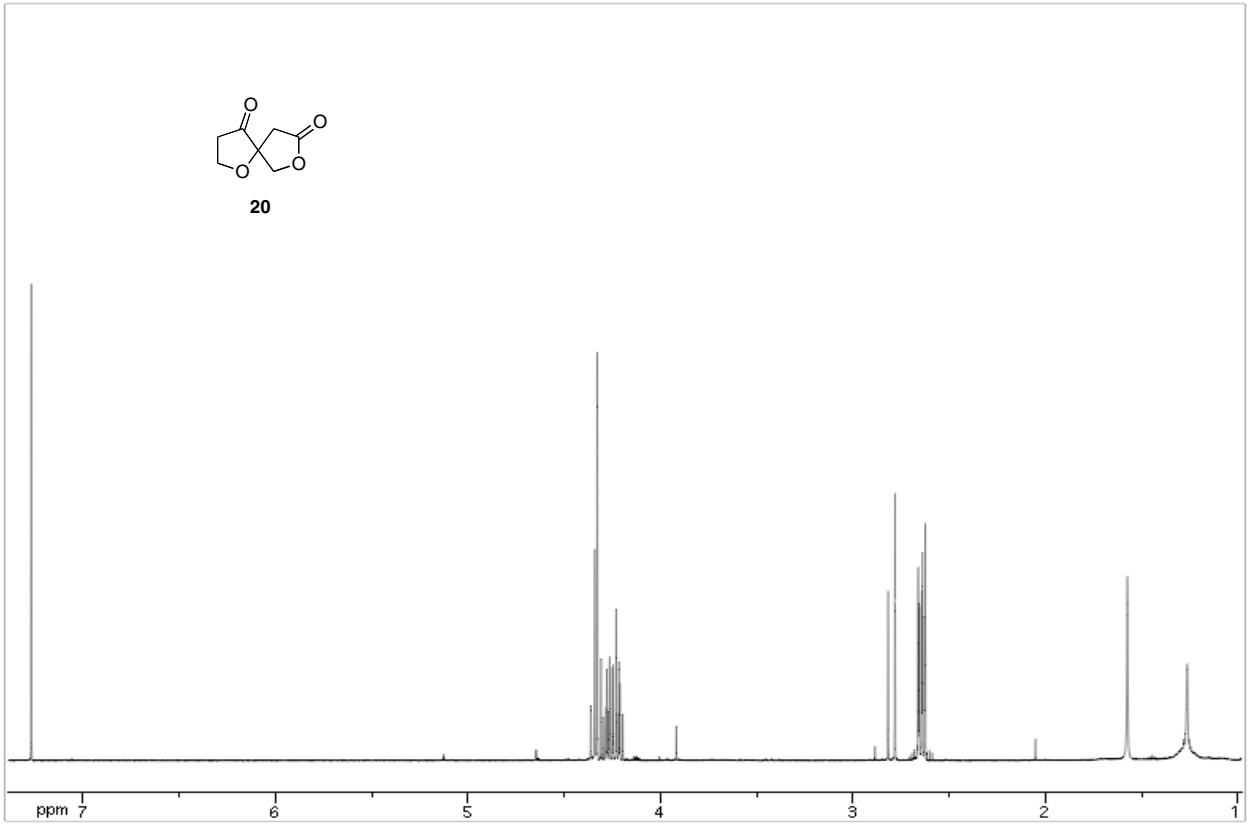
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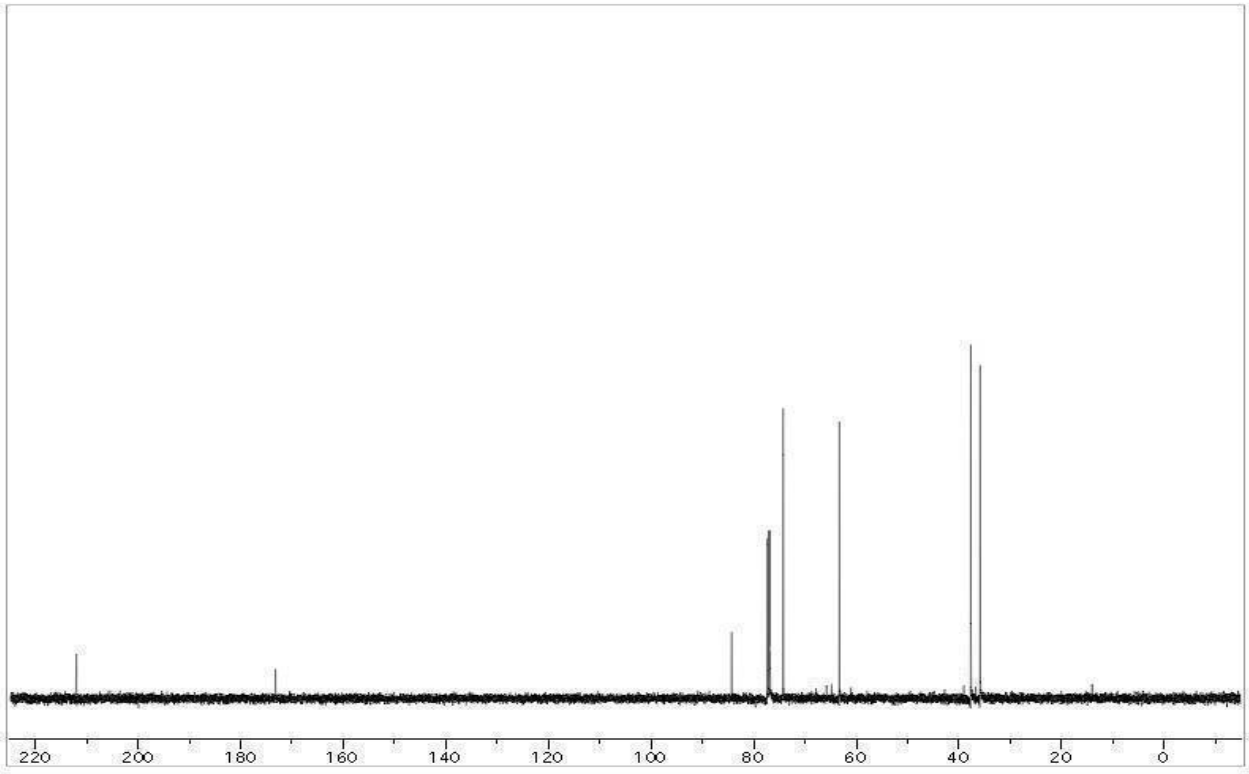
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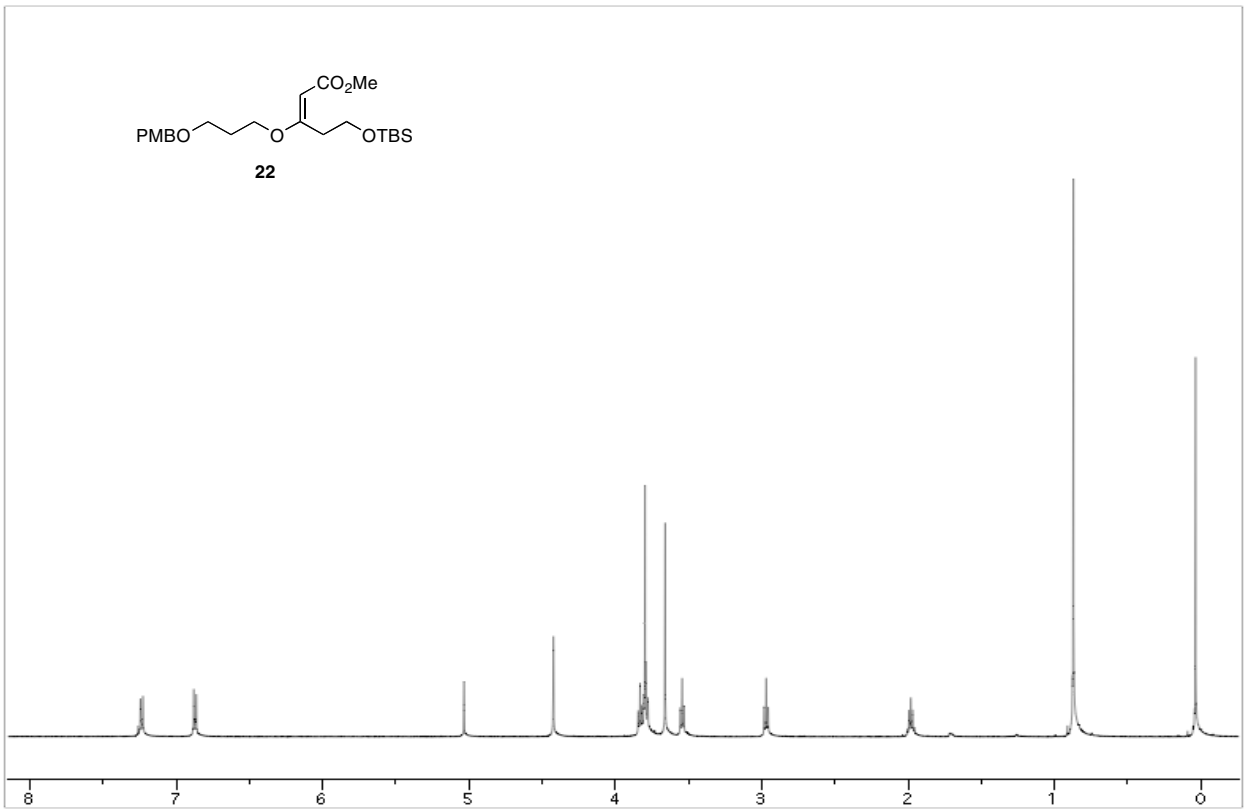
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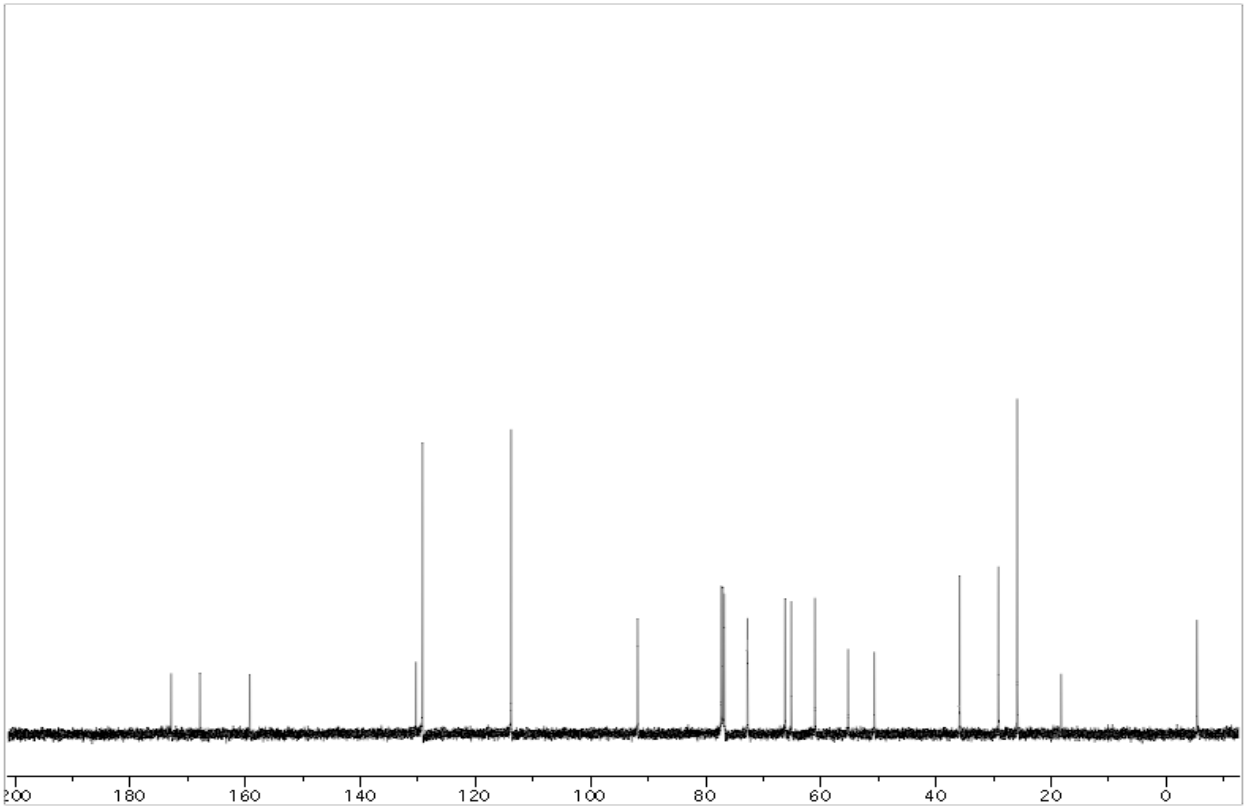
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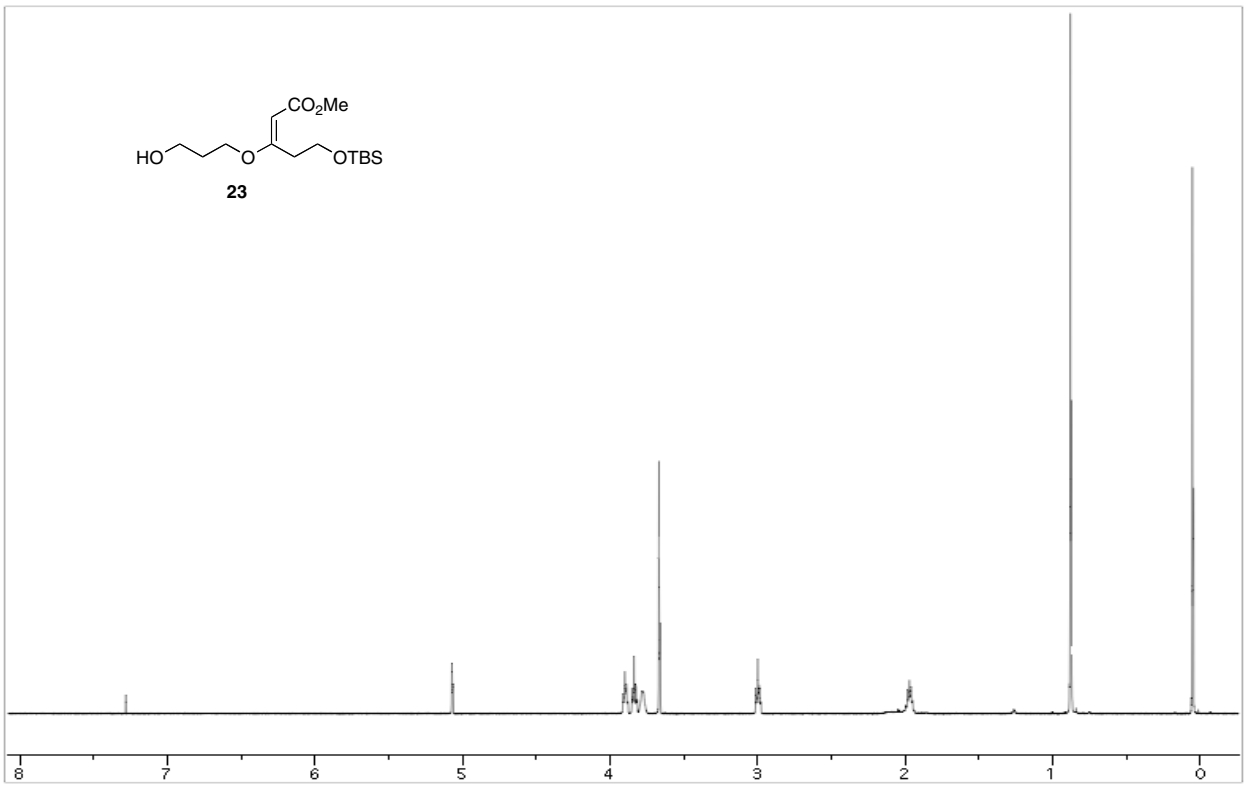
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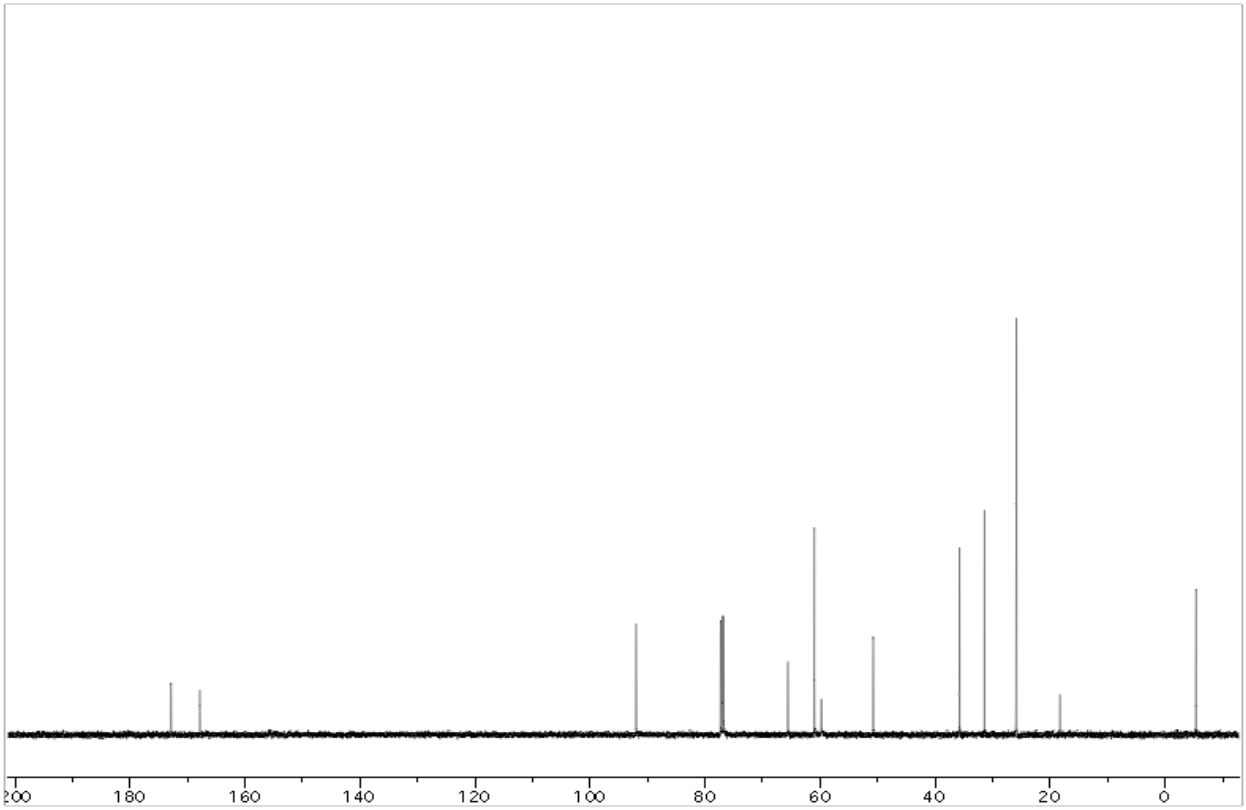
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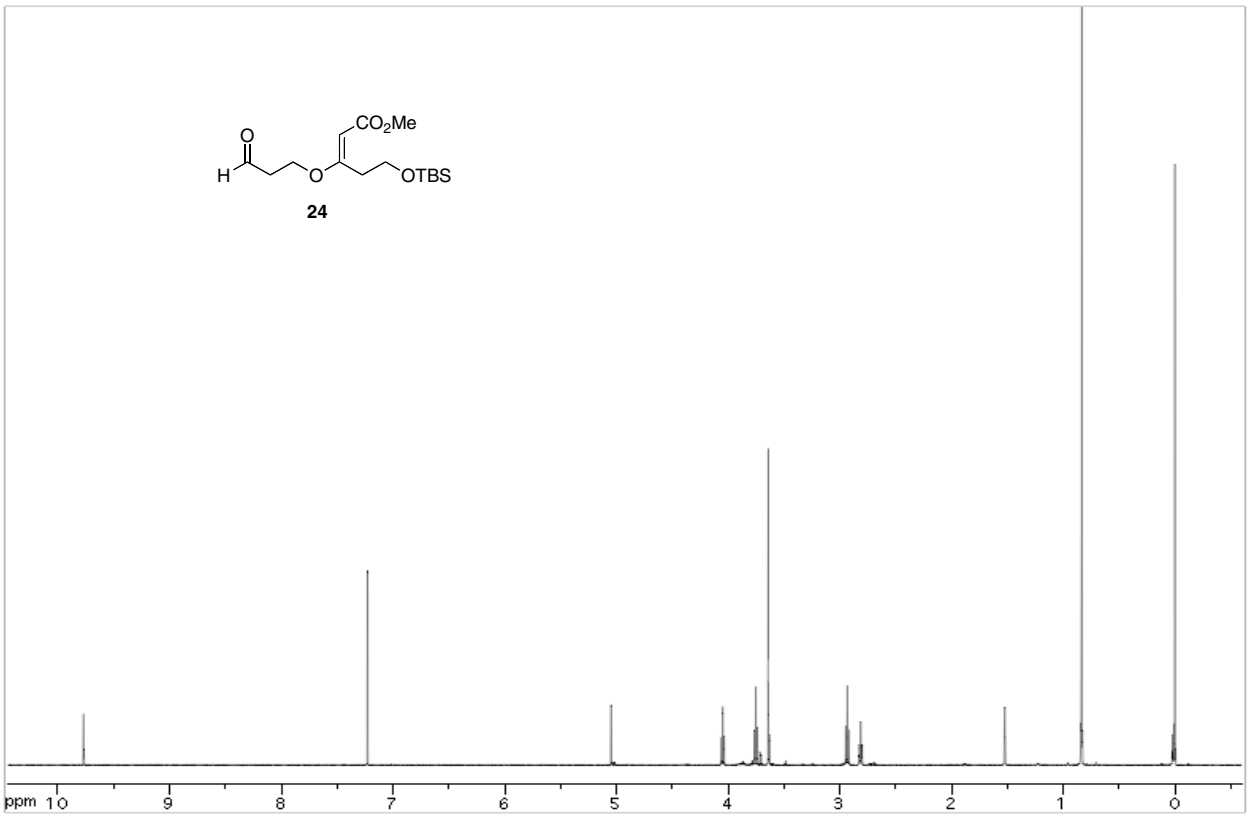
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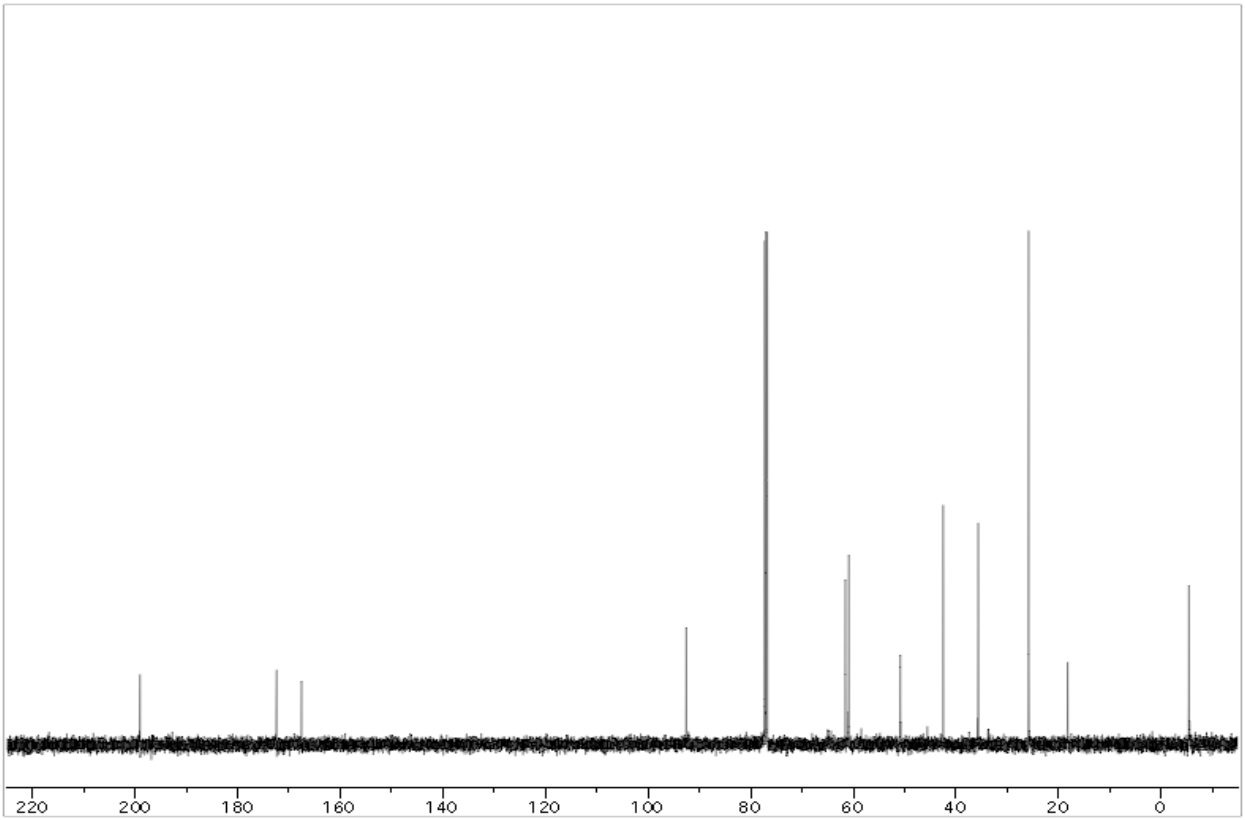
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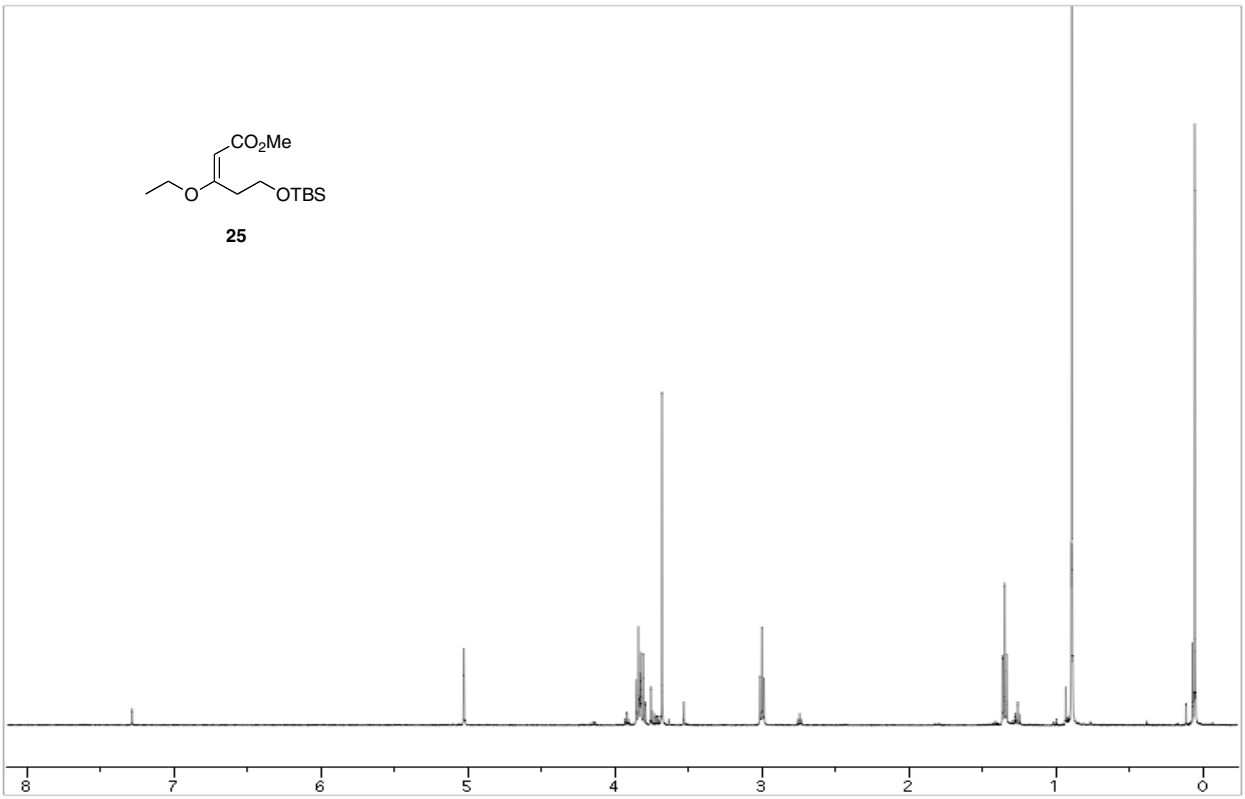
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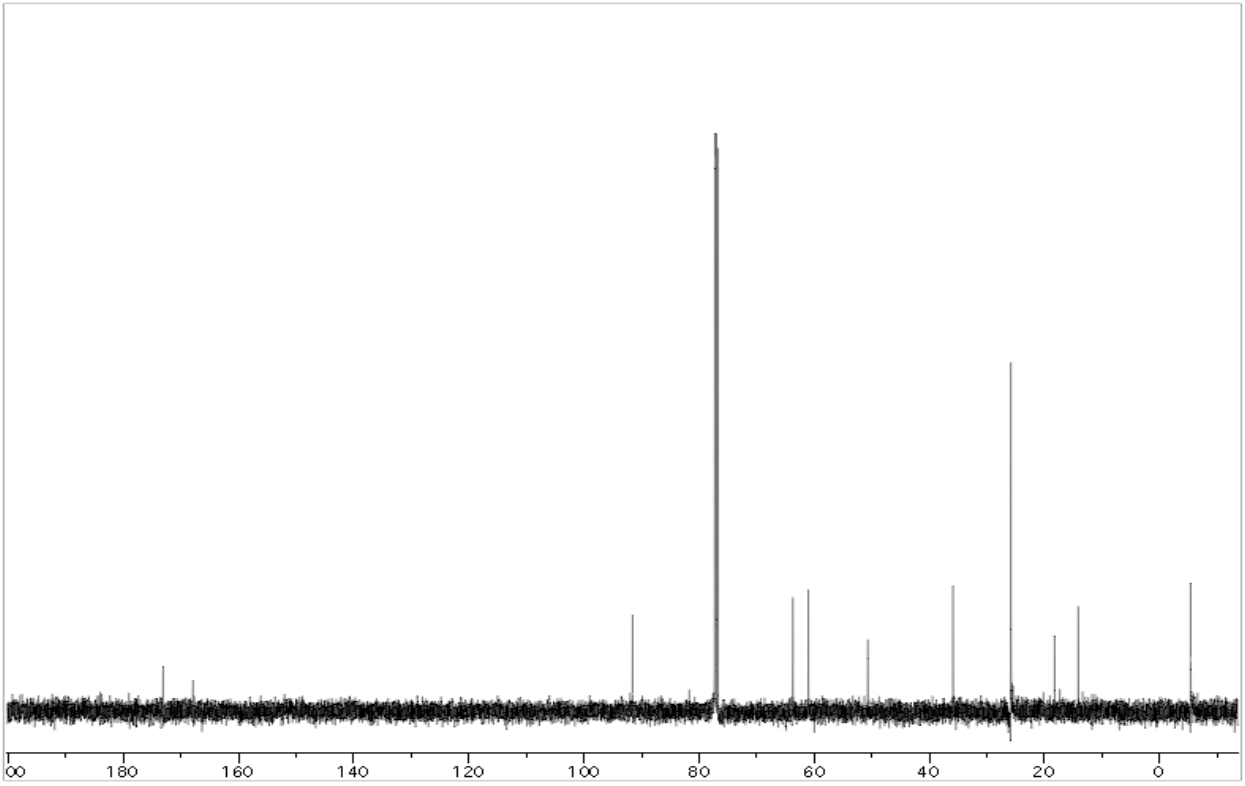
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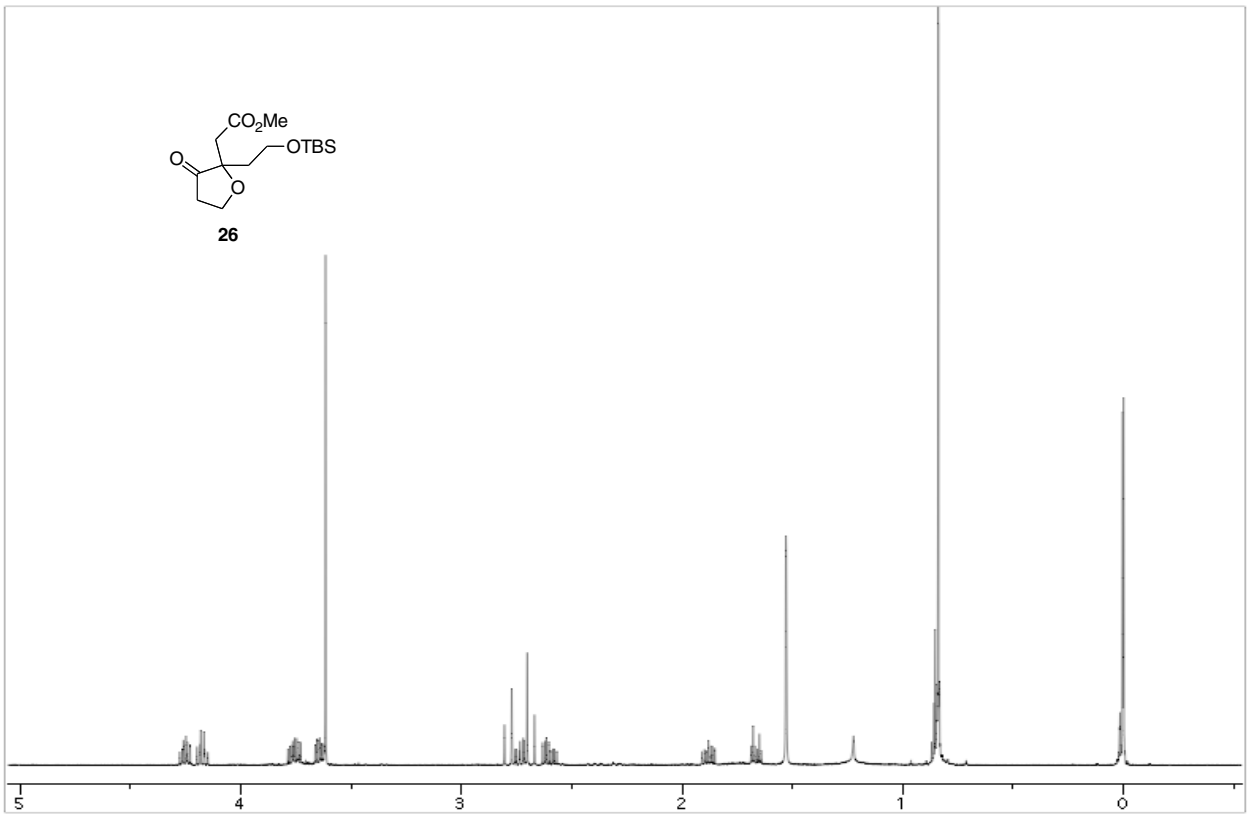
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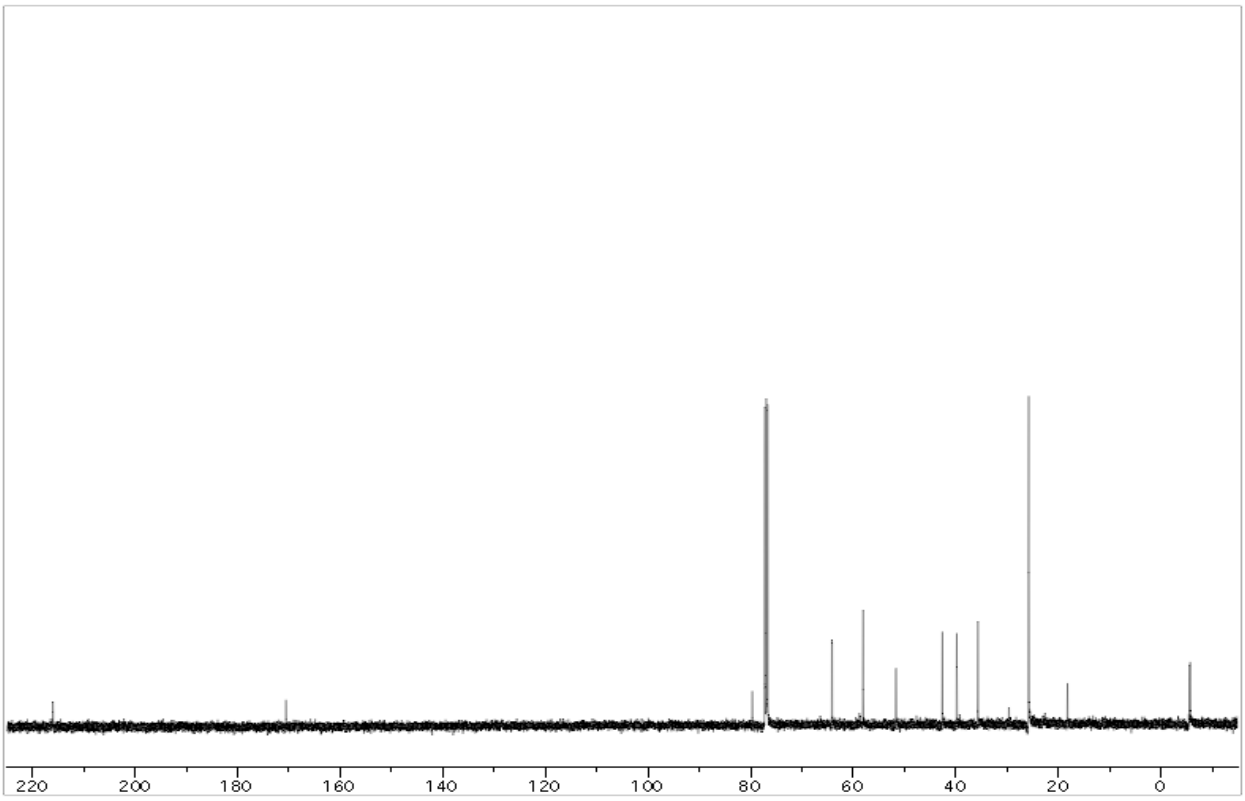
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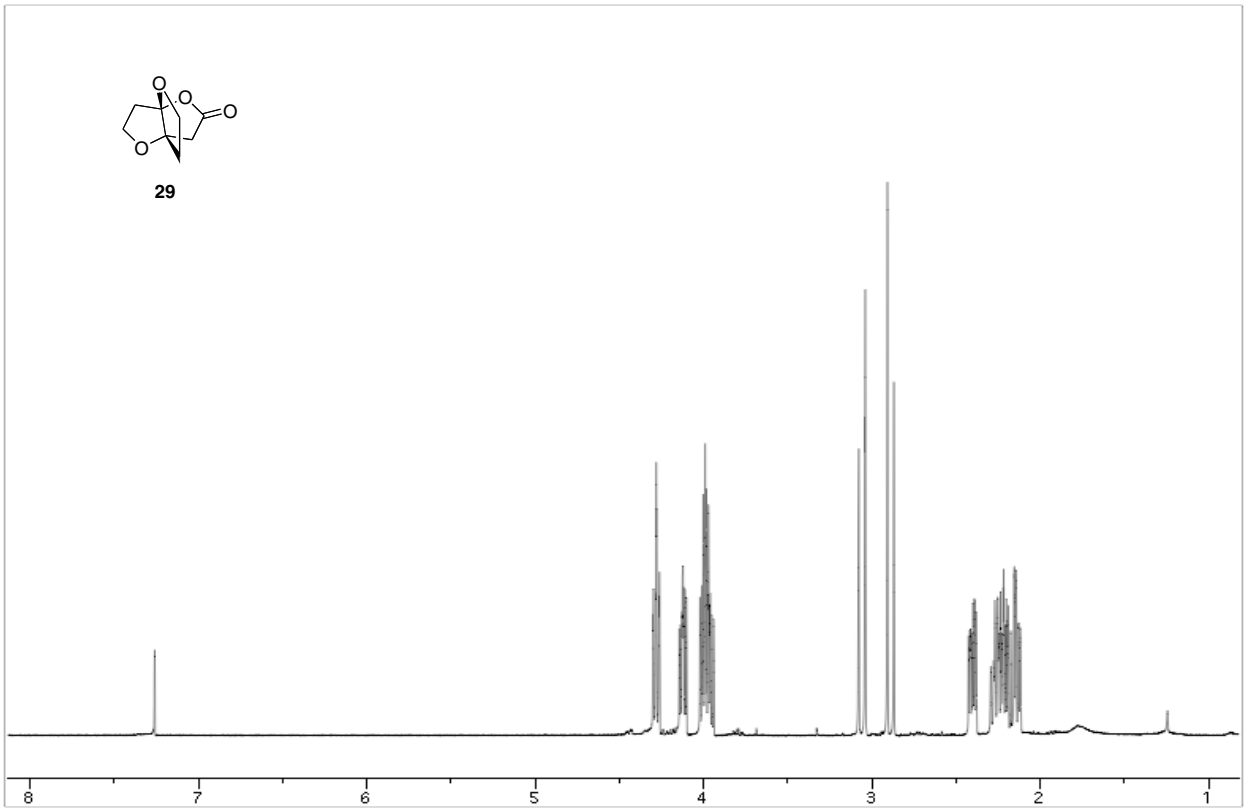
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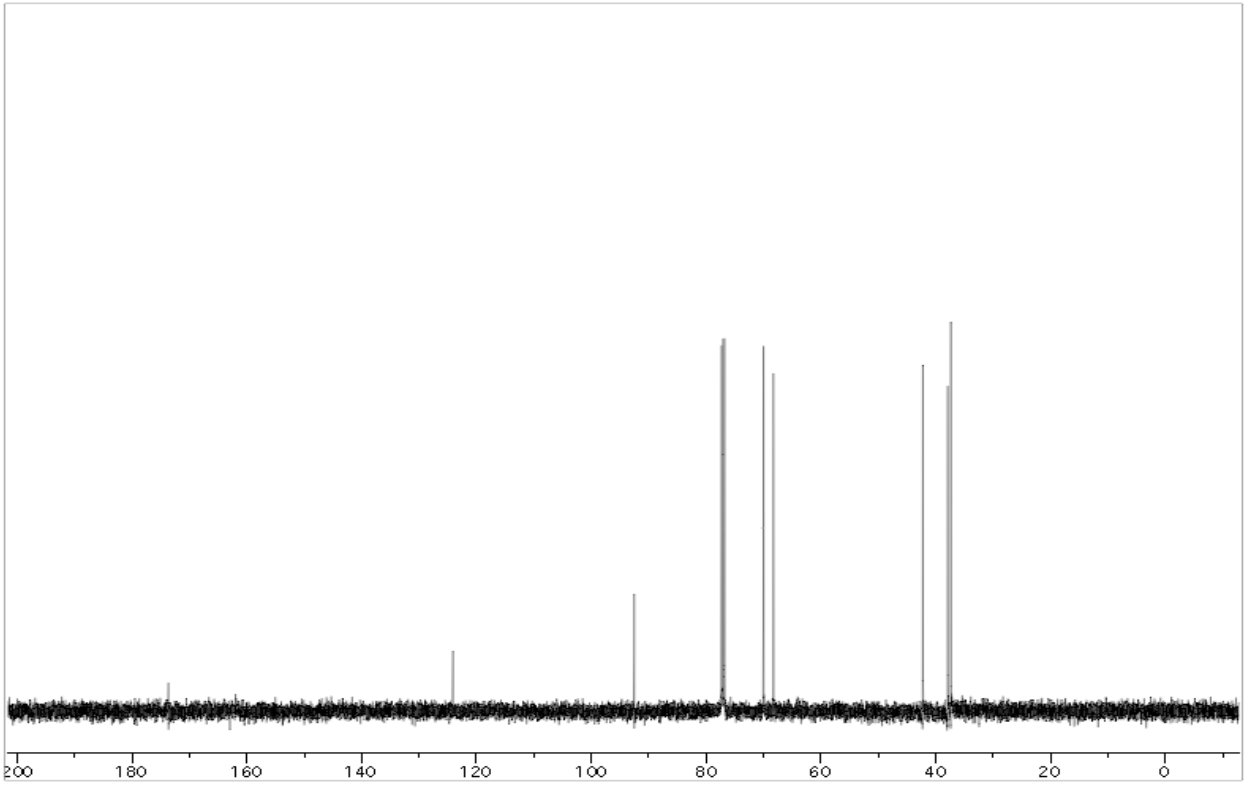
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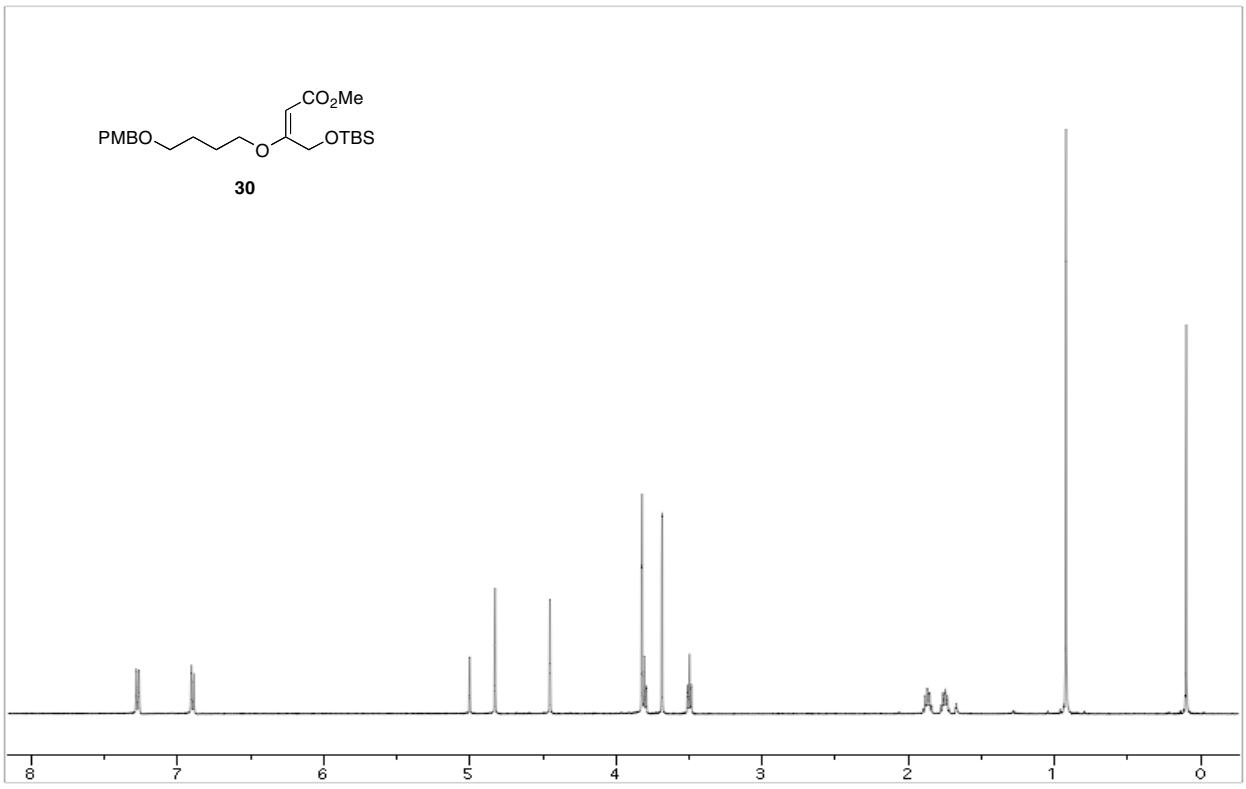
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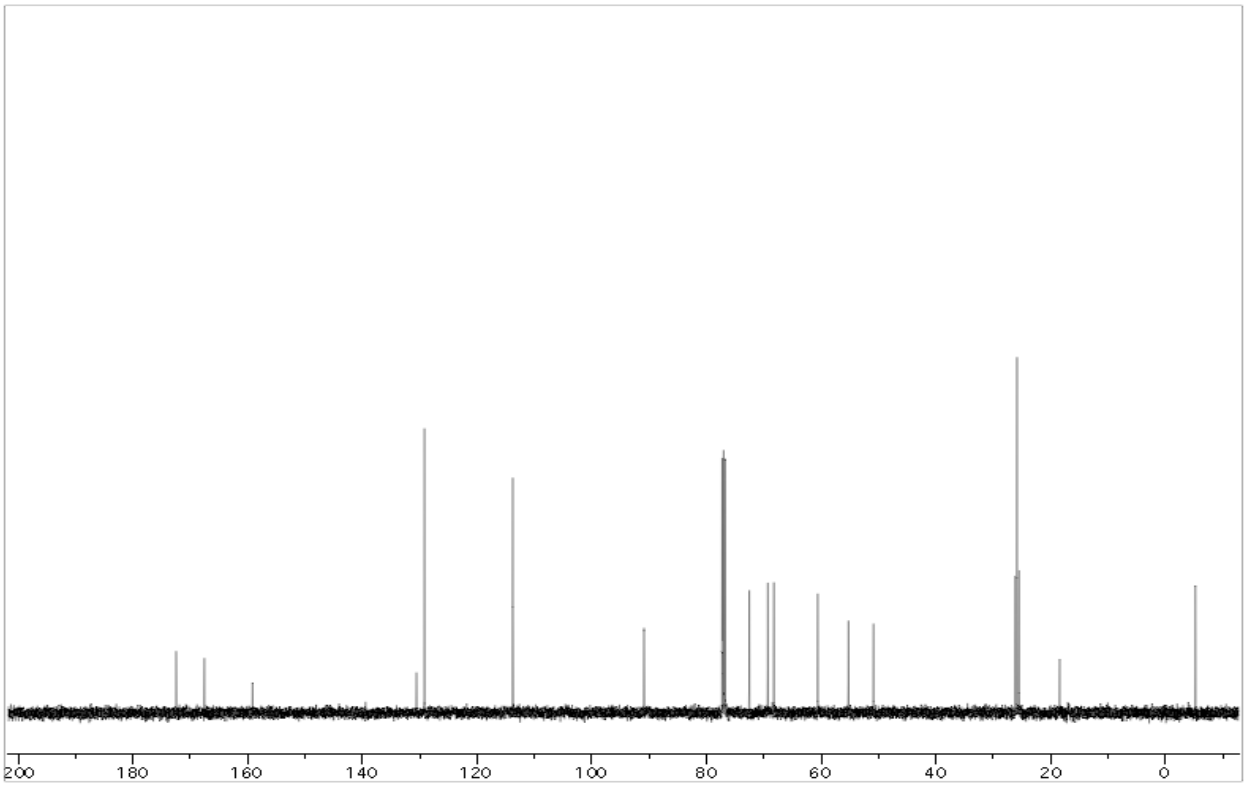
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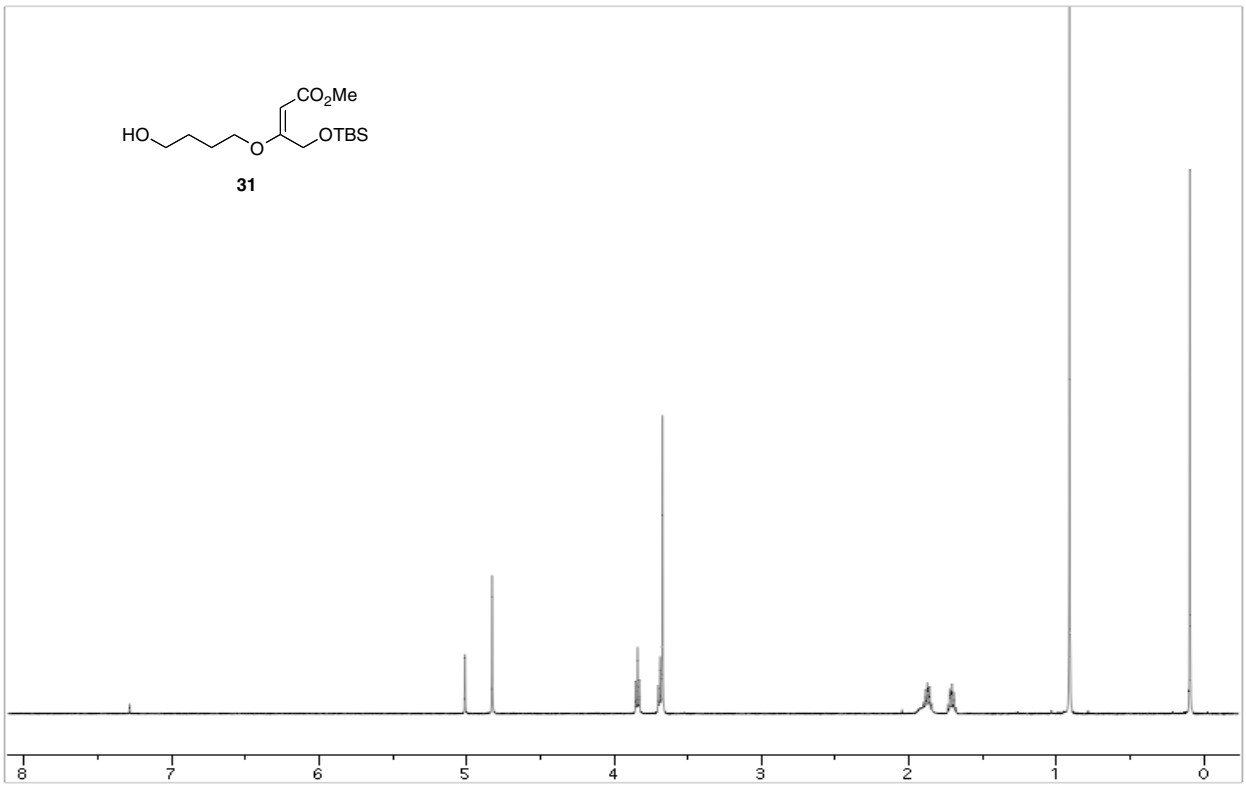
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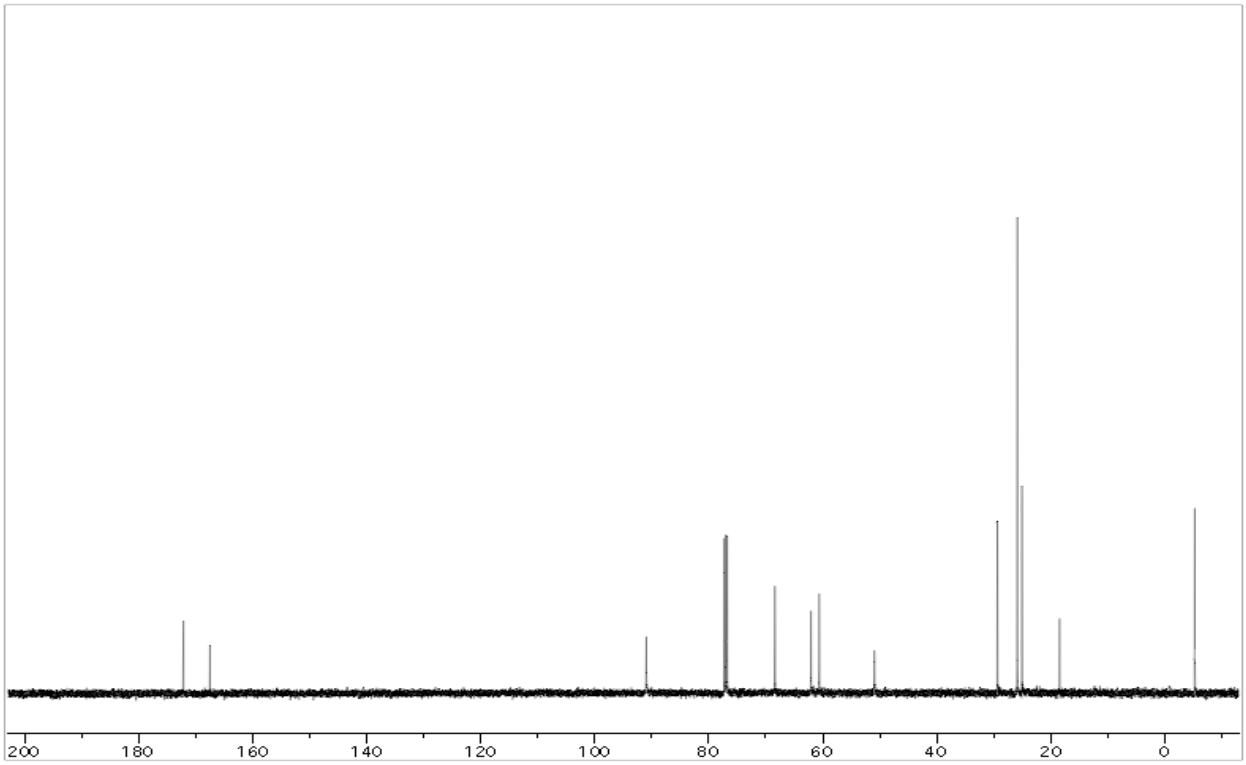
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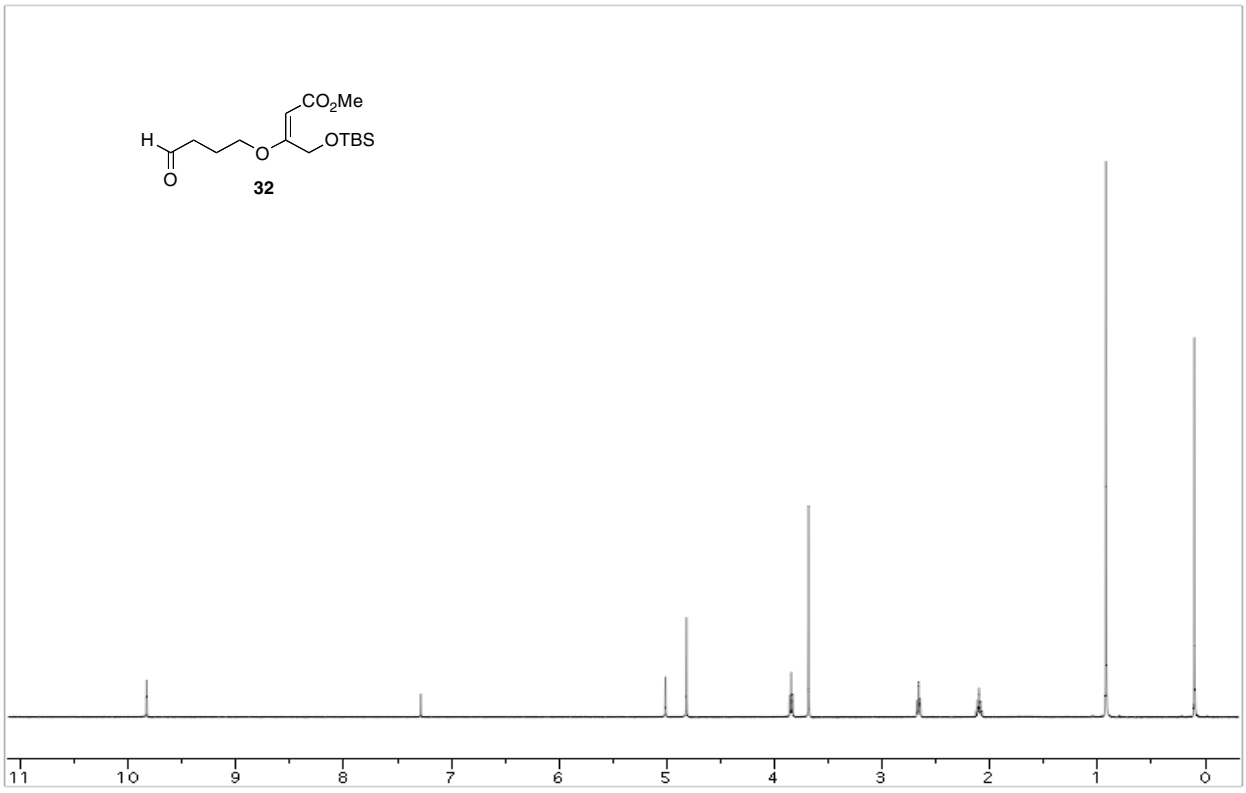
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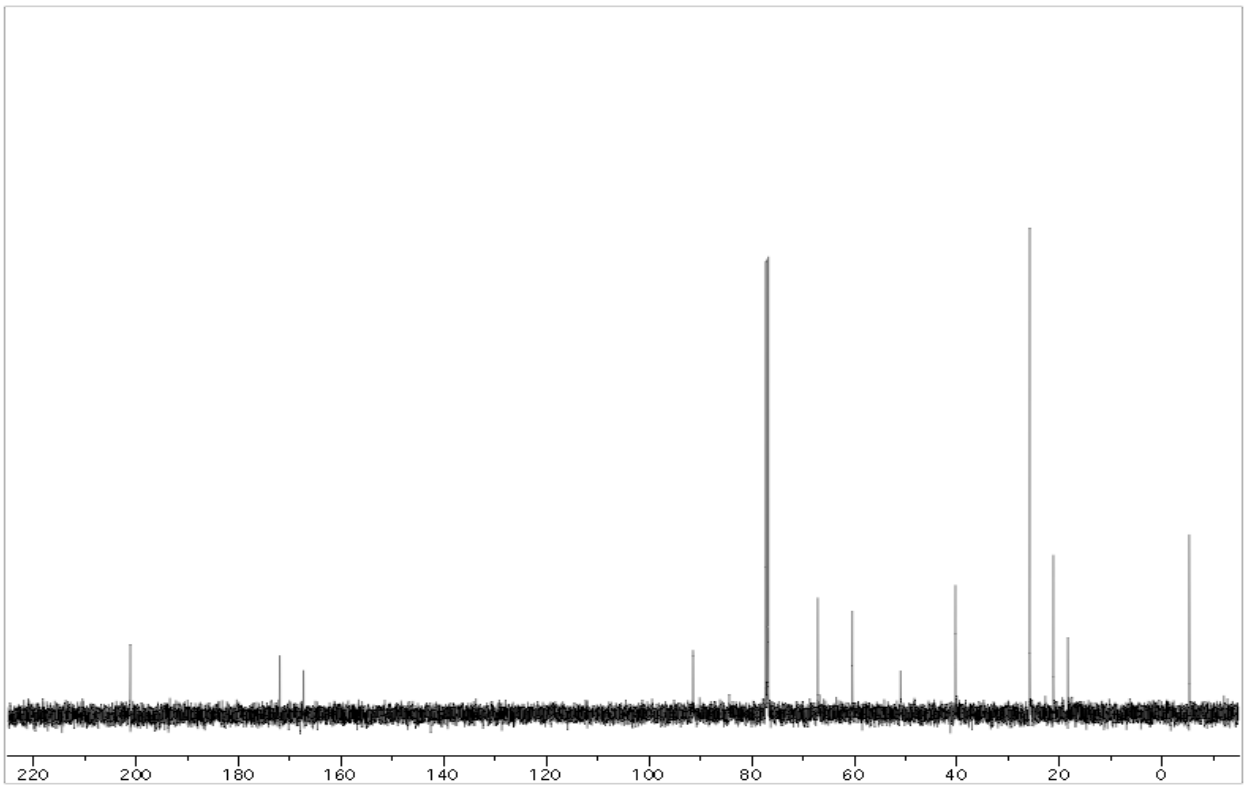
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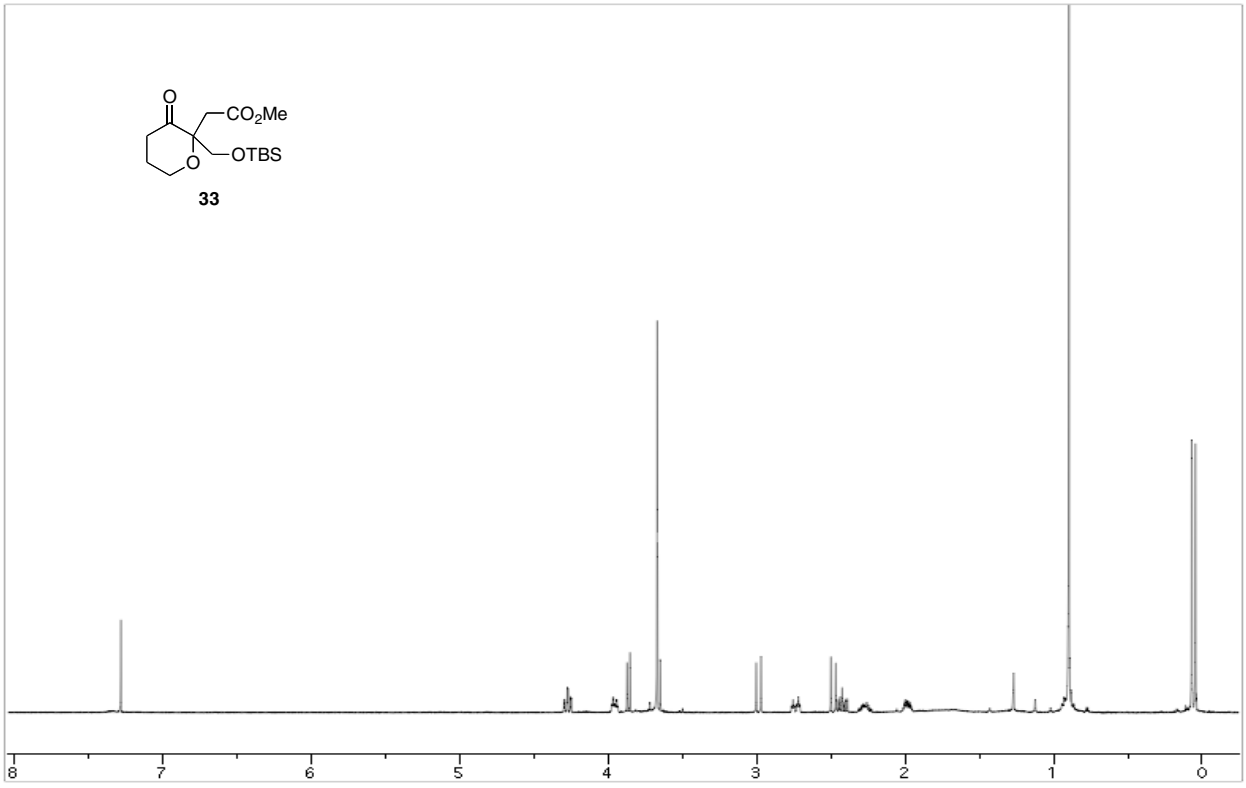
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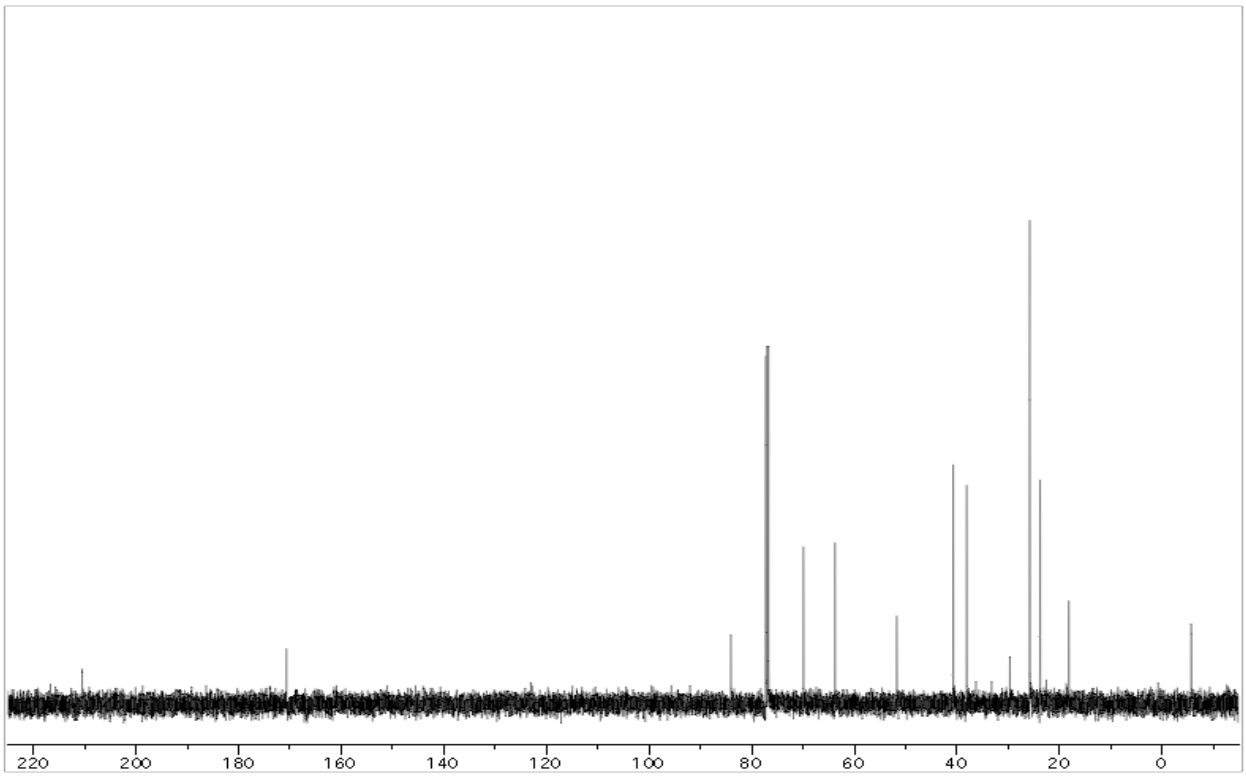
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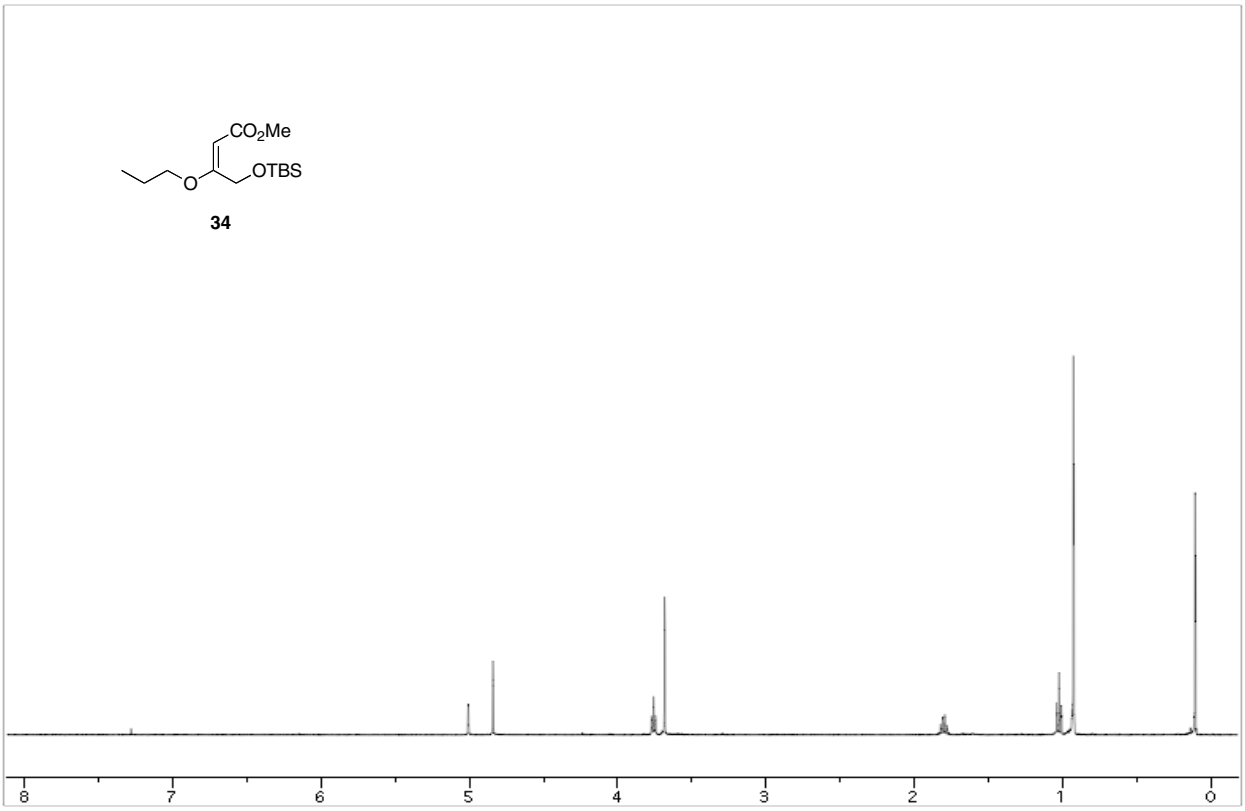
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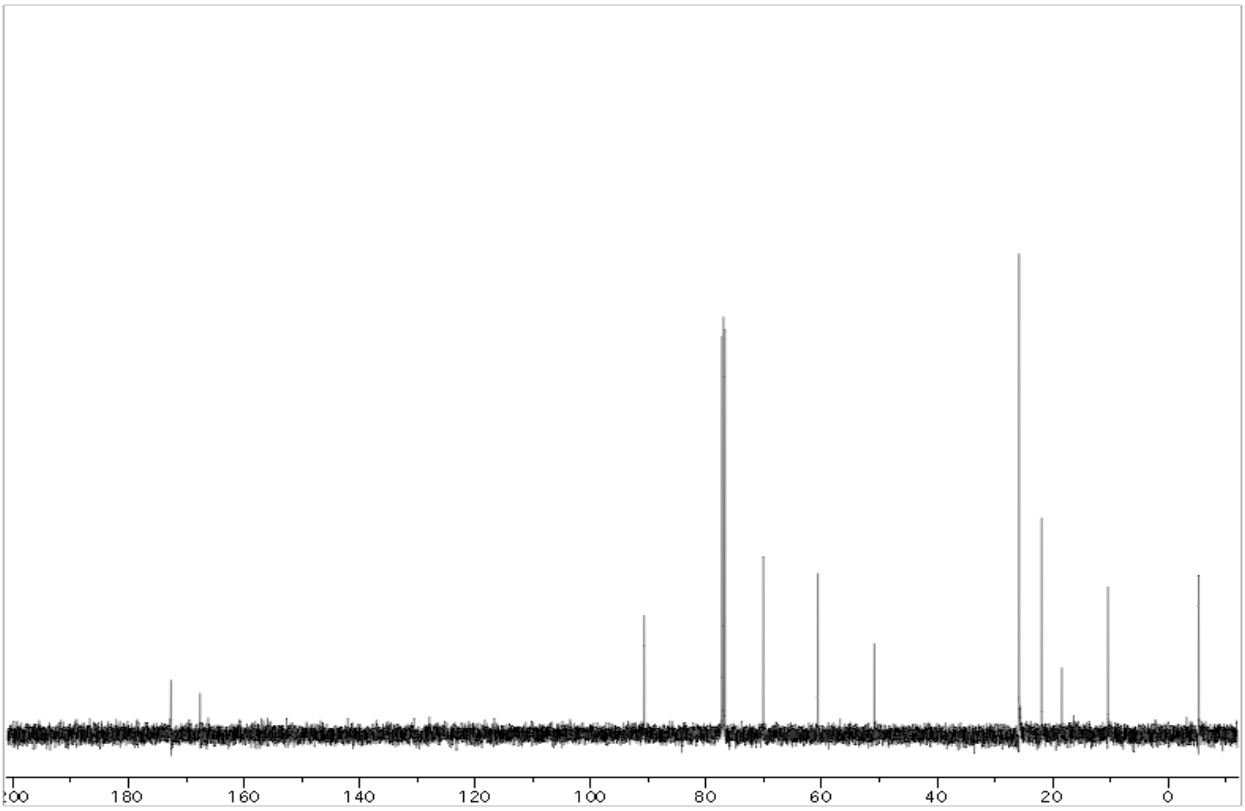
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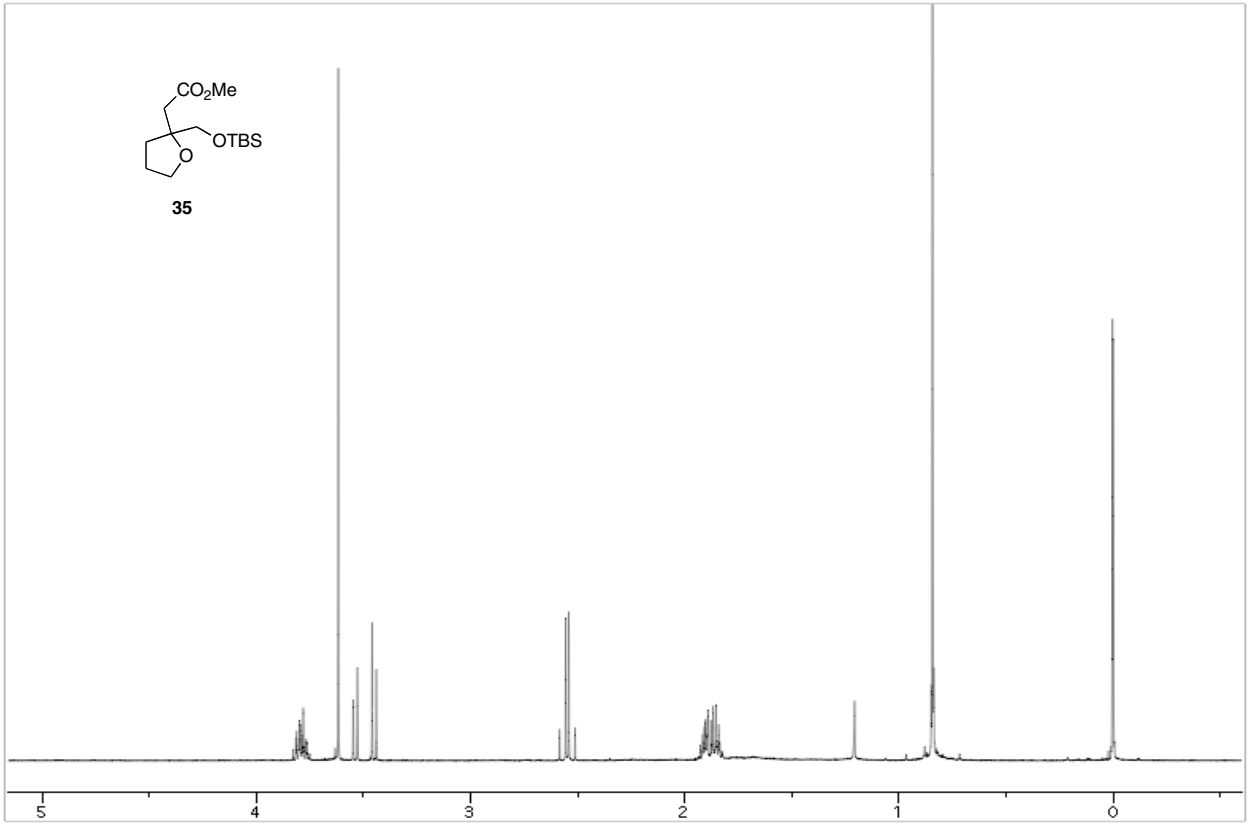
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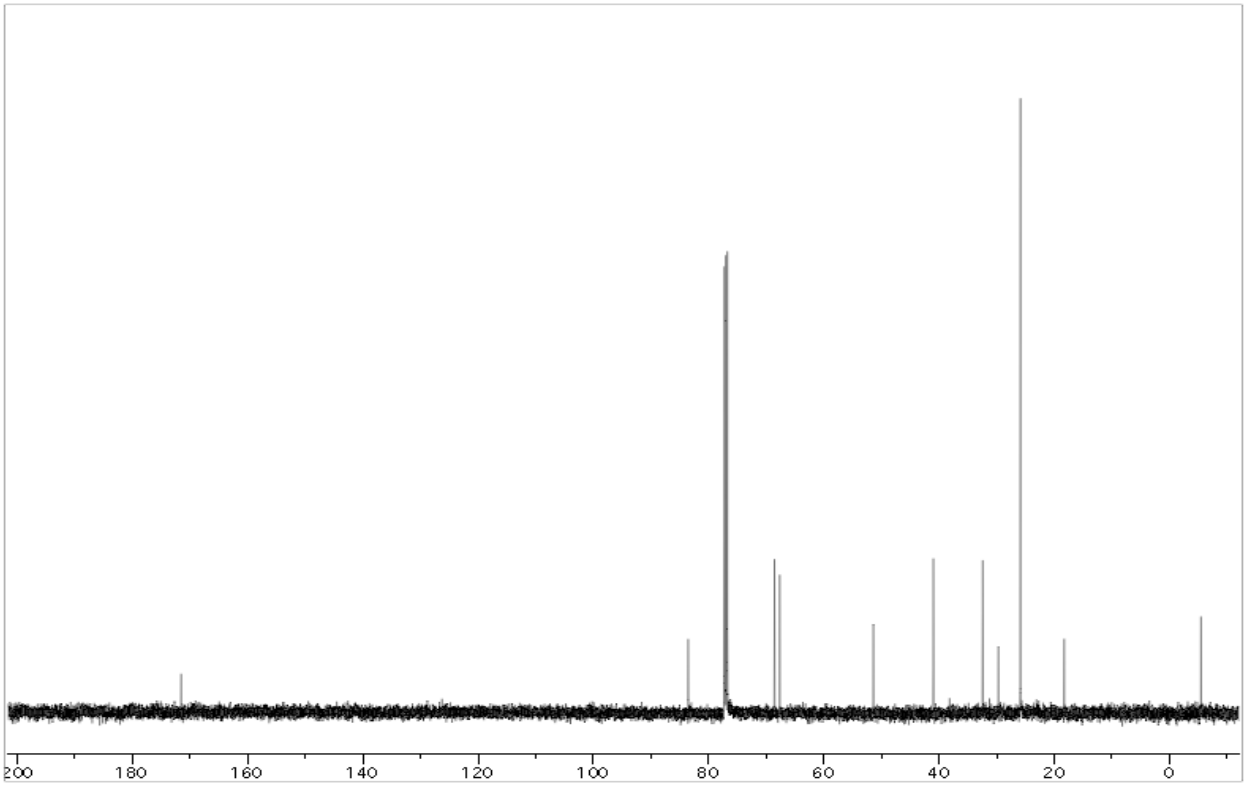
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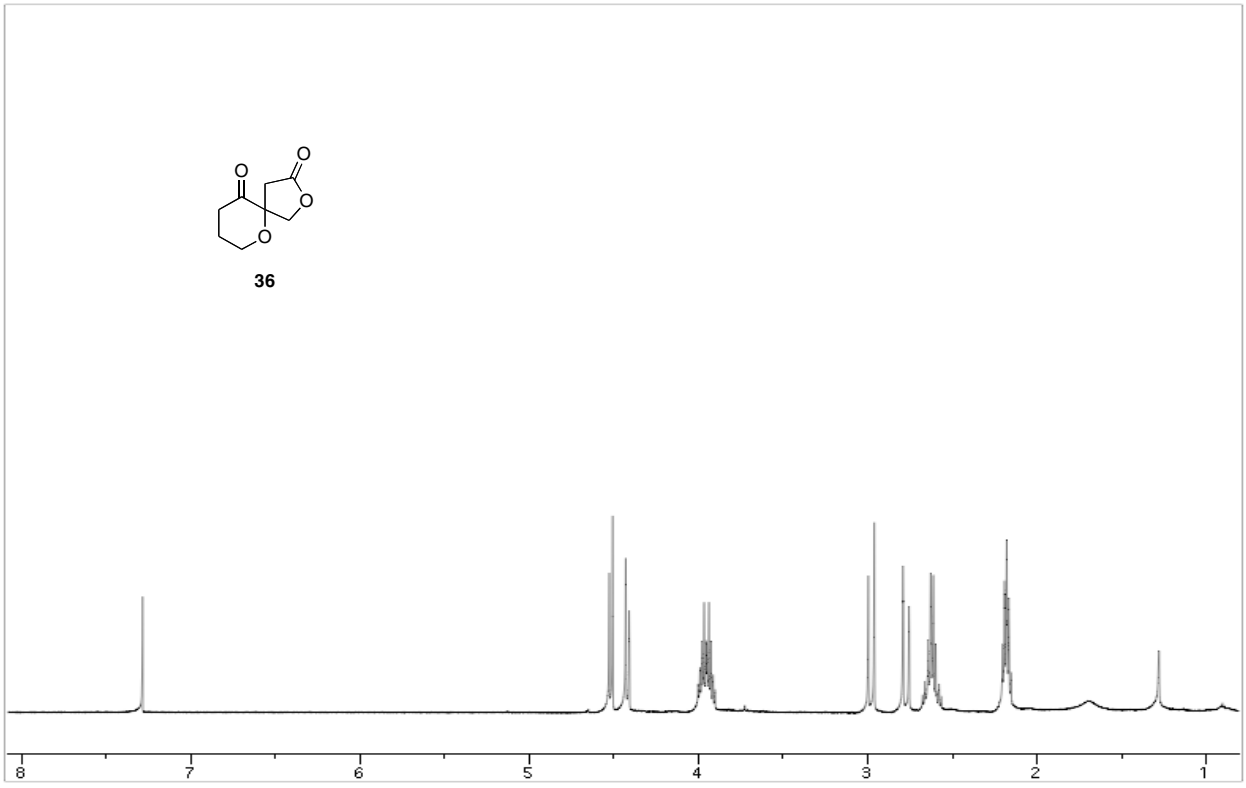
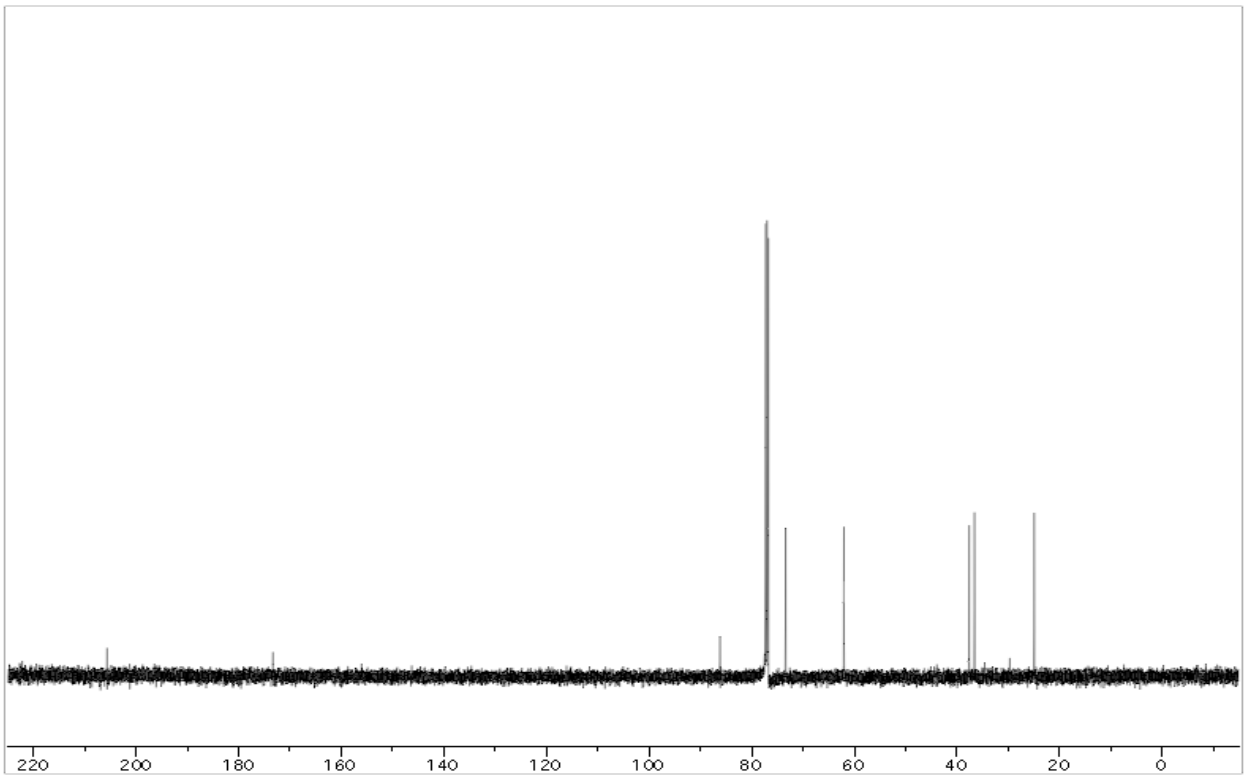
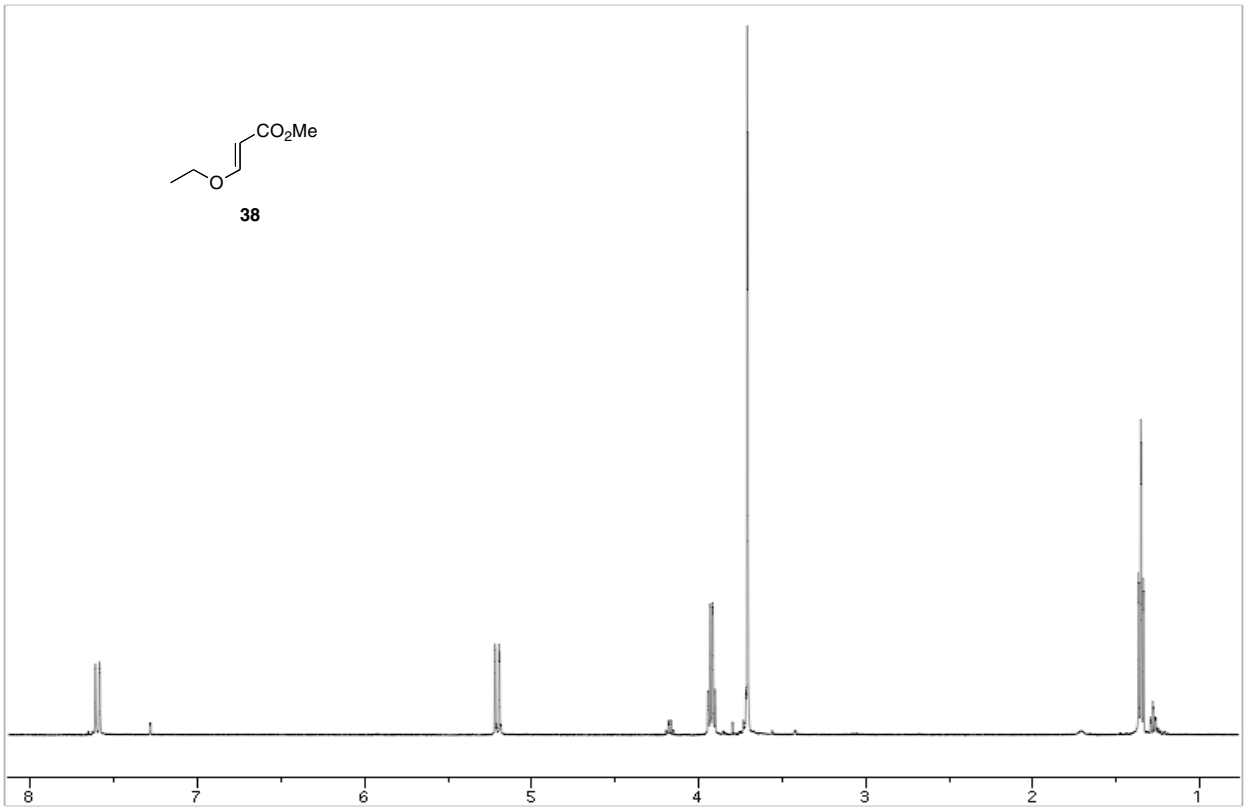
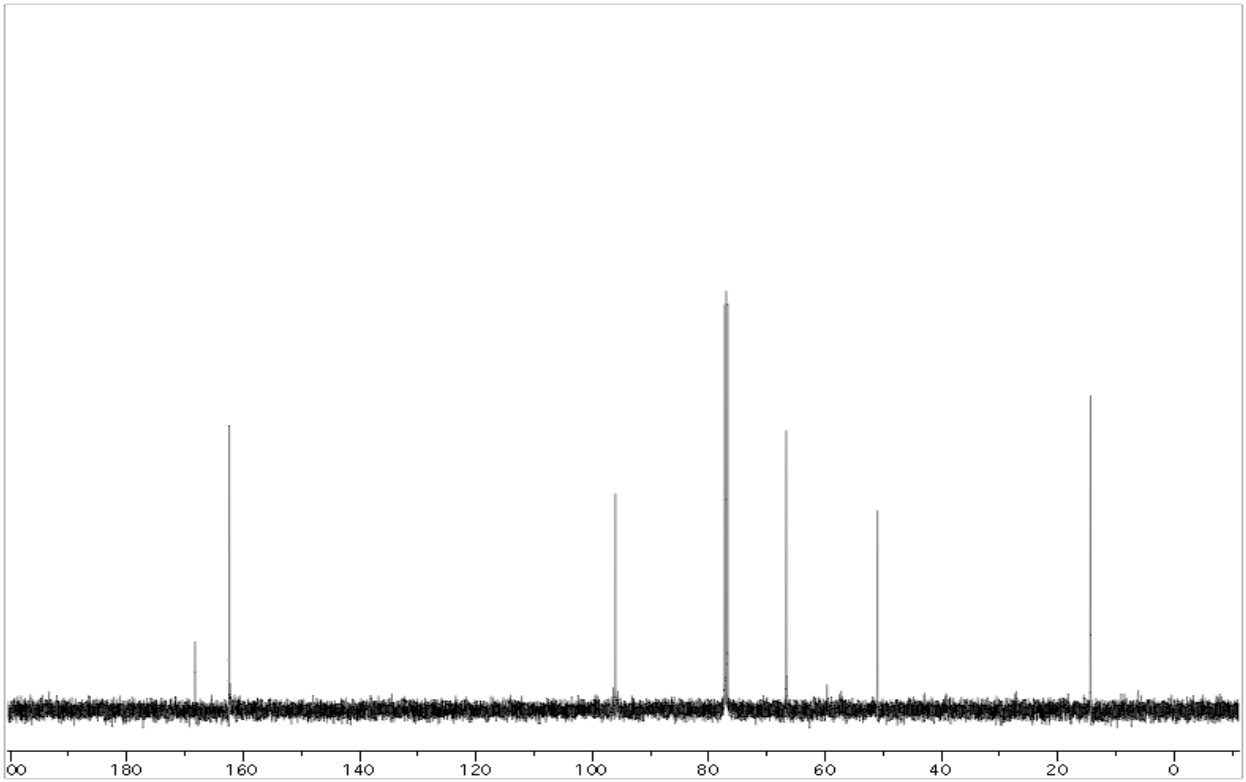
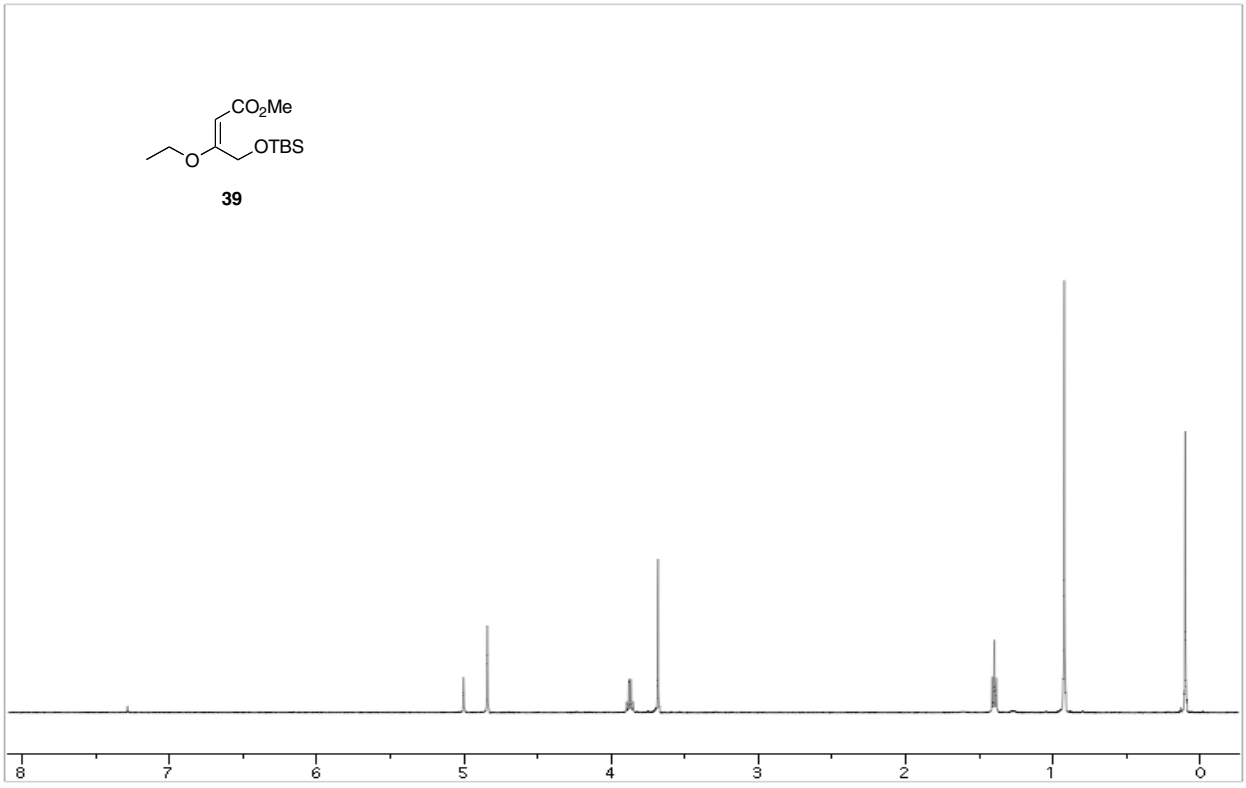

O
O
O
O
36
8
7
6
5
4
3
2
1

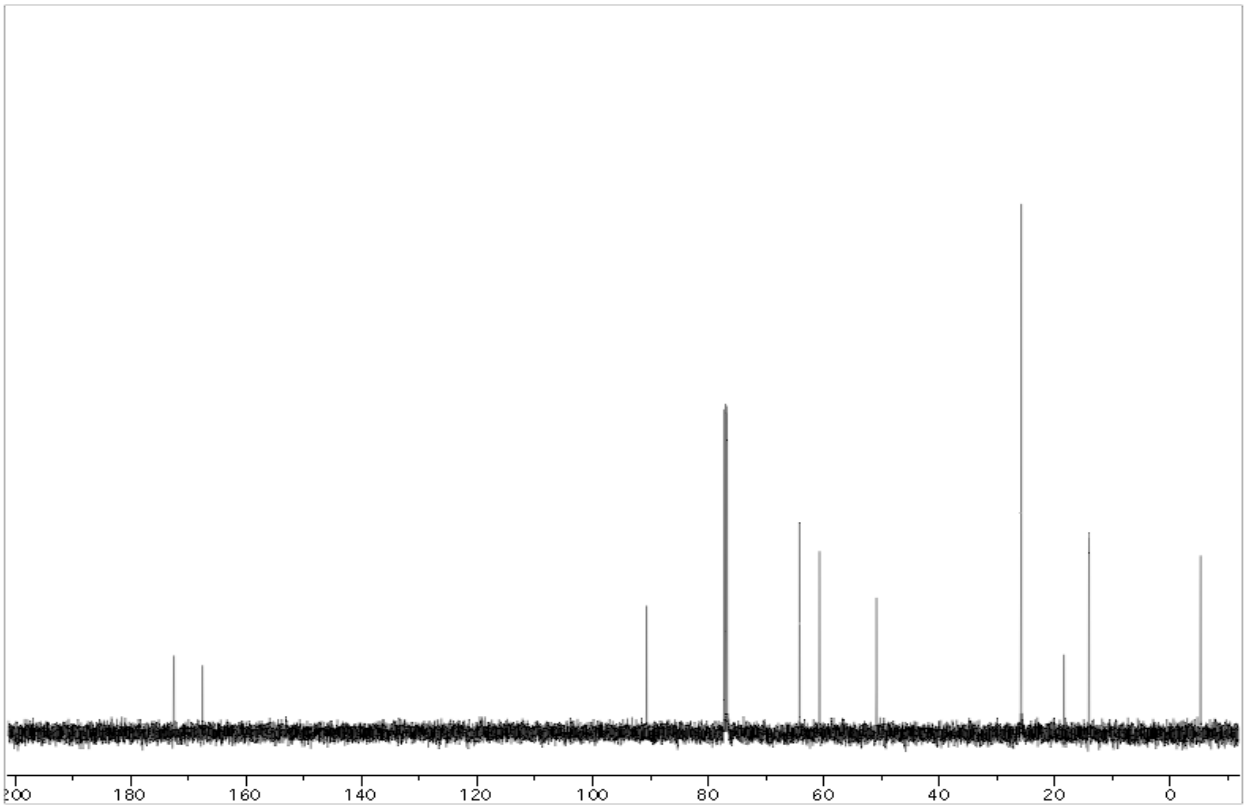

220
200
180
160
140
120
100
80
60
40
20
0


CO2Me
O
38
8
7
6
5
4
3
2
1


00
180
160
140
120
100
80
60
40
20
0



39



1.4 COMPUTATIONAL DATA

Gaussian Archive entries for *ab initio* and DFT optimised structures (**40**-**49**).

5-Membered parent system 40 (n=1, R=H)

Acyl radical 40 (n=1, R=H)

HF/3-21G*

1\1\GINC-GOMBERG01\POpt\UHF\3-21G*\C5H7O2(2)\HMAITKEN\07-Oct-2010\1\\#
HF/3-21G* opt=(grad)\\calc of 5 exo starting radical\\0,2\O\C,1,B1\C,2
,B2,1,A1\C,3,B3,2,A2,1,D1,0\O,4,B4,3,A3,2,D2,0\C,5,B5,4,A4,3,D3,0\C,6,
B6,5,A5,4,D4,0\H,7,B7,6,A6,5,D5,0\H,7,B8,6,A7,5,D6,0\H,6,B9,5,A8,4,D7,
0\H,4,B10,3,A9,2,D8,0\H,4,B11,3,A10,2,D9,0\H,3,B12,4,A11,5,D10,0\H,3,B
13,4,A12,5,D11,0\\B1=1.18614471\B2=1.50912597\B3=1.52694762\B4=1.43590
99\B5=1.37414064\B6=1.31484692\B7=1.07031043\B8=1.07072037\B9=1.070115
02\B10=1.08185828\B11=1.08185828\B12=1.08231421\B13=1.08231421\A1=130.
19023444\A2=111.32610613\A3=105.38258671\A4=119.72012652\A5=127.770708
33\A6=119.49551521\A7=123.61020176\A8=109.81097055\A9=110.77612972\A10
=110.77612972\A11=110.09660809\A12=110.09660809\D1=0.\D2=180.\D3=-180.
\D4=0.\D5=180.\D6=0.\D7=180.\D8=60.31836182\D9=-60.31836182\D10=59.210
47756\D11=-59.21047756\\Version=AM64L-G03RevE.01\State=2-A'\HF=-341.14
50959\S2=0.769763\S2-1=0.\S2A=0.750192\RMSD=2.719e-09\RMSF=6.928e-05\T
hermal=0.\Dipole=0.5056641,0.,0.5649685\PG=CS [SG(C5H3O2),X(H4)]\\@

HF/6-31G*

1\1\GINC-GOMBERG15\POpt\UHF\6-31G(d)\C5H7O2(2)\HMAITKEN\29-Sep-2010\1\
\#HF/6-31G* opt=(grad,readfc) geom=checkpoint guess=read\\calc of 5 ex
o starting radical\\0,2\O\C,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\O,4,B4
,3,A3,2,D2,0\C,5,B5,4,A4,3,D3,0\C,6,B6,5,A5,4,D4,0\H,7,B7,6,A6,5,D5,0\
H,7,B8,6,A7,5,D6,0\H,6,B9,5,A8,4,D7,0\H,4,B10,3,A9,2,D8,0\H,4,B11,3,A1
0,2,D9,0\H,3,B12,4,A11,5,D10,0\H,3,B13,4,A12,5,D11,0\\B1=1.16605202\B2
=1.51399368\B3=1.5215602\B4=1.40143012\B5=1.34506573\B6=1.31936324\B7=
1.07300442\B8=1.07302412\B9=1.07372429\B10=1.08405062\B11=1.08405062\B
12=1.08459205\B13=1.08459205\A1=128.88738653\A2=112.59154563\A3=106.72
426216\A4=118.48748437\A5=128.40570005\A6=118.82470368\A7=123.94348924
\A8=109.95343701\A9=110.62677985\A10=110.62677985\A11=110.75708237\A12
=110.75708237\D1=0.\D2=180.\D3=-180.\D4=0.\D5=180.\D6=0.\D7=180.\D8=59
.89458699\D9=-59.89458698\D10=59.01601493\D11=-59.01601493\\Version=AM
64L-G03RevE.01\State=2-A'\HF=-343.0596823\S2=0.761466\S2-1=0.\S2A=0.75
0097\RMSD=8.767e-09\RMSF=1.548e-05\Thermal=0.\Dipole=0.408639,0.,0.610
6742\PG=CS [SG(C5H3O2),X(H4)]\\@

HF/6-311G**

1\1\GINC-GOMBERG15\POpt\UHF\6-311G(d,p)\C5H7O2(2)\HMAITKEN\29-Sep-2010
\1\\#HF/6-311G** opt=(grad,readfc) geom=checkpoint guess=read\\calc of
5 exo starting radical\\0,2\O\C,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\O
,4,B4,3,A3,2,D2,0\C,5,B5,4,A4,3,D3,0\C,6,B6,5,A5,4,D4,0\H,7,B7,6,A6,5,
D5,0\H,7,B8,6,A7,5,D6,0\H,6,B9,5,A8,4,D7,0\H,4,B10,3,A9,2,D8,0\H,4,B11
,3,A10,2,D9,0\H,3,B12,4,A11,5,D10,0\H,3,B13,4,A12,5,D11,0\\B1=1.158810
5\B2=1.51335946\B3=1.52019049\B4=1.40078789\B5=1.34216872\B6=1.3192651
2\B7=1.07330101\B8=1.07333715\B9=1.0745465\B10=1.08525095\B11=1.085250
95\B12=1.08478817\B13=1.08478817\A1=129.35854999\A2=112.78187916\A3=10
6.77877013\A4=118.67377441\A5=128.38803552\A6=118.58528222\A7=123.9216

9633\A8=110.11710985\A9=110.53774596\A10=110.53774596\A11=110.86829888
\A12=110.86829888\D1=0.\D2=180.\D3=-180.\D4=0.\D5=180.\D6=0.\D7=180.\D
8=59.84843983\D9=-59.84843983\D10=59.16091942\D11=-59.16091942\\Versio
n=AM64L-G03RevE.01\State=2-A'\HF=-343.1490046\S2=0.761623\S2-1=0.\S2A=
0.750097\RMSD=4.168e-09\RMSF=6.460e-05\Thermal=0.\Dipole=0.4374896,0.,
0.6031374\PG=CS [SG(C5H3O2),X(H4)]\\@

BHandHLYP/6-311G**

1\1\GINC-GOMBERG15\POpt\UBHandHLYP\6-311G(d,p)\C5H7O2(2)\HMAITKEN\29-S
ep-2010\1\\#BHandHLYP/6-311G** opt=(grad,readfc) geom=checkpoint guess
=read\\calc of 5 exo starting radical\\0,2\O\C,1,B1\C,2,B2,1,A1\C,3,B3
,2,A2,1,D1,0\O,4,B4,3,A3,2,D2,0\C,5,B5,4,A4,3,D3,0\C,6,B6,5,A5,4,D4,0\
H,7,B7,6,A6,5,D5,0\H,7,B8,6,A7,5,D6,0\H,6,B9,5,A8,4,D7,0\H,4,B10,3,A9,
2,D8,0\H,4,B11,3,A10,2,D9,0\H,3,B12,4,A11,5,D10,0\H,3,B13,4,A12,5,D11,
0\\B1=1.16815993\B2=1.50631895\B3=1.51524965\B4=1.4056914\B5=1.3456342
3\B6=1.32150402\B7=1.07380799\B8=1.07401309\B9=1.07621926\B10=1.087538
04\B11=1.08753804\B12=1.08601839\B13=1.08601839\A1=128.18208343\A2=112
.95192769\A3=106.88766918\A4=117.65365713\A5=128.05965349\A6=118.75110
254\A7=123.71453559\A8=109.99371254\A9=110.60241069\A10=110.60241069\A
11=110.97081604\A12=110.97081604\D1=0.\D2=180.\D3=-180.\D4=0.\D5=180.\
D6=0.\D7=180.\D8=59.7764479\D9=-59.7764479\D10=58.99630506\D11=-58.996
30506\\Version=AM64L-G03RevE.01\State=2-A'\HF=-344.9897763\S2=0.754838
\S2-1=0.\S2A=0.750014\RMSD=9.122e-09\RMSF=9.136e-05\Thermal=0.\Dipole=
0.4461392,0.,0.5036152\PG=CS [SG(C5H3O2),X(H4)]\\@

BHandHLYP/6-311++G**

1\1\GINC-GOMBERG03\POpt\UBHandHLYP\6-311++G(d,p)\C5H7O2(2)\HMAITKEN\09
-Oct-2010\1\\#BHandHLYP/6-311++G(d,p) opt=(grad,readfc) geom=checkpoin
t guess=read\\calc of 5 exo starting radical\\0,2\O\C,1,B1\C,2,B2,1,A1
\C,3,B3,2,A2,1,D1,0\O,4,B4,3,A3,2,D2,0\C,5,B5,4,A4,3,D3,0\C,6,B6,5,A5,
4,D4,0\H,7,B7,6,A6,5,D5,0\H,7,B8,6,A7,5,D6,0\H,6,B9,5,A8,4,D7,0\H,4,B1
0,3,A9,2,D8,0\H,4,B11,3,A10,2,D9,0\H,3,B12,4,A11,5,D10,0\H,3,B13,4,A12
,5,D11,0\\B1=1.16811665\B2=1.5047788\B3=1.5158375\B4=1.40628919\B5=1.3
458143\B6=1.32324538\B7=1.0738882\B8=1.07421567\B9=1.07617597\B10=1.08
744523\B11=1.08744523\B12=1.0861989\B13=1.0861989\A1=128.71487208\A2=1
13.0778557\A3=106.91686747\A4=117.74775105\A5=127.90320216\A6=118.6215
7583\A7=123.81197714\A8=110.11797654\A9=110.66910647\A10=110.66910647\
A11=111.07042942\A12=111.07042942\D1=0.\D2=180.\D3=-180.\D4=0.\D5=180.
\D6=0.\D7=180.\D8=59.88887523\D9=-59.88887522\D10=59.03851948\D11=-59.
03851948\\Version=AM64L-G03RevE.01\State=2-A'\HF=-344.9974478\S2=0.755
029\S2-1=0.\S2A=0.750015\RMSD=7.503e-09\RMSF=1.288e-04\Thermal=0.\Dipo
le=0.4821363,0.,0.5156878\PG=CS [SG(C5H3O2),X(H4)]\\@

Cyclization transition state 44

HF/3-21G*

1\1\GINC-GOMBERG15\FTS\UHF\3-21G*\C5H7O2(2)\HMAITKEN\29-Sep-2010\1\\#H
F/3-21G* opt=(grad,maxcyc=500,ts,nofreeze,noeigentest) geom=checkpoint
guess=read\\calc of 5-exo benchmark ts\\0,2\C\C,1,B1\C,2,B2,1,A1\O,3,
B3,2,A2,1,D1,0\C,1,B4,3,A3,2,D2,0\C,5,B5,4,A4,3,D3,0\O,1,B6,2,A5,3,D4,
0\H,2,B7,1,A6,4,D5,0\H,2,B8,1,A7,4,D6,0\H,3,B9,2,A8,1,D7,0\H,3,B10,2,A
9,1,D8,0\H,5,B11,4,A10,3,D9,0\H,6,B12,5,A11,4,D10,0\H,6,B13,5,A12,4,D1
1,0\\B1=1.51511204\B2=1.52793048\B3=1.44256549\B6=1.18830218\B7=1.0844

2828\B8=1.0821966\B9=1.07647787\B10=1.08392163\B11=1.07444046\B12=1.07
084865\B13=1.07054332\A1=105.84467067\A2=107.49422179\A3=62.2932733\A4
=117.73195317\A5=132.56936355\A6=108.11734684\A7=110.60836061\A8=112.7
0647831\A9=110.29565761\A10=115.6383251\A11=119.96932639\A12=120.52072
763\D1=47.33209843\D2=153.06942335\D3=142.47402714\D4=-195.4494289\D5=
92.48395053\D6=-147.73707385\D7=164.3492718\D8=-72.88357578\D9=-63.695
00647\D10=-14.57434129\D11=169.99347494\B4=2.18344097\B5=1.37547777\\V
ersion=AM64L-G03RevE.01\State=2-A\HF=-341.125959\S2=1.021666\S2-1=0.\S
2A=0.77273\RMSD=8.361e-09\RMSF=2.061e-05\Thermal=0.\Dipole=0.114034,-0
.3597978,0.81868\PG=C01 [X(C5H7O2)]\\@

HF/6-31G*

1\1\GINC-GOMBERG01\FTS\UHF\6-31G(d)\C5H7O2(2)\HMAITKEN\07-Oct-2010\1\\
#HF/6-31G* opt=(grad,maxcyc=500,ts,nofreeze,noeigentest,readfc) scf=qc
scfcyc=500 geom=checkpoint guess=read\\calc of 5-exo benchmark\\0,2\C
\C,1,B1\C,2,B2,1,A1\O,3,B3,2,A2,1,D1,0\C,1,B4,3,A3,2,D2,0\C,5,B5,4,A4,
3,D3,0\O,1,B6,2,A5,3,D4,0\H,2,B7,1,A6,4,D5,0\H,2,B8,1,A7,4,D6,0\H,3,B9
,2,A8,1,D7,0\H,3,B10,2,A9,1,D8,0\H,5,B11,4,A10,3,D9,0\H,6,B12,5,A11,4,
D10,0\H,6,B13,5,A12,4,D11,0\\B1=1.51219846\B2=1.52310769\B3=1.40272163
\B6=1.16836215\B7=1.08587365\B8=1.08419475\B9=1.07965323\B10=1.0880639
5\B11=1.07898264\B12=1.07348406\B13=1.07280003\A1=105.99236352\A2=108.
26426199\A3=60.58280919\A4=118.03982396\A5=130.93411009\A6=107.7069011
\A7=110.14292583\A8=112.55532853\A9=110.53440238\A10=114.98605248\A11=
120.59823598\A12=120.00832823\D1=44.22277675\D2=158.28891697\D3=149.37
72035\D4=-192.99090414\D5=95.08299526\D6=-146.48860284\D7=162.23785302
\D8=-76.46544744\D9=-60.42773504\D10=-17.91056283\D11=169.65760531\B4=
2.16435377\B5=1.38522593\\Version=AM64L-G03RevE.01\State=2-A\HF=-343.0
349072\S2=1.008414\S2-1=0.\S2A=0.762276\RMSD=0.000e+00\RMSF=4.990e-05\
Thermal=0.\Dipole=-0.2345857,0.877681,0.1317932\PG=C01 [X(C5H7O2)]\\@

HF/6-311G**

1\1\GINC-GOMBERG01\FTS\UHF\6-311G(d,p)\C5H7O2(2)\HMAITKEN\06-Oct-2010\
1\\#HF/6-311G** opt=(grad,maxcyc=500,ts,nofreeze,noeigentest,readfc) g
eom=checkpoint guess=read\\calc of 5-exo benchmark\\0,2\C\C,1,B1\C,2,B
2,1,A1\O,3,B3,2,A2,1,D1,0\C,1,B4,3,A3,2,D2,0\C,5,B5,4,A4,3,D3,0\O,1,B6
,2,A5,3,D4,0\H,2,B7,1,A6,4,D5,0\H,2,B8,1,A7,4,D6,0\H,3,B9,2,A8,1,D7,0\
H,3,B10,2,A9,1,D8,0\H,5,B11,4,A10,3,D9,0\H,6,B12,5,A11,4,D10,0\H,6,B13
,5,A12,4,D11,0\\B1=1.51095614\B2=1.52222296\B3=1.40197339\B6=1.1615191
3\B7=1.08618083\B8=1.08438409\B9=1.0798046\B10=1.08913007\B11=1.079838
95\B12=1.07415988\B13=1.07335701\A1=105.91052819\A2=108.19180092\A3=60
.66761155\A4=118.07239547\A5=131.42145209\A6=107.47779394\A7=110.05068
15\A8=112.55605475\A9=110.46736012\A10=115.00410955\A11=120.44581472\A
12=119.86973566\D1=44.30315225\D2=158.07959591\D3=149.20864153\D4=-193
.5601363\D5=94.88996303\D6=-146.62033628\D7=162.426449\D8=-76.26082704
\D9=-60.82293345\D10=-18.07366877\D11=169.82483332\B4=2.15425134\B5=1.
38464284\\Version=AM64L-G03RevE.01\State=2-A\HF=-343.1215054\S2=0.9991
98\S2-1=0.\S2A=0.761437\RMSD=5.439e-09\RMSF=4.873e-05\Thermal=0.\Dipol
e=0.1970722,-0.3184589,0.8488552\PG=C01 [X(C5H7O2)]\\@

BHandHLYP/6-311G**

1\1\GINC-GOMBERG03\FTS\UBHandHLYP\6-311G(d,p)\C5H7O2(2)\HMAITKEN\09-Oc
t-2010\1\\#BHandHLYP/6-311G** opt=(grad,maxcyc=500,ts,nofreeze,noeigen
test,readfc) geom=checkpoint guess=read\\calc of 5-exo benchmark\\0,2\

C\C,1,B1\C,2,B2,1,A1\O,3,B3,2,A2,1,D1,0\C,1,B4,3,A3,2,D2,0\C,5,B5,4,A4
,3,D3,0\O,1,B6,2,A5,3,D4,0\H,2,B7,1,A6,4,D5,0\H,2,B8,1,A7,4,D6,0\H,3,B
9,2,A8,1,D7,0\H,3,B10,2,A9,1,D8,0\H,5,B11,4,A10,3,D9,0\H,6,B12,5,A11,4
,D10,0\H,6,B13,5,A12,4,D11,0\\B1=1.50605725\B2=1.51732387\B3=1.4073487
4\B6=1.16769715\B7=1.08739584\B8=1.08552735\B9=1.0811113\B10=1.0906733
5\B11=1.08184948\B12=1.07465015\B13=1.0734564\A1=105.96349043\A2=108.0
2782282\A3=60.76154198\A4=118.82459767\A5=131.38891867\A6=107.66295469
\A7=109.61851488\A8=112.72500645\A9=110.44129373\A10=115.06904\A11=120
.46424741\A12=120.10806844\D1=44.81290635\D2=157.99718922\D3=148.81322
459\D4=-189.69659532\D5=94.8658689\D6=-146.99301601\D7=162.67763092\D8
=-75.77489932\D9=-57.72926952\D10=-16.17168937\D11=168.95892619\B4=2.1
603985\B5=1.36055002\\Version=AM64L-G03RevE.01\State=2-A\HF=-344.96588
08\S2=0.819781\S2-1=0.\S2A=0.750722\RMSD=2.754e-09\RMSF=8.627e-05\Ther
mal=0.\Dipole=0.0632578,-0.4217693,0.8613759\PG=C01 [X(C5H7O2)]\\@

BHandHLYP/6-311++G(d,p)

1\1\GINC-GOMBERG03\FTS\UBHandHLYP\6-311++G(d,p)\C5H7O2(2)\HMAITKEN\09-
Oct-2010\1\\#BHandHLYP/6-311++G** opt=(grad,maxcyc=500,ts,nofreeze,noe
igentest,readfc) geom=checkpoint guess=read\\calc of 5-exo benchmark\\
0,2\C\C,1,B1\C,2,B2,1,A1\O,3,B3,2,A2,1,D1,0\C,1,B4,3,A3,2,D2,0\C,5,B5,
4,A4,3,D3,0\O,1,B6,2,A5,3,D4,0\H,2,B7,1,A6,4,D5,0\H,2,B8,1,A7,4,D6,0\H
,3,B9,2,A8,1,D7,0\H,3,B10,2,A9,1,D8,0\H,5,B11,4,A10,3,D9,0\H,6,B12,5,A
11,4,D10,0\H,6,B13,5,A12,4,D11,0\\B1=1.50415825\B2=1.51721975\B3=1.408
16264\B6=1.16832362\B7=1.08751567\B8=1.08569026\B9=1.08119199\B10=1.09
044456\B11=1.08165161\B12=1.07482824\B13=1.07361797\A1=106.12315787\A2
=108.06570776\A3=60.77005719\A4=118.96688304\A5=131.3909129\A6=107.667
40672\A7=109.49268957\A8=112.70191537\A9=110.5374977\A10=114.99290812\
A11=120.6769346\A12=119.92401746\D1=44.48199743\D2=158.29568003\D3=148
.78564879\D4=-189.4641284\D5=95.23780668\D6=-146.70515174\D7=162.35182
599\D8=-76.04149076\D9=-57.67343766\D10=-16.44737281\D11=169.02959604\
B4=2.16326752\B5=1.36043529\\Version=AM64L-G03RevE.01\State=2-A\HF=-34
4.973973\S2=0.818435\S2-1=0.\S2A=0.750697\RMSD=9.844e-09\RMSF=4.595e-0
5\Thermal=0.\Dipole=0.0911494,-0.4368517,0.9086788\PG=C01 [X(C5H7O2)]\\@

Cyclization product 41 (n=1, R=H)

HF/3-21G*

1\1\GINC-GOMBERG01\FOpt\UHF\3-21G*\C5H7O2(2)\HMAITKEN\08-Oct-2010\1\\#
HF/3-21G* opt=(grad)\\calc of 5 exo radical product\\0,2\C\O,1,B1\C,2,
B2,1,A1\C,1,B3,2,A2,3,D1,0\H,1,B4,2,A3,3,D2,0\H,1,B5,2,A4,3,D3,0\H,3,B
6,2,A5,1,D4,0\H,4,B7,1,A6,2,D5,0\H,4,B8,1,A7,2,D6,0\C,4,B9,1,A8,2,D7,0
\O,10,B10,4,A9,1,D8,0\C,3,B11,2,A10,1,D9,0\H,12,B12,3,A11,2,D10,0\H,12
,B13,3,A12,2,D11,0\\B1=1.45399781\B2=1.43926372\B3=1.53334462\B4=1.076
20043\B5=1.08249227\B6=1.08616315\B7=1.07932311\B8=1.08505001\B9=1.520
47192\B10=1.20374421\B11=1.49310368\B12=1.0709447\B13=1.07026775\A1=10
9.47219191\A2=104.12503729\A3=107.57079443\A4=110.12168942\A5=110.9345
6088\A6=114.4420939\A7=110.45007238\A8=102.5794611\A9=127.90296206\A10
=109.5888338\A11=119.67460426\A12=118.29646472\D1=34.6585981\D2=155.94
462273\D3=-84.36445405\D4=94.88310286\D5=-153.50606405\D6=82.62103213\
D7=-32.3412193\D8=-160.89248486\D9=-141.79500124\D10=185.60586588\D11=
14.75658751\\Version=AM64L-G03RevE.01\State=2-A\HF=-341.1660581\S2=0.7
63775\S2-1=0.\S2A=0.750145\RMSD=2.367e-09\RMSF=1.846e-05\Thermal=0.\Di
pole=-0.5474034,0.0039999,-0.5426578\PG=C01 [X(C5H7O2)]\\@

HF/6-31G*

1\1\GINC-GOMBERG01\FOpt\UHF\6-31G(d)\C5H7O2(2)\HMAITKEN\08-Oct-2010\1\
\#HF/6-31G* opt=(grad,readfc) geom=checkpoint guess=read\\calc of 5 ex
o radical product\\0,2\C\O,1,B1\C,2,B2,1,A1\C,1,B3,2,A2,3,D1,0\H,1,B4,
2,A3,3,D2,0\H,1,B5,2,A4,3,D3,0\H,3,B6,2,A5,1,D4,0\H,4,B7,1,A6,2,D5,0\H
,4,B8,1,A7,2,D6,0\C,4,B9,1,A8,2,D7,0\O,10,B10,4,A9,1,D8,0\C,3,B11,2,A1
0,1,D9,0\H,12,B12,3,A11,2,D10,0\H,12,B13,3,A12,2,D11,0\\B1=1.40923349\
B2=1.4021902\B3=1.52677335\B4=1.07968258\B5=1.08783545\B6=1.09215765\B
7=1.0820306\B8=1.08613978\B9=1.51672179\B10=1.1857083\B11=1.49062583\B
12=1.07296318\B13=1.07309897\A1=109.46216077\A2=104.90522984\A3=107.86
72332\A4=110.15462517\A5=110.41704955\A6=115.19558548\A7=111.22921059\
A8=101.72081718\A9=127.71605181\A10=110.75327649\A11=119.25809341\A12=
118.95921988\D1=37.8503771\D2=159.93216853\D3=-81.76065629\D4=86.34189
288\D5=-151.11787567\D6=84.81635525\D7=-30.34258897\D8=-165.11783013\D
9=-151.22929904\D10=186.89345617\D11=22.87132081\\Version=AM64L-G03Rev
E.01\State=2-A\HF=-343.0805572\S2=0.762524\S2-1=0.\S2A=0.750109\RMSD=9
.802e-09\RMSF=1.069e-05\Thermal=0.\Dipole=-0.6281006,0.1471692,-0.4986
364\PG=C01 [X(C5H7O2)]\\@

HF/6-311G**

1\1\GINC-GOMBERG01\FOpt\UHF\6-311G(d,p)\C5H7O2(2)\HMAITKEN\08-Oct-2010
\1\\#HF/6-311G** opt=(grad,readfc) geom=checkpoint guess=read\\calc of
5 exo radical product\\0,2\C\O,1,B1\C,2,B2,1,A1\C,1,B3,2,A2,3,D1,0\H,
1,B4,2,A3,3,D2,0\H,1,B5,2,A4,3,D3,0\H,3,B6,2,A5,1,D4,0\H,4,B7,1,A6,2,D
5,0\H,4,B8,1,A7,2,D6,0\C,4,B9,1,A8,2,D7,0\O,10,B10,4,A9,1,D8,0\C,3,B11
,2,A10,1,D9,0\H,12,B12,3,A11,2,D10,0\H,12,B13,3,A12,2,D11,0\\B1=1.4079
0157\B2=1.400454\B3=1.52559853\B4=1.07988026\B5=1.08905453\B6=1.093284
49\B7=1.0819602\B8=1.08641033\B9=1.51584774\B10=1.1801113\B11=1.489606
53\B12=1.07360231\B13=1.0735993\A1=109.29546874\A2=104.84081399\A3=108
.0258864\A4=110.14741077\A5=110.43738965\A6=115.36332542\A7=111.076350
08\A8=101.71215727\A9=127.85343079\A10=110.90356888\A11=119.28543645\A
12=118.94102151\D1=38.20115024\D2=160.30018741\D3=-81.2621269\D4=86.07
377131\D5=-151.89664394\D6=83.75551536\D7=-30.97029037\D8=-164.4938661
\D9=-151.44371509\D10=185.32390507\D11=19.53896926\\Version=AM64L-G03R
evE.01\State=2-A\HF=-343.1658967\S2=0.762895\S2-1=0.\S2A=0.750114\RMSD
=9.201e-09\RMSF=5.447e-06\Thermal=0.\Dipole=-0.642323,0.1564819,-0.506
4705\PG=C01 [X(C5H7O2)]\\@

BHandHLYP/6-311G**

1\1\GINC-GOMBERG01\FOpt\UBHandHLYP\6-311G(d,p)\C5H7O2(2)\HMAITKEN\08-O
ct-2010\1\\#BHandHLYP/6-311G** opt=(grad,readfc) geom=checkpoint guess
=read\\calc of 5 exo radical product\\0,2\C\O,1,B1\C,2,B2,1,A1\C,1,B3,
2,A2,3,D1,0\H,1,B4,2,A3,3,D2,0\H,1,B5,2,A4,3,D3,0\H,3,B6,2,A5,1,D4,0\H
,4,B7,1,A6,2,D5,0\H,4,B8,1,A7,2,D6,0\C,4,B9,1,A8,2,D7,0\O,10,B10,4,A9,
1,D8,0\C,3,B11,2,A10,1,D9,0\H,12,B12,3,A11,2,D10,0\H,12,B13,3,A12,2,D1
1,0\\B1=1.41515113\B2=1.40633451\B3=1.51974638\B4=1.08125833\B5=1.0908
744\B6=1.09783725\B7=1.08257361\B8=1.08742795\B9=1.51263443\B10=1.1876
8842\B11=1.47412138\B12=1.07355737\B13=1.07342327\A1=108.74300478\A2=1
04.9933413\A3=107.71501112\A4=110.26469949\A5=110.60224528\A6=115.6463
2774\A7=111.01252626\A8=101.89428543\A9=128.09373561\A10=111.09669273\
A11=119.65063929\A12=119.12143789\D1=38.06283555\D2=160.23804752\D3=-8
1.4187786\D4=86.72110284\D5=-153.08788564\D6=82.50223899\D7=-32.128318

07\D8=-162.79880865\D9=-149.94675121\D10=184.3284879\D11=11.97528506\\
Version=AM64L-G03RevE.01\State=2-A\HF=-345.0025221\S2=0.75576\S2-1=0.\
S2A=0.750023\RMSD=9.586e-09\RMSF=1.339e-05\Thermal=0.\Dipole=-0.602051
7,0.1200524,-0.4900822\PG=C01 [X(C5H7O2)]\\@

BHandHLYP/6-311++G**

1\1\GINC-GOMBERG01\FOpt\UBHandHLYP\6-311++G(d,p)\C5H7O2(2)\HMAITKEN\08
-Oct-2010\1\\#BHandHLYP/6-311++G(d,p) opt=(grad,readfc) geom=checkpoin
t guess=read\\calc of 5 exo radical product\\0,2\C\O,1,B1\C,2,B2,1,A1\
C,1,B3,2,A2,3,D1,0\H,1,B4,2,A3,3,D2,0\H,1,B5,2,A4,3,D3,0\H,3,B6,2,A5,1
,D4,0\H,4,B7,1,A6,2,D5,0\H,4,B8,1,A7,2,D6,0\C,4,B9,1,A8,2,D7,0\O,10,B1
0,4,A9,1,D8,0\C,3,B11,2,A10,1,D9,0\H,12,B12,3,A11,2,D10,0\H,12,B13,3,A
12,2,D11,0\\B1=1.41551948\B2=1.4066192\B3=1.52030959\B4=1.08132288\B5=
1.09062532\B6=1.09819286\B7=1.08277636\B8=1.0873923\B9=1.51187275\B10=
1.18875108\B11=1.47345775\B12=1.07359721\B13=1.07355089\A1=108.7326809
5\A2=104.98584751\A3=107.72092145\A4=110.10274198\A5=110.34913756\A6=1
15.46629116\A7=111.22418144\A8=102.06524648\A9=127.91230045\A10=111.25
885901\A11=119.64365143\A12=119.29332272\D1=38.15270497\D2=160.3195281
5\D3=-81.39118024\D4=85.19277847\D5=-151.93856973\D6=83.73229293\D7=-3
1.182431\D8=-164.0632649\D9=-151.59363278\D10=184.0181557\D11=9.962066
25\\Version=AM64L-G03RevE.01\State=2-A\HF=-345.0111034\S2=0.755766\S2-
1=0.\S2A=0.750023\RMSD=4.260e-09\RMSF=7.402e-05\Thermal=0.\Dipole=-0.6
489358,0.1820974,-0.5272741\PG=C01 [X(C5H7O2)]\\@

Decarbonylation transition state 40 → 42 (n=1, R=H)

HF/3-21G*

1\1\GINC-GOMBERG01\FTS\UHF\3-21G*\C5H7O2(2)\HMAITKEN\12-Nov-2010\1\\#H
F/3-21G* opt=(grad,ts,noeigentest,nofreeze,readfc) geom=checkpoint gue
ss=read\\5 membered decarbonylation ts\\0,2\C\H,1,B1\H,1,B2,2,A1\C,1,B
3,2,A2,3,D1,0\H,4,B4,1,A3,2,D2,0\H,4,B5,1,A4,2,D3,0\O,1,B6,4,A5,5,D4,0
\C,4,B7,1,A6,7,D5,0\O,8,B8,4,A7,1,D6,0\C,7,B9,1,A8,4,D7,0\H,10,B10,7,A
9,1,D8,0\C,10,B11,7,A10,1,D9,0\H,12,B12,10,A11,7,D10,0\H,12,B13,10,A12
,7,D11,0\\B1=1.08184825\B2=1.08184988\B3=1.50347089\B4=1.07622377\B5=1
.07622346\B6=1.44308662\B9=1.37238554\B10=1.07043143\B11=1.3154343\B12
=1.0706881\B13=1.07038042\A1=108.61362044\A2=110.89542823\A3=116.04368
49\A4=116.0413044\A5=106.30325115\A6=102.18365267\A7=119.06462507\A8=1
19.54906602\A9=109.82355402\A10=127.95291476\A11=123.64679804\A12=119.
49010718\D1=-122.10316706\D2=170.73870259\D3=-49.99512247\D4=-69.64219
295\D5=-180.00918163\D6=-180.0257816\D7=179.9984592\D8=180.00147995\D9
=0.00151972\D10=0.00012167\D11=179.99999827\B7=2.00553911\B8=1.1498257
9\\Version=AM64L-G03RevE.01\State=2-A\HF=-341.1225309\S2=0.807134\S2-1
=0.\S2A=0.750883\RMSD=6.966e-09\RMSF=1.641e-05\Thermal=0.\Dipole=0.146
5007,-0.4902127,0.1052652\PG=C01 [X(C5H7O2)]\\@

HF/6-31G*

1\1\GINC-GOMBERG01\FTS\UHF\6-31G(d)\C5H7O2(2)\HMAITKEN\12-Nov-2010\1\\
#HF/6-31G* opt=(grad,ts,noeigentest,nofreeze,readfc) geom=checkpoint g
uess=read\\5 membered decarbonylation ts\\0,2\C\H,1,B1\H,1,B2,2,A1\C,1
,B3,2,A2,3,D1,0\H,4,B4,1,A3,2,D2,0\H,4,B5,1,A4,2,D3,0\O,1,B6,4,A5,5,D4
,0\C,4,B7,1,A6,7,D5,0\O,8,B8,4,A7,1,D6,0\C,7,B9,1,A8,4,D7,0\H,10,B10,7
,A9,1,D8,0\C,10,B11,7,A10,1,D9,0\H,12,B12,10,A11,7,D10,0\H,12,B13,10,A
12,7,D11,0\\B1=1.08460035\B2=1.08460159\B3=1.50170186\B4=1.0782311\B5=

1.07823063\B6=1.40611112\B9=1.34357124\B10=1.07393208\B11=1.31994864\B
12=1.07299103\B13=1.07304306\A1=108.13371014\A2=110.62243754\A3=116.07
71982\A4=116.07786769\A5=107.66809407\A6=105.79261076\A7=116.82748508\
A8=118.44522046\A9=109.97603179\A10=128.54067408\A11=123.96210336\A12=
118.83550065\D1=-121.2803446\D2=171.1903426\D3=-51.39166186\D4=-68.708
0301\D5=-179.99821644\D6=-179.98260893\D7=179.98887982\D8=180.00854296
\D9=0.00860951\D10=0.00052193\D11=180.00012217\B7=1.99272296\B8=1.1333
2886\\Version=AM64L-G03RevE.01\State=2-A\HF=-343.0360291\S2=0.80935\S2
-1=0.\S2A=0.750969\RMSD=7.082e-09\RMSF=5.640e-06\Thermal=0.\Dipole=0.0
969624,-0.4387431,0.0701177\PG=C01 [X(C5H7O2)]\\@

HF/6-311G**

1\1\GINC-GOMBERG03\FTS\UHF\6-311G(d,p)\C5H7O2(2)\HMAITKEN\12-Nov-2010\
1\\#HF/6-311G** opt=(grad,ts,noeigentest,nofreeze,readfc) geom=checkpo
int guess=read\\5 membered decarbonylation ts\\0,2\C\H,1,B1\H,1,B2,2,A
1\C,1,B3,2,A2,3,D1,0\H,4,B4,1,A3,2,D2,0\H,4,B5,1,A4,2,D3,0\O,1,B6,4,A5
,5,D4,0\C,4,B7,1,A6,7,D5,0\O,8,B8,4,A7,1,D6,0\C,7,B9,1,A8,4,D7,0\H,10,
B10,7,A9,1,D8,0\C,10,B11,7,A10,1,D9,0\H,12,B12,10,A11,7,D10,0\H,12,B13
,10,A12,7,D11,0\\B1=1.08562772\B2=1.08562559\B3=1.50116611\B4=1.078872
23\B5=1.07887465\B6=1.40550782\B9=1.34073717\B10=1.07479148\B11=1.3198
0947\B12=1.07325761\B13=1.07331194\A1=108.23562843\A2=110.51176647\A3=
115.95854838\A4=115.95904821\A5=107.68008421\A6=106.18788732\A7=116.93
300431\A8=118.62392052\A9=110.14487335\A10=128.52762356\A11=123.925894
09\A12=118.58876299\D1=-121.14142974\D2=171.238775\D3=-51.48875049\D4=
-68.65125325\D5=-180.0152958\D6=-179.98256396\D7=179.99689618\D8=180.0
0498138\D9=0.0051843\D10=-0.0000951\D11=179.99929225\B7=1.9841944\B8=1
.12555229\\Version=AM64L-G03RevE.01\State=2-A\HF=-343.1265926\S2=0.808
63\S2-1=0.\S2A=0.751014\RMSD=7.787e-09\RMSF=2.482e-05\Thermal=0.\Dipol
e=0.0623253,-0.4211481,0.044801\PG=C01 [X(C5H7O2)]\\@

BHandHLYP/6-311G**

1\1\GINC-GOMBERG01\FTS\UBHandHLYP\6-311G(d,p)\C5H7O2(2)\HMAITKEN\12-No
v-2010\1\\#BHandHLYP/6-311G** opt=(grad,ts,noeigentest,nofreeze,readfc
) geom=checkpoint guess=read\\5 membered decarbonylation ts\\0,2\C\H,1
,B1\H,1,B2,2,A1\C,1,B3,2,A2,3,D1,0\H,4,B4,1,A3,2,D2,0\H,4,B5,1,A4,2,D3
,0\O,1,B6,4,A5,5,D4,0\C,4,B7,1,A6,7,D5,0\O,8,B8,4,A7,1,D6,0\C,7,B9,1,A
8,4,D7,0\H,10,B10,7,A9,1,D8,0\C,10,B11,7,A10,1,D9,0\H,12,B12,10,A11,7,
D10,0\H,12,B13,10,A12,7,D11,0\\B1=1.08776202\B2=1.0877692\B3=1.4877120
4\B4=1.07786612\B5=1.07786076\B6=1.41541182\B9=1.34356252\B10=1.076679
34\B11=1.32259594\B12=1.0739189\B13=1.07389838\A1=108.04586518\A2=110.
80645257\A3=117.68572984\A4=117.69112585\A5=108.01682671\A6=103.347008
5\A7=115.3416825\A8=117.40622394\A9=110.00162531\A10=128.29615803\A11=
123.74951334\A12=118.73497235\D1=-121.56331775\D2=167.33285018\D3=-47.
3346934\D4=-72.62939692\D5=-179.95934719\D6=-180.0633653\D7=179.993946
23\D8=179.99919757\D9=-0.00084425\D10=0.00086459\D11=180.00054398\B7=2
.14246212\B8=1.12793106\\Version=AM64L-G03RevE.01\State=2-A\HF=-344.96
0767\S2=0.771409\S2-1=0.\S2A=0.750146\RMSD=9.186e-09\RMSF=2.870e-05\Th
ermal=0.\Dipole=0.0411451,-0.1666733,0.0303716\PG=C01 [X(C5H7O2)]\\@

BHandHLYP/6-311++G**

1\1\GINC-GOMBERG01\FTS\UBHandHLYP\6-311++G(d,p)\C5H7O2(2)\HMAITKEN\12-
Nov-2010\1\\#BHandHLYP/6-311++G(d,p) opt=(grad,ts,noeigentest,nofreeze
,readfc) geom=checkpoint guess=read\\5 membered decarbonylation ts\\0,

2\C\H,1,B1\H,1,B2,2,A1\C,1,B3,2,A2,3,D1,0\H,4,B4,1,A3,2,D2,0\H,4,B5,1,
A4,2,D3,0\O,1,B6,4,A5,5,D4,0\C,4,B7,1,A6,7,D5,0\O,8,B8,4,A7,1,D6,0\C,7
,B9,1,A8,4,D7,0\H,10,B10,7,A9,1,D8,0\C,10,B11,7,A10,1,D9,0\H,12,B12,10
,A11,7,D10,0\H,12,B13,10,A12,7,D11,0\\B1=1.08765333\B2=1.08764473\B3=1
.48740788\B4=1.07783789\B5=1.07783796\B6=1.41614605\B9=1.3437145\B10=1
.07649285\B11=1.32385045\B12=1.0739513\B13=1.07397882\A1=108.12917337\
A2=110.81822091\A3=117.87599474\A4=117.8784811\A5=108.15500486\A6=103.
1518892\A7=115.25565391\A8=117.53611166\A9=110.1256062\A10=128.1392000
5\A11=123.78701839\A12=118.63779122\D1=-121.64101048\D2=166.87641498\D
3=-46.83137373\D4=-73.14980746\D5=-180.00450108\D6=-179.89228587\D7=18
0.00224887\D8=179.9976235\D9=-0.00282275\D10=0.00081075\D11=180.000117
5\B7=2.15162924\B8=1.12849554\\Version=AM64L-G03RevE.01\State=2-A\HF=-
344.9676446\S2=0.77135\S2-1=0.\S2A=0.750149\RMSD=7.437e-09\RMSF=5.595e
-05\Thermal=0.\Dipole=0.0595364,-0.1845132,0.0428305\PG=C01 [X(C5H7O2)]\\@

Decarbonylation product 42 (n=1, R=H)

HF/3-21G*

1\1\GINC-GOMBERG01\FOpt\UHF\3-21G*\C4H7O1(2)\HMAITKEN\24-Nov-2010\1\\#
HF/3-21G* opt=grad\\benchmark calc of decarbonylation radical product\
\0,2\C\C,1,B1\O,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\H,5,B5
,4,A4,3,D3,0\H,5,B6,4,A5,3,D4,0\H,4,B7,3,A6,2,D5,0\H,2,B8,1,A7,3,D6,0\
H,2,B9,1,A8,3,D7,0\H,1,B10,2,A9,3,D8,0\H,1,B11,2,A10,3,D9,0\\B1=1.4950
5238\B2=1.44143699\B3=1.36952432\B4=1.31595834\B5=1.07042525\B6=1.0705
5456\B7=1.07057601\B8=1.08572302\B9=1.08758068\B10=1.07003569\B11=1.07
195702\A1=106.99787039\A2=119.65035672\A3=128.1308016\A4=119.4740406\A
5=123.65700056\A6=109.82148095\A7=111.31453412\A8=111.51771145\A9=118.
74706285\A10=120.06654357\D1=179.88377718\D2=0.16647571\D3=180.0036511
2\D4=0.0389756\D5=180.16333247\D6=-120.12591335\D7=119.65201455\D8=-14
.80800394\D9=-186.57907485\\Version=AM64L-G03RevE.01\State=2-A\HF=-229
.0464807\S2=0.763055\S2-1=0.\S2A=0.750123\RMSD=7.262e-09\RMSF=1.466e-0
5\Thermal=0.\Dipole=-0.4551581,0.0472363,0.0684631\PG=C01 [X(C4H7O1)]\\@

HF/6-31G*

1\1\GINC-GOMBERG10\FOpt\UHF\6-31G(d)\C4H7O1(2)\HMAITKEN\09-Nov-2010\1\
\#HF/6-31G* opt=(grad,readfc) geom=checkpoint guess=read\\benchmark ca
lc of decarbonylation radical product\\0,2\C\C,1,B1\O,2,B2,1,A1\C,3,B3
,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\H,5,B5,4,A4,3,D3,0\H,5,B6,4,A5,3,D4,0\
H,4,B7,3,A6,2,D5,0\H,2,B8,1,A7,3,D6,0\H,2,B9,1,A8,3,D7,0\H,1,B10,2,A9,
3,D8,0\H,1,B11,2,A10,3,D9,0\\B1=1.49112178\B2=1.40471034\B3=1.34094488
\B4=1.3204959\B5=1.07308224\B6=1.0729417\B7=1.07411824\B8=1.08705502\B
9=1.09025897\B10=1.07334165\B11=1.07431499\A1=108.33195898\A2=118.5401
976\A3=128.69907052\A4=118.83110323\A5=123.95883116\A6=109.99962198\A7
=110.77479896\A8=111.26162236\A9=119.42904415\A10=119.45247049\D1=179.
52176555\D2=0.5117679\D3=179.97805488\D4=0.0317909\D5=180.46200157\D6=
-120.68294211\D7=120.12879094\D8=-29.58027468\D9=-192.79188311\\Versio
n=AM64L-G03RevE.01\State=2-A\HF=-230.3218919\S2=0.76184\S2-1=0.\S2A=0.
750092\RMSD=7.280e-09\RMSF=3.033e-05\Thermal=0.\Dipole=-0.3919256,0.07
52296,-0.0101285\PG=C01 [X(C4H7O1)]\\@

HF/6-311G**

1\1\GINC-GOMBERG10\FOpt\UHF\6-311G(d,p)\C4H7O1(2)\HMAITKEN\09-Nov-2010
\1\\#HF/6-311G** opt=(grad,readfc) geom=checkpoint guess=read\\benchma

rk calc of decarbonylation radical product\\0,2\C\C,1,B1\O,2,B2,1,A1\C
,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\H,5,B5,4,A4,3,D3,0\H,5,B6,4,A5,3,
D4,0\H,4,B7,3,A6,2,D5,0\H,2,B8,1,A7,3,D6,0\H,2,B9,1,A8,3,D7,0\H,1,B10,
2,A9,3,D8,0\H,1,B11,2,A10,3,D9,0\\B1=1.49005307\B2=1.40388719\B3=1.337
96646\B4=1.32050232\B5=1.07336159\B6=1.07317057\B7=1.07499799\B8=1.088
16698\B9=1.09133581\B10=1.07397043\B11=1.0749966\A1=108.42762889\A2=11
8.71916717\A3=128.70737573\A4=118.58248876\A5=123.92122218\A6=110.1555
3845\A7=110.69201908\A8=111.00389626\A9=119.36461265\A10=119.39622501\
D1=179.48418775\D2=0.53662766\D3=179.97888236\D4=0.0303075\D5=180.4816
5327\D6=-120.7696904\D7=120.12024817\D8=-27.8739317\D9=-191.97280102\\
Version=AM64L-G03RevE.01\State=2-A\HF=-230.3834784\S2=0.762122\S2-1=0.
\S2A=0.750096\RMSD=7.971e-09\RMSF=6.814e-06\Thermal=0.\Dipole=-0.38616
63,0.0702198,-0.0172158\PG=C01 [X(C4H7O1)]\\@

BHandHLYP/6-311G**

1\1\GINC-GOMBERG10\FOpt\UBHandHLYP\6-311G(d,p)\C4H7O1(2)\HMAITKEN\09-N
ov-2010\1\\#BHandHLYP/6-311G** opt=(grad,readfc) geom=checkpoint guess
=read\\benchmark calc of decarbonylation radical product\\0,2\C\C,1,B1
\O,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\H,5,B5,4,A4,3,D3,0\
H,5,B6,4,A5,3,D4,0\H,4,B7,3,A6,2,D5,0\H,2,B8,1,A7,3,D6,0\H,2,B9,1,A8,3
,D7,0\H,1,B10,2,A9,3,D8,0\H,1,B11,2,A10,3,D9,0\\B1=1.47570563\B2=1.409
17943\B3=1.34118626\B4=1.3230766\B5=1.073854\B6=1.07376876\B7=1.076669
58\B8=1.09227798\B9=1.09553497\B10=1.07363502\B11=1.0743469\A1=108.696
42127\A2=117.67290939\A3=128.40369757\A4=118.72413746\A5=123.75842831\
A6=110.01487896\A7=111.16825265\A8=111.30731394\A9=119.66065492\A10=11
9.95316396\D1=179.27774468\D2=0.47487355\D3=179.99012206\D4=0.04189125
\D5=180.42446638\D6=-121.07126137\D7=120.28129842\D8=-18.33212684\D9=-
190.29047494\\Version=AM64L-G03RevE.01\State=2-A\HF=-231.6819323\S2=0.
7552\S2-1=0.\S2A=0.750017\RMSD=7.022e-09\RMSF=4.552e-06\Thermal=0.\Dip
ole=-0.3676253,0.0402166,-0.0231174\PG=C01 [X(C4H7O1)]\\@

BHandHLYP/6-311++G**

1\1\GINC-GOMBERG02\FOpt\UBHandHLYP\6-311++G(d,p)\C4H7O1(2)\HMAITKEN\09
-Nov-2010\1\\#BHandHLYP/6-311++G(d,p) opt=(grad,readfc) geom=checkpoin
t guess=read\\benchmark calc of decarbonylation radical product\\0,2\C
\C,1,B1\O,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\H,5,B5,4,A4,
3,D3,0\H,5,B6,4,A5,3,D4,0\H,4,B7,3,A6,2,D5,0\H,2,B8,1,A7,3,D6,0\H,2,B9
,1,A8,3,D7,0\H,1,B10,2,A9,3,D8,0\H,1,B11,2,A10,3,D9,0\\B1=1.47529266\B
2=1.40940539\B3=1.34128113\B4=1.32446154\B5=1.07392946\B6=1.07378377\B
7=1.07638718\B8=1.09230957\B9=1.09516073\B10=1.07370476\B11=1.07444722
\A1=108.85341912\A2=117.82168371\A3=128.24396086\A4=118.61984379\A5=12
3.80632696\A6=110.13683757\A7=111.15165055\A8=111.27463563\A9=119.9529
0496\A10=119.79375013\D1=179.52622515\D2=0.33313957\D3=179.98523779\D4
=0.03425521\D5=180.29570035\D6=-120.99383569\D7=120.31438829\D8=-15.65
804806\D9=-188.98719805\\Version=AM64L-G03RevE.01\State=2-A\HF=-231.68
69691\S2=0.755242\S2-1=0.\S2A=0.750018\RMSD=9.241e-09\RMSF=3.472e-05\T
hermal=0.\Dipole=-0.4056157,0.0369501,-0.004339\PG=C01 [X(C4H7O1)]\\@

6-Membered parent system 40 (n=2, R=H)

Acyl radical 40 (n=2, R=H)

HF/3-21G*

1\1\GINC-GOMBERG07\FOpt\UHF\3-21G*\C6H9O2(2)\HMAITKEN\11-Oct-2010\1\\#
HF/3-21G* opt=(grad) scf=qc\\6 membered starting radical\\0,2\C\C,1,B1
\O,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\H,5,B5,4,A4,3,D3,0\
H,5,B6,4,A5,3,D4,0\H,4,B7,3,A6,2,D5,0\H,2,B8,1,A7,3,D6,0\H,2,B9,1,A8,3
,D7,0\H,1,B10,2,A9,3,D8,0\H,1,B11,2,A10,3,D9,0\C,1,B12,2,A11,3,D10,0\H
,13,B13,1,A12,2,D11,0\H,13,B14,1,A13,2,D12,0\C,13,B15,1,A14,2,D13,0\O,
16,B16,13,A15,1,D14,0\\B1=1.52398655\B2=1.43810586\B3=1.37148062\B4=1.
31556272\B5=1.07035262\B6=1.07067779\B7=1.07031005\B8=1.0841015\B9=1.0
8432018\B10=1.08151152\B11=1.08140855\B12=1.5384792\B13=1.08506829\B14
=1.0849738\B15=1.51432902\B16=1.18510399\A1=105.89276063\A2=119.977020
51\A3=127.94873469\A4=119.52532696\A5=123.59020987\A6=109.79928694\A7=
111.14111953\A8=111.16550967\A9=108.89579951\A10=108.75097308\A11=111.
46676663\A12=111.48698471\A13=111.50090492\A14=111.78996599\A15=130.65
841668\D1=-179.94971082\D2=0.09253609\D3=-180.00847747\D4=-0.0458746\D
5=180.08907333\D6=-119.46052762\D7=119.50698535\D8=58.37203122\D9=-58.
53447175\D10=-180.05524031\D11=-59.91037805\D12=59.88960353\D13=-179.9
7930975\D14=0.23702428\\Version=AM64L-G03RevE.01\State=2-A\HF=-379.964
3979\S2=0.770302\S2-1=0.\S2A=0.750197\RMSD=0.000e+00\RMSF=1.004e-04\Th
ermal=0.\Dipole=-0.7525994,0.0020059,1.1626392\PG=C01 [X(C6H9O2)]\\@

HF/6-31G*

1\1\GINC-GOMBERG04\FOpt\UHF\6-31G(d)\C6H9O2(2)\HMAITKEN\11-Oct-2010\1\
\#HF/6-31G* opt=(grad,readfc) geom=checkpoint guess=read\\6 membered s
tarting radical\\0,2\C\C,1,B1\O,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\C,4,B4,3,
A3,2,D2,0\H,5,B5,4,A4,3,D3,0\H,5,B6,4,A5,3,D4,0\H,4,B7,3,A6,2,D5,0\H,2
,B8,1,A7,3,D6,0\H,2,B9,1,A8,3,D7,0\H,1,B10,2,A9,3,D8,0\H,1,B11,2,A10,3
,D9,0\C,1,B12,2,A11,3,D10,0\H,13,B13,1,A12,2,D11,0\H,13,B14,1,A13,2,D1
2,0\C,13,B15,1,A14,2,D13,0\O,16,B16,13,A15,1,D14,0\\B1=1.51888349\B2=1
.40208879\B3=1.34246003\B4=1.32011372\B5=1.07302071\B6=1.0730086\B7=1.
073919\B8=1.08679539\B9=1.08679446\B10=1.08366966\B11=1.08367403\B12=1
.53020875\B13=1.08660958\B14=1.08659723\B15=1.51737151\B16=1.16488453\
A1=107.59397811\A2=118.72987636\A3=128.57515596\A4=118.85938008\A5=123
.92795748\A6=109.98940092\A7=110.93352092\A8=110.93349241\A9=109.19546
681\A10=109.19553614\A11=111.63097492\A12=111.80778753\A13=111.8103069
6\A14=113.29767813\A15=129.28195548\D1=-180.0006447\D2=0.00074819\D3=-
179.99924101\D4=0.00100886\D5=180.00119747\D6=-120.0708097\D7=120.0712
3618\D8=58.27764919\D9=-58.28207789\D10=-180.00235442\D11=-59.37359991
\D12=59.37448439\D13=-179.9933662\D14=0.03759365\\Version=AM64L-G03Rev
E.01\State=2-A\HF=-382.0944867\S2=0.76149\S2-1=0.\S2A=0.750098\RMSD=9.
361e-09\RMSF=2.233e-06\Thermal=0.\Dipole=-0.6674902,0.000351,1.0066326
\PG=C01 [X(C6H9O2)]\\@

HF/6-311G**

1\1\GINC-GOMBERG04\FOpt\UHF\6-311G(d,p)\C6H9O2(2)\HMAITKEN\11-Oct-2010
\1\\#HF/6-311G** opt=(grad,readfc) geom=checkpoint guess=read\\6 membe
red starting radical\\0,2\C\C,1,B1\O,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\C,4,
B4,3,A3,2,D2,0\H,5,B5,4,A4,3,D3,0\H,5,B6,4,A5,3,D4,0\H,4,B7,3,A6,2,D5,
0\H,2,B8,1,A7,3,D6,0\H,2,B9,1,A8,3,D7,0\H,1,B10,2,A9,3,D8,0\H,1,B11,2,

A10,3,D9,0\C,1,B12,2,A11,3,D10,0\H,13,B13,1,A12,2,D11,0\H,13,B14,1,A13
,2,D12,0\C,13,B15,1,A14,2,D13,0\O,16,B16,13,A15,1,D14,0\\B1=1.51733452
\B2=1.40153933\B3=1.33951916\B4=1.32006169\B5=1.07329323\B6=1.07328413
\B7=1.0747976\B8=1.0879789\B9=1.08798604\B10=1.08426438\B11=1.08426472
\B12=1.52915552\B13=1.08688708\B14=1.08687728\B15=1.51679577\B16=1.157
55334\A1=107.65806927\A2=118.92443889\A3=128.56943676\A4=118.61584267\
A5=123.90195545\A6=110.1550429\A7=110.8291196\A8=110.82939343\A9=109.1
7074525\A10=109.16382909\A11=111.65377371\A12=111.93485067\A13=111.935
01951\A14=113.49657581\A15=129.68960795\D1=-179.99036336\D2=0.0018324\
D3=-180.01528782\D4=-0.01934892\D5=179.98944663\D6=-120.06194641\D7=12
0.06105282\D8=58.31709169\D9=-58.25584873\D10=-179.96725383\D11=-59.54
040617\D12=59.49817217\D13=-180.01539172\D14=0.03929501\\Version=AM64L
-G03RevE.01\State=2-A\HF=-382.1932502\S2=0.76161\S2-1=0.\S2A=0.750098\
RMSD=5.159e-09\RMSF=1.569e-05\Thermal=0.\Dipole=-0.6097333,0.000055,1.
0106027\PG=C01 [X(C6H9O2)]\\@

BHandHLYP/6-311G**

1\1\GINC-GOMBERG04\FOpt\UBHandHLYP\6-311G(d,p)\C6H9O2(2)\HMAITKEN\11-O
ct-2010\1\\#BHandHLYP/6-311G** opt=(grad,readfc) geom=checkpoint guess
=read\\6 membered starting radical\\0,2\C\C,1,B1\O,2,B2,1,A1\C,3,B3,2,
A2,1,D1,0\C,4,B4,3,A3,2,D2,0\H,5,B5,4,A4,3,D3,0\H,5,B6,4,A5,3,D4,0\H,4
,B7,3,A6,2,D5,0\H,2,B8,1,A7,3,D6,0\H,2,B9,1,A8,3,D7,0\H,1,B10,2,A9,3,D
8,0\H,1,B11,2,A10,3,D9,0\C,1,B12,2,A11,3,D10,0\H,13,B13,1,A12,2,D11,0\
H,13,B14,1,A13,2,D12,0\C,13,B15,1,A14,2,D13,0\O,16,B16,13,A15,1,D14,0\
\B1=1.51069948\B2=1.40698907\B3=1.34303886\B4=1.32255885\B5=1.07380475
\B6=1.07390236\B7=1.07648008\B8=1.09010979\B9=1.09011457\B10=1.0851572
4\B11=1.08516358\B12=1.52321759\B13=1.08795702\B14=1.08794158\B15=1.51
03586\B16=1.1668157\A1=107.66129605\A2=117.85826487\A3=128.24611881\A4
=118.7820477\A5=123.69484879\A6=110.01506434\A7=110.98003119\A8=110.97
657287\A9=109.20373285\A10=109.20628846\A11=111.7213392\A12=112.084588
66\A13=112.08461821\A14=113.68049106\A15=128.45325816\D1=-180.01734744
\D2=0.00526993\D3=-179.98046275\D4=0.00789073\D5=180.01126979\D6=-120.
06885424\D7=120.07055722\D8=58.25924433\D9=-58.20935895\D10=-179.97618
974\D11=-59.26550267\D12=59.46780715\D13=-179.89069226\D14=0.02788691\
\Version=AM64L-G03RevE.01\State=2-A\HF=-384.2875275\S2=0.754789\S2-1=0
.\S2A=0.750014\RMSD=7.104e-09\RMSF=4.298e-05\Thermal=0.\Dipole=-0.5206
786,0.0022204,0.9283365\PG=C01 [X(C6H9O2)]\\@

BHandHLYP/6-311++G**

1\1\GINC-GOMBERG04\FOpt\UBHandHLYP\6-311++G(d,p)\C6H9O2(2)\HMAITKEN\11
-Oct-2010\1\\#BHandHLYP/6-311++G(d,p) opt=(grad,readfc) geom=checkpoin
t guess=read\\6 membered starting radical\\0,2\C\C,1,B1\O,2,B2,1,A1\C,
3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\H,5,B5,4,A4,3,D3,0\H,5,B6,4,A5,3,D
4,0\H,4,B7,3,A6,2,D5,0\H,2,B8,1,A7,3,D6,0\H,2,B9,1,A8,3,D7,0\H,1,B10,2
,A9,3,D8,0\H,1,B11,2,A10,3,D9,0\C,1,B12,2,A11,3,D10,0\H,13,B13,1,A12,2
,D11,0\H,13,B14,1,A13,2,D12,0\C,13,B15,1,A14,2,D13,0\O,16,B16,13,A15,1
,D14,0\\B1=1.51129355\B2=1.40747709\B3=1.34295937\B4=1.32399492\B5=1.0
738779\B6=1.07397204\B7=1.0763425\B8=1.08998511\B9=1.0899888\B10=1.085
24806\B11=1.08524395\B12=1.52373489\B13=1.0880666\B14=1.08805445\B15=1
.50799473\B16=1.16683733\A1=107.90588381\A2=117.96830428\A3=128.085864
8\A4=118.66105599\A5=123.75418082\A6=110.16257858\A7=110.96289764\A8=1
10.95767822\A9=109.31469317\A10=109.30977532\A11=111.37575878\A12=112.
09052\A13=112.09391003\A14=113.95712169\A15=129.1088552\D1=-180.017135

68\D2=-0.0240271\D3=-179.98961194\D4=0.01164933\D5=179.98398141\D6=-12
0.04677729\D7=120.03906447\D8=58.37907564\D9=-58.29201568\D10=-179.956
30154\D11=-59.28724198\D12=59.38770427\D13=-179.94246731\D14=0.0221676
3\\Version=AM64L-G03RevE.01\State=2-A\HF=-384.2954112\S2=0.754971\S2-1
=0.\S2A=0.750015\RMSD=3.047e-09\RMSF=2.052e-05\Thermal=0.\Dipole=-0.54
13986,0.0012888,1.0024967\PG=C01 [X(C6H9O2)]\\@

Cyclization transition state 46

HF/3-21G*

1\1\GINC-GOMBERG02\FTS\UHF\3-21G*\C6H9O2(2)\HMAITKEN\23-Nov-2010\1\\#H
F/3-21G* opt=(grad,readfc,ts,noeigentest,nofreeze) geom=checkpoint gue
ss=read\\calc 6-exo radical ts benchmark\\0,2\O\C,1,B1\C,2,B2,1,A1\C,3
,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\O,5,B5,4,A4,3,D3,0\C,2,B6,1,A5,3,D4
,0\C,7,B7,3,A6,4,D5,0\H,3,B8,4,A7,5,D6,0\H,3,B9,4,A8,5,D7,0\H,4,B10,3,
A9,5,D8,0\H,4,B11,3,A10,5,D9,0\H,5,B12,7,A11,3,D10,0\H,5,B13,7,A12,3,D
11,0\H,7,B14,3,A13,4,D12,0\H,8,B15,7,A14,3,D13,0\H,8,B16,7,A15,3,D14,0
\\B1=1.19235168\B2=1.51493092\B3=1.54009286\B4=1.52953856\B5=1.4381639
2\B8=1.08675648\B9=1.08435572\B10=1.08271356\B11=1.08408393\B12=1.0789
4524\B13=1.08668665\B14=1.07660166\B15=1.07043461\B16=1.07054976\A1=12
9.69374932\A2=111.06717354\A3=112.52947485\A4=111.52897704\A5=122.5553
8271\A6=131.95051822\A7=109.4576708\A8=111.50539947\A9=109.91354582\A1
0=108.94298815\A11=134.53230251\A12=88.29717538\A13=82.06470367\A14=12
0.39260485\A15=119.94567242\D1=138.5150399\D2=60.115755\D3=-69.5108334
3\D4=-176.20799279\D5=118.91538954\D6=-58.28115319\D7=182.00317302\D8=
-120.84745861\D9=120.86846404\D10=155.97300467\D11=-89.17035311\D12=-1
16.40335646\D13=88.3480335\D14=-84.55968174\B6=2.21122515\B7=1.3730589
\\Version=AM64L-G03RevE.01\State=2-A\HF=-379.9424243\S2=1.051837\S2-1=
0.\S2A=0.784847\RMSD=6.009e-09\RMSF=2.120e-05\Thermal=0.\Dipole=0.8108
881,-0.4113087,1.0837541\PG=C01 [X(C6H9O2)]\\@

HF/6-31G*

1\1\GINC-GOMBERG08\FTS\UHF\6-31G(d)\C6H9O2(2)\HMAITKEN\11-Oct-2010\1\\
#HF/6-31G* opt=(grad,readfc,ts,nofreeze,noeigentest) geom=checkpoint g
uess=read\\calc 6-exo radical product benchmark\\0,2\O\C,1,B1\C,2,B2,1
,A1\C,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\O,5,B5,4,A4,3,D3,0\C,2,B6,1,
A5,3,D4,0\C,7,B7,3,A6,4,D5,0\H,3,B8,4,A7,5,D6,0\H,3,B9,4,A8,5,D7,0\H,4
,B10,3,A9,5,D8,0\H,4,B11,3,A10,5,D9,0\H,5,B12,7,A11,3,D10,0\H,5,B13,7,
A12,3,D11,0\H,7,B14,3,A13,4,D12,0\H,8,B15,7,A14,3,D13,0\H,8,B16,7,A15,
3,D14,0\\B1=1.17053856\B2=1.51531374\B3=1.53139474\B4=1.52412404\B5=1.
40176717\B8=1.08857408\B9=1.08569593\B10=1.08559177\B11=1.08649657\B12
=1.08148237\B13=1.08936815\B14=1.07969918\B15=1.07263375\B16=1.0733957
\A1=127.75040024\A2=112.51226788\A3=113.40193881\A4=112.46416909\A5=12
3.44658016\A6=131.97343226\A7=109.82751689\A8=112.01361213\A9=109.9703
4447\A10=108.95194546\A11=134.95014483\A12=87.80271776\A13=85.81395412
\A14=119.7917284\A15=120.49483421\D1=145.05218685\D2=53.44865248\D3=-6
8.76693796\D4=-177.28486477\D5=120.31958264\D6=-64.33238283\D7=176.301
77402\D8=-121.43490791\D9=121.49557151\D10=156.43835112\D11=-90.527813
\D12=-112.97135996\D13=88.47777771\D14=-80.8793214\B6=2.19199587\B7=1.
38554124\\Version=AM64L-G03RevE.01\State=2-A\HF=-382.0675952\S2=1.0277
06\S2-1=0.\S2A=0.76471\RMSD=4.845e-09\RMSF=5.046e-05\Thermal=0.\Dipole
=0.688873,-0.3497934,1.0497748\PG=C01 [X(C6H9O2)]\\@

HF.6-311G**

1\1\GINC-GOMBERG01\FTS\UHF\6-311G(d,p)\C6H9O2(2)\HMAITKEN\11-Oct-2010\
1\\#HF/6-311G** opt=(grad,readfc,ts,nofreeze,noeigentest) geom=checkpo
int guess=read\\calc 6-exo radical product benchmark\\0,2\O\C,1,B1\C,2
,B2,1,A1\C,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\O,5,B5,4,A4,3,D3,0\C,2,
B6,1,A5,3,D4,0\C,7,B7,3,A6,4,D5,0\H,3,B8,4,A7,5,D6,0\H,3,B9,4,A8,5,D7,
0\H,4,B10,3,A9,5,D8,0\H,4,B11,3,A10,5,D9,0\H,5,B12,7,A11,3,D10,0\H,5,B
13,7,A12,3,D11,0\H,7,B14,3,A13,4,D12,0\H,8,B15,7,A14,3,D13,0\H,8,B16,7
,A15,3,D14,0\\B1=1.16399159\B2=1.51435402\B3=1.53107689\B4=1.52332429\
B5=1.40092435\B8=1.08881783\B9=1.08600754\B10=1.08620685\B11=1.0868253
7\B12=1.081717\B13=1.09053688\B14=1.08040202\B15=1.07312477\B16=1.0740
1348\A1=128.16047884\A2=112.43023745\A3=113.47071325\A4=112.46376751\A
5=123.23724831\A6=132.36397617\A7=109.91723919\A8=112.11030005\A9=109.
86213377\A10=108.97050793\A11=135.1055612\A12=87.77574\A13=85.50157915
\A14=119.673846\A15=120.37564901\D1=142.81994196\D2=53.45889458\D3=-67
.93616518\D4=-178.80127549\D5=121.12542618\D6=-64.01002738\D7=176.1828
1046\D8=-121.42136904\D9=121.45262989\D10=155.99788422\D11=-90.9087081
4\D12=-112.54088936\D13=87.75111717\D14=-81.65518218\B6=2.17960804\B7=
1.38513414\\Version=AM64L-G03RevE.01\State=2-A\HF=-382.163768\S2=1.018
853\S2-1=0.\S2A=0.763636\RMSD=9.597e-09\RMSF=5.288e-05\Thermal=0.\Dipo
le=0.7176583,-0.3463343,1.0633742\PG=C01 [X(C6H9O2)]\\@

BHandHLYP/6-311G**

1\1\GINC-GOMBERG06\FTS\UBHandHLYP\6-311G(d,p)\C6H9O2(2)\HMAITKEN\11-Oc
t-2010\1\\#BHandHLYP/6-311G** opt=(grad,readfc,ts,nofreeze,noeigentest
) geom=checkpoint guess=read\\calc 6-exo radical product benchmark\\0,
2\O\C,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\O,5,B5,4,
A4,3,D3,0\C,2,B6,1,A5,3,D4,0\C,7,B7,3,A6,4,D5,0\H,3,B8,4,A7,5,D6,0\H,3
,B9,4,A8,5,D7,0\H,4,B10,3,A9,5,D8,0\H,4,B11,3,A10,5,D9,0\H,5,B12,7,A11
,3,D10,0\H,5,B13,7,A12,3,D11,0\H,7,B14,3,A13,4,D12,0\H,8,B15,7,A14,3,D
13,0\H,8,B16,7,A15,3,D14,0\\B1=1.16935749\B2=1.50921318\B3=1.52491325\
B4=1.51714891\B5=1.40651162\B8=1.08992591\B9=1.08780689\B10=1.08663134
\B11=1.08733767\B12=1.08323341\B13=1.09225122\B14=1.08269248\B15=1.073
16267\B16=1.07451021\A1=127.96648588\A2=112.72029131\A3=113.17717177\A
4=112.30618907\A5=122.89801232\A6=132.52426009\A7=109.79851057\A8=112.
38048299\A9=109.88958307\A10=109.14408991\A11=134.81546276\A12=87.0008
5687\A13=82.93406873\A14=119.84953772\A15=120.49384086\D1=143.24111191
\D2=52.58966632\D3=-68.06110035\D4=-178.93689851\D5=123.11420616\D6=-6
4.46958725\D7=175.7922479\D8=-121.14418429\D9=121.69057512\D10=156.886
49581\D11=-90.88061648\D12=-112.2217372\D13=88.0591\D14=-83.61996852\B
6=2.17270015\B7=1.36056832\\Version=AM64L-G03RevE.01\State=2-A\HF=-384
.2613665\S2=0.822837\S2-1=0.\S2A=0.750728\RMSD=5.603e-09\RMSF=3.643e-0
5\Thermal=0.\Dipole=0.8499768,-0.3474527,0.990864\PG=C01 [X(C6H9O2)]\\@

BHandHLYP/6-311++G**

1\1\GINC-GOMBERG08\FTS\UBHandHLYP\6-311++G(d,p)\C6H9O2(2)\HMAITKEN\11-
Oct-2010\1\\#BHandHLYP/6-311++G(d,p) opt=(grad,readfc,ts,nofreeze,noei
gentest) geom=checkpoint guess=read\\calc 6-exo radical product benchm
ark\\0,2\O\C,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\O,
5,B5,4,A4,3,D3,0\C,2,B6,1,A5,3,D4,0\C,7,B7,3,A6,4,D5,0\H,3,B8,4,A7,5,D
6,0\H,3,B9,4,A8,5,D7,0\H,4,B10,3,A9,5,D8,0\H,4,B11,3,A10,5,D9,0\H,5,B1
2,7,A11,3,D10,0\H,5,B13,7,A12,3,D11,0\H,7,B14,3,A13,4,D12,0\H,8,B15,7,
A14,3,D13,0\H,8,B16,7,A15,3,D14,0\\B1=1.17012663\B2=1.50776966\B3=1.52

493634\B4=1.51678602\B5=1.40725958\B8=1.09009299\B9=1.08798008\B10=1.0
8677556\B11=1.08741982\B12=1.08336498\B13=1.0920258\B14=1.08245348\B15
=1.07329608\B16=1.07463644\A1=128.01138047\A2=112.7620848\A3=113.23595
077\A4=112.39183688\A5=123.00609226\A6=132.65962843\A7=109.85291697\A8
=112.27319787\A9=109.94276585\A10=109.06207308\A11=134.74147985\A12=86
.98809043\A13=82.632435\A14=119.69143931\A15=120.71098478\D1=142.80468
212\D2=52.67624582\D3=-67.56609157\D4=-178.83637599\D5=123.53978076\D6
=-64.39131264\D7=175.94554908\D8=-121.47412592\D9=121.46896526\D10=156
.65675537\D11=-91.15720141\D12=-112.07307852\D13=87.80874634\D14=-83.9
6351537\B6=2.17506358\B7=1.36081148\\Version=AM64L-G03RevE.01\State=2-
A\HF=-384.2691973\S2=0.821648\S2-1=0.\S2A=0.750707\RMSD=4.539e-09\RMSF
=4.617e-05\Thermal=0.\Dipole=0.8971697,-0.3554195,1.066654\PG=C01 [X(C
6H9O2)]\\@

Cyclization product 41 (n=2, R=H)

HF/3-21G*

1\1\GINC-GOMBERG01\FOpt\UHF\3-21G*\C6H9O2(2)\HMAITKEN\08-Oct-2010\1\\#
HF/3-21G* opt=grad\\calc 6-exo radical product benchmark\\0,2\C\C,1,B1
\C,2,B2,1,A1\C,1,B3,3,A2,2,D1,0\H,1,B4,4,A3,3,D2,0\H,1,B5,4,A4,3,D3,0\
H,3,B6,2,A5,1,D4,0\H,3,B7,2,A6,1,D5,0\H,4,B8,1,A7,3,D6,0\H,4,B9,1,A8,3
,D7,0\H,2,B10,1,A9,4,D8,0\O,3,B11,2,A10,1,D9,0\C,2,B12,1,A11,4,D10,0\H
,13,B13,2,A12,1,D11,0\H,13,B14,2,A13,1,D12,0\C,1,B15,4,A14,3,D13,0\O,1
6,B16,1,A15,4,D14,0\\B1=2.56313489\B2=2.4286696\B3=1.54258373\B4=1.088
27125\B5=1.0809526\B6=1.07874321\B7=1.08683592\B8=1.08284056\B9=1.0829
822\B10=1.09329555\B11=1.44113148\B12=1.49043184\B13=1.06922687\B14=1.
07006843\B15=1.5146518\B16=1.2100503\A1=60.26420379\A2=35.02097393\A3=
109.00802739\A4=112.01141515\A5=138.5557273\A6=91.55193022\A7=109.6273
8628\A8=110.13398816\A9=94.0219153\A10=32.72618931\A11=143.75454129\A1
2=120.0374453\A13=118.42000521\A14=111.19651813\A15=123.14210316\D1=14
5.19925204\D2=-66.92899724\D3=173.2119564\D4=147.14037519\D5=-91.18448
465\D6=-119.02632915\D7=121.62588047\D8=-108.01443442\D9=141.78175438\
D10=117.71964938\D11=31.38440617\D12=-147.87134287\D13=51.61162894\D14
=137.37174501\\Version=AM64L-G03RevE.01\State=2-A\HF=-379.9880518\S2=0
.765901\S2-1=0.\S2A=0.750206\RMSD=5.422e-09\RMSF=1.312e-05\Thermal=0.\
Dipole=0.8798227,-0.7705578,-0.5799872\PG=C01 [X(C6H9O2)]\\@

HF/6-31G*

1\1\GINC-GOMBERG01\FOpt\UHF\6-31G(d)\C6H9O2(2)\HMAITKEN\08-Oct-2010\1\
\#HF/6-31G* opt=(grad,readfc) geom=checkpoint guess=read\\calc 6-exo r
adical product benchmark\\0,2\C\C,1,B1\C,2,B2,1,A1\C,1,B3,3,A2,2,D1,0\
H,1,B4,4,A3,3,D2,0\H,1,B5,4,A4,3,D3,0\H,3,B6,2,A5,1,D4,0\H,3,B7,2,A6,1
,D5,0\H,4,B8,1,A7,3,D6,0\H,4,B9,1,A8,3,D7,0\H,2,B10,1,A9,4,D8,0\O,3,B1
1,2,A10,1,D9,0\C,2,B12,1,A11,4,D10,0\H,13,B13,2,A12,1,D11,0\H,13,B14,2
,A13,1,D12,0\C,1,B15,4,A14,3,D13,0\O,16,B16,1,A15,4,D14,0\\B1=2.581475
95\B2=2.36818919\B3=1.53236833\B4=1.08995616\B5=1.08251169\B6=1.081314
96\B7=1.0906227\B8=1.08565424\B9=1.08575927\B10=1.09791701\B11=1.40116
549\B12=1.49076586\B13=1.07070268\B14=1.07281379\B15=1.5171812\B16=1.1
9077886\A1=60.51837255\A2=34.8555467\A3=109.41814481\A4=112.67386993\A
5=138.55651913\A6=90.89465824\A7=109.89736486\A8=110.33124828\A9=95.93
705238\A10=32.48733993\A11=142.96353518\A12=120.21553909\A13=118.35548
806\A14=112.71317199\A15=122.16693424\D1=148.30866042\D2=-72.92476468\
D3=167.93293934\D4=147.80745222\D5=-93.24472793\D6=-119.36209687\D7=12

2.2916514\D8=-104.96969627\D9=138.63252505\D10=119.55629248\D11=44.704
1649\D12=-146.38503115\D13=44.90534958\D14=146.64691414\\Version=AM64L
-G03RevE.01\State=2-A\HF=-382.1168097\S2=0.762268\S2-1=0.\S2A=0.7501\R
MSD=5.050e-09\RMSF=3.586e-05\Thermal=0.\Dipole=0.9693307,-0.6467931,-0
.4451156\PG=C01 [X(C6H9O2)]\\@

HF/6-311G**

1\1\GINC-GOMBERG01\FOpt\UHF\6-311G(d,p)\C6H9O2(2)\HMAITKEN\08-Oct-2010
\1\\#HF/6-311G** opt=(grad,readfc) geom=checkpoint guess=read\\calc 6-
exo radical product benchmark\\0,2\C\C,1,B1\C,2,B2,1,A1\C,1,B3,3,A2,2,
D1,0\H,1,B4,4,A3,3,D2,0\H,1,B5,4,A4,3,D3,0\H,3,B6,2,A5,1,D4,0\H,3,B7,2
,A6,1,D5,0\H,4,B8,1,A7,3,D6,0\H,4,B9,1,A8,3,D7,0\H,2,B10,1,A9,4,D8,0\O
,3,B11,2,A10,1,D9,0\C,2,B12,1,A11,4,D10,0\H,13,B13,2,A12,1,D11,0\H,13,
B14,2,A13,1,D12,0\C,1,B15,4,A14,3,D13,0\O,16,B16,1,A15,4,D14,0\\B1=2.5
7826991\B2=2.36665618\B3=1.53165369\B4=1.09025457\B5=1.08250959\B6=1.0
8151872\B7=1.09181382\B8=1.08624526\B9=1.08603585\B10=1.09900065\B11=1
.40040107\B12=1.48963503\B13=1.0713258\B14=1.07333749\B15=1.51670637\B
16=1.1852859\A1=60.55943449\A2=34.83632408\A3=109.48339884\A4=112.7664
4134\A5=138.62484654\A6=90.92912153\A7=109.8461298\A8=110.34526621\A9=
95.50504592\A10=32.46732619\A11=143.37477137\A12=120.1057433\A13=118.2
5999798\A14=112.64318504\A15=122.32574988\D1=148.22603858\D2=-72.26841
03\D3=168.26330365\D4=147.75885125\D5=-93.17162556\D6=-119.33322968\D7
=122.2268167\D8=-105.21887537\D9=138.92632253\D10=120.06125716\D11=43.
71765589\D12=-146.46653151\D13=45.28148209\D14=145.81182092\\Version=A
M64L-G03RevE.01\State=2-A\HF=-382.2114268\S2=0.762514\S2-1=0.\S2A=0.75
0103\RMSD=7.230e-09\RMSF=1.825e-05\Thermal=0.\Dipole=0.9844344,-0.6569
741,-0.4646448\PG=C01 [X(C6H9O2)]\\@

BHandHLYP/6-311G**

1\1\GINC-GOMBERG01\FOpt\UBHandHLYP\6-311G(d,p)\C6H9O2(2)\HMAITKEN\08-O
ct-2010\1\\#BHandHLYP/6-311G** opt=(grad,readfc) geom=checkpoint guess
=read\\calc 6-exo radical product benchmark\\0,2\C\C,1,B1\C,2,B2,1,A1\
C,1,B3,3,A2,2,D1,0\H,1,B4,4,A3,3,D2,0\H,1,B5,4,A4,3,D3,0\H,3,B6,2,A5,1
,D4,0\H,3,B7,2,A6,1,D5,0\H,4,B8,1,A7,3,D6,0\H,4,B9,1,A8,3,D7,0\H,2,B10
,1,A9,4,D8,0\O,3,B11,2,A10,1,D9,0\C,2,B12,1,A11,4,D10,0\H,13,B13,2,A12
,1,D11,0\H,13,B14,2,A13,1,D12,0\C,1,B15,4,A14,3,D13,0\O,16,B16,1,A15,4
,D14,0\\B1=2.57125211\B2=2.3646262\B3=1.52667051\B4=1.0912357\B5=1.083
52201\B6=1.08300569\B7=1.09390552\B8=1.08668963\B9=1.0866562\B10=1.103
81635\B11=1.40601769\B12=1.47490552\B13=1.07192158\B14=1.07337994\B15=
1.51050993\B16=1.19430624\A1=60.49274009\A2=34.8100071\A3=109.34857264
\A4=112.9792986\A5=138.9712442\A6=90.48401732\A7=109.82910847\A8=110.4
3454302\A9=94.84847532\A10=33.05309087\A11=143.44053916\A12=119.974291
34\A13=118.66295485\A14=112.8966898\A15=122.52022129\D1=148.23142393\D
2=-72.25004708\D3=168.46464706\D4=148.13107541\D5=-93.0888891\D6=-119.
25574533\D7=122.35319967\D8=-104.50989002\D9=138.86279117\D10=121.6662
7153\D11=35.9693507\D12=-146.85838682\D13=45.24432627\D14=145.83325517
\\Version=AM64L-G03RevE.01\State=2-A\HF=-384.3020364\S2=0.755189\S2-1=
0.\S2A=0.750017\RMSD=8.351e-09\RMSF=7.228e-06\Thermal=0.\Dipole=0.9222
706,-0.600384,-0.4810083\PG=C01 [X(C6H9O2)]\\@

BHandHLYP/6-311++G**

1\1\GINC-GOMBERG03\FOpt\UBHandHLYP\6-311++G(d,p)\C6H9O2(2)\HMAITKEN\09
-Oct-2010\0\\#BHandHLYP/6-311++G(d,p) opt=(readfc) geom=checkpoint gue

ss=read\\calc 6-exo radical product benchmark\\0,2\C,-0.0117423856,-0.
0035824793,-0.0009323595\C,0.007758908,0.0091317646,2.5725524293\C,2.0
581872822,0.0210518216,1.3896441541\C,1.4389422109,0.4640268656,0.0804
203434\H,-0.0368167111,-1.0818677454,-0.1682561285\H,-0.5585382497,0.4
572543026,-0.8151489095\H,3.0630117566,0.4090233776,1.5034732403\H,2.1
084425395,-1.07001841,1.4448008934\H,1.4824155723,1.5486135594,0.02682
96978\H,2.0089251968,0.0740384756,-0.7586526498\H,0.075416994,-1.08795
23883,2.6742026215\O,1.3197702178,0.5222806194,2.4772074194\C,-0.65123
25515,0.5839064541,3.760654736\H,-1.7123000498,0.7382388628,3.76434282
03\H,-0.0570106728,0.7851365638,4.6318459169\C,-0.7812104266,0.2265001
168,1.2774166309\O,-1.94896527,0.4820099709,1.2857728939\\Version=AM64
L-G03RevE.01\State=2-A\HF=-384.3101061\S2=0.755231\S2-1=0.\S2A=0.75001
7\RMSD=5.495e-09\RMSF=2.065e-06\Thermal=0.\Dipole=1.0055766,-0.6253265
,-0.5204014\PG=C01 [X(C6H9O2)]\\@

Decarbonylation transition state 40 → 42 (n=2, R=H)

HF/3-21G*

1\1\GINC-GOMBERG01\FTS\UHF\3-21G*\C6H9O2(2)\HMAITKEN\21-Nov-2010\1\\#H
F/3-21G* opt=(grad,ts,readfc,noeigentest,nofreeze) geom=checkpoint gue
ss=read\\decarbonylation transition state\\0,2\C\C,1,B1\O,2,B2,1,A1\C,
3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\H,5,B5,4,A4,3,D3,0\H,5,B6,4,A5,3,D
4,0\H,4,B7,3,A6,2,D5,0\H,2,B8,1,A7,3,D6,0\H,2,B9,1,A8,3,D7,0\H,1,B10,2
,A9,3,D8,0\H,1,B11,2,A10,3,D9,0\C,1,B12,2,A11,3,D10,0\H,13,B13,1,A12,2
,D11,0\H,13,B14,1,A13,2,D12,0\C,13,B15,1,A14,2,D13,0\O,16,B16,13,A15,1
,D14,0\\B1=1.53100108\B2=1.43924481\B3=1.37122768\B4=1.31550424\B5=1.0
7035453\B6=1.07069631\B7=1.07043531\B8=1.08351995\B9=1.08351862\B10=1.
08150334\B11=1.0815016\B12=1.51805658\B13=1.07720583\B14=1.07722442\A1
=105.81349202\A2=119.93542549\A3=127.9513665\A4=119.5192976\A5=123.579
76065\A6=109.85914044\A7=111.06478908\A8=111.06284182\A9=108.24586584\
A10=108.24813783\A11=111.23053995\A12=116.77643041\A13=116.77181048\A1
4=106.0060211\A15=117.94904774\D1=-180.00546412\D2=0.00162111\D3=-180.
0003955\D4=0.00002037\D5=180.00062157\D6=-119.44508859\D7=119.4454586\
D8=58.14792753\D9=-58.15561493\D10=-180.00325073\D11=-69.48311546\D12=
69.40831225\D13=-180.04346996\D14=-0.10530903\B15=1.99961483\B16=1.152
22053\\Version=AM64L-G03RevE.01\State=2-A\HF=-379.9433781\S2=0.807731\
S2-1=0.\S2A=0.75088\RMSD=1.986e-09\RMSF=1.267e-05\Thermal=0.\Dipole=0.
5065795,0.9077348,0.0000921\PG=C01 [X(C6H9O2)]\\@

HF/6-31G*

1\1\GINC-GOMBERG01\FTS\UHF\6-31G(d)\C6H9O2(2)\HMAITKEN\21-Nov-2010\1\\
#HF/6-31G* opt=(grad,ts,readfc,noeigentest,nofreeze) geom=checkpoint g
uess=read\\decarbonylation transition state\\0,2\C\C,1,B1\O,2,B2,1,A1\
C,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\H,5,B5,4,A4,3,D3,0\H,5,B6,4,A5,3
,D4,0\H,4,B7,3,A6,2,D5,0\H,2,B8,1,A7,3,D6,0\H,2,B9,1,A8,3,D7,0\H,1,B10
,2,A9,3,D8,0\H,1,B11,2,A10,3,D9,0\C,1,B12,2,A11,3,D10,0\H,13,B13,1,A12
,2,D11,0\H,13,B14,1,A13,2,D12,0\C,13,B15,1,A14,2,D13,0\O,16,B16,13,A15
,1,D14,0\\B1=1.52367578\B2=1.40303035\B3=1.3422219\B4=1.32024273\B5=1.
07305789\B6=1.07297961\B7=1.07401646\B8=1.08620851\B9=1.08620049\B10=1
.08406675\B11=1.08408002\B12=1.51102047\B13=1.07920275\B14=1.07918449\
A1=107.48772998\A2=118.71080125\A3=128.60776841\A4=118.85854919\A5=123
.91503999\A6=109.99492853\A7=110.88321067\A8=110.88417252\A9=108.69793
259\A10=108.70446869\A11=111.64651703\A12=116.52164333\A13=116.5278567

2\A14=108.03601384\A15=117.63665039\D1=-179.96355138\D2=-0.00774312\D3
=-179.99737498\D4=0.00161525\D5=179.99207909\D6=-120.02809095\D7=120.0
2399934\D8=58.04301868\D9=-58.0832449\D10=-180.02033739\D11=-67.993848
97\D12=68.05132644\D13=-179.96120537\D14=0.09390853\B15=1.989886\B16=1
.1345983\\Version=AM64L-G03RevE.01\State=2-A\HF=-382.0716164\S2=0.8096
97\S2-1=0.\S2A=0.750963\RMSD=4.815e-09\RMSF=3.974e-05\Thermal=0.\Dipol
e=-0.5716498,0.0006098,0.6319031\PG=C01 [X(C6H9O2)]\\@

HF/6-311G**

1\1\GINC-GOMBERG02\FTS\UHF\6-311G(d,p)\C6H9O2(2)\HMAITKEN\21-Nov-2010\
1\\#HF/6-311G** opt=(grad,ts,readfc,noeigentest,nofreeze) geom=checkpo
int guess=read\\decarbonylation transition state\\0,2\C\C,1,B1\O,2,B2,
1,A1\C,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\H,5,B5,4,A4,3,D3,0\H,5,B6,4
,A5,3,D4,0\H,4,B7,3,A6,2,D5,0\H,2,B8,1,A7,3,D6,0\H,2,B9,1,A8,3,D7,0\H,
1,B10,2,A9,3,D8,0\H,1,B11,2,A10,3,D9,0\C,1,B12,2,A11,3,D10,0\H,13,B13,
1,A12,2,D11,0\H,13,B14,1,A13,2,D12,0\C,13,B15,1,A14,2,D13,0\O,16,B16,1
3,A15,1,D14,0\\B1=1.52196997\B2=1.40263964\B3=1.33924494\B4=1.32015172
\B5=1.0733152\B6=1.07325833\B7=1.07489607\B8=1.08736427\B9=1.08736276\
B10=1.08462091\B11=1.08463673\B12=1.51075405\B13=1.0799048\B14=1.07987
028\A1=107.53574366\A2=118.90328279\A3=128.59472148\A4=118.60645975\A5
=123.88313309\A6=110.16737736\A7=110.79023871\A8=110.79223976\A9=108.6
4693776\A10=108.64706481\A11=111.70726109\A12=116.47280244\A13=116.479
93287\A14=108.28364639\A15=117.72907338\D1=-180.00282398\D2=0.00061269
\D3=-179.99967729\D4=0.00100597\D5=180.00172814\D6=-120.01452252\D7=12
0.01222923\D8=58.08343077\D9=-58.08574785\D10=-180.00121094\D11=-67.97
019899\D12=68.0206008\D13=-179.94954062\D14=0.34282786\B15=1.9804128\B
16=1.12683946\\Version=AM64L-G03RevE.01\State=2-A\HF=-382.1715111\S2=0
.808837\S2-1=0.\S2A=0.751005\RMSD=5.503e-09\RMSF=4.875e-06\Thermal=0.\
Dipole=-0.5181855,0.0017075,0.6323163\PG=C01 [X(C6H9O2)]\\@

BHandHLYP/6-311G**

1\1\GINC-GOMBERG02\FTS\UBHandHLYP\6-311G(d,p)\C6H9O2(2)\HMAITKEN\22-No
v-2010\1\\#BHandHLYP/6-311G** opt=(grad,ts,readfc,noeigentest,nofreeze
) geom=checkpoint guess=read\\decarbonylation transition state\\0,2\C\
C,1,B1\O,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\H,5,B5,4,A4,3
,D3,0\H,5,B6,4,A5,3,D4,0\H,4,B7,3,A6,2,D5,0\H,2,B8,1,A7,3,D6,0\H,2,B9,
1,A8,3,D7,0\H,1,B10,2,A9,3,D8,0\H,1,B11,2,A10,3,D9,0\C,1,B12,2,A11,3,D
10,0\H,13,B13,1,A12,2,D11,0\H,13,B14,1,A13,2,D12,0\C,13,B15,1,A14,2,D1
3,0\O,16,B16,13,A15,1,D14,0\\B1=1.51903785\B2=1.40852064\B3=1.34263874
\B4=1.3226128\B5=1.07382847\B6=1.07388458\B7=1.07663545\B8=1.08906929\
B9=1.08907275\B10=1.08603228\B11=1.08604665\B12=1.49437722\B13=1.07855
964\B14=1.07865967\A1=107.45310333\A2=117.83245759\A3=128.27815522\A4=
118.76417283\A5=123.67832258\A6=110.03601929\A7=110.91743344\A8=110.90
36183\A9=108.28318072\A10=108.27111769\A11=111.97611128\A12=118.204650
01\A13=118.18000745\A14=105.99549984\A15=114.93851064\D1=-180.0463575\
D2=0.02829202\D3=-180.00023055\D4=0.00103593\D5=180.0255883\D6=-119.99
234617\D7=119.9825553\D8=57.86146633\D9=-57.83160429\D10=-179.97594159
\D11=-72.33061717\D12=71.77417143\D13=-180.38685291\D14=-1.01822113\B1
5=2.12758244\B16=1.1299306\\Version=AM64L-G03RevE.01\State=2-A\HF=-384
.2600102\S2=0.771736\S2-1=0.\S2A=0.75015\RMSD=7.716e-09\RMSF=9.703e-06
\Thermal=0.\Dipole=-0.4332651,-0.0049394,0.4728335\PG=C01 [X(C6H9O2)]\\@

BHandHLYP/6-31++G**

1\1\GINC-GOMBERG03\FTS\UBHandHLYP\6-311++G(d,p)\C6H9O2(2)\HMAITKEN\22-
Nov-2010\1\\#BHandHLYP/6-311++G(d,p) opt=(grad,ts,readfc,noeigentest,n
ofreeze) geom=checkpoint guess=read\\decarbonylation transition state\
\0,2\C\C,1,B1\O,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\H,5,B5
,4,A4,3,D3,0\H,5,B6,4,A5,3,D4,0\H,4,B7,3,A6,2,D5,0\H,2,B8,1,A7,3,D6,0\
H,2,B9,1,A8,3,D7,0\H,1,B10,2,A9,3,D8,0\H,1,B11,2,A10,3,D9,0\C,1,B12,2,
A11,3,D10,0\H,13,B13,1,A12,2,D11,0\H,13,B14,1,A13,2,D12,0\C,13,B15,1,A
14,2,D13,0\O,16,B16,13,A15,1,D14,0\\B1=1.51946996\B2=1.40907807\B3=1.3
4254088\B4=1.32409889\B5=1.07390651\B6=1.07391237\B7=1.07646356\B8=1.0
8889346\B9=1.08892625\B10=1.08615248\B11=1.08611676\B12=1.49407419\B13
=1.07830756\B14=1.078777\A1=107.67459653\A2=117.93659328\A3=128.124743
74\A4=118.65384191\A5=123.72593134\A6=110.17782579\A7=110.89459106\A8=
110.8579378\A9=108.37703809\A10=108.38733264\A11=111.72312718\A12=118.
38667281\A13=118.26672438\A14=106.11962062\A15=115.07830205\D1=-180.03
141727\D2=-0.05419333\D3=-180.00045652\D4=-0.00511931\D5=179.94866153\
D6=-119.96544377\D7=119.95469319\D8=57.98825398\D9=-57.91328789\D10=-1
79.95585889\D11=-73.13516958\D12=71.67946237\D13=-181.1247221\D14=-5.1
2638373\B15=2.13786103\B16=1.13029034\\Version=AM64L-G03RevE.01\State=
2-A\HF=-384.2667401\S2=0.771515\S2-1=0.\S2A=0.750152\RMSD=6.815e-09\RM
SF=5.149e-06\Thermal=0.\Dipole=-0.4734801,-0.0204404,0.504946\PG=C01 [
X(C6H9O2)]\\@

Decarbonylation product 42 (n=2, R=H)

HF/3-21G*

1\1\GINC-GOMBERG01\FOpt\UHF\3-21G*\C5H9O1(2)\HMAITKEN\23-Nov-2010\1\\#
HF/3-21G* opt=(grad)\\6 membered decarbonylation radical\\0,2\C\O,1,B1
\C,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\H,4,B4,3,A3,2,D2,0\H,4,B5,3,A4,2,D3,0\
H,3,B6,2,A5,1,D4,0\H,1,B7,2,A6,3,D5,0\H,1,B8,2,A7,3,D6,0\C,1,B9,2,A8,3
,D7,0\H,10,B10,1,A9,2,D8,0\H,10,B11,1,A10,2,D9,0\C,10,B12,1,A11,2,D10,
0\H,13,B13,10,A12,1,D11,0\H,13,B14,10,A13,1,D12,0\\B1=1.44070721\B2=1.
36977072\B3=1.31584321\B4=1.07043778\B5=1.07062964\B6=1.07069294\B7=1.
08284764\B8=1.08391138\B9=1.52919177\B10=1.08203099\B11=1.08695417\B12
=1.50638138\B13=1.07239976\B14=1.07475618\A1=119.96033847\A2=128.03816
\A3=119.52504903\A4=123.54229694\A5=109.92450265\A6=110.13931837\A7=10
9.96232951\A8=106.21326158\A9=108.40099775\A10=107.44528534\A11=111.56
228128\A12=121.05917889\A13=119.99191632\D1=-0.21417371\D2=180.0166182
5\D3=0.04139299\D4=179.81612362\D5=-59.42803825\D6=60.38002595\D7=-179
.56648866\D8=60.0378373\D9=-55.59577596\D10=182.51173483\D11=220.78434
417\D12=51.30887271\\Version=AM64L-G03RevE.01\State=2-A\HF=-267.868824
8\S2=0.763221\S2-1=0.\S2A=0.750128\RMSD=8.770e-09\RMSF=3.937e-06\Therm
al=0.\Dipole=0.1145185,-0.0185308,-0.3760262\PG=C01 [X(C5H9O1)]\\@

HF/6-31G*

1\1\GINC-GOMBERG07\FOpt\UHF\6-31G(d)\C5H9O1(2)\HMAITKEN\09-Nov-2010\1\
\#HF/6-31G* opt=(grad,readfc) geom=checkpoint guess=read\\6 membered d
ecarbonylation radical\\0,2\C\O,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\H,
4,B4,3,A3,2,D2,0\H,4,B5,3,A4,2,D3,0\H,3,B6,2,A5,1,D4,0\H,1,B7,2,A6,3,D
5,0\H,1,B8,2,A7,3,D6,0\C,1,B9,2,A8,3,D7,0\H,10,B10,1,A9,2,D8,0\H,10,B1
1,1,A10,2,D9,0\C,10,B12,1,A11,2,D10,0\H,13,B13,10,A12,1,D11,0\H,13,B14
,10,A13,1,D12,0\\B1=1.4044964\B2=1.34109785\B3=1.32048655\B4=1.0731350

9\B5=1.07292963\B6=1.07423453\B7=1.08557719\B8=1.08652473\B9=1.5205147
5\B10=1.08515706\B11=1.09016813\B12=1.49989123\B13=1.07441458\B14=1.07
63521\A1=118.74898659\A2=128.67011723\A3=118.86081257\A4=123.8807931\A
5=110.04003888\A6=109.87617551\A7=109.70706088\A8=107.81343894\A9=108.
893593\A10=108.10151055\A11=112.19252495\A12=120.4289084\A13=120.35837
664\D1=-0.10045702\D2=180.01756087\D3=0.052431\D4=179.92354699\D5=-59.
04895761\D6=59.55336821\D7=-179.82251593\D8=59.72913057\D9=-55.4540259
3\D10=182.18507307\D11=206.91576291\D12=43.43841082\\Version=AM64L-G03
RevE.01\State=2-A\HF=-269.3587613\S2=0.762155\S2-1=0.\S2A=0.750098\RMS
D=4.841e-09\RMSF=1.210e-05\Thermal=0.\Dipole=0.0068073,-0.043459,-0.31
83401\PG=C01 [X(C5H9O1)]\\@

HF/6-311G**

1\1\GINC-GOMBERG03\FOpt\UHF\6-311G(d,p)\C5H9O1(2)\HMAITKEN\10-Nov-2010
\1\\#HF/6-311G** opt=(grad,readfc) geom=checkpoint guess=read\\6 membe
red decarbonylation radical\\0,2\C\O,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,1,D1
,0\H,4,B4,3,A3,2,D2,0\H,4,B5,3,A4,2,D3,0\H,3,B6,2,A5,1,D4,0\H,1,B7,2,A
6,3,D5,0\H,1,B8,2,A7,3,D6,0\C,1,B9,2,A8,3,D7,0\H,10,B10,1,A9,2,D8,0\H,
10,B11,1,A10,2,D9,0\C,10,B12,1,A11,2,D10,0\H,13,B13,10,A12,1,D11,0\H,1
3,B14,10,A13,1,D12,0\\B1=1.40403156\B2=1.33803534\B3=1.32043268\B4=1.0
7338909\B5=1.07319989\B6=1.07511777\B7=1.08677575\B8=1.08767833\B9=1.5
1862831\B10=1.08572148\B11=1.09085645\B12=1.49927642\B13=1.07502707\B1
4=1.07707394\A1=118.92671928\A2=128.65570788\A3=118.60672948\A4=123.84
430376\A5=110.21496278\A6=109.88668278\A7=109.72533423\A8=107.87467187
\A9=108.93177996\A10=108.11605891\A11=112.31045405\A12=120.32311962\A1
3=120.4151285\D1=-0.08162427\D2=180.01432605\D3=0.059818\D4=179.941069
54\D5=-59.06950597\D6=59.67489458\D7=-179.77668563\D8=59.33541664\D9=-
55.9054097\D10=181.8779528\D11=204.53666568\D12=40.58171388\\Version=A
M64L-G03RevE.01\State=2-A\HF=-269.4297142\S2=0.762338\S2-1=0.\S2A=0.75
0101\RMSD=5.224e-09\RMSF=4.448e-06\Thermal=0.\Dipole=-0.0113638,-0.048
837,-0.3037323\PG=C01 [X(C5H9O1)]\\@

BHandHLYP/6-311G**

1\1\GINC-GOMBERG02\FOpt\UBHandHLYP\6-311G(d,p)\C5H9O1(2)\HMAITKEN\10-N
ov-2010\1\\#BHandHLYP/6-311G** opt=(grad,readfc) geom=checkpoint guess
=read\\6 membered decarbonylation radical\\0,2\C\O,1,B1\C,2,B2,1,A1\C,
3,B3,2,A2,1,D1,0\H,4,B4,3,A3,2,D2,0\H,4,B5,3,A4,2,D3,0\H,3,B6,2,A5,1,D
4,0\H,1,B7,2,A6,3,D5,0\H,1,B8,2,A7,3,D6,0\C,1,B9,2,A8,3,D7,0\H,10,B10,
1,A9,2,D8,0\H,10,B11,1,A10,2,D9,0\C,10,B12,1,A11,2,D10,0\H,13,B13,10,A
12,1,D11,0\H,13,B14,10,A13,1,D12,0\\B1=1.40898632\B2=1.34153663\B3=1.3
2288238\B4=1.07387395\B5=1.07382792\B6=1.07678068\B7=1.08864692\B8=1.0
8972668\B9=1.51358616\B10=1.0870339\B11=1.09391844\B12=1.48426189\B13=
1.07465847\B14=1.0767683\A1=117.89523644\A2=128.33723339\A3=118.755882
69\A4=123.65682672\A5=110.07693385\A6=109.85753925\A7=109.69700948\A8=
107.85929809\A9=109.04220782\A10=107.67574871\A11=112.59714742\A12=120
.7964266\A13=120.72199233\D1=-0.25454896\D2=180.02465284\D3=0.06405036
\D4=179.79265043\D5=-58.78081696\D6=59.77768454\D7=-179.6513967\D8=59.
58836589\D9=-54.82352998\D10=182.91117914\D11=205.36160156\D12=35.6199
5131\\Version=AM64L-G03RevE.01\State=2-A\HF=-270.9814105\S2=0.755227\S
2-1=0.\S2A=0.750017\RMSD=6.487e-09\RMSF=7.766e-06\Thermal=0.\Dipole=-0
.0184695,-0.0327711,-0.2889167\PG=C01 [X(C5H9O1)]\\@

BHandHLYP/6-311++G**

1\1\GINC-GOMBERG07\FOpt\UBHandHLYP\6-311++G(d,p)\C5H9O1(2)\HMAITKEN\10
-Nov-2010\1\\#BHandHLYP/6-311++G(d,p) opt=(grad,readfc) geom=checkpoin
t guess=read\\6 membered decarbonylation radical\\0,2\C\O,1,B1\C,2,B2,
1,A1\C,3,B3,2,A2,1,D1,0\H,4,B4,3,A3,2,D2,0\H,4,B5,3,A4,2,D3,0\H,3,B6,2
,A5,1,D4,0\H,1,B7,2,A6,3,D5,0\H,1,B8,2,A7,3,D6,0\C,1,B9,2,A8,3,D7,0\H,
10,B10,1,A9,2,D8,0\H,10,B11,1,A10,2,D9,0\C,10,B12,1,A11,2,D10,0\H,13,B
13,10,A12,1,D11,0\H,13,B14,10,A13,1,D12,0\\B1=1.40964666\B2=1.34142066
\B3=1.32440966\B4=1.07394426\B5=1.07385193\B6=1.07658771\B7=1.08850378
\B8=1.08954104\B9=1.51366479\B10=1.08708272\B11=1.09391778\B12=1.48435
241\B13=1.07479651\B14=1.07684583\A1=118.00174803\A2=128.18230089\A3=1
18.64592202\A4=123.70499352\A5=110.22085252\A6=109.70760611\A7=109.579
92884\A8=108.0641119\A9=109.23116489\A10=107.84042135\A11=112.49008382
\A12=120.77081242\A13=120.80360242\D1=-0.26211717\D2=180.02638672\D3=0
.06203951\D4=179.78147413\D5=-58.79980402\D6=59.70315913\D7=-179.70010
909\D8=60.00935272\D9=-54.61214247\D10=183.29528345\D11=205.09274692\D
12=34.9721262\\Version=AM64L-G03RevE.01\State=2-A\HF=-270.9863983\S2=0
.755272\S2-1=0.\S2A=0.750018\RMSD=3.950e-09\RMSF=7.944e-06\Thermal=0.\
Dipole=-0.0132366,-0.0360514,-0.3123105\PG=C01 [X(C5H9O1)]\\@

Alkyl cyclization transition state 42 →43 (n=2, R=H)

HF/3-21G*

1\1\GINC-GOMBERG01\FTS\UHF\3-21G*\C5H9O1(2)\HMAITKEN\12-Oct-2010\1\\#H
F/3-21G* opt=(grad,ts,nofreeze,noeigentest,readfc) geom=checkpoint gue
ss=read\\6 membered decarbonylation cyclic radical ts\\0,2\C\O,1,B1\C,
2,B2,1,A1\C,1,B3,2,A2,3,D1,0\H,1,B4,2,A3,3,D2,0\H,1,B5,2,A4,3,D3,0\H,3
,B6,2,A5,1,D4,0\H,4,B7,1,A6,2,D5,0\H,4,B8,1,A7,2,D6,0\C,3,B9,2,A8,1,D7
,0\H,10,B10,3,A9,2,D8,0\H,10,B11,3,A10,2,D9,0\C,3,B12,2,A11,1,D10,0\H,
13,B13,3,A12,2,D11,0\H,13,B14,3,A13,2,D12,0\\B1=1.4398932\B2=1.4019861
5\B3=1.53732748\B4=1.07828076\B5=1.08536854\B6=1.07424904\B7=1.0857001
8\B8=1.0822092\B10=1.07128364\B11=1.0710056\B13=1.07344745\B14=1.07731
381\A1=113.50038619\A2=107.16292362\A3=106.72618516\A4=110.22387814\A5
=115.3470949\A6=109.89073105\A7=108.64961987\A8=117.75657751\A9=120.65
21747\A10=119.94611885\A11=94.39926894\A12=105.66341961\A13=101.627433
57\D1=52.1707862\D2=173.4637634\D3=-67.69533862\D4=65.51033572\D5=-172
.59397366\D6=68.68367222\D7=-142.18993222\D8=190.98272223\D9=15.453949
51\D10=-28.09344292\D11=-122.21094777\D12=117.01280257\B9=1.37759077\B
12=2.20382191\\Version=AM64L-G03RevE.01\State=2-A\HF=-267.8511715\S2=1
.013568\S2-1=0.\S2A=0.760963\RMSD=5.688e-09\RMSF=1.596e-05\Thermal=0.\
Dipole=0.4915804,-0.0677641,-0.5903663\PG=C01 [X(C5H9O1)]\\@

HF/6-31G*

1\1\GINC-GOMBERG02\FTS\UHF\6-31G(d)\C5H9O1(2)\HMAITKEN\12-Oct-2010\1\\
#HF/6-31G* opt=(grad,ts,nofreeze,noeigentest,readfc) geom=checkpoint g
uess=read\\6 membered decarbonylation cyclic radical ts\\0,2\C\O,1,B1\
C,2,B2,1,A1\C,1,B3,2,A2,3,D1,0\H,1,B4,2,A3,3,D2,0\H,1,B5,2,A4,3,D3,0\H
,3,B6,2,A5,1,D4,0\H,4,B7,1,A6,2,D5,0\H,4,B8,1,A7,2,D6,0\C,3,B9,2,A8,1,
D7,0\H,10,B10,3,A9,2,D8,0\H,10,B11,3,A10,2,D9,0\C,3,B12,2,A11,1,D10,0\
H,13,B13,3,A12,2,D11,0\H,13,B14,3,A13,2,D12,0\\B1=1.4001226\B2=1.36591
192\B3=1.52734068\B4=1.08131721\B5=1.08941755\B6=1.07850679\B7=1.08805
934\B8=1.08465343\B10=1.0735429\B11=1.07371998\B13=1.07586282\B14=1.07
900275\A1=112.8437775\A2=107.83365487\A3=107.16072364\A4=110.05820766\
A5=114.73913994\A6=110.1989283\A7=108.79877167\A8=118.0518438\A9=120.1

4038184\A10=120.58730945\A11=94.58854774\A12=107.75632302\A13=102.5331
309\D1=54.76266769\D2=176.6367101\D3=-65.78019687\D4=62.90611133\D5=-1
71.81344098\D6=70.3013116\D7=-148.16300563\D8=191.06746284\D9=18.82055
589\D10=-31.75494191\D11=-118.30276619\D12=121.09452738\B9=1.38698332\
B12=2.1891444\\Version=AM64L-G03RevE.01\State=2-A\HF=-269.3376753\S2=1
.016618\S2-1=0.\S2A=0.760437\RMSD=7.816e-09\RMSF=3.661e-05\Thermal=0.\
Dipole=0.381021,-0.0532624,-0.5004388\PG=C01 [X(C5H9O1)]\\@

HF/6-311G**

1\1\GINC-GOMBERG02\FTS\UHF\6-311G(d,p)\C5H9O1(2)\HMAITKEN\12-Oct-2010\
1\\#HF/6-311G** opt=(grad,ts,nofreeze,noeigentest,readfc) geom=checkpo
int guess=read\\6 membered decarbonylation cyclic radical ts\\0,2\C\O,
1,B1\C,2,B2,1,A1\C,1,B3,2,A2,3,D1,0\H,1,B4,2,A3,3,D2,0\H,1,B5,2,A4,3,D
3,0\H,3,B6,2,A5,1,D4,0\H,4,B7,1,A6,2,D5,0\H,4,B8,1,A7,2,D6,0\C,3,B9,2,
A8,1,D7,0\H,10,B10,3,A9,2,D8,0\H,10,B11,3,A10,2,D9,0\C,3,B12,2,A11,1,D
10,0\H,13,B13,3,A12,2,D11,0\H,13,B14,3,A13,2,D12,0\\B1=1.39962879\B2=1
.36415591\B3=1.52600934\B4=1.08159698\B5=1.0906195\B6=1.07917637\B7=1.
08837335\B8=1.0851541\B10=1.07403485\B11=1.07434565\B13=1.07658574\B14
=1.07979399\A1=112.82973052\A2=107.69666946\A3=107.24662993\A4=110.036
4095\A5=114.80470327\A6=110.21131078\A7=108.83925581\A8=117.94944539\A
9=120.0297144\A10=120.41984759\A11=94.85646345\A12=108.00056687\A13=10
2.48394915\D1=54.43430232\D2=176.28303262\D3=-66.04340193\D4=63.404063
24\D5=-171.64045249\D6=70.3366754\D7=-148.06704659\D8=191.05049838\D9=
18.69215513\D10=-31.49760265\D11=-118.61465441\D12=120.7542261\B9=1.38
739375\B12=2.1754271\\Version=AM64L-G03RevE.01\State=2-A\HF=-269.40599
41\S2=1.006972\S2-1=0.\S2A=0.760054\RMSD=9.150e-09\RMSF=3.521e-05\Ther
mal=0.\Dipole=0.3635337,-0.0396742,-0.5108929\PG=C01 [X(C5H9O1)]\\@

BHandHLYP/6-311G**

1\1\GINC-GOMBERG02\FTS\UBHandHLYP\6-311G(d,p)\C5H9O1(2)\HMAITKEN\12-Oc
t-2010\1\\#BHandHLYP/6-311G** opt=(grad,ts,nofreeze,noeigentest,readfc
) geom=checkpoint guess=read\\6 membered decarbonylation cyclic radica
l ts\\0,2\C\O,1,B1\C,2,B2,1,A1\C,1,B3,2,A2,3,D1,0\H,1,B4,2,A3,3,D2,0\H
,1,B5,2,A4,3,D3,0\H,3,B6,2,A5,1,D4,0\H,4,B7,1,A6,2,D5,0\H,4,B8,1,A7,2,
D6,0\C,3,B9,2,A8,1,D7,0\H,10,B10,3,A9,2,D8,0\H,10,B11,3,A10,2,D9,0\C,3
,B12,2,A11,1,D10,0\H,13,B13,3,A12,2,D11,0\H,13,B14,3,A13,2,D12,0\\B1=1
.40483501\B2=1.36174873\B3=1.52551045\B4=1.08259979\B5=1.09201974\B6=1
.08110953\B7=1.08973127\B8=1.08541599\B10=1.0739146\B11=1.07483797\B13
=1.07571592\B14=1.07927935\A1=112.29938259\A2=107.53576182\A3=107.1418
2009\A4=110.05673432\A5=114.95066113\A6=109.6461994\A7=108.66795557\A8
=119.26580062\A9=120.19634733\A10=120.4717356\A11=93.97331776\A12=106.
2324457\A13=101.29935778\D1=56.54005313\D2=178.38170427\D3=-63.7465493
9\D4=57.2936398\D5=-172.27436687\D6=70.20856115\D7=-149.15779266\D8=19
1.17054431\D9=15.8469101\D10=-33.42898914\D11=-117.04530092\D12=122.97
694806\B9=1.36101084\B12=2.20538325\\Version=AM64L-G03RevE.01\State=2-
A\HF=-270.9623668\S2=0.825939\S2-1=0.\S2A=0.750768\RMSD=6.922e-09\RMSF
=1.970e-05\Thermal=0.\Dipole=0.2938222,-0.0100019,-0.5572896\PG=C01 [X
(C5H9O1)]\\@

BHandHLYP/6-311++G**

1\1\GINC-GOMBERG02\FTS\UBHandHLYP\6-311++G(d,p)\C5H9O1(2)\HMAITKEN\12-
Oct-2010\1\\#BHandHLYP/6-311++G(d,p) opt=(grad,ts,nofreeze,noeigentest
,readfc) geom=checkpoint guess=read\\6 membered decarbonylation cyclic

radical ts\\0,2\C\O,1,B1\C,2,B2,1,A1\C,1,B3,2,A2,3,D1,0\H,1,B4,2,A3,3
,D2,0\H,1,B5,2,A4,3,D3,0\H,3,B6,2,A5,1,D4,0\H,4,B7,1,A6,2,D5,0\H,4,B8,
1,A7,2,D6,0\C,3,B9,2,A8,1,D7,0\H,10,B10,3,A9,2,D8,0\H,10,B11,3,A10,2,D
9,0\C,3,B12,2,A11,1,D10,0\H,13,B13,3,A12,2,D11,0\H,13,B14,3,A13,2,D12,
0\\B1=1.4055116\B2=1.36189099\B3=1.5252972\B4=1.08269682\B5=1.09174394
\B6=1.08090633\B7=1.08976107\B8=1.08546401\B10=1.0740417\B11=1.0749769
2\B13=1.07577151\B14=1.07925256\A1=112.42944179\A2=107.56787235\A3=107
.14056948\A4=109.93110381\A5=114.87321987\A6=109.51950853\A7=108.75287
234\A8=119.39145944\A9=119.99687609\A10=120.70898094\A11=93.87604251\A
12=106.04520356\A13=101.08338051\D1=56.43230674\D2=178.2758274\D3=-63.
92022081\D4=57.20910691\D5=-171.83217884\D6=70.71950997\D7=-149.240930
79\D8=191.24204086\D9=15.88806413\D10=-33.4902207\D11=-116.88886104\D1
2=123.27350687\B9=1.36132164\B12=2.20724218\\Version=AM64L-G03RevE.01\
State=2-A\HF=-270.9670947\S2=0.824468\S2-1=0.\S2A=0.750749\RMSD=7.704e
-09\RMSF=2.515e-05\Thermal=0.\Dipole=0.3209061,-0.0252127,-0.6006025\P
G=C01 [X(C5H9O1)]\\@

Alkyl cyclization product 43 (R=H)

HF/3-21G*

1\1\GINC-GOMBERG04\FOpt\UHF\3-21G*\C5H9O1(2)\HMAITKEN\11-Oct-2010\1\\#
HF/3-21G* opt=(grad)\\6 membered decarbonylation radical\\0,2\C\O,1,B1
\C,2,B2,1,A1\C,1,B3,2,A2,3,D1,0\H,1,B4,2,A3,3,D2,0\H,1,B5,2,A4,3,D3,0\
H,3,B6,2,A5,1,D4,0\H,4,B7,1,A6,2,D5,0\H,4,B8,1,A7,2,D6,0\C,3,B9,2,A8,1
,D7,0\H,10,B10,3,A9,2,D8,0\H,10,B11,3,A10,2,D9,0\C,3,B12,2,A11,1,D10,0
\H,13,B13,3,A12,2,D11,0\H,13,B14,3,A13,2,D12,0\\B1=1.45299224\B2=1.454
22482\B3=1.54139898\B4=1.07928024\B5=1.08170904\B6=1.08318337\B7=1.081
04787\B8=1.08228076\B9=1.49902301\B10=1.07370583\B11=1.07140797\B12=1.
54672328\B13=1.08038002\B14=1.08352454\A1=110.59211614\A2=105.7603395\
A3=108.8404923\A4=108.93543988\A5=107.44649998\A6=112.28670826\A7=110.
38829992\A8=109.15719761\A9=119.82968074\A10=118.86601685\A11=104.8100
8027\A12=112.34999614\A13=109.9995407\D1=9.04233911\D2=130.60995673\D3
=-110.15522909\D4=134.20016188\D5=-150.96861391\D6=86.8891956\D7=-105.
055239\D8=-183.23785459\D9=-17.47214991\D10=15.5499344\D11=-154.834051
87\D12=83.11175443\\Version=AM64L-G03RevE.01\State=2-A\HF=-267.8932573
\S2=0.762687\S2-1=0.\S2A=0.750118\RMSD=4.273e-09\RMSF=3.669e-05\Therma
l=0.\Dipole=0.6759837,0.019663,-0.4590743\PG=C01 [X(C5H9O1)]\\@

HF/6-31G*

1\1\GINC-GOMBERG04\FOpt\UHF\6-31G(d)\C5H9O1(2)\HMAITKEN\11-Oct-2010\1\
\#HF/6-31G* opt=(grad,readfc) geom=checkpoint guess=read\\6 membered d
ecarbonylation radical\\0,2\C\O,1,B1\C,2,B2,1,A1\C,1,B3,2,A2,3,D1,0\H,
1,B4,2,A3,3,D2,0\H,1,B5,2,A4,3,D3,0\H,3,B6,2,A5,1,D4,0\H,4,B7,1,A6,2,D
5,0\H,4,B8,1,A7,2,D6,0\C,3,B9,2,A8,1,D7,0\H,10,B10,3,A9,2,D8,0\H,10,B1
1,3,A10,2,D9,0\C,3,B12,2,A11,1,D10,0\H,13,B13,3,A12,2,D11,0\H,13,B14,3
,A13,2,D12,0\\B1=1.40876778\B2=1.41371512\B3=1.52624634\B4=1.08291798\
B5=1.08723975\B6=1.08826173\B7=1.08374729\B8=1.08509166\B9=1.4998734\B
10=1.07624461\B11=1.07409839\B12=1.53782644\B13=1.08308214\B14=1.08582
941\A1=111.69612001\A2=105.94630599\A3=108.74988178\A4=109.38181412\A5
=107.53515123\A6=112.80020315\A7=110.49016188\A8=109.89176749\A9=119.6
7090237\A10=119.09648718\A11=105.42626038\A12=112.79737757\A13=110.071
3394\D1=14.19948285\D2=136.52819004\D3=-105.56899742\D4=127.797308\D5=
-153.47494393\D6=85.24430074\D7=-113.02208679\D8=-183.59418375\D9=-22.

85340844\D10=9.63853713\D11=-151.40092882\D12=87.79644297\\Version=AM6
4L-G03RevE.01\State=2-A\HF=-269.3830091\S2=0.761799\S2-1=0.\S2A=0.7500
93\RMSD=6.122e-09\RMSF=1.659e-05\Thermal=0.\Dipole=0.5727304,0.0244188
,-0.3686751\PG=C01 [X(C5H9O1)]\\@

HF/6-311G**

1\1\GINC-GOMBERG04\FOpt\UHF\6-311G(d,p)\C5H9O1(2)\HMAITKEN\11-Oct-2010
\1\\#HF/6-311G** opt=(grad,readfc) geom=checkpoint guess=read\\6 membe
red decarbonylation radical\\0,2\C\O,1,B1\C,2,B2,1,A1\C,1,B3,2,A2,3,D1
,0\H,1,B4,2,A3,3,D2,0\H,1,B5,2,A4,3,D3,0\H,3,B6,2,A5,1,D4,0\H,4,B7,1,A
6,2,D5,0\H,4,B8,1,A7,2,D6,0\C,3,B9,2,A8,1,D7,0\H,10,B10,3,A9,2,D8,0\H,
10,B11,3,A10,2,D9,0\C,3,B12,2,A11,1,D10,0\H,13,B13,3,A12,2,D11,0\H,13,
B14,3,A13,2,D12,0\\B1=1.40846202\B2=1.41284257\B3=1.52518209\B4=1.0832
7309\B5=1.08829135\B6=1.08888701\B7=1.08397632\B8=1.08561103\B9=1.4994
5899\B10=1.0770638\B11=1.07476493\B12=1.53746858\B13=1.08324272\B14=1.
08635837\A1=111.66332527\A2=105.9321967\A3=108.80099942\A4=109.4253724
7\A5=107.62140847\A6=112.75238338\A7=110.46210353\A8=109.93090248\A9=1
19.6802896\A10=118.98226347\A11=105.48658251\A12=112.72848356\A13=109.
99957553\D1=14.68168496\D2=136.91817799\D3=-105.00722685\D4=127.324870
82\D5=-153.70345557\D6=84.95963194\D7=-113.70832041\D8=-184.07132163\D
9=-22.76563326\D10=9.16106012\D11=-151.18358523\D12=88.00207315\\Versi
on=AM64L-G03RevE.01\State=2-A\HF=-269.45005\S2=0.762038\S2-1=0.\S2A=0.
750096\RMSD=3.283e-09\RMSF=2.387e-05\Thermal=0.\Dipole=0.5673807,0.042
8763,-0.3719142\PG=C01 [X(C5H9O1)]\\@

BHandHLYP/6-311G**

1\1\GINC-GOMBERG06\FOpt\UBHandHLYP\6-311G(d,p)\C5H9O1(2)\HMAITKEN\11-O
ct-2010\0\\#BHandHLYP/6-311G** opt=(readfc) geom=checkpoint guess=read
\\6 membered decarbonylation radical\\0,2\C,0.,0.,0.\O,0.,0.,1.4145246
018\C,1.3278508362,0.,1.9205906389\C,1.3913198994,-0.4464254272,-0.414
7988354\H,-0.7880068635,-0.6608504636,-0.3438940544\H,-0.211230854,1.0
046077544,-0.368071917\H,1.4328064158,0.8637674594,2.5812487276\H,1.66
48263295,-0.1053860739,-1.4069579073\H,1.4640241488,-1.5297689619,-0.3
914635704\C,1.5755094501,-1.2449570238,2.6901666141\H,2.5322807288,-1.
4125675411,3.154371675\H,0.7510564717,-1.8898471568,2.9318500466\C,2.2
402515585,0.1650007646,0.6927959423\H,3.2017368939,-0.3167977443,0.822
8690706\H,2.4111786817,1.2197967744,0.4954693329\\Version=AM64L-G03Rev
E.01\State=2-A\HF=-271.0031359\S2=0.755215\S2-1=0.\S2A=0.750017\RMSD=4
.099e-09\RMSF=2.300e-05\Thermal=0.\Dipole=0.208803,0.6407675,0.0340478
\PG=C01 [X(C5H9O1)]\\@

BHandHLYP/6-311++G**

1\1\GINC-GOMBERG01\FOpt\UBHandHLYP\6-311++G(d,p)\C5H9O1(2)\HMAITKEN\12
-Oct-2010\0\\#BHandHLYP/6-311++G(d,p) opt=(readfc) geom=checkpoint gue
ss=read\\6 membered decarbonylation radical\\0,2\C,1.3432149235,-0.722
9625505,0.0778487477\O,0.0407819656,-1.1629277936,-0.2615822973\C,-0.8
302601682,-0.0605356159,-0.4767507109\C,1.1892292632,0.7246674241,0.51
10318673\H,1.7304067902,-1.372806256,0.8547984391\H,1.9950684137,-0.80
26507246,-0.7925319265\H,-1.2485572866,-0.1605825664,-1.4808903346\H,2
.1020537181,1.2982465648,0.3952521843\H,0.8804635921,0.7760779884,1.55
10805396\C,-1.9315073534,-0.0774850104,0.5174105803\H,-2.6865405674,0.
6897229351,0.4967301823\H,-2.0669847968,-0.935848883,1.149069356\C,0.0
613882457,1.191121665,-0.4021449264\H,-0.4719035849,2.0581516526,-0.03

20392719\H,0.4511477729,1.4266887402,-1.3887604772\\Version=AM64L-G03R
evE.01\State=2-A\HF=-271.0076569\S2=0.755274\S2-1=0.\S2A=0.750018\RMSD
=8.129e-09\RMSF=1.287e-04\Thermal=0.\Dipole=0.2300396,0.7012954,0.0332
938\PG=C01 [X(C5H9O1)]\\@

5-Membered ester system 40 (n=1, R=CO_2Me)

Acyl radical 40 (n=1, R=CO_2Me)

HF/3-21G*

1\1\GINC-GOMBERG01\FOpt\UHF\3-21G*\C7H9O4(2)\HMAITKEN\12-Oct-2010\1\\#
HF/3-21G* opt=(grad)\\start CO2Me and H\\0,2\O\C,1,B1\C,2,B2,1,A1\C,3,
B3,2,A2,1,D1,0\O,4,B4,3,A3,2,D2,0\C,5,B5,4,A4,3,D3,0\C,6,B6,5,A5,4,D4,
0\H,7,B7,6,A6,5,D5,0\H,6,B8,5,A7,4,D6,0\H,4,B9,3,A8,2,D7,0\H,4,B10,3,A
9,2,D8,0\H,3,B11,2,A10,1,D9,0\H,3,B12,2,A11,1,D10,0\C,7,B13,6,A12,5,D1
1,0\O,14,B14,7,A13,6,D12,0\O,14,B15,7,A14,6,D13,0\C,16,B16,14,A15,7,D1
4,0\H,17,B17,16,A16,14,D15,0\H,17,B18,16,A17,14,D16,0\H,17,B19,16,A18,
14,D17,0\\B1=1.18571529\B2=1.50944846\B3=1.52604338\B4=1.44293585\B5=1
.35413922\B6=1.32264809\B7=1.06796515\B8=1.06776649\B9=1.08103889\B10=
1.08103897\B11=1.08226664\B12=1.08226635\B13=1.45841014\B14=1.20638383
\B15=1.35789131\B16=1.45113614\B17=1.07924028\B18=1.07651055\B19=1.079
24075\A1=130.03957019\A2=111.10752218\A3=105.29860672\A4=120.77770767\
A5=127.23380035\A6=123.78846264\A7=111.38390458\A8=111.03263984\A9=111
.03267947\A10=108.85554936\A11=108.85573806\A12=121.06612136\A13=125.5
9324927\A14=112.54014984\A15=117.78501378\A16=110.35253189\A17=105.273
57612\A18=110.3527761\D1=-0.00193055\D2=179.99926703\D3=180.00012135\D
4=-0.00115534\D5=-0.00044564\D6=179.99889949\D7=60.68690318\D8=-60.688
31495\D9=121.47303845\D10=-121.47716352\D11=180.00201852\D12=180.03093
327\D13=0.02674802\D14=179.99984947\D15=60.32220018\D16=179.99922792\D
17=-60.32362573\\Version=AM64L-G03RevE.01\State=2-A\HF=-566.5291985\S2
=0.770505\S2-1=0.\S2A=0.750201\RMSD=7.707e-09\RMSF=5.408e-05\Thermal=0
.\Dipole=0.0746764,-0.0003403,1.4837912\PG=C01 [X(C7H9O4)]\\@

HF/6-31G*

1\1\GINC-GOMBERG01\FOpt\UHF\6-31G(d)\C7H9O4(2)\HMAITKEN\12-Oct-2010\1\
\#HF/6-31G* opt=(grad,readfc) geom=checkpoint guess=read\\start CO2Me
and H\\0,2\O\C,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\O,4,B4,3,A3,2,D2,0\
C,5,B5,4,A4,3,D3,0\C,6,B6,5,A5,4,D4,0\H,7,B7,6,A6,5,D5,0\H,6,B8,5,A7,4
,D6,0\H,4,B9,3,A8,2,D7,0\H,4,B10,3,A9,2,D8,0\H,3,B11,2,A10,1,D9,0\H,3,
B12,2,A11,1,D10,0\C,7,B13,6,A12,5,D11,0\O,14,B14,7,A13,6,D12,0\O,14,B1
5,7,A14,6,D13,0\C,16,B16,14,A15,7,D14,0\H,17,B17,16,A16,14,D15,0\H,17,
B18,16,A17,14,D16,0\H,17,B19,16,A18,14,D17,0\\B1=1.16547225\B2=1.51444
344\B3=1.52092787\B4=1.40867808\B5=1.32903519\B6=1.32866052\B7=1.07149
233\B8=1.07167602\B9=1.08296832\B10=1.08296068\B11=1.08446046\B12=1.08
44885\B13=1.47146812\B14=1.19122051\B15=1.33031372\B16=1.41587889\B17=
1.08025763\B18=1.07903358\B19=1.08025319\A1=128.73181544\A2=112.357361
82\A3=106.55356269\A4=119.44859381\A5=127.69400432\A6=123.37568525\A7=
110.89283054\A8=110.85608014\A9=110.85448622\A10=108.00369916\A11=107.
99773011\A12=122.2401453\A13=123.3116297\A14=113.78888746\A15=116.7196
4084\A16=110.57727088\A17=105.82173474\A18=110.57572877\D1=0.03818485\
D2=180.00688383\D3=180.00146635\D4=-0.00707295\D5=-0.01966493\D6=179.9
8971733\D7=60.232152\D8=-60.22523168\D9=122.54309715\D10=-122.46403912
\D11=180.01564492\D12=179.92475749\D13=-0.09883394\D14=179.96460744\D1

5=60.55582533\D16=179.99248253\D17=-60.57164172\\Version=AM64L-G03RevE
.01\State=2-A\HF=-569.7104422\S2=0.761602\S2-1=0.\S2A=0.750099\RMSD=7.
060e-09\RMSF=1.814e-05\Thermal=0.\Dipole=0.0150563,-0.0001635,1.595095
9\PG=C01 [X(C7H9O4)]\\@

HF/6-311G**

1\1\GINC-GOMBERG04\FOpt\UHF\6-311G(d,p)\C7H9O4(2)\HMAITKEN\13-Oct-2010
\1\\#HF/6-311G** opt=(grad,readfc) geom=checkpoint guess=read\\start C
O2Me and H\\0,2\O\C,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\O,4,B4,3,A3,2,
D2,0\C,5,B5,4,A4,3,D3,0\C,6,B6,5,A5,4,D4,0\H,7,B7,6,A6,5,D5,0\H,6,B8,5
,A7,4,D6,0\H,4,B9,3,A8,2,D7,0\H,4,B10,3,A9,2,D8,0\H,3,B11,2,A10,1,D9,0
\H,3,B12,2,A11,1,D10,0\C,7,B13,6,A12,5,D11,0\O,14,B14,7,A13,6,D12,0\O,
14,B15,7,A14,6,D13,0\C,16,B16,14,A15,7,D14,0\H,17,B17,16,A16,14,D15,0\
H,17,B18,16,A17,14,D16,0\H,17,B19,16,A18,14,D17,0\\B1=1.15819854\B2=1.
51388382\B3=1.51949009\B4=1.40797045\B5=1.32680936\B6=1.32768492\B7=1.
07157799\B8=1.07241128\B9=1.08413375\B10=1.08415961\B11=1.08470769\B12
=1.08464499\B13=1.47226676\B14=1.18554845\B15=1.32778452\B16=1.4158233
7\B17=1.08157757\B18=1.07952127\B19=1.0815783\A1=129.21092012\A2=112.5
6459621\A3=106.62031475\A4=119.48346292\A5=127.73508636\A6=123.5164503
4\A7=111.1790694\A8=110.78096055\A9=110.78333176\A10=107.69197729\A11=
107.74642025\A12=122.1663793\A13=123.25406682\A14=113.76776942\A15=117
.00976861\A16=110.60373909\A17=105.82707115\A18=110.60397311\D1=-0.339
92494\D2=179.95330215\D3=179.99029434\D4=0.00664782\D5=0.01178027\D6=1
80.00959704\D7=60.12370758\D8=-60.22473785\D9=122.20939066\D10=-122.95
172419\D11=179.99488552\D12=180.01678255\D13=0.02470928\D14=180.006511
37\D15=60.55137138\D16=180.00903041\D17=-60.53320478\\Version=AM64L-G0
3RevE.01\State=2-A\HF=-569.8555578\S2=0.761729\S2-1=0.\S2A=0.750099\RM
SD=6.093e-09\RMSF=2.814e-05\Thermal=0.\Dipole=0.0615231,0.0052818,1.56
73574\PG=C01 [X(C7H9O4)]\\@

BHandHLYP/6-311G**

1\1\GINC-GOMBERG03\FOpt\UBHandHLYP\6-311G(d,p)\C7H9O4(2)\HMAITKEN\13-O
ct-2010\1\\#BHandHLYP/6-311G** opt=(grad,readfc) geom=checkpoint guess
=read\\start CO2Me and H\\0,2\O\C,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\
O,4,B4,3,A3,2,D2,0\C,5,B5,4,A4,3,D3,0\C,6,B6,5,A5,4,D4,0\H,7,B7,6,A6,5
,D5,0\H,6,B8,5,A7,4,D6,0\H,4,B9,3,A8,2,D7,0\H,4,B10,3,A9,2,D8,0\H,3,B1
1,2,A10,1,D9,0\H,3,B12,2,A11,1,D10,0\C,7,B13,6,A12,5,D11,0\O,14,B14,7,
A13,6,D12,0\O,14,B15,7,A14,6,D13,0\C,16,B16,14,A15,7,D14,0\H,17,B17,16
,A16,14,D15,0\H,17,B18,16,A17,14,D16,0\H,17,B19,16,A18,14,D17,0\\B1=1.
16761854\B2=1.5070254\B3=1.51405889\B4=1.41294016\B5=1.33024812\B6=1.3
3090574\B7=1.07300346\B8=1.0747381\B9=1.08647677\B10=1.08646565\B11=1.
08596944\B12=1.0860174\B13=1.46307123\B14=1.19564594\B15=1.33835757\B1
6=1.41960366\B17=1.08324531\B18=1.08041411\B19=1.08324775\A1=127.98942
776\A2=112.71544845\A3=106.81403038\A4=118.45407297\A5=127.56071727\A6
=123.4147468\A7=111.28877222\A8=110.81917494\A9=110.822671\A10=107.723
55496\A11=107.65350889\A12=122.20532991\A13=123.74696379\A14=113.40889
305\A15=115.86751433\A16=110.62321839\A17=105.79448615\A18=110.6280674
6\D1=0.30995236\D2=180.05114609\D3=180.00906686\D4=0.01402915\D5=-0.01
057102\D6=180.01544764\D7=60.12741823\D8=-60.02108044\D9=123.17881336\
D10=-122.48604788\D11=180.03038476\D12=179.87477634\D13=-0.12900651\D1
4=180.04368617\D15=60.39130867\D16=180.00943313\D17=-60.36889017\\Vers
ion=AM64L-G03RevE.01\State=2-A\HF=-572.8117764\S2=0.754865\S2-1=0.\S2A
=0.750014\RMSD=6.016e-09\RMSF=5.418e-05\Thermal=0.\Dipole=0.0784398,-0

.0034285,1.4094258\PG=C01 [X(C7H9O4)]\\@

BHandHLYP/6-311++G**

1\1\GINC-GOMBERG04\FOpt\UBHandHLYP\6-311++G(d,p)\C7H9O4(2)\HMAITKEN\13
-Oct-2010\1\\#BHandHLYP/6-311++G(d,p) opt=(grad,readfc) geom=checkpoin
t guess=read\\start CO2Me and H\\0,2\O\C,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,
1,D1,0\O,4,B4,3,A3,2,D2,0\C,5,B5,4,A4,3,D3,0\C,6,B6,5,A5,4,D4,0\H,7,B7
,6,A6,5,D5,0\H,6,B8,5,A7,4,D6,0\H,4,B9,3,A8,2,D7,0\H,4,B10,3,A9,2,D8,0
\H,3,B11,2,A10,1,D9,0\H,3,B12,2,A11,1,D10,0\C,7,B13,6,A12,5,D11,0\O,14
,B14,7,A13,6,D12,0\O,14,B15,7,A14,6,D13,0\C,16,B16,14,A15,7,D14,0\H,17
,B17,16,A16,14,D15,0\H,17,B18,16,A17,14,D16,0\H,17,B19,16,A18,14,D17,0
\\B1=1.16755539\B2=1.50535463\B3=1.51462197\B4=1.413497\B5=1.33044161\
B6=1.33175101\B7=1.07317092\B8=1.07484188\B9=1.08632567\B10=1.08631292
\B11=1.08608771\B12=1.08614666\B13=1.46274686\B14=1.19733387\B15=1.337
65741\B16=1.42031403\B17=1.08307352\B18=1.08046726\B19=1.08307608\A1=1
28.56977175\A2=112.85961778\A3=106.80263432\A4=118.59397107\A5=127.388
05477\A6=123.37136615\A7=111.30406733\A8=110.87845545\A9=110.87711406\
A10=107.52200603\A11=107.47248912\A12=122.19261645\A13=123.63999649\A1
4=113.61739059\A15=116.18647433\A16=110.56696837\A17=105.74653763\A18=
110.56626234\D1=0.25334146\D2=180.02629365\D3=180.01061283\D4=0.003148
35\D5=-0.00089006\D6=180.00624692\D7=60.23426495\D8=-60.17045045\D9=12
3.20642922\D10=-122.64525701\D11=180.01126128\D12=179.97472339\D13=-0.
01749325\D14=180.01131736\D15=60.44559223\D16=180.00993237\D17=-60.425
9487\\Version=AM64L-G03RevE.01\State=2-A\HF=-572.8244919\S2=0.755047\S
2-1=0.\S2A=0.750015\RMSD=5.543e-09\RMSF=7.031e-05\Thermal=0.\Dipole=0.
0963361,-0.0037616,1.4723174\PG=C01 [X(C7H9O4)]\\@

Cyclization transition state 45

HF/3-21G*

1\1\GINC-GOMBERG11\FTS\UHF\3-21G*\C7H9O4(2)\HMAITKEN\15-Oct-2010\1\\#H
F/3-21G* opt=(grad,readfc,ts,noeigentest,nofreeze) geom=checkpoint gue
ss=read\\5exo ts CO2Me and H\\0,2\C\C,1,B1\C,2,B2,1,A1\O,3,B3,2,A2,1,D
1,0\C,1,B4,3,A3,2,D2,0\C,5,B5,4,A4,3,D3,0\O,1,B6,2,A5,3,D4,0\H,2,B7,1,
A6,7,D5,0\H,2,B8,1,A7,7,D6,0\H,3,B9,2,A8,1,D7,0\H,3,B10,2,A9,1,D8,0\H,
5,B11,4,A10,3,D9,0\H,6,B12,5,A11,4,D10,0\C,6,B13,5,A12,4,D11,0\O,14,B1
4,6,A13,5,D12,0\O,14,B15,6,A14,5,D13,0\C,16,B16,14,A15,6,D14,0\H,17,B1
7,16,A16,14,D15,0\H,17,B18,16,A17,14,D16,0\H,17,B19,16,A18,14,D17,0\\B
1=1.51585063\B2=1.52845105\B3=1.44405214\B6=1.18457997\B7=1.08438869\B
8=1.08209679\B9=1.07595027\B10=1.08340493\B11=1.07098106\B12=1.0683457
6\B13=1.44471473\B14=1.21499994\B15=1.35889321\B16=1.44999266\B17=1.07
956712\B18=1.07649831\B19=1.07940438\A1=106.36542594\A2=107.31025217\A
3=61.51965862\A4=117.75860617\A5=133.07427711\A6=107.84235925\A7=110.4
3913668\A8=112.68129378\A9=110.47884951\A10=116.99775597\A11=120.86176
446\A12=121.40140741\A13=125.30152936\A14=112.73152863\A15=117.8717896
2\A16=110.45119996\A17=105.29932662\A18=110.38519622\D1=46.49207556\D2
=155.29582932\D3=143.83203609\D4=164.37917969\D5=-77.71093046\D6=41.78
754824\D7=163.36799599\D8=-73.51969596\D9=-59.53006258\D10=-11.9100463
3\D11=170.83160248\D12=178.15982402\D13=-1.86332572\D14=178.14993443\D
15=61.17775649\D16=-179.17007374\D17=-59.64438335\B4=2.20473228\B5=1.3
7265872\\Version=AM64L-G03RevE.01\State=2-A\HF=-566.5110072\S2=1.06799
8\S2-1=0.\S2A=0.804228\RMSD=7.526e-09\RMSF=1.146e-05\Thermal=0.\Dipole
=0.0535698,-1.2096027,1.2189454\PG=C01 [X(C7H9O4)]\\@

HF/6-31G*

1\1\GINC-GOMBERG04\FTS\UHF\6-31G(d)\C7H9O4(2)\HMAITKEN\15-Oct-2010\1\\
#HF/6-31G* opt=(grad,readfc,ts,noeigentest,nofreeze) geom=checkpoint g
uess=read\\5exo ts CO2Me and H\\0,2\C\C,1,B1\C,2,B2,1,A1\O,3,B3,2,A2,1
,D1,0\C,1,B4,3,A3,2,D2,0\C,5,B5,4,A4,3,D3,0\O,1,B6,2,A5,3,D4,0\H,2,B7,
1,A6,7,D5,0\H,2,B8,1,A7,7,D6,0\H,3,B9,2,A8,1,D7,0\H,3,B10,2,A9,1,D8,0\
H,5,B11,4,A10,3,D9,0\H,6,B12,5,A11,4,D10,0\C,6,B13,5,A12,4,D11,0\O,14,
B14,6,A13,5,D12,0\O,14,B15,6,A14,5,D13,0\C,16,B16,14,A15,6,D14,0\H,17,
B17,16,A16,14,D15,0\H,17,B18,16,A17,14,D16,0\H,17,B19,16,A18,14,D17,0\
\B1=1.51266603\B2=1.52343244\B3=1.40495678\B6=1.16509389\B7=1.08567636
\B8=1.0839223\B9=1.07909532\B10=1.08723643\B11=1.07616522\B12=1.072400
75\B13=1.46312642\B14=1.19364936\B15=1.32973577\B16=1.41548993\B17=1.0
8050973\B18=1.07889989\B19=1.08026632\A1=106.30965896\A2=108.06276232\
A3=60.24683594\A4=117.64730984\A5=131.54853434\A6=107.45242737\A7=109.
99980249\A8=112.55428853\A9=110.71523535\A10=115.92799613\A11=120.2417
2774\A12=123.32757375\A13=123.30432883\A14=113.44045166\A15=116.781474
12\A16=110.58313006\A17=105.83354467\A18=110.51945915\D1=43.26664588\D
2=159.87162438\D3=149.546568\D4=166.53047239\D5=-74.93989927\D6=43.310
73215\D7=161.07976968\D8=-77.27609535\D9=-58.04170768\D10=-15.15138717
\D11=169.61140982\D12=177.64091842\D13=-2.60902678\D14=178.84215313\D1
5=61.21213004\D16=-179.33188006\D17=-59.97160955\B4=2.16602665\B5=1.38
648631\\Version=AM64L-G03RevE.01\State=2-A\HF=-569.6863314\S2=1.010437
\S2-1=0.\S2A=0.769741\RMSD=5.339e-09\RMSF=1.343e-05\Thermal=0.\Dipole=
0.0813668,-1.2081526,1.3460741\PG=C01 [X(C7H9O4)]\\@

HF/6-311G**

1\1\GINC-GOMBERG04\FTS\UHF\6-311G(d,p)\C7H9O4(2)\HMAITKEN\15-Oct-2010\
1\\#HF/6-311G** opt=(grad,readfc,ts,noeigentest,nofreeze) geom=checkpo
int guess=read\\5exo ts CO2Me and H\\0,2\C\C,1,B1\C,2,B2,1,A1\O,3,B3,2
,A2,1,D1,0\C,1,B4,3,A3,2,D2,0\C,5,B5,4,A4,3,D3,0\O,1,B6,2,A5,3,D4,0\H,
2,B7,1,A6,7,D5,0\H,2,B8,1,A7,7,D6,0\H,3,B9,2,A8,1,D7,0\H,3,B10,2,A9,1,
D8,0\H,5,B11,4,A10,3,D9,0\H,6,B12,5,A11,4,D10,0\C,6,B13,5,A12,4,D11,0\
O,14,B14,6,A13,5,D12,0\O,14,B15,6,A14,5,D13,0\C,16,B16,14,A15,6,D14,0\
H,17,B17,16,A16,14,D15,0\H,17,B18,16,A17,14,D16,0\H,17,B19,16,A18,14,D
17,0\\B1=1.51107749\B2=1.52269009\B3=1.40387888\B6=1.15822783\B7=1.085
98603\B8=1.08410553\B9=1.07927686\B10=1.08836924\B11=1.07676669\B12=1.
07268298\B13=1.46313457\B14=1.18816549\B15=1.32779009\B16=1.41515514\B
17=1.08183755\B18=1.07943467\B19=1.08157661\A1=106.22295224\A2=108.052
82965\A3=60.29211808\A4=117.75965211\A5=132.0648829\A6=107.21519138\A7
=109.94023513\A8=112.51276633\A9=110.61738771\A10=116.05253741\A11=120
.3610916\A12=123.18236241\A13=123.35228617\A14=113.37187821\A15=117.05
297005\A16=110.61911487\A17=105.85803226\A18=110.54258322\D1=43.470212
88\D2=159.53480541\D3=149.3170832\D4=165.86018733\D5=-75.73789284\D6=4
2.58090405\D7=161.43017894\D8=-76.98625337\D9=-58.41221221\D10=-15.049
5852\D11=169.80617517\D12=177.52222802\D13=-2.65343393\D14=178.6480248
9\D15=61.14431609\D16=-179.36309032\D17=-60.00107935\B4=2.15769716\B5=
1.3852443\\Version=AM64L-G03RevE.01\State=2-A\HF=-569.829341\S2=1.0016
67\S2-1=0.\S2A=0.768352\RMSD=7.060e-09\RMSF=9.095e-06\Thermal=0.\Dipol
e=0.0505204,-1.2197712,1.3494478\PG=C01 [X(C7H9O4)]\\@

BHandHLYP/6-311G**

1\1\GINC-GOMBERG12\FTS\UBHandHLYP\6-311G(d,p)\C7H9O4(2)\HMAITKEN\15-Oc

t-2010\1\\#BHandHLYP/6-311G** opt=(grad,readfc,ts,noeigentest,nofreeze
) geom=checkpoint guess=read\\5exo ts CO2Me and H\\0,2\C\C,1,B1\C,2,B2
,1,A1\O,3,B3,2,A2,1,D1,0\C,1,B4,3,A3,2,D2,0\C,5,B5,4,A4,3,D3,0\O,1,B6,
2,A5,3,D4,0\H,2,B7,1,A6,7,D5,0\H,2,B8,1,A7,7,D6,0\H,3,B9,2,A8,1,D7,0\H
,3,B10,2,A9,1,D8,0\H,5,B11,4,A10,3,D9,0\H,6,B12,5,A11,4,D10,0\C,6,B13,
5,A12,4,D11,0\O,14,B14,6,A13,5,D12,0\O,14,B15,6,A14,5,D13,0\C,16,B16,1
4,A15,6,D14,0\H,17,B17,16,A16,14,D15,0\H,17,B18,16,A17,14,D16,0\H,17,B
19,16,A18,14,D17,0\\B1=1.50467632\B2=1.51847833\B3=1.40914522\B6=1.163
07203\B7=1.08722461\B8=1.08538632\B9=1.08054033\B10=1.08967307\B11=1.0
7939584\B12=1.07379442\B13=1.45066017\B14=1.19845547\B15=1.34237899\B1
6=1.41806474\B17=1.08349604\B18=1.08064537\B19=1.0833863\A1=106.513131
48\A2=107.81256856\A3=59.88138485\A4=118.99576629\A5=132.47350258\A6=1
07.1410445\A7=109.6368167\A8=112.56400968\A9=110.63480863\A10=116.2898
8946\A11=120.53180422\A12=122.92390652\A13=124.36648337\A14=112.964145
55\A15=115.80317343\A16=110.70048468\A17=105.86234372\A18=110.63017588
\D1=44.96261221\D2=158.86896018\D3=150.30527742\D4=167.82965951\D5=-73
.65609738\D6=44.31597144\D7=162.64350289\D8=-75.49983959\D9=-53.349004
92\D10=-13.75285415\D11=169.52884657\D12=178.52515445\D13=-1.34371246\
D14=179.02207603\D15=60.33930004\D16=-179.98914683\D17=-60.44276208\B4
=2.19317419\B5=1.36248761\\Version=AM64L-G03RevE.01\State=2-A\HF=-572.
7915426\S2=0.8126\S2-1=0.\S2A=0.750885\RMSD=8.329e-09\RMSF=2.675e-05\T
hermal=0.\Dipole=-0.1990717,-1.3290707,1.5667692\PG=C01 [X(C7H9O4)]\\@

BHandHLYP/6-311++G**

1\1\GINC-GOMBERG03\FTS\UBHandHLYP\6-311++G(d,p)\C7H9O4(2)\HMAITKEN\15-
Oct-2010\1\\#BHandHLYP/6-311++G(d,p) opt=(grad,readfc,ts,noeigentest,n
ofreeze) geom=checkpoint guess=read\\5exo ts CO2Me and H\\0,2\C\C,1,B1
\C,2,B2,1,A1\O,3,B3,2,A2,1,D1,0\C,1,B4,3,A3,2,D2,0\C,5,B5,4,A4,3,D3,0\
O,1,B6,2,A5,3,D4,0\H,2,B7,1,A6,7,D5,0\H,2,B8,1,A7,7,D6,0\H,3,B9,2,A8,1
,D7,0\H,3,B10,2,A9,1,D8,0\H,5,B11,4,A10,3,D9,0\H,6,B12,5,A11,4,D10,0\C
,6,B13,5,A12,4,D11,0\O,14,B14,6,A13,5,D12,0\O,14,B15,6,A14,5,D13,0\C,1
6,B16,14,A15,6,D14,0\H,17,B17,16,A16,14,D15,0\H,17,B18,16,A17,14,D16,0
\H,17,B19,16,A18,14,D17,0\\B1=1.50318837\B2=1.51849969\B3=1.40960806\B
6=1.16357582\B7=1.08741175\B8=1.08554459\B9=1.08071557\B10=1.08951952\
B11=1.07943766\B12=1.07405707\B13=1.45067822\B14=1.20035115\B15=1.3412
104\B16=1.4189832\B17=1.0833076\B18=1.0806653\B19=1.08321779\A1=106.75
350255\A2=107.88225534\A3=59.88510525\A4=118.97957882\A5=132.42095146\
A6=107.11839169\A7=109.48181387\A8=112.50779589\A9=110.7584374\A10=116
.15876995\A11=120.49652627\A12=123.07464559\A13=124.18838061\A14=113.2
0720478\A15=116.13395678\A16=110.64016141\A17=105.79910347\A18=110.575
91227\D1=43.91487399\D2=160.066844\D3=150.83148225\D4=168.94228896\D5=
-72.24374529\D6=45.54102637\D7=161.58407436\D8=-76.54715517\D9=-52.927
20699\D10=-14.24392058\D11=169.07853104\D12=177.68494364\D13=-2.275283
08\D14=178.84515464\D15=60.48642716\D16=-179.90192117\D17=-60.40440876
\B4=2.19426663\B5=1.36281918\\Version=AM64L-G03RevE.01\State=2-A\HF=-5
72.8045615\S2=0.812497\S2-1=0.\S2A=0.750868\RMSD=8.260e-09\RMSF=2.762e
-05\Thermal=0.\Dipole=-0.183532,-1.3806103,1.6581824\PG=C01 [X(C7H9O4)]\\@

Cyclization product 41 (n=1, R=CO_2Me)

HF/3-21G*

1\1\GINC-GOMBERG01\FOpt\UHF\3-21G*\C7H9O4(2)\HMAITKEN\12-Oct-2010\1\\#
HF/3-21G* opt=(grad)\\CO2Me and H radical product\\0,2\C\O,1,B1\C,2,B2

,1,A1\C,1,B3,2,A2,3,D1,0\H,1,B4,2,A3,3,D2,0\H,1,B5,2,A4,3,D3,0\H,3,B6,
2,A5,1,D4,0\H,4,B7,1,A6,2,D5,0\H,4,B8,1,A7,2,D6,0\C,4,B9,1,A8,2,D7,0\O
,10,B10,4,A9,1,D8,0\C,3,B11,2,A10,1,D9,0\H,12,B12,3,A11,2,D10,0\C,12,B
13,3,A12,2,D11,0\O,14,B14,12,A13,3,D12,0\O,14,B15,12,A14,3,D13,0\C,16,
B16,14,A15,12,D14,0\H,17,B17,16,A16,14,D15,0\H,17,B18,16,A17,14,D16,0\
H,17,B19,16,A18,14,D17,0\\B1=1.45812724\B2=1.43871557\B3=1.53234991\B4
=1.07591644\B5=1.082359\B6=1.082469\B7=1.07914581\B8=1.0817839\B9=1.51
517481\B10=1.20295365\B11=1.49120664\B12=1.06757957\B13=1.43768597\B14
=1.22296558\B15=1.35208608\B16=1.45094606\B17=1.07974741\B18=1.0761455
6\B19=1.07964469\A1=109.48623326\A2=104.51092371\A3=107.20161793\A4=10
9.72232784\A5=110.92135751\A6=114.28026215\A7=110.12340293\A8=103.1075
4434\A9=128.43364516\A10=109.29149566\A11=122.5856111\A12=118.45083232
\A13=124.70691156\A14=113.01808119\A15=118.11013275\A16=110.46157882\A
17=105.19119041\A18=110.44884774\D1=32.81933314\D2=153.89327486\D3=-86
.68666614\D4=96.22981752\D5=-152.13548409\D6=82.8383838\D7=-30.4070561
1\D8=-161.86051002\D9=-141.78452296\D10=246.33556184\D11=61.03146021\D
12=9.64370524\D13=-172.0349886\D14=181.67533198\D15=60.31040673\D16=17
9.87248725\D17=-60.59187211\\Version=AM64L-G03RevE.01\State=2-A\HF=-56
6.5535127\S2=0.840243\S2-1=0.\S2A=0.752362\RMSD=2.132e-09\RMSF=2.760e-
05\Thermal=0.\Dipole=-0.5597314,-0.0111175,0.0337632\PG=C01 [X(C7H9O4)]\\@

HF/6-31G*

1\1\GINC-GOMBERG01\FOpt\UHF\6-31G(d)\C7H9O4(2)\HMAITKEN\12-Oct-2010\1\
\#HF/6-31G* opt=(grad,readfc) geom=checkpoint guess=read\\CO2Me and H
radical product\\0,2\C\O,1,B1\C,2,B2,1,A1\C,1,B3,2,A2,3,D1,0\H,1,B4,2,
A3,3,D2,0\H,1,B5,2,A4,3,D3,0\H,3,B6,2,A5,1,D4,0\H,4,B7,1,A6,2,D5,0\H,4
,B8,1,A7,2,D6,0\C,4,B9,1,A8,2,D7,0\O,10,B10,4,A9,1,D8,0\C,3,B11,2,A10,
1,D9,0\H,12,B12,3,A11,2,D10,0\C,12,B13,3,A12,2,D11,0\O,14,B14,12,A13,3
,D12,0\O,14,B15,12,A14,3,D13,0\C,16,B16,14,A15,12,D14,0\H,17,B17,16,A1
6,14,D15,0\H,17,B18,16,A17,14,D16,0\H,17,B19,16,A18,14,D17,0\\B1=1.413
38652\B2=1.40134572\B3=1.52635148\B4=1.07936132\B5=1.08758829\B6=1.088
20386\B7=1.081978\B8=1.08378441\B9=1.51226307\B10=1.18506198\B11=1.496
83111\B12=1.07208005\B13=1.46198347\B14=1.19639078\B15=1.32345348\B16=
1.41681665\B17=1.0804372\B18=1.07848806\B19=1.08046465\A1=110.0014804\
A2=105.5161814\A3=107.54375221\A4=109.78637717\A5=110.38460177\A6=114.
75987952\A7=111.29799653\A8=102.04764202\A9=128.37631006\A10=110.47260
765\A11=121.28070356\A12=119.64878533\A13=123.62026699\A14=112.5755682
7\A15=116.92951546\A16=110.49527284\A17=105.78558327\A18=110.49827738\
D1=33.97781023\D2=156.03329796\D3=-85.97315617\D4=91.93167747\D5=-149.
66765438\D6=85.59412942\D7=-28.91731342\D8=-162.54197437\D9=-147.07015
61\D10=247.61617511\D11=65.10766611\D12=7.15397562\D13=-173.52366522\D
14=181.00492993\D15=60.2953586\D16=179.72590117\D17=-60.86431484\\Vers
ion=AM64L-G03RevE.01\State=2-A\HF=-569.7330189\S2=0.781301\S2-1=0.\S2A
=0.750577\RMSD=7.342e-09\RMSF=1.159e-05\Thermal=0.\Dipole=-0.6341043,0
.1904008,0.2292209\PG=C01 [X(C7H9O4)]\\@

HF/6-311G**

1\1\GINC-GOMBERG03\FOpt\UHF\6-311G(d,p)\C7H9O4(2)\HMAITKEN\13-Oct-2010
\1\\#HF/6-311G** opt=(grad,readfc) geom=checkpoint guess=read\\CO2Me a
nd H radical product\\0,2\C\O,1,B1\C,2,B2,1,A1\C,1,B3,2,A2,3,D1,0\H,1,
B4,2,A3,3,D2,0\H,1,B5,2,A4,3,D3,0\H,3,B6,2,A5,1,D4,0\H,4,B7,1,A6,2,D5,
0\H,4,B8,1,A7,2,D6,0\C,4,B9,1,A8,2,D7,0\O,10,B10,4,A9,1,D8,0\C,3,B11,2
,A10,1,D9,0\H,12,B12,3,A11,2,D10,0\C,12,B13,3,A12,2,D11,0\O,14,B14,12,

A13,3,D12,0\O,14,B15,12,A14,3,D13,0\C,16,B16,14,A15,12,D14,0\H,17,B17,
16,A16,14,D15,0\H,17,B18,16,A17,14,D16,0\H,17,B19,16,A18,14,D17,0\\B1=
1.4123271\B2=1.3996832\B3=1.52529283\B4=1.07964898\B5=1.08884105\B6=1.
08889303\B7=1.08201027\B8=1.08399642\B9=1.51138959\B10=1.17950351\B11=
1.49615973\B12=1.07220826\B13=1.462864\B14=1.19067311\B15=1.32115911\B
16=1.41668726\B17=1.08173905\B18=1.07897855\B19=1.08174478\A1=109.8687
5819\A2=105.48236576\A3=107.69333084\A4=109.80126819\A5=110.47084811\A
6=114.89091647\A7=111.17385529\A8=102.03480138\A9=128.48108525\A10=110
.55302226\A11=121.33618469\A12=119.67906782\A13=123.67221061\A14=112.4
6378624\A15=117.14926906\A16=110.51423427\A17=105.79161763\A18=110.523
84531\D1=34.2504306\D2=156.28818568\D3=-85.59259898\D4=91.79297493\D5=
-150.3073055\D6=84.64368571\D7=-29.46005208\D8=-161.95237224\D9=-147.1
810726\D10=247.05948915\D11=64.73981432\D12=7.43149754\D13=-173.257260
94\D14=181.0702795\D15=60.37159153\D16=179.82066459\D17=-60.73986053\\
Version=AM64L-G03RevE.01\State=2-A\HF=-569.874332\S2=0.779813\S2-1=0.\
S2A=0.75055\RMSD=5.903e-09\RMSF=1.108e-05\Thermal=0.\Dipole=-0.6387589
,0.1869326,0.2345993\PG=C01 [X(C7H9O4)]\\@

BHandHLYP/6-311G**

1\1\GINC-GOMBERG04\FOpt\UBHandHLYP\6-311G(d,p)\C7H9O4(2)\HMAITKEN\13-O
ct-2010\1\\#BHandHLYP/6-311G** opt=(grad,readfc) geom=checkpoint guess
=read\\CO2Me and H radical product\\0,2\C\O,1,B1\C,2,B2,1,A1\C,1,B3,2,
A2,3,D1,0\H,1,B4,2,A3,3,D2,0\H,1,B5,2,A4,3,D3,0\H,3,B6,2,A5,1,D4,0\H,4
,B7,1,A6,2,D5,0\H,4,B8,1,A7,2,D6,0\C,4,B9,1,A8,2,D7,0\O,10,B10,4,A9,1,
D8,0\C,3,B11,2,A10,1,D9,0\H,12,B12,3,A11,2,D10,0\C,12,B13,3,A12,2,D11,
0\O,14,B14,12,A13,3,D12,0\O,14,B15,12,A14,3,D13,0\C,16,B16,14,A15,12,D
14,0\H,17,B17,16,A16,14,D15,0\H,17,B18,16,A17,14,D16,0\H,17,B19,16,A18
,14,D17,0\\B1=1.42048648\B2=1.40720452\B3=1.51815344\B4=1.08114645\B5=
1.09044278\B6=1.09093611\B7=1.08258605\B8=1.0852507\B9=1.50801207\B10=
1.18709704\B11=1.48234599\B12=1.07356513\B13=1.44959524\B14=1.20230826
\B15=1.33130822\B16=1.42067391\B17=1.08342282\B18=1.07993482\B19=1.083
33779\A1=109.51774852\A2=105.70993819\A3=107.27794106\A4=109.8572891\A
5=110.74075382\A6=115.21874012\A7=111.08993961\A8=102.3381539\A9=128.5
2930694\A10=110.41262026\A11=121.63517732\A12=119.29606456\A13=124.155
19571\A14=112.28075759\A15=115.98988832\A16=110.51088727\A17=105.76382
955\A18=110.51959218\D1=33.53225812\D2=155.58638871\D3=-86.44900217\D4
=93.64298391\D5=-151.12366722\D6=83.4863487\D7=-30.15385376\D8=-160.75
153366\D9=-144.46355723\D10=241.90612949\D11=62.17470841\D12=8.8517525
5\D13=-172.21349043\D14=181.2144223\D15=60.51008355\D16=180.13904335\D
17=-60.22949729\\Version=AM64L-G03RevE.01\State=2-A\HF=-572.8278205\S2
=0.761019\S2-1=0.\S2A=0.750076\RMSD=8.596e-09\RMSF=2.838e-05\Thermal=0
.\Dipole=-0.5612485,0.1105334,0.2107538\PG=C01 [X(C7H9O4)]\\@

BHandHLYP/6-311++G**

1\1\GINC-GOMBERG03\FOpt\UBHandHLYP\6-311++G(d,p)\C7H9O4(2)\HMAITKEN\13
-Oct-2010\1\\#BHandHLYP/6-311++G(d,p) opt=(grad,readfc) geom=checkpoin
t guess=read\\CO2Me and H radical product\\0,2\C\O,1,B1\C,2,B2,1,A1\C,
1,B3,2,A2,3,D1,0\H,1,B4,2,A3,3,D2,0\H,1,B5,2,A4,3,D3,0\H,3,B6,2,A5,1,D
4,0\H,4,B7,1,A6,2,D5,0\H,4,B8,1,A7,2,D6,0\C,4,B9,1,A8,2,D7,0\O,10,B10,
4,A9,1,D8,0\C,3,B11,2,A10,1,D9,0\H,12,B12,3,A11,2,D10,0\C,12,B13,3,A12
,2,D11,0\O,14,B14,12,A13,3,D12,0\O,14,B15,12,A14,3,D13,0\C,16,B16,14,A
15,12,D14,0\H,17,B17,16,A16,14,D15,0\H,17,B18,16,A17,14,D16,0\H,17,B19
,16,A18,14,D17,0\\B1=1.42114961\B2=1.40868494\B3=1.51890234\B4=1.08126

445\B5=1.09012754\B6=1.09089617\B7=1.0826564\B8=1.08559401\B9=1.507070
12\B10=1.18830408\B11=1.4829917\B12=1.07383157\B13=1.44971412\B14=1.20
305882\B15=1.33150601\B16=1.4211363\B17=1.08325489\B18=1.08001847\B19=
1.08320322\A1=109.51880954\A2=105.65040425\A3=107.30043583\A4=109.7407
4896\A5=110.48032686\A6=115.11131805\A7=111.21146875\A8=102.40839464\A
9=128.36662893\A10=110.54075464\A11=121.35730007\A12=119.61309977\A13=
124.09765982\A14=112.32606433\A15=116.27743456\A16=110.44521422\A17=10
5.72455927\A18=110.46498464\D1=33.6501569\D2=155.71135828\D3=-86.33360
41\D4=92.75212433\D5=-150.63450487\D6=84.13812131\D7=-29.75998731\D8=-
160.96035922\D9=-145.58933456\D10=244.05132678\D11=64.59070071\D12=7.9
2793048\D13=-172.950005\D14=181.02407261\D15=60.66693703\D16=180.23408
553\D17=-60.19327909\\Version=AM64L-G03RevE.01\State=2-A\HF=-572.84093
13\S2=0.76084\S2-1=0.\S2A=0.750075\RMSD=6.090e-09\RMSF=2.493e-05\Therm
al=0.\Dipole=-0.6231596,0.1607539,0.178952\PG=C01 [X(C7H9O4)]\\@

Decarbonylation transition state 40 → 42 (n=1, R=CO_2Me)

HF/3-21G*

1\1\GINC-GOMBERG01\FTS\UHF\3-21G*\C7H9O4(2)\HMAITKEN\18-Nov-2010\1\\#H
F/3-21G* opt=(grad,ts,readfc,noeigentest,nofreeze) geom=checkpoint gue
ss=read\\decarbonylation ts CO2Me and H\\0,2\C\H,1,B1\H,1,B2,2,A1\C,1,
B3,3,A2,2,D1,0\H,4,B4,1,A3,3,D2,0\H,4,B5,1,A4,3,D3,0\O,1,B6,4,A5,5,D4,
0\C,4,B7,1,A6,7,D5,0\O,8,B8,4,A7,1,D6,0\C,7,B9,1,A8,4,D7,0\H,10,B10,7,
A9,1,D8,0\C,10,B11,7,A10,1,D9,0\H,12,B12,10,A11,7,D10,0\C,12,B13,10,A1
2,7,D11,0\O,14,B14,12,A13,10,D12,0\O,14,B15,12,A14,10,D13,0\C,16,B16,1
4,A15,12,D14,0\H,17,B17,16,A16,14,D15,0\H,17,B18,16,A17,14,D16,0\H,17,
B19,16,A18,14,D17,0\\B1=1.080954\B2=1.080954\B3=1.50226521\B4=1.076127
7\B5=1.07612772\B6=1.45080008\B8=1.14941655\B9=1.35202216\B10=1.068027
81\B11=1.32374113\B12=1.06778381\B13=1.45734638\B14=1.20679643\B15=1.3
5826956\B16=1.45102561\B17=1.07923873\B18=1.07653758\B19=1.07923873\A1
=108.95564906\A2=111.16882542\A3=116.01934166\A4=116.01931495\A5=106.2
7980098\A6=101.93476008\A7=119.38249397\A8=120.6038711\A9=111.43355873
\A10=127.37873354\A11=123.79244839\A12=121.13650158\A13=125.62428863\A
14=112.58752417\A15=117.77901501\A16=110.36673854\A17=105.29115809\A18
=110.36673827\D1=122.85113724\D2=49.56185705\D3=-171.1302396\D4=-69.65
413616\D5=179.99990558\D6=-180.00005436\D7=180.00001754\D8=-180.000005
51\D9=-0.00000606\D10=-0.00000025\D11=180.00000015\D12=-180.00000147\D
13=-0.00000141\D14=179.99999934\D15=60.32165349\D16=-180.0000086\D17=-
60.32167102\B7=1.99748137\\Version=AM64L-G03RevE.01\State=2-A\HF=-566.
5072915\S2=0.806706\S2-1=0.\S2A=0.750859\RMSD=5.436e-09\RMSF=4.169e-07
\Thermal=0.\Dipole=-0.6595146,-0.2026717,-0.4708134\PG=C01 [X(C7H9O4)]\\@

HF/6-31G*

1\1\GINC-GOMBERG02\FTS\UHF\6-31G(d)\C7H9O4(2)\HMAITKEN\18-Nov-2010\1\\
#HF/6-31G* opt=(grad,ts,readfc,noeigentest,nofreeze) geom=checkpoint g
uess=read\\decarbonylation ts CO2Me and H\\0,2\C\H,1,B1\H,1,B2,2,A1\C,
1,B3,3,A2,2,D1,0\H,4,B4,1,A3,3,D2,0\H,4,B5,1,A4,3,D3,0\O,1,B6,4,A5,5,D
4,0\C,4,B7,1,A6,7,D5,0\O,8,B8,4,A7,1,D6,0\C,7,B9,1,A8,4,D7,0\H,10,B10,
7,A9,1,D8,0\C,10,B11,7,A10,1,D9,0\H,12,B12,10,A11,7,D10,0\C,12,B13,10,
A12,7,D11,0\O,14,B14,12,A13,10,D12,0\O,14,B15,12,A14,10,D13,0\C,16,B16
,14,A15,12,D14,0\H,17,B17,16,A16,14,D15,0\H,17,B18,16,A17,14,D16,0\H,1
7,B19,16,A18,14,D17,0\\B1=1.08341867\B2=1.08341838\B3=1.50083432\B4=1.
07808943\B5=1.07808788\B6=1.41390086\B8=1.13288585\B9=1.32730035\B10=1

.07185249\B11=1.32957392\B12=1.07134554\B13=1.47066817\B14=1.19159153\
B15=1.33042445\B16=1.41562559\B17=1.08028305\B18=1.07905999\B19=1.0802
8293\A1=108.45286576\A2=110.8496309\A3=116.03069779\A4=116.03289963\A5
=107.55173958\A6=105.61578712\A7=117.0384778\A8=119.38666245\A9=110.92
93813\A10=127.78759596\A11=123.37108408\A12=122.30684841\A13=123.32657
824\A14=113.82203668\A15=116.73654471\A16=110.58732033\A17=105.8209550
1\A18=110.58736431\D1=121.91086786\D2=51.07184012\D3=-171.52647472\D4=
-68.67942464\D5=180.0213315\D6=-179.98506838\D7=179.9989953\D8=-179.99
979581\D9=0.00013525\D10=0.00001789\D11=180.00010013\D12=-180.00009718
\D13=-0.00006051\D14=179.99995956\D15=60.56914906\D16=-179.99658992\D1
7=-60.56215147\B7=1.98626712\\Version=AM64L-G03RevE.01\State=2-A\HF=-5
69.6873228\S2=0.80916\S2-1=0.\S2A=0.75096\RMSD=5.732e-09\RMSF=7.480e-0
6\Thermal=0.\Dipole=-0.7512512,-0.1903601,-0.5411462\PG=C01 [X(C7H9O4)]\\@

HF/6-311G**

1\1\GINC-GOMBERG01\FTS\UHF\6-311G(d,p)\C7H9O4(2)\HMAITKEN\18-Nov-2010\
1\\#HF/6-311G** opt=(grad,ts,readfc,noeigentest,nofreeze) geom=checkpo
int guess=read\\decarbonylation ts CO2Me and H\\0,2\C\H,1,B1\H,1,B2,2,
A1\C,1,B3,3,A2,2,D1,0\H,4,B4,1,A3,3,D2,0\H,4,B5,1,A4,3,D3,0\O,1,B6,4,A
5,5,D4,0\C,4,B7,1,A6,7,D5,0\O,8,B8,4,A7,1,D6,0\C,7,B9,1,A8,4,D7,0\H,10
,B10,7,A9,1,D8,0\C,10,B11,7,A10,1,D9,0\H,12,B12,10,A11,7,D10,0\C,12,B1
3,10,A12,7,D11,0\O,14,B14,12,A13,10,D12,0\O,14,B15,12,A14,10,D13,0\C,1
6,B16,14,A15,12,D14,0\H,17,B17,16,A16,14,D15,0\H,17,B18,16,A17,14,D16,
0\H,17,B19,16,A18,14,D17,0\\B1=1.08450145\B2=1.08450334\B3=1.50033746\
B4=1.0787285\B5=1.07873048\B6=1.4130072\B8=1.12512893\B9=1.32498537\B1
0=1.07259844\B11=1.32861511\B12=1.07141803\B13=1.47156425\B14=1.185983
51\B15=1.32809664\B16=1.41546605\B17=1.08160761\B18=1.07955617\B19=1.0
8160646\A1=108.50921877\A2=110.74133291\A3=115.92364049\A4=115.9114590
8\A5=107.58945732\A6=106.01162983\A7=117.12661127\A8=119.41876861\A9=1
11.21939764\A10=127.83115797\A11=123.50766379\A12=122.23255271\A13=123
.27405155\A14=113.79354287\A15=117.01815673\A16=110.61046075\A17=105.8
367632\A18=110.61087884\D1=121.73933927\D2=51.08577038\D3=-171.6527555
\D4=-68.70493182\D5=179.9267172\D6=-180.04174129\D7=180.00131262\D8=-1
79.99969882\D9=0.00047527\D10=0.00026122\D11=179.99984438\D12=-179.999
51235\D13=0.00076338\D14=179.9993944\D15=60.55925845\D16=-179.98293472
\D17=-60.52417689\B7=1.9785276\\Version=AM64L-G03RevE.01\State=2-A\HF=
-569.8336602\S2=0.808491\S2-1=0.\S2A=0.751008\RMSD=4.312e-09\RMSF=1.58
1e-05\Thermal=0.\Dipole=-0.7682659,-0.1944606,-0.5535936\PG=C01 [X(C7H
9O4)]\\@

BHandHLYP/6-311G**

1\1\GINC-GOMBERG02\FTS\UBHandHLYP\6-311G(d,p)\C7H9O4(2)\HMAITKEN\18-No
v-2010\1\\#BHandHLYP/6-311G** opt=(grad,ts,readfc,noeigentest,nofreeze
) geom=checkpoint guess=read\\decarbonylation ts CO2Me and H\\0,2\C\H,
1,B1\H,1,B2,2,A1\C,1,B3,3,A2,2,D1,0\H,4,B4,1,A3,3,D2,0\H,4,B5,1,A4,3,D
3,0\O,1,B6,4,A5,5,D4,0\C,4,B7,1,A6,7,D5,0\O,8,B8,4,A7,1,D6,0\C,7,B9,1,
A8,4,D7,0\H,10,B10,7,A9,1,D8,0\C,10,B11,7,A10,1,D9,0\H,12,B12,10,A11,7
,D10,0\C,12,B13,10,A12,7,D11,0\O,14,B14,12,A13,10,D12,0\O,14,B15,12,A1
4,10,D13,0\C,16,B16,14,A15,12,D14,0\H,17,B17,16,A16,14,D15,0\H,17,B18,
16,A17,14,D16,0\H,17,B19,16,A18,14,D17,0\\B1=1.0865598\B2=1.0865653\B3
=1.48665119\B4=1.07771399\B5=1.0777062\B6=1.42358137\B8=1.12756967\B9=
1.32759628\B10=1.07510425\B11=1.33226343\B12=1.0727943\B13=1.46176492\
B14=1.19607559\B15=1.33909722\B16=1.41903704\B17=1.08331998\B18=1.0805

0485\B19=1.08332395\A1=108.35477747\A2=111.02755603\A3=117.63580535\A4
=117.64572249\A5=107.96584911\A6=103.12193667\A7=115.61307381\A8=118.2
4601332\A9=111.32256796\A10=127.76386405\A11=123.43367192\A12=122.2497
824\A13=123.82200916\A14=113.46305954\A15=115.86842827\A16=110.6497406
4\A17=105.81290511\A18=110.65057964\D1=122.18154605\D2=47.11138642\D3=
-167.61122999\D4=-72.57922412\D5=180.0543268\D6=-180.03519988\D7=179.9
9656903\D8=-179.99682868\D9=0.00307473\D10=0.00010743\D11=180.00196131
\D12=-180.00255452\D13=-0.00117327\D14=179.99662449\D15=60.41421017\D1
6=-179.96465129\D17=-60.34306176\B7=2.13226571\\Version=AM64L-G03RevE.
01\State=2-A\HF=-572.7835034\S2=0.771613\S2-1=0.\S2A=0.750147\RMSD=4.2
51e-09\RMSF=2.751e-05\Thermal=0.\Dipole=-0.7447304,0.0864977,-0.537136
4\PG=C01 [X(C7H9O4)]\\@

BHandHLYP/6-311++G**

1\1\GINC-GOMBERG01\FTS\UBHandHLYP\6-311++G(d,p)\C7H9O4(2)\HMAITKEN\18-
Nov-2010\1\\#BHandHLYP/6-311++G(d,p) opt=(grad,ts,readfc,noeigentest,n
ofreeze) geom=checkpoint guess=read\\decarbonylation ts CO2Me and H\\0
,2\C\H,1,B1\H,1,B2,2,A1\C,1,B3,3,A2,2,D1,0\H,4,B4,1,A3,3,D2,0\H,4,B5,1
,A4,3,D3,0\O,1,B6,4,A5,5,D4,0\C,4,B7,1,A6,7,D5,0\O,8,B8,4,A7,1,D6,0\C,
7,B9,1,A8,4,D7,0\H,10,B10,7,A9,1,D8,0\C,10,B11,7,A10,1,D9,0\H,12,B12,1
0,A11,7,D10,0\C,12,B13,10,A12,7,D11,0\O,14,B14,12,A13,10,D12,0\O,14,B1
5,12,A14,10,D13,0\C,16,B16,14,A15,12,D14,0\H,17,B17,16,A16,14,D15,0\H,
17,B18,16,A17,14,D16,0\H,17,B19,16,A18,14,D17,0\\B1=1.08645021\B2=1.08
645022\B3=1.48639716\B4=1.07766648\B5=1.07767022\B6=1.42434718\B8=1.12
803841\B9=1.32786183\B10=1.07521266\B11=1.33310686\B12=1.07291531\B13=
1.46149896\B14=1.19801845\B15=1.33802976\B16=1.41991\B17=1.08312191\B1
8=1.08052445\B19=1.08311824\A1=108.45437906\A2=111.03408333\A3=117.829
30453\A4=117.82361825\A5=108.07656782\A6=102.94516165\A7=115.54679628\
A8=118.39956804\A9=111.33928487\A10=127.57453859\A11=123.37851424\A12=
122.23678704\A13=123.68564052\A14=113.6833154\A15=116.20526858\A16=110
.59340665\A17=105.74605983\A18=110.59396358\D1=122.25496359\D2=46.4173
6692\D3=-167.26313192\D4=-73.21179094\D5=179.94929033\D6=-180.03322635
\D7=179.99879515\D8=-179.9990101\D9=0.00116036\D10=0.00003467\D11=179.
99960639\D12=-180.00005226\D13=0.00000485\D14=179.99918951\D15=60.4661
4065\D16=-179.97423662\D17=-60.41286294\B7=2.14211333\\Version=AM64L-G
03RevE.01\State=2-A\HF=-572.7954577\S2=0.77156\S2-1=0.\S2A=0.75015\RMS
D=9.862e-09\RMSF=2.707e-05\Thermal=0.\Dipole=-0.7740799,0.0605258,-0.5
580632\PG=C01 [X(C7H9O4)]\\@

Decarbonylation product 42 (n=1, R=CO_2Me)

HF/3-21G*

1\1\GINC-GOMBERG01\FOpt\UHF\3-21G*\C6H9O3(2)\HMAITKEN\23-Nov-2010\1\\#
HF/3-21G* opt=(grad)\\decarbonylation radical CO2Me and H\\0,2\C\C,1,B
1\O,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\H,5,B5,4,A4,3,D3,0
\H,4,B6,3,A5,2,D4,0\H,2,B7,1,A6,3,D5,0\H,2,B8,1,A7,3,D6,0\H,1,B9,2,A8,
3,D7,0\H,1,B10,2,A9,3,D8,0\C,5,B11,4,A10,3,D9,0\O,12,B12,5,A11,4,D10,0
\O,12,B13,5,A12,4,D11,0\C,14,B14,12,A13,5,D12,0\H,15,B15,14,A14,12,D13
,0\H,15,B16,14,A15,12,D14,0\H,15,B17,14,A16,12,D15,0\\B1=1.49361586\B2
=1.4491415\B3=1.34914639\B4=1.3245062\B5=1.06761226\B6=1.06809182\B7=1
.08655431\B8=1.08444586\B9=1.07164093\B10=1.06999462\B11=1.45642491\B1
2=1.20712406\B13=1.35883306\B14=1.45059505\B15=1.079278\B16=1.07658886
\B17=1.07927635\A1=106.82881562\A2=120.69891979\A3=127.51141871\A4=123

.78106407\A5=111.43545872\A6=111.84177384\A7=111.58405499\A8=119.85849
288\A9=118.77810707\A10=121.16356303\A11=125.67817496\A12=112.61503776
\A13=117.75859911\A14=110.38650062\A15=105.29770752\A16=110.38580311\D
1=-179.9944876\D2=-0.12617257\D3=-0.03975871\D4=-180.12847467\D5=-119.
13893288\D6=119.71621558\D7=-171.47184823\D8=17.85019141\D9=-180.00305
775\D10=179.98172884\D11=-0.03781235\D12=179.98172224\D13=60.33548778\
D14=-179.98623506\D15=-60.30975011\\Version=AM64L-G03RevE.01\State=2-A
\HF=-454.4318311\S2=0.762925\S2-1=0.\S2A=0.750121\RMSD=9.543e-09\RMSF=
1.884e-05\Thermal=0.\Dipole=0.1665746,-0.0541627,-0.7700304\PG=C01 [X(
C6H9O3)]\\@

HF/6-31G*

1\1\GINC-GOMBERG11\FOpt\UHF\6-31G(d)\C6H9O3(2)\HMAITKEN\09-Nov-2010\1\
\#HF/6-31G* opt=(grad) geom=checkpoint guess=read\\decarbonylation rad
ical CO2Me and H\\0,2\C\C,1,B1\O,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\C,4,B4,3
,A3,2,D2,0\H,5,B5,4,A4,3,D3,0\H,4,B6,3,A5,2,D4,0\H,2,B7,1,A6,3,D5,0\H,
2,B8,1,A7,3,D6,0\H,1,B9,2,A8,3,D7,0\H,1,B10,2,A9,3,D8,0\C,5,B11,4,A10,
3,D9,0\O,12,B12,5,A11,4,D10,0\O,12,B13,5,A12,4,D11,0\C,14,B14,12,A13,5
,D12,0\H,15,B15,14,A14,12,D13,0\H,15,B16,14,A15,12,D14,0\H,15,B17,14,A
16,12,D15,0\\B1=1.49011458\B2=1.41248098\B3=1.32470237\B4=1.3304428\B5
=1.07119633\B6=1.07195174\B7=1.08886308\B8=1.08559962\B9=1.07389978\B1
0=1.07324241\B11=1.46973719\B12=1.19197446\B13=1.33096765\B14=1.415167
03\B15=1.0803172\B16=1.07912529\B17=1.08035225\A1=108.10041072\A2=119.
46984656\A3=127.9187511\A4=123.35664727\A5=110.94221366\A6=111.5384705
1\A7=111.00517144\A8=119.29499495\A9=119.45993035\A10=122.32791793\A11
=123.3862708\A12=113.8536394\A13=116.72834267\A14=110.61084065\A15=105
.8283958\A16=110.60454575\D1=-179.51689363\D2=-0.51941551\D3=-0.036019
51\D4=-180.45719214\D5=-119.71582899\D6=120.27886573\D7=-165.27930267\
D8=31.4516582\D9=-179.98024201\D10=179.96527903\D11=-0.04323448\D12=17
9.99382401\D13=60.44401495\D14=-180.1162517\D15=-60.6900414\\Version=A
M64L-G03RevE.01\State=2-A\HF=-456.9737803\S2=0.761778\S2-1=0.\S2A=0.75
0091\RMSD=5.927e-09\RMSF=8.921e-06\Thermal=0.\Dipole=0.3105185,-0.0742
52,-0.8456322\PG=C01 [X(C6H9O3)]\\@

HF/6-311G**

1\1\GINC-GOMBERG11\FOpt\UHF\6-311G(d,p)\C6H9O3(2)\HMAITKEN\09-Nov-2010
\1\\#HF/6-311G** opt=(grad,readfc) geom=checkpoint guess=read\\decarbo
nylation radical CO2Me and H\\0,2\C\C,1,B1\O,2,B2,1,A1\C,3,B3,2,A2,1,D
1,0\C,4,B4,3,A3,2,D2,0\H,5,B5,4,A4,3,D3,0\H,4,B6,3,A5,2,D4,0\H,2,B7,1,
A6,3,D5,0\H,2,B8,1,A7,3,D6,0\H,1,B9,2,A8,3,D7,0\H,1,B10,2,A9,3,D8,0\C,
5,B11,4,A10,3,D9,0\O,12,B12,5,A11,4,D10,0\O,12,B13,5,A12,4,D11,0\C,14,
B14,12,A13,5,D12,0\H,15,B15,14,A14,12,D13,0\H,15,B16,14,A15,12,D14,0\H
,15,B17,14,A16,12,D15,0\\B1=1.48908081\B2=1.41146721\B3=1.32220398\B4=
1.32957127\B5=1.07124238\B6=1.07272096\B7=1.09003078\B8=1.08678575\B9=
1.07460313\B10=1.0738493\B11=1.47064317\B12=1.18636725\B13=1.32857154\
B14=1.41499683\B15=1.08167206\B16=1.07962251\B17=1.08166638\A1=108.229
42486\A2=119.51017822\A3=127.97390773\A4=123.4947527\A5=111.23263387\A
6=111.2790348\A7=110.91973419\A8=119.24554491\A9=119.39921797\A10=122.
25293844\A11=123.33495217\A12=113.83029197\A13=117.01335426\A14=110.63
206287\A15=105.84160704\A16=110.63161043\D1=-179.59353236\D2=-0.463655
27\D3=-0.03686084\D4=-180.41155097\D5=-119.74879541\D6=120.40872171\D7
=-166.54484231\D8=29.44045976\D9=-179.98437043\D10=179.94332305\D11=-0
.05950827\D12=179.93779055\D13=60.6047973\D14=-179.93993911\D15=-60.48

495946\\Version=AM64L-G03RevE.01\State=2-A\HF=-457.0911277\S2=0.762075
\S2-1=0.\S2A=0.750095\RMSD=4.217e-09\RMSF=1.281e-05\Thermal=0.\Dipole=
0.3157291,-0.0700057,-0.820008\PG=C01 [X(C6H9O3)]\\@

BHandHLYP/6-311G**

1\1\GINC-GOMBERG06\FOpt\UBHandHLYP\6-311G(d,p)\C6H9O3(2)\HMAITKEN\09-N
ov-2010\1\\#BHandHLYP/6-311G** opt=(grad,readfc) geom=checkpoint guess
=read\\decarbonylation radical CO2Me and H\\0,2\C\C,1,B1\O,2,B2,1,A1\C
,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\H,5,B5,4,A4,3,D3,0\H,4,B6,3,A5,2,
D4,0\H,2,B7,1,A6,3,D5,0\H,2,B8,1,A7,3,D6,0\H,1,B9,2,A8,3,D7,0\H,1,B10,
2,A9,3,D8,0\C,5,B11,4,A10,3,D9,0\O,12,B12,5,A11,4,D10,0\O,12,B13,5,A12
,4,D11,0\C,14,B14,12,A13,5,D12,0\H,15,B15,14,A14,12,D13,0\H,15,B16,14,
A15,12,D14,0\H,15,B17,14,A16,12,D15,0\\B1=1.47473992\B2=1.41714211\B3=
1.32550084\B4=1.33280397\B5=1.07269808\B6=1.07504071\B7=1.09425269\B8=
1.0905853\B9=1.07405916\B10=1.07363237\B11=1.46125131\B12=1.19629858\B
13=1.33917741\B14=1.41893382\B15=1.08335435\B16=1.08052156\B17=1.08333
89\A1=108.4804703\A2=118.4803416\A3=127.81639343\A4=123.40382649\A5=11
1.31057396\A6=111.58862491\A7=111.39540277\A8=119.81077163\A9=119.6872
0465\A10=122.27321906\A11=123.8435745\A12=113.47006909\A13=115.8908565
2\A14=110.65968011\A15=105.80933109\A16=110.6626242\D1=-179.3118816\D2
=-0.50541838\D3=-0.053282\D4=-180.44401018\D5=-119.81696007\D6=120.713
63154\D7=-167.30671975\D8=21.46009927\D9=-179.98795483\D10=179.9296956
2\D11=-0.07190568\D12=179.96807185\D13=60.43511729\D14=-179.9472085\D1
5=-60.32668185\\Version=AM64L-G03RevE.01\State=2-A\HF=-459.5049775\S2=
0.75517\S2-1=0.\S2A=0.750017\RMSD=6.118e-09\RMSF=1.047e-05\Thermal=0.\
Dipole=0.2726816,-0.0396747,-0.805901\PG=C01 [X(C6H9O3)]\\@

BHandHLYP/6-311++G**

1\1\GINC-GOMBERG07\FOpt\UBHandHLYP\6-311++G(d,p)\C6H9O3(2)\HMAITKEN\09
-Nov-2010\1\\#BHandHLYP/6-311++G(d,p) opt=(grad,readfc) geom=checkpoin
t guess=read\\decarbonylation radical CO2Me and H\\0,2\C\C,1,B1\O,2,B2
,1,A1\C,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\H,5,B5,4,A4,3,D3,0\H,4,B6,
3,A5,2,D4,0\H,2,B7,1,A6,3,D5,0\H,2,B8,1,A7,3,D6,0\H,1,B9,2,A8,3,D7,0\H
,1,B10,2,A9,3,D8,0\C,5,B11,4,A10,3,D9,0\O,12,B12,5,A11,4,D10,0\O,12,B1
3,5,A12,4,D11,0\C,14,B14,12,A13,5,D12,0\H,15,B15,14,A14,12,D13,0\H,15,
B16,14,A15,12,D14,0\H,15,B17,14,A16,12,D15,0\\B1=1.47464119\B2=1.41727
893\B3=1.32581351\B4=1.33363449\B5=1.07283747\B6=1.07513707\B7=1.09395
727\B8=1.09050003\B9=1.07419385\B10=1.0737486\B11=1.46096651\B12=1.198
19757\B13=1.33818417\B14=1.4197124\B15=1.08315498\B16=1.08054905\B17=1
.08315393\A1=108.64121566\A2=118.64682978\A3=127.62714839\A4=123.34222
992\A5=111.32720911\A6=111.53775737\A7=111.33436768\A8=119.6498747\A9=
119.94741721\A10=122.26364129\A11=123.71496286\A12=113.68362994\A13=11
6.2303688\A14=110.60807675\A15=105.74400953\A16=110.60721658\D1=-179.5
3070094\D2=-0.47911462\D3=-0.03599861\D4=-180.42448232\D5=-119.8334949
2\D6=120.66786419\D7=-167.78205369\D8=20.05237429\D9=-180.02744705\D10
=179.95456112\D11=-0.05199604\D12=179.96384865\D13=60.45593057\D14=-17
9.98654289\D15=-60.43101052\\Version=AM64L-G03RevE.01\State=2-A\HF=-45
9.5150615\S2=0.755206\S2-1=0.\S2A=0.750017\RMSD=7.856e-09\RMSF=1.915e-
05\Thermal=0.\Dipole=0.2878392,-0.042418,-0.8174809\PG=C01 [X(C6H9O3)]\\@

6-Membered ester system 40 (n=2, R=CO_2Me)

Acyl radical 40 (n=2, R=CO_2Me)

HF/3-21G*

1\1\GINC-GOMBERG03\FOpt\UHF\3-21G*\C8H11O4(2)\HMAITKEN\13-Oct-2010\1\\
#HF/3-21G* opt=(grad)\\radical starting material 6 membered\\0,2\C\C,1
,B1\O,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\H,5,B5,4,A4,3,D3
,0\H,4,B6,3,A5,2,D4,0\H,2,B7,1,A6,3,D5,0\H,2,B8,1,A7,3,D6,0\H,1,B9,2,A
8,3,D7,0\H,1,B10,2,A9,3,D8,0\C,1,B11,2,A10,3,D9,0\H,12,B12,1,A11,2,D10
,0\H,12,B13,1,A12,2,D11,0\C,12,B14,1,A13,2,D12,0\O,15,B15,12,A14,1,D13
,0\C,5,B16,4,A15,3,D14,0\O,17,B17,5,A16,4,D15,0\O,17,B18,5,A17,4,D16,0
\C,19,B19,17,A18,5,D17,0\H,20,B20,19,A19,17,D18,0\H,20,B21,19,A20,17,D
19,0\H,20,B22,19,A21,17,D20,0\\B1=1.52286302\B2=1.44603877\B3=1.351379
23\B4=1.32377262\B5=1.06773085\B6=1.06797436\B7=1.0831206\B8=1.0831380
1\B9=1.08140141\B10=1.08138836\B11=1.53872913\B12=1.08487304\B13=1.084
87085\B14=1.5146792\B15=1.18465445\B16=1.45717649\B17=1.20693553\B18=1
.3579378\B19=1.45109122\B20=1.07651126\B21=1.07923188\B22=1.07923843\A
1=105.82738794\A2=120.9625409\A3=127.32061674\A4=123.73329384\A5=111.4
5571222\A6=111.44038426\A7=111.44765106\A8=108.90037971\A9=108.8906406
5\A10=111.36725583\A11=111.54240949\A12=111.54092438\A13=111.59185217\
A14=130.4954976\A15=121.19782533\A16=125.597749\A17=112.58974273\A18=1
17.81339147\A19=105.29076864\A20=110.36473626\A21=110.36088922\D1=-180
.01170839\D2=0.01594197\D3=0.00088982\D4=180.01559358\D5=-119.05478869
\D6=119.06343136\D7=58.50102179\D8=-58.51626485\D9=-180.00742294\D10=-
59.99251956\D11=59.94101379\D12=-180.02626732\D13=-0.00434925\D14=-179
.98606744\D15=-180.02844094\D16=-0.03242622\D17=179.99321538\D18=-179.
97863285\D19=-60.29874317\D20=60.34660394\\Version=AM64L-G03RevE.01\St
ate=2-A\HF=-605.3493014\S2=0.770693\S2-1=0.\S2A=0.750201\RMSD=3.659e-0
9\RMSF=1.300e-05\Thermal=0.\Dipole=-0.1513205,-0.0005157,0.3048007\PG=
C01 [X(C8H11O4)]\\@

HF/6-31G*

1\1\GINC-GOMBERG05\FOpt\UHF\6-31G(d)\C8H11O4(2)\HMAITKEN\13-Oct-2010\1
\\#HF/6-31G* opt=(grad,readfc) geom=checkpoint guess=read\\radical sta
rting material 6 membered\\0,2\C\C,1,B1\O,2,B2,1,A1\C,3,B3,2,A2,1,D1,0
\C,4,B4,3,A3,2,D2,0\H,5,B5,4,A4,3,D3,0\H,4,B6,3,A5,2,D4,0\H,2,B7,1,A6,
3,D5,0\H,2,B8,1,A7,3,D6,0\H,1,B9,2,A8,3,D7,0\H,1,B10,2,A9,3,D8,0\C,1,B
11,2,A10,3,D9,0\H,12,B12,1,A11,2,D10,0\H,12,B13,1,A12,2,D11,0\C,12,B14
,1,A13,2,D12,0\O,15,B15,12,A14,1,D13,0\C,5,B16,4,A15,3,D14,0\O,17,B17,
5,A16,4,D15,0\O,17,B18,5,A17,4,D16,0\C,19,B19,17,A18,5,D17,0\H,20,B20,
19,A19,17,D18,0\H,20,B21,19,A20,17,D19,0\H,20,B22,19,A21,17,D20,0\\B1=
1.51810523\B2=1.40981502\B3=1.32624408\B4=1.32979838\B5=1.07129251\B6=
1.07186429\B7=1.08543061\B8=1.08544089\B9=1.08357191\B10=1.08357199\B1
1=1.53038936\B12=1.08647602\B13=1.08646199\B14=1.51757627\B15=1.164667
97\B16=1.47032406\B17=1.19179622\B18=1.3302788\B19=1.41564756\B20=1.07
903303\B21=1.08029376\B22=1.08027027\A1=107.41794053\A2=119.61049667\A
3=127.77536633\A4=123.31613277\A5=110.95630166\A6=111.17030969\A7=111.
17880501\A8=109.22921637\A9=109.22413024\A10=111.52262714\A11=111.8397
227\A12=111.83914699\A13=113.09887287\A14=129.1588671\A15=122.37467384
\A16=123.31020963\A17=113.83006169\A18=116.7496857\A19=105.81652692\A2
0=110.58734117\A21=110.58864891\D1=-179.99673358\D2=0.03738333\D3=-0.0

0263788\D4=180.04070869\D5=-119.70164025\D6=119.69935368\D7=58.3828114
6\D8=-58.2570218\D9=-179.93685836\D10=-59.42656062\D11=59.42309993\D12
=-179.99730291\D13=0.02877926\D14=-179.99422867\D15=-180.01291192\D16=
-0.01219284\D17=180.01663517\D18=-180.09904224\D19=-60.66916523\D20=60
.46633786\\Version=AM64L-G03RevE.01\State=2-A\HF=-608.7460242\S2=0.761
571\S2-1=0.\S2A=0.750099\RMSD=6.151e-09\RMSF=1.537e-05\Thermal=0.\Dipo
le=0.0185921,0.0010065,0.1593156\PG=C01 [X(C8H11O4)]\\@

HF/6-311G**

1\1\GINC-GOMBERG06\FOpt\UHF\6-311G(d,p)\C8H11O4(2)\HMAITKEN\13-Oct-201
0\1\\#HF/6-311G** opt=(grad,readfc) geom=checkpoint guess=read\\radica
l starting material 6 membered\\0,2\C\C,1,B1\O,2,B2,1,A1\C,3,B3,2,A2,1
,D1,0\C,4,B4,3,A3,2,D2,0\H,5,B5,4,A4,3,D3,0\H,4,B6,3,A5,2,D4,0\H,2,B7,
1,A6,3,D5,0\H,2,B8,1,A7,3,D6,0\H,1,B9,2,A8,3,D7,0\H,1,B10,2,A9,3,D8,0\
C,1,B11,2,A10,3,D9,0\H,12,B12,1,A11,2,D10,0\H,12,B13,1,A12,2,D11,0\C,1
2,B14,1,A13,2,D12,0\O,15,B15,12,A14,1,D13,0\C,5,B16,4,A15,3,D14,0\O,17
,B17,5,A16,4,D15,0\O,17,B18,5,A17,4,D16,0\C,19,B19,17,A18,5,D17,0\H,20
,B20,19,A19,17,D18,0\H,20,B21,19,A20,17,D19,0\H,20,B22,19,A21,17,D20,0
\\B1=1.51652917\B2=1.40902463\B3=1.3239669\B4=1.32897958\B5=1.07134644
\B6=1.07260345\B7=1.08668209\B8=1.08666896\B9=1.084167\B10=1.08416705\
B11=1.52934412\B12=1.08675378\B13=1.08675436\B14=1.51696603\B15=1.1572
1568\B16=1.47138787\B17=1.18626065\B18=1.32787302\B19=1.41555376\B20=1
.07952345\B21=1.08160264\B22=1.08160569\A1=107.49040804\A2=119.6745933
3\A3=127.84345109\A4=123.45761899\A5=111.22972901\A6=111.07486461\A7=1
11.08119315\A8=109.20151316\A9=109.20107331\A10=111.54209415\A11=111.9
6031384\A12=111.96021555\A13=113.30647709\A14=129.56971622\A15=122.305
61142\A16=123.25226057\A17=113.80721044\A18=117.04831393\A19=105.81387
824\A20=110.61814484\A21=110.61715605\D1=-179.93229435\D2=-0.04053669\
D3=-0.00496273\D4=179.96802732\D5=-119.70866966\D6=119.72122997\D7=58.
31243795\D8=-58.34145402\D9=-180.01174833\D10=-59.59406602\D11=59.5414
6948\D12=-180.02470519\D13=0.02231045\D14=-179.97493628\D15=-180.06968
77\D16=-0.07037186\D17=179.987588\D18=-180.00091703\D19=-60.55156539\D
20=60.55091677\\Version=AM64L-G03RevE.01\State=2-A\HF=-608.9005463\S2=
0.761668\S2-1=0.\S2A=0.750099\RMSD=5.571e-09\RMSF=4.390e-05\Thermal=0.
\Dipole=0.0746954,-0.0007425,0.1960101\PG=C01 [X(C8H11O4)]\\@

BHandHLYP/6-311G**

1\1\GINC-GOMBERG13\FOpt\UBHandHLYP\6-311G(d,p)\C8H11O4(2)\HMAITKEN\13-
Oct-2010\1\\#BHandHLYP/6-311G** opt=(grad,readfc) geom=checkpoint gues
s=read\\radical starting material 6 membered\\0,2\C\C,1,B1\O,2,B2,1,A1
\C,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\H,5,B5,4,A4,3,D3,0\H,4,B6,3,A5,
2,D4,0\H,2,B7,1,A6,3,D5,0\H,2,B8,1,A7,3,D6,0\H,1,B9,2,A8,3,D7,0\H,1,B1
0,2,A9,3,D8,0\C,1,B11,2,A10,3,D9,0\H,12,B12,1,A11,2,D10,0\H,12,B13,1,A
12,2,D11,0\C,12,B14,1,A13,2,D12,0\O,15,B15,12,A14,1,D13,0\C,5,B16,4,A1
5,3,D14,0\O,17,B17,5,A16,4,D15,0\O,17,B18,5,A17,4,D16,0\C,19,B19,17,A1
8,5,D17,0\H,20,B20,19,A19,17,D18,0\H,20,B21,19,A20,17,D19,0\H,20,B22,1
9,A21,17,D20,0\\B1=1.50993094\B2=1.41486377\B3=1.32731287\B4=1.3320516
1\B5=1.07282116\B6=1.07497051\B7=1.08875489\B8=1.08875566\B9=1.08509\B
10=1.08508809\B11=1.52360252\B12=1.08783224\B13=1.08784602\B14=1.51062
652\B15=1.16660615\B16=1.46183759\B17=1.19616345\B18=1.3382937\B19=1.4
1944873\B20=1.08044536\B21=1.08326918\B22=1.08328988\A1=107.51971923\A
2=118.64727296\A3=127.65196191\A4=123.34183836\A5=111.32879273\A6=111.
23755419\A7=111.23989629\A8=109.25579428\A9=109.2565161\A10=111.624861

44\A11=112.11297345\A12=112.10617404\A13=113.49963123\A14=128.34398173
\A15=122.31448997\A16=123.77496137\A17=113.44232077\A18=115.91778195\A
19=105.80113872\A20=110.63218052\A21=110.62817563\D1=-179.96634107\D2=
-0.04457349\D3=0.00083805\D4=179.95727447\D5=-119.70018396\D6=119.6974
3531\D7=58.33540472\D8=-58.22837159\D9=-179.9477733\D10=-59.33044547\D
11=59.49123633\D12=-179.93123924\D13=-0.04430466\D14=-179.9926639\D15=
-180.02815442\D16=-0.02398339\D17=179.9777445\D18=-179.88672766\D19=-6
0.26104557\D20=60.49714067\\Version=AM64L-G03RevE.01\State=2-A\HF=-612
.1102303\S2=0.754799\S2-1=0.\S2A=0.750014\RMSD=8.079e-09\RMSF=3.631e-0
5\Thermal=0.\Dipole=0.0991968,0.0008686,0.131333\PG=C01 [X(C8H11O4)]\\@

BHandHLYP/6-311++G**

1\1\GINC-GOMBERG04\FOpt\UBHandHLYP\6-311++G(d,p)\C8H11O4(2)\HMAITKEN\1
4-Oct-2010\1\\#BHandHLYP/6-311++G(d,p) opt=(grad,readfc) geom=checkpoi
nt guess=read\\radical starting material 6 membered\\0,2\C\C,1,B1\O,2,
B2,1,A1\C,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\H,5,B5,4,A4,3,D3,0\H,4,B
6,3,A5,2,D4,0\H,2,B7,1,A6,3,D5,0\H,2,B8,1,A7,3,D6,0\H,1,B9,2,A8,3,D7,0
\H,1,B10,2,A9,3,D8,0\C,1,B11,2,A10,3,D9,0\H,12,B12,1,A11,2,D10,0\H,12,
B13,1,A12,2,D11,0\C,12,B14,1,A13,2,D12,0\O,15,B15,12,A14,1,D13,0\C,5,B
16,4,A15,3,D14,0\O,17,B17,5,A16,4,D15,0\O,17,B18,5,A17,4,D16,0\C,19,B1
9,17,A18,5,D17,0\H,20,B20,19,A19,17,D18,0\H,20,B21,19,A20,17,D19,0\H,2
0,B22,19,A21,17,D20,0\\B1=1.51046537\B2=1.41511748\B3=1.32735238\B4=1.
33301926\B5=1.07298591\B6=1.07514112\B7=1.08866974\B8=1.08867554\B9=1.
08517884\B10=1.08518198\B11=1.52401904\B12=1.08790506\B13=1.08793164\B
14=1.50852958\B15=1.1665517\B16=1.46166978\B17=1.1980105\B18=1.3377260
9\B19=1.42017931\B20=1.0804991\B21=1.08311971\B22=1.08313645\A1=107.70
584767\A2=118.77485363\A3=127.45874103\A4=123.27360717\A5=111.3673211\
A6=111.21015174\A7=111.22156808\A8=109.3445855\A9=109.34003071\A10=111
.3067274\A11=112.12958173\A12=112.12187001\A13=113.74626864\A14=128.95
944196\A15=122.31762327\A16=123.65585925\A17=113.65281261\A18=116.2751
5034\A19=105.73872332\A20=110.60014624\A21=110.59689226\D1=-179.896383
77\D2=-0.03320731\D3=-0.02913829\D4=179.97240475\D5=-119.66854486\D6=1
19.68447862\D7=58.29522403\D8=-58.44472284\D9=-180.06877537\D10=-59.57
621119\D11=59.21230048\D12=-180.1897375\D13=-0.00204147\D14=-179.96020
805\D15=-180.16282007\D16=-0.1586018\D17=179.93190385\D18=-179.9754096
1\D19=-60.41772641\D20=60.47491331\\Version=AM64L-G03RevE.01\State=2-A
\HF=-612.1232261\S2=0.754977\S2-1=0.\S2A=0.750015\RMSD=8.222e-09\RMSF=
5.481e-05\Thermal=0.\Dipole=0.1289482,-0.0037009,0.1756196\PG=C01 [X(C
8H11O4)]\\@

Cyclization transition state 47

HF/3-21G*

1\1\GINC-GOMBERG11\FTS\UHF\3-21G*\C7H9O4(2)\HMAITKEN\15-Oct-2010\1\\#H
F/3-21G* opt=(grad,readfc,ts,noeigentest,nofreeze) geom=checkpoint gue
ss=read\\5exo ts CO2Me and H\\0,2\C\C,1,B1\C,2,B2,1,A1\O,3,B3,2,A2,1,D
1,0\C,1,B4,3,A3,2,D2,0\C,5,B5,4,A4,3,D3,0\O,1,B6,2,A5,3,D4,0\H,2,B7,1,
A6,7,D5,0\H,2,B8,1,A7,7,D6,0\H,3,B9,2,A8,1,D7,0\H,3,B10,2,A9,1,D8,0\H,
5,B11,4,A10,3,D9,0\H,6,B12,5,A11,4,D10,0\C,6,B13,5,A12,4,D11,0\O,14,B1
4,6,A13,5,D12,0\O,14,B15,6,A14,5,D13,0\C,16,B16,14,A15,6,D14,0\H,17,B1
7,16,A16,14,D15,0\H,17,B18,16,A17,14,D16,0\H,17,B19,16,A18,14,D17,0\\B
1=1.51585063\B2=1.52845105\B3=1.44405214\B6=1.18457997\B7=1.08438869\B
8=1.08209679\B9=1.07595027\B10=1.08340493\B11=1.07098106\B12=1.0683457

6\B13=1.44471473\B14=1.21499994\B15=1.35889321\B16=1.44999266\B17=1.07
956712\B18=1.07649831\B19=1.07940438\A1=106.36542594\A2=107.31025217\A
3=61.51965862\A4=117.75860617\A5=133.07427711\A6=107.84235925\A7=110.4
3913668\A8=112.68129378\A9=110.47884951\A10=116.99775597\A11=120.86176
446\A12=121.40140741\A13=125.30152936\A14=112.73152863\A15=117.8717896
2\A16=110.45119996\A17=105.29932662\A18=110.38519622\D1=46.49207556\D2
=155.29582932\D3=143.83203609\D4=164.37917969\D5=-77.71093046\D6=41.78
754824\D7=163.36799599\D8=-73.51969596\D9=-59.53006258\D10=-11.9100463
3\D11=170.83160248\D12=178.15982402\D13=-1.86332572\D14=178.14993443\D
15=61.17775649\D16=-179.17007374\D17=-59.64438335\B4=2.20473228\B5=1.3
7265872\\Version=AM64L-G03RevE.01\State=2-A\HF=-566.5110072\S2=1.06799
8\S2-1=0.\S2A=0.804228\RMSD=7.526e-09\RMSF=1.146e-05\Thermal=0.\Dipole
=0.0535698,-1.2096027,1.2189454\PG=C01 [X(C7H9O4)]\\@

HF/6-31G*

1\1\GINC-GOMBERG04\FTS\UHF\6-31G(d)\C7H9O4(2)\HMAITKEN\15-Oct-2010\1\\
#HF/6-31G* opt=(grad,readfc,ts,noeigentest,nofreeze) geom=checkpoint g
uess=read\\5exo ts CO2Me and H\\0,2\C\C,1,B1\C,2,B2,1,A1\O,3,B3,2,A2,1
,D1,0\C,1,B4,3,A3,2,D2,0\C,5,B5,4,A4,3,D3,0\O,1,B6,2,A5,3,D4,0\H,2,B7,
1,A6,7,D5,0\H,2,B8,1,A7,7,D6,0\H,3,B9,2,A8,1,D7,0\H,3,B10,2,A9,1,D8,0\
H,5,B11,4,A10,3,D9,0\H,6,B12,5,A11,4,D10,0\C,6,B13,5,A12,4,D11,0\O,14,
B14,6,A13,5,D12,0\O,14,B15,6,A14,5,D13,0\C,16,B16,14,A15,6,D14,0\H,17,
B17,16,A16,14,D15,0\H,17,B18,16,A17,14,D16,0\H,17,B19,16,A18,14,D17,0\
\B1=1.51266603\B2=1.52343244\B3=1.40495678\B6=1.16509389\B7=1.08567636
\B8=1.0839223\B9=1.07909532\B10=1.08723643\B11=1.07616522\B12=1.072400
75\B13=1.46312642\B14=1.19364936\B15=1.32973577\B16=1.41548993\B17=1.0
8050973\B18=1.07889989\B19=1.08026632\A1=106.30965896\A2=108.06276232\
A3=60.24683594\A4=117.64730984\A5=131.54853434\A6=107.45242737\A7=109.
99980249\A8=112.55428853\A9=110.71523535\A10=115.92799613\A11=120.2417
2774\A12=123.32757375\A13=123.30432883\A14=113.44045166\A15=116.781474
12\A16=110.58313006\A17=105.83354467\A18=110.51945915\D1=43.26664588\D
2=159.87162438\D3=149.546568\D4=166.53047239\D5=-74.93989927\D6=43.310
73215\D7=161.07976968\D8=-77.27609535\D9=-58.04170768\D10=-15.15138717
\D11=169.61140982\D12=177.64091842\D13=-2.60902678\D14=178.84215313\D1
5=61.21213004\D16=-179.33188006\D17=-59.97160955\B4=2.16602665\B5=1.38
648631\\Version=AM64L-G03RevE.01\State=2-A\HF=-569.6863314\S2=1.010437
\S2-1=0.\S2A=0.769741\RMSD=5.339e-09\RMSF=1.343e-05\Thermal=0.\Dipole=
0.0813668,-1.2081526,1.3460741\PG=C01 [X(C7H9O4)]\\@

HF/6-311G**

1\1\GINC-GOMBERG04\FTS\UHF\6-311G(d,p)\C7H9O4(2)\HMAITKEN\15-Oct-2010\
1\\#HF/6-311G** opt=(grad,readfc,ts,noeigentest,nofreeze) geom=checkpo
int guess=read\\5exo ts CO2Me and H\\0,2\C\C,1,B1\C,2,B2,1,A1\O,3,B3,2
,A2,1,D1,0\C,1,B4,3,A3,2,D2,0\C,5,B5,4,A4,3,D3,0\O,1,B6,2,A5,3,D4,0\H,
2,B7,1,A6,7,D5,0\H,2,B8,1,A7,7,D6,0\H,3,B9,2,A8,1,D7,0\H,3,B10,2,A9,1,
D8,0\H,5,B11,4,A10,3,D9,0\H,6,B12,5,A11,4,D10,0\C,6,B13,5,A12,4,D11,0\
O,14,B14,6,A13,5,D12,0\O,14,B15,6,A14,5,D13,0\C,16,B16,14,A15,6,D14,0\
H,17,B17,16,A16,14,D15,0\H,17,B18,16,A17,14,D16,0\H,17,B19,16,A18,14,D
17,0\\B1=1.51107749\B2=1.52269009\B3=1.40387888\B6=1.15822783\B7=1.085
98603\B8=1.08410553\B9=1.07927686\B10=1.08836924\B11=1.07676669\B12=1.
07268298\B13=1.46313457\B14=1.18816549\B15=1.32779009\B16=1.41515514\B
17=1.08183755\B18=1.07943467\B19=1.08157661\A1=106.22295224\A2=108.052
82965\A3=60.29211808\A4=117.75965211\A5=132.0648829\A6=107.21519138\A7

=109.94023513\A8=112.51276633\A9=110.61738771\A10=116.05253741\A11=120
.3610916\A12=123.18236241\A13=123.35228617\A14=113.37187821\A15=117.05
297005\A16=110.61911487\A17=105.85803226\A18=110.54258322\D1=43.470212
88\D2=159.53480541\D3=149.3170832\D4=165.86018733\D5=-75.73789284\D6=4
2.58090405\D7=161.43017894\D8=-76.98625337\D9=-58.41221221\D10=-15.049
5852\D11=169.80617517\D12=177.52222802\D13=-2.65343393\D14=178.6480248
9\D15=61.14431609\D16=-179.36309032\D17=-60.00107935\B4=2.15769716\B5=
1.3852443\\Version=AM64L-G03RevE.01\State=2-A\HF=-569.829341\S2=1.0016
67\S2-1=0.\S2A=0.768352\RMSD=7.060e-09\RMSF=9.095e-06\Thermal=0.\Dipol
e=0.0505204,-1.2197712,1.3494478\PG=C01 [X(C7H9O4)]\\@

BHandHLYP/6-311G**

1\1\GINC-GOMBERG12\FTS\UBHandHLYP\6-311G(d,p)\C7H9O4(2)\HMAITKEN\15-Oc
t-2010\1\\#BHandHLYP/6-311G** opt=(grad,readfc,ts,noeigentest,nofreeze
) geom=checkpoint guess=read\\5exo ts CO2Me and H\\0,2\C\C,1,B1\C,2,B2
,1,A1\O,3,B3,2,A2,1,D1,0\C,1,B4,3,A3,2,D2,0\C,5,B5,4,A4,3,D3,0\O,1,B6,
2,A5,3,D4,0\H,2,B7,1,A6,7,D5,0\H,2,B8,1,A7,7,D6,0\H,3,B9,2,A8,1,D7,0\H
,3,B10,2,A9,1,D8,0\H,5,B11,4,A10,3,D9,0\H,6,B12,5,A11,4,D10,0\C,6,B13,
5,A12,4,D11,0\O,14,B14,6,A13,5,D12,0\O,14,B15,6,A14,5,D13,0\C,16,B16,1
4,A15,6,D14,0\H,17,B17,16,A16,14,D15,0\H,17,B18,16,A17,14,D16,0\H,17,B
19,16,A18,14,D17,0\\B1=1.50467632\B2=1.51847833\B3=1.40914522\B6=1.163
07203\B7=1.08722461\B8=1.08538632\B9=1.08054033\B10=1.08967307\B11=1.0
7939584\B12=1.07379442\B13=1.45066017\B14=1.19845547\B15=1.34237899\B1
6=1.41806474\B17=1.08349604\B18=1.08064537\B19=1.0833863\A1=106.513131
48\A2=107.81256856\A3=59.88138485\A4=118.99576629\A5=132.47350258\A6=1
07.1410445\A7=109.6368167\A8=112.56400968\A9=110.63480863\A10=116.2898
8946\A11=120.53180422\A12=122.92390652\A13=124.36648337\A14=112.964145
55\A15=115.80317343\A16=110.70048468\A17=105.86234372\A18=110.63017588
\D1=44.96261221\D2=158.86896018\D3=150.30527742\D4=167.82965951\D5=-73
.65609738\D6=44.31597144\D7=162.64350289\D8=-75.49983959\D9=-53.349004
92\D10=-13.75285415\D11=169.52884657\D12=178.52515445\D13=-1.34371246\
D14=179.02207603\D15=60.33930004\D16=-179.98914683\D17=-60.44276208\B4
=2.19317419\B5=1.36248761\\Version=AM64L-G03RevE.01\State=2-A\HF=-572.
7915426\S2=0.8126\S2-1=0.\S2A=0.750885\RMSD=8.329e-09\RMSF=2.675e-05\T
hermal=0.\Dipole=-0.1990717,-1.3290707,1.5667692\PG=C01 [X(C7H9O4)]\\@

BHandHLYP/6-311++G**

1\1\GINC-GOMBERG03\FTS\UBHandHLYP\6-311++G(d,p)\C7H9O4(2)\HMAITKEN\15-
Oct-2010\1\\#BHandHLYP/6-311++G(d,p) opt=(grad,readfc,ts,noeigentest,n
ofreeze) geom=checkpoint guess=read\\5exo ts CO2Me and H\\0,2\C\C,1,B1
\C,2,B2,1,A1\O,3,B3,2,A2,1,D1,0\C,1,B4,3,A3,2,D2,0\C,5,B5,4,A4,3,D3,0\
O,1,B6,2,A5,3,D4,0\H,2,B7,1,A6,7,D5,0\H,2,B8,1,A7,7,D6,0\H,3,B9,2,A8,1
,D7,0\H,3,B10,2,A9,1,D8,0\H,5,B11,4,A10,3,D9,0\H,6,B12,5,A11,4,D10,0\C
,6,B13,5,A12,4,D11,0\O,14,B14,6,A13,5,D12,0\O,14,B15,6,A14,5,D13,0\C,1
6,B16,14,A15,6,D14,0\H,17,B17,16,A16,14,D15,0\H,17,B18,16,A17,14,D16,0
\H,17,B19,16,A18,14,D17,0\\B1=1.50318837\B2=1.51849969\B3=1.40960806\B
6=1.16357582\B7=1.08741175\B8=1.08554459\B9=1.08071557\B10=1.08951952\
B11=1.07943766\B12=1.07405707\B13=1.45067822\B14=1.20035115\B15=1.3412
104\B16=1.4189832\B17=1.0833076\B18=1.0806653\B19=1.08321779\A1=106.75
350255\A2=107.88225534\A3=59.88510525\A4=118.97957882\A5=132.42095146\
A6=107.11839169\A7=109.48181387\A8=112.50779589\A9=110.7584374\A10=116
.15876995\A11=120.49652627\A12=123.07464559\A13=124.18838061\A14=113.2
0720478\A15=116.13395678\A16=110.64016141\A17=105.79910347\A18=110.575

91227\D1=43.91487399\D2=160.066844\D3=150.83148225\D4=168.94228896\D5=
-72.24374529\D6=45.54102637\D7=161.58407436\D8=-76.54715517\D9=-52.927
20699\D10=-14.24392058\D11=169.07853104\D12=177.68494364\D13=-2.275283
08\D14=178.84515464\D15=60.48642716\D16=-179.90192117\D17=-60.40440876
\B4=2.19426663\B5=1.36281918\\Version=AM64L-G03RevE.01\State=2-A\HF=-5
72.8045615\S2=0.812497\S2-1=0.\S2A=0.750868\RMSD=8.260e-09\RMSF=2.762e
-05\Thermal=0.\Dipole=-0.183532,-1.3806103,1.6581824\PG=C01 [X(C7H9O4)]\\@

Cyclization product 41 (n=2, R=CO_2Me)

HF/3-21G*

1\1\GINC-GOMBERG05\FOpt\UHF\3-21G*\C8H11O4(2)\HMAITKEN\13-Oct-2010\1\\
#HF/3-21G* opt=(grad)\\6exo radical product\\0,2\C\C,1,B1\C,2,B2,1,A1\
C,3,B3,2,A2,1,D1,0\H,1,B4,4,A3,3,D2,0\H,1,B5,4,A4,3,D3,0\H,3,B6,2,A5,1
,D4,0\H,3,B7,2,A6,1,D5,0\H,4,B8,3,A7,2,D6,0\H,4,B9,3,A8,2,D7,0\H,2,B10
,1,A9,4,D8,0\O,3,B11,2,A10,1,D9,0\C,2,B12,1,A11,4,D10,0\H,13,B13,2,A12
,1,D11,0\C,1,B14,4,A13,3,D12,0\O,15,B15,1,A14,4,D13,0\C,13,B16,2,A15,1
,D14,0\O,17,B17,13,A16,2,D15,0\O,17,B18,13,A17,2,D16,0\C,19,B19,17,A18
,13,D17,0\H,20,B20,19,A19,17,D18,0\H,20,B21,19,A20,17,D19,0\H,20,B22,1
9,A21,17,D20,0\\B1=2.5543099\B2=2.42446148\B3=1.52801815\B4=1.08775218
\B5=1.0808345\B6=1.07847286\B7=1.08608493\B8=1.08289724\B9=1.08287548\
B10=1.08654361\B11=1.44323736\B12=1.48552513\B13=1.06660568\B14=1.5123
9538\B15=1.20857949\B16=1.42924464\B17=1.22637735\B18=1.35447987\B19=1
.44937691\B20=1.07998978\B21=1.07637459\B22=1.07982075\A1=60.51392073\
A2=92.76830267\A3=109.18376834\A4=111.84902895\A5=138.42404221\A6=91.3
2351628\A7=108.69376383\A8=110.2580254\A9=94.37285392\A10=32.70133186\
A11=143.28767088\A12=120.38542727\A13=110.62816284\A14=123.80236613\A1
5=118.46771276\A16=123.92546712\A17=113.83377262\A18=117.89969751\A19=
110.604675\A20=105.229943\A21=110.50641909\D1=18.71554772\D2=-66.51395
166\D3=173.35774476\D4=146.72903327\D5=-91.86231147\D6=90.3363229\D7=-
150.84024293\D8=-109.30117086\D9=141.25348557\D10=117.658624\D11=-82.8
6247216\D12=52.14349046\D13=132.86515276\D14=-268.1144385\D15=5.410050
98\D16=-175.43592459\D17=178.98745713\D18=60.87549256\D19=180.43824948
\D20=-60.04926732\\Version=AM64L-G03RevE.01\State=2-A\HF=-605.3753946\
S2=0.857696\S2-1=0.\S2A=0.753994\RMSD=6.090e-09\RMSF=2.535e-05\Thermal
=0.\Dipole=0.9051088,-0.377673,-0.4196501\PG=C01 [X(C8H11O4)]\\@

HF/6-31G*

1\1\GINC-GOMBERG04\FOpt\UHF\6-31G(d)\C8H11O4(2)\HMAITKEN\13-Oct-2010\1
\\#HF/6-31G* opt=(grad,readfc) geom=checkpoint guess=read\\6exo radica
l product\\0,2\C\C,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\H,1,B4,4,A3,3,D
2,0\H,1,B5,4,A4,3,D3,0\H,3,B6,2,A5,1,D4,0\H,3,B7,2,A6,1,D5,0\H,4,B8,3,
A7,2,D6,0\H,4,B9,3,A8,2,D7,0\H,2,B10,1,A9,4,D8,0\O,3,B11,2,A10,1,D9,0\
C,2,B12,1,A11,4,D10,0\H,13,B13,2,A12,1,D11,0\C,1,B14,4,A13,3,D12,0\O,1
5,B15,1,A14,4,D13,0\C,13,B16,2,A15,1,D14,0\O,17,B17,13,A16,2,D15,0\O,1
7,B18,13,A17,2,D16,0\C,19,B19,17,A18,13,D17,0\H,20,B20,19,A19,17,D18,0
\H,20,B21,19,A20,17,D19,0\H,20,B22,19,A21,17,D20,0\\B1=2.56674823\B2=2
.36248904\B3=1.52171422\B4=1.08945706\B5=1.08229667\B6=1.0810403\B7=1.
08962351\B8=1.08570947\B9=1.0855725\B10=1.08905388\B11=1.40436027\B12=
1.49147817\B13=1.07190967\B14=1.51464893\B15=1.1896428\B16=1.45659465\
B17=1.19738771\B18=1.32529381\B19=1.41539694\B20=1.08076963\B21=1.0786
9045\B22=1.08045784\A1=60.98888351\A2=94.53431584\A3=109.51717417\A4=1
12.4853471\A5=138.71793253\A6=90.74779609\A7=108.63615792\A8=110.39664

961\A9=95.1638186\A10=32.73171756\A11=143.53164763\A12=119.62056478\A1
3=111.51184043\A14=123.21325695\A15=119.96606002\A16=123.6607853\A17=1
12.65023966\A18=116.82996259\A19=110.5986028\A20=105.81351323\A21=110.
53632613\D1=16.86338412\D2=-71.46876282\D3=168.8810991\D4=146.90021099
\D5=-94.06907342\D6=93.35610136\D7=-149.04385067\D8=-105.67700145\D9=1
38.46405823\D10=121.430947\D11=-75.57247789\D12=46.5204688\D13=138.274
361\D14=-261.74684264\D15=6.48167455\D16=-174.23453056\D17=179.5300643
1\D18=61.3286597\D19=180.74198082\D20=-59.84481832\\Version=AM64L-G03R
evE.01\State=2-A\HF=-608.7704735\S2=0.784215\S2-1=0.\S2A=0.750654\RMSD
=9.223e-09\RMSF=3.341e-05\Thermal=0.\Dipole=0.9649996,-0.1018577,-0.27
78253\PG=C01 [X(C8H11O4)]\\@

HF/6-311G**

1\1\GINC-GOMBERG03\FOpt\UHF\6-311G(d,p)\C8H11O4(2)\HMAITKEN\13-Oct-201
0\1\\#HF/6-311G** opt=(grad,readfc) geom=checkpoint guess=read\\6exo r
adical product\\0,2\C\C,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\H,1,B4,4,A
3,3,D2,0\H,1,B5,4,A4,3,D3,0\H,3,B6,2,A5,1,D4,0\H,3,B7,2,A6,1,D5,0\H,4,
B8,3,A7,2,D6,0\H,4,B9,3,A8,2,D7,0\H,2,B10,1,A9,4,D8,0\O,3,B11,2,A10,1,
D9,0\C,2,B12,1,A11,4,D10,0\H,13,B13,2,A12,1,D11,0\C,1,B14,4,A13,3,D12,
0\O,15,B15,1,A14,4,D13,0\C,13,B16,2,A15,1,D14,0\O,17,B17,13,A16,2,D15,
0\O,17,B18,13,A17,2,D16,0\C,19,B19,17,A18,13,D17,0\H,20,B20,19,A19,17,
D18,0\H,20,B21,19,A20,17,D19,0\H,20,B22,19,A21,17,D20,0\\B1=2.56475526
\B2=2.36054685\B3=1.52065082\B4=1.08979311\B5=1.08233036\B6=1.08127731
\B7=1.09087524\B8=1.08632311\B9=1.08585484\B10=1.08974696\B11=1.403333
6\B12=1.49044545\B13=1.07229094\B14=1.5140675\B15=1.1842568\B16=1.4571
7449\B17=1.19180091\B18=1.32303439\B19=1.4152217\B20=1.08203832\B21=1.
07917444\B22=1.08180685\A1=61.00616231\A2=94.51125363\A3=109.57800062\
A4=112.58958385\A5=138.80681953\A6=90.72939268\A7=108.62008436\A8=110.
3238732\A9=94.94239927\A10=32.72285701\A11=143.70731356\A12=119.717244
65\A13=111.52317362\A14=123.30516351\A15=120.04031071\A16=123.76656247
\A17=112.5276696\A18=117.07832327\A19=110.63302785\A20=105.81721992\A2
1=110.55617912\D1=16.8959923\D2=-70.99074415\D3=169.06999824\D4=146.96
271386\D5=-93.97869808\D6=93.24841839\D7=-149.09730684\D8=-105.8816606
2\D9=138.64171471\D10=121.77630668\D11=-74.94652024\D12=46.68501105\D1
3=138.05391224\D14=-260.77632249\D15=6.24943662\D16=-174.38346186\D17=
179.53970207\D18=60.86160842\D19=180.31182142\D20=-60.271035\\Version=
AM64L-G03RevE.01\State=2-A\HF=-608.9212521\S2=0.782728\S2-1=0.\S2A=0.7
50625\RMSD=9.103e-09\RMSF=1.519e-05\Thermal=0.\Dipole=0.9587321,-0.105
8028,-0.2841382\PG=C01 [X(C8H11O4)]\\@

BHandHLYP/6-311G**

1\1\GINC-GOMBERG10\FOpt\UBHandHLYP\6-311G(d,p)\C8H11O4(2)\HMAITKEN\13-
Oct-2010\1\\#BHandHLYP/6-311G** opt=(grad,readfc) geom=checkpoint gues
s=read\\6exo radical product\\0,2\C\C,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,1,D
1,0\H,1,B4,4,A3,3,D2,0\H,1,B5,4,A4,3,D3,0\H,3,B6,2,A5,1,D4,0\H,3,B7,2,
A6,1,D5,0\H,4,B8,3,A7,2,D6,0\H,4,B9,3,A8,2,D7,0\H,2,B10,1,A9,4,D8,0\O,
3,B11,2,A10,1,D9,0\C,2,B12,1,A11,4,D10,0\H,13,B13,2,A12,1,D11,0\C,1,B1
4,4,A13,3,D12,0\O,15,B15,1,A14,4,D13,0\C,13,B16,2,A15,1,D14,0\O,17,B17
,13,A16,2,D15,0\O,17,B18,13,A17,2,D16,0\C,19,B19,17,A18,13,D17,0\H,20,
B20,19,A19,17,D18,0\H,20,B21,19,A20,17,D19,0\H,20,B22,19,A21,17,D20,0\
\B1=2.55881265\B2=2.35910154\B3=1.51514256\B4=1.09072909\B5=1.08338521
\B6=1.08280044\B7=1.09289306\B8=1.08675071\B9=1.08649795\B10=1.0940319
9\B11=1.40881007\B12=1.4762352\B13=1.0736696\B14=1.50824019\B15=1.1927

1961\B16=1.44335182\B17=1.20329373\B18=1.33325551\B19=1.41926725\B20=1
.08362552\B21=1.08013564\B22=1.08350914\A1=60.85043046\A2=94.52884877\
A3=109.44063418\A4=112.78146507\A5=139.0045398\A6=90.30418393\A7=108.5
9639046\A8=110.36262673\A9=94.48911824\A10=33.21099728\A11=143.7066502
1\A12=119.79102337\A13=111.84474176\A14=123.46637392\A15=119.61251847\
A16=124.06628656\A17=112.43079643\A18=115.87717279\A19=110.63678147\A2
0=105.79170513\A21=110.5400288\D1=16.95148113\D2=-70.74812961\D3=169.3
9318338\D4=147.48068083\D5=-93.82887679\D6=93.13997176\D7=-149.2650480
1\D8=-105.90707359\D9=138.59847209\D10=122.8309831\D11=-79.60370553\D1
2=46.91590348\D13=137.86438036\D14=-263.87281888\D15=5.6622424\D16=-17
4.87889067\D17=179.49565331\D18=60.08822441\D19=179.75467209\D20=-60.6
5808334\\Version=AM64L-G03RevE.01\State=2-A\HF=-612.1284537\S2=0.76196
7\S2-1=0.\S2A=0.750082\RMSD=6.834e-09\RMSF=2.714e-05\Thermal=0.\Dipole
=0.9279673,-0.0944391,-0.2956812\PG=C01 [X(C8H11O4)]\\@

BHandHLYP/6-311++G**

1\1\GINC-GOMBERG08\FOpt\UBHandHLYP\6-311++G(d,p)\C8H11O4(2)\HMAITKEN\1
4-Oct-2010\1\\#BHandHLYP/6-311++G(d,p) opt=(grad,readfc) geom=checkpoi
nt guess=read\\6exo radical product\\0,2\C\C,1,B1\C,2,B2,1,A1\C,3,B3,2
,A2,1,D1,0\H,1,B4,4,A3,3,D2,0\H,1,B5,4,A4,3,D3,0\H,3,B6,2,A5,1,D4,0\H,
3,B7,2,A6,1,D5,0\H,4,B8,3,A7,2,D6,0\H,4,B9,3,A8,2,D7,0\H,2,B10,1,A9,4,
D8,0\O,3,B11,2,A10,1,D9,0\C,2,B12,1,A11,4,D10,0\H,13,B13,2,A12,1,D11,0
\C,1,B14,4,A13,3,D12,0\O,15,B15,1,A14,4,D13,0\C,13,B16,2,A15,1,D14,0\O
,17,B17,13,A16,2,D15,0\O,17,B18,13,A17,2,D16,0\C,19,B19,17,A18,13,D17,
0\H,20,B20,19,A19,17,D18,0\H,20,B21,19,A20,17,D19,0\H,20,B22,19,A21,17
,D20,0\\B1=2.55703633\B2=2.36090059\B3=1.51499522\B4=1.0908905\B5=1.08
346644\B6=1.08295954\B7=1.09261876\B8=1.08682589\B9=1.08658031\B10=1.0
9360097\B11=1.4099187\B12=1.47701447\B13=1.07401727\B14=1.5070959\B15=
1.1939221\B16=1.44348332\B17=1.20457036\B18=1.33334583\B19=1.4198615\B
20=1.08348308\B21=1.08018971\B22=1.08329837\A1=60.94067434\A2=94.48024
943\A3=109.5050796\A4=112.68308101\A5=138.99052282\A6=90.38039269\A7=1
08.76267539\A8=110.15901025\A9=94.0285005\A10=33.20350732\A11=144.1037
291\A12=119.68361493\A13=111.77362303\A14=123.50895466\A15=120.0506689
7\A16=124.1984174\A17=112.38827704\A18=116.2071343\A19=110.56974967\A2
0=105.73368231\A21=110.47945818\D1=16.60460566\D2=-70.90453661\D3=169.
30404523\D4=146.98562003\D5=-94.26404672\D6=93.96514666\D7=-148.568736
\D8=-105.41934407\D9=138.67390561\D10=123.56128079\D11=-77.17053416\D1
2=46.66461862\D13=137.46832295\D14=-260.80083931\D15=5.21515017\D16=-1
75.26404043\D17=179.3934383\D18=60.81132283\D19=180.39895143\D20=-60.0
568076\\Version=AM64L-G03RevE.01\State=2-A\HF=-612.14165\S2=0.761767\S
2-1=0.\S2A=0.750081\RMSD=8.018e-09\RMSF=8.943e-06\Thermal=0.\Dipole=0.
9854237,-0.1246846,-0.3488834\PG=C01 [X(C8H11O4)]\\@

Decarbonylation transition state 40 → 42 (n=2, R=CO_2Me)

HF/3-21G*

1\1\GINC-GOMBERG02\FTS\UHF\3-21G*\C8H11O4(2)\HMAITKEN\21-Nov-2010\1\\#
HF/3-21G* opt=(grad,readfc,noeigentest,nofreeze,ts) geom=checkpoint gu
ess=read\\decarbonylation ts\\0,2\C\C,1,B1\O,2,B2,1,A1\C,3,B3,2,A2,1,D
1,0\C,4,B4,3,A3,2,D2,0\H,5,B5,4,A4,3,D3,0\H,4,B6,3,A5,2,D4,0\H,2,B7,1,
A6,3,D5,0\H,2,B8,1,A7,3,D6,0\H,1,B9,2,A8,3,D7,0\H,1,B10,2,A9,3,D8,0\C,
1,B11,2,A10,3,D9,0\H,12,B12,1,A11,2,D10,0\H,12,B13,1,A12,2,D11,0\C,12,
B14,1,A13,2,D12,0\O,15,B15,12,A14,1,D13,0\C,5,B16,4,A15,3,D14,0\O,17,B

17,5,A16,4,D15,0\O,17,B18,5,A17,4,D16,0\C,19,B19,17,A18,5,D17,0\H,20,B
20,19,A19,17,D18,0\H,20,B21,19,A20,17,D19,0\H,20,B22,19,A21,17,D20,0\\
B1=1.52804959\B2=1.44747935\B3=1.35070338\B4=1.32396378\B5=1.06770667\
B6=1.06806847\B7=1.08265937\B8=1.08265927\B9=1.0816419\B10=1.0816418\B
11=1.51325275\B12=1.07844966\B13=1.07844947\B15=1.15108227\B16=1.45685
551\B17=1.20698902\B18=1.35839036\B19=1.45089696\B20=1.07654857\B21=1.
07925153\B22=1.07925146\A1=105.80055899\A2=120.93800329\A3=127.3597651
1\A4=123.71337637\A5=111.48943464\A6=111.39008767\A7=111.39016707\A8=1
08.37351375\A9=108.37370765\A10=111.53355778\A11=116.82313942\A12=116.
82325965\A13=104.61441691\A14=119.56747386\A15=121.19037578\A16=125.63
744429\A17=112.60059067\A18=117.78080073\A19=105.29312126\A20=110.3736
3108\A21=110.37364779\D1=-179.99992694\D2=-0.00008071\D3=-0.00000617\D
4=-180.00008394\D5=-119.02617855\D6=119.02629539\D7=58.30171067\D8=-58
.30334351\D9=179.99909924\D10=-69.9142417\D11=69.91822465\D12=-179.997
98164\D13=-180.00074924\D14=179.99998715\D15=-179.99996212\D16=0.00001
85\D17=-179.99992389\D18=-180.00067175\D19=-60.32298265\D20=60.3216013
9\B14=1.98754103\\Version=AM64L-G03RevE.01\State=2-A\HF=-605.3288012\S
2=0.8068\S2-1=0.\S2A=0.750858\RMSD=4.163e-09\RMSF=8.627e-06\Thermal=0.
\Dipole=0.4128292,0.0000261,-0.0582821\PG=C01 [X(C8H11O4)]\\@

HF/6-31G*

1\1\GINC-GOMBERG02\FTS\UHF\6-31G(d)\C8H11O4(2)\HMAITKEN\21-Nov-2010\1\
\#HF/6-31G* opt=(grad,readfc,noeigentest,nofreeze,ts) geom=checkpoint
guess=read\\decarbonylation ts\\0,2\C\C,1,B1\O,2,B2,1,A1\C,3,B3,2,A2,1
,D1,0\C,4,B4,3,A3,2,D2,0\H,5,B5,4,A4,3,D3,0\H,4,B6,3,A5,2,D4,0\H,2,B7,
1,A6,3,D5,0\H,2,B8,1,A7,3,D6,0\H,1,B9,2,A8,3,D7,0\H,1,B10,2,A9,3,D8,0\
C,1,B11,2,A10,3,D9,0\H,12,B12,1,A11,2,D10,0\H,12,B13,1,A12,2,D11,0\C,1
2,B14,1,A13,2,D12,0\O,15,B15,12,A14,1,D13,0\C,5,B16,4,A15,3,D14,0\O,17
,B17,5,A16,4,D15,0\O,17,B18,5,A17,4,D16,0\C,19,B19,17,A18,5,D17,0\H,20
,B20,19,A19,17,D18,0\H,20,B21,19,A20,17,D19,0\H,20,B22,19,A21,17,D20,0
\\B1=1.52175515\B2=1.41101351\B3=1.32594062\B4=1.32992144\B5=1.0713059
8\B6=1.07194311\B7=1.08497531\B8=1.08497466\B9=1.08432997\B10=1.084329
69\B11=1.50852002\B12=1.07966974\B13=1.07966893\B15=1.1340283\B16=1.47
004259\B17=1.19187874\B18=1.33087543\B19=1.41534806\B20=1.07907187\B21
=1.08029664\B22=1.08029657\A1=107.36987286\A2=119.61580718\A3=127.8052
3488\A4=123.32056842\A5=110.97038185\A6=111.12327095\A7=111.12345691\A
8=108.74969631\A9=108.75042856\A10=111.94824837\A11=116.68899769\A12=1
16.68933825\A13=107.73361153\A14=117.08152387\A15=122.33247751\A16=123
.36605272\A17=113.83959995\A18=116.71429373\A19=105.8323722\A20=110.59
676313\A21=110.59679981\D1=-179.99960683\D2=-0.00028847\D3=-0.00007761
\D4=-180.00031219\D5=-119.68404072\D6=119.6843669\D7=58.13748182\D8=-5
8.14245495\D9=179.99734319\D10=-68.741666\D11=68.74907148\D12=-179.997
13172\D13=-180.00319347\D14=179.99999054\D15=-180.00004805\D16=-0.0002
0574\D17=-179.99983457\D18=-180.00297019\D19=-60.55891872\D20=60.55282
311\B14=1.98153604\\Version=AM64L-G03RevE.01\State=2-A\HF=-608.7239584
\S2=0.808999\S2-1=0.\S2A=0.750963\RMSD=4.307e-09\RMSF=6.689e-05\Therma
l=0.\Dipole=0.5819848,0.0000488,-0.2103617\PG=C01 [X(C8H11O4)]\\@

HF/6-311G**

1\1\GINC-GOMBERG02\FTS\UHF\6-311G(d,p)\C8H11O4(2)\HMAITKEN\21-Nov-2010
\1\\#HF/6-311G** opt=(grad,readfc,noeigentest,nofreeze,ts) geom=checkp
oint guess=read\\decarbonylation ts\\0,2\C\C,1,B1\O,2,B2,1,A1\C,3,B3,2
,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\H,5,B5,4,A4,3,D3,0\H,4,B6,3,A5,2,D4,0\H,

2,B7,1,A6,3,D5,0\H,2,B8,1,A7,3,D6,0\H,1,B9,2,A8,3,D7,0\H,1,B10,2,A9,3,
D8,0\C,1,B11,2,A10,3,D9,0\H,12,B12,1,A11,2,D10,0\H,12,B13,1,A12,2,D11,
0\C,12,B14,1,A13,2,D12,0\O,15,B15,12,A14,1,D13,0\C,5,B16,4,A15,3,D14,0
\O,17,B17,5,A16,4,D15,0\O,17,B18,5,A17,4,D16,0\C,19,B19,17,A18,5,D17,0
\H,20,B20,19,A19,17,D18,0\H,20,B21,19,A20,17,D19,0\H,20,B22,19,A21,17,
D20,0\\B1=1.51998284\B2=1.41044808\B3=1.32342751\B4=1.32908846\B5=1.07
132965\B6=1.07270751\B7=1.08620909\B8=1.08620945\B9=1.08483385\B10=1.0
8483354\B11=1.50814414\B12=1.08043308\B13=1.08043397\B15=1.12636455\B1
6=1.47105418\B17=1.18623337\B18=1.32822882\B19=1.41534881\B20=1.079577
8\B21=1.0816335\B22=1.08163261\A1=107.42420254\A2=119.67386767\A3=127.
8681151\A4=123.4504204\A5=111.25881077\A6=111.0474627\A7=111.0476852\A
8=108.73509316\A9=108.73546402\A10=112.01803279\A11=116.62068413\A12=1
16.62024199\A13=108.22590772\A14=117.26874811\A15=122.28258678\A16=123
.28947432\A17=113.81282801\A18=117.02545328\A19=105.83796793\A20=110.6
1836887\A21=110.61841498\D1=-179.99994092\D2=-0.00016842\D3=0.00003332
\D4=-180.00017611\D5=-119.69028048\D6=119.69059469\D7=58.17103059\D8=-
58.17563662\D9=179.99755627\D10=-68.70906851\D11=68.71335945\D12=-179.
99744994\D13=-180.02094554\D14=179.99996045\D15=-179.99983748\D16=0.00
036126\D17=-179.99953699\D18=-179.99668264\D19=-60.54064882\D20=60.547
41052\B14=1.97260336\\Version=AM64L-G03RevE.01\State=2-A\HF=-608.87972
9\S2=0.808118\S2-1=0.\S2A=0.751004\RMSD=7.929e-09\RMSF=2.674e-05\Therm
al=0.\Dipole=0.5633967,0.0001103,-0.1880483\PG=C01 [X(C8H11O4)]\\@

BHandHLYP/6-311G**

1\1\GINC-GOMBERG02\FTS\UBHandHLYP\6-311G(d,p)\C8H11O4(2)\HMAITKEN\21-N
ov-2010\1\\#BHandHLYP/6-311G** opt=(grad,readfc,noeigentest,nofreeze,t
s) geom=checkpoint guess=read\\decarbonylation ts\\0,2\C\C,1,B1\O,2,B2
,1,A1\C,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\H,5,B5,4,A4,3,D3,0\H,4,B6,
3,A5,2,D4,0\H,2,B7,1,A6,3,D5,0\H,2,B8,1,A7,3,D6,0\H,1,B9,2,A8,3,D7,0\H
,1,B10,2,A9,3,D8,0\C,1,B11,2,A10,3,D9,0\H,12,B12,1,A11,2,D10,0\H,12,B1
3,1,A12,2,D11,0\C,12,B14,1,A13,2,D12,0\O,15,B15,12,A14,1,D13,0\C,5,B16
,4,A15,3,D14,0\O,17,B17,5,A16,4,D15,0\O,17,B18,5,A17,4,D16,0\C,19,B19,
17,A18,5,D17,0\H,20,B20,19,A19,17,D18,0\H,20,B21,19,A20,17,D19,0\H,20,
B22,19,A21,17,D20,0\\B1=1.51676241\B2=1.41671187\B3=1.32651274\B4=1.33
242295\B5=1.07280982\B6=1.07511383\B7=1.08793001\B8=1.08793072\B9=1.08
588294\B10=1.08588111\B11=1.49302628\B12=1.07917077\B13=1.07917163\B15
=1.12912274\B16=1.46139643\B17=1.19621074\B18=1.33905156\B19=1.4190256
4\B20=1.08050228\B21=1.08332973\B22=1.0833307\A1=107.38687784\A2=118.6
337669\A3=127.70362984\A4=123.32330035\A5=111.36749675\A6=111.18993517
\A7=111.19012876\A8=108.4728394\A9=108.47336596\A10=112.1195792\A11=11
8.22119721\A12=118.22143348\A13=105.9925144\A14=115.55466848\A15=122.2
9615162\A16=123.8338033\A17=113.45416386\A18=115.88752602\A19=105.8097
6629\A20=110.65402583\A21=110.65379088\D1=-180.00177743\D2=0.00130822\
D3=0.00007013\D4=-179.99875619\D5=-119.64199998\D6=119.64226278\D7=57.
99183937\D8=-57.99274863\D9=179.99913979\D10=-72.62376499\D11=72.62958
89\D12=-179.99761006\D13=-179.98832083\D14=179.99963085\D15=-179.99967
868\D16=0.0003488\D17=-180.00014389\D18=-179.99087399\D19=-60.37040385
\D20=60.38920854\B14=2.1217379\\Version=AM64L-G03RevE.01\State=2-A\HF=
-612.0832488\S2=0.771412\S2-1=0.\S2A=0.750148\RMSD=6.819e-09\RMSF=5.05
5e-06\Thermal=0.\Dipole=0.387378,-0.000001,-0.3610599\PG=C01 [X(C8H11O4)]\\@

BHandHLYP/6-311++G**

1\1\GINC-GOMBERG04\FTS\UBHandHLYP\6-311++G(d,p)\C8H11O4(2)\HMAITKEN\22
-Nov-2010\1\\#BHandHLYP/6-311++G(d,p) opt=(grad,readfc,noeigentest,nof
reeze,ts) geom=checkpoint guess=read\\decarbonylation ts\\0,2\C\C,1,B1
\O,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\H,5,B5,4,A4,3,D3,0\
H,4,B6,3,A5,2,D4,0\H,2,B7,1,A6,3,D5,0\H,2,B8,1,A7,3,D6,0\H,1,B9,2,A8,3
,D7,0\H,1,B10,2,A9,3,D8,0\C,1,B11,2,A10,3,D9,0\H,12,B12,1,A11,2,D10,0\
H,12,B13,1,A12,2,D11,0\C,12,B14,1,A13,2,D12,0\O,15,B15,12,A14,1,D13,0\
C,5,B16,4,A15,3,D14,0\O,17,B17,5,A16,4,D15,0\O,17,B18,5,A17,4,D16,0\C,
19,B19,17,A18,5,D17,0\H,20,B20,19,A19,17,D18,0\H,20,B21,19,A20,17,D19,
0\H,20,B22,19,A21,17,D20,0\\B1=1.51713896\B2=1.41722358\B3=1.32654318\
B4=1.33338951\B5=1.07291895\B6=1.07525628\B7=1.0877844\B8=1.08778399\B
9=1.08597944\B10=1.08597742\B11=1.49273264\B12=1.07908786\B13=1.079087
97\B15=1.1295185\B16=1.46102272\B17=1.19820304\B18=1.33805331\B19=1.41
985647\B20=1.08053243\B21=1.0831353\B22=1.0831332\A1=107.55853627\A2=1
18.77060114\A3=127.51905722\A4=123.25795294\A5=111.39654062\A6=111.154
01608\A7=111.15400268\A8=108.5849809\A9=108.58573028\A10=111.91036043\
A11=118.35130185\A12=118.35041042\A13=105.89505455\A14=115.50422055\A1
5=122.29096805\A16=123.70210225\A17=113.67878833\A18=116.22738817\A19=
105.7428216\A20=110.60001064\A21=110.60022223\D1=-179.99958788\D2=-0.0
0040889\D3=-0.00002626\D4=-180.00037406\D5=-119.61218101\D6=119.612047
67\D7=58.08314203\D8=-58.08346549\D9=179.99996342\D10=-73.03026747\D11
=73.02945056\D12=-180.00060035\D13=-180.02471144\D14=180.00005518\D15=
-180.00016553\D16=-0.00006423\D17=-179.99958016\D18=-180.00879392\D19=
-60.45108654\D20=60.43275731\B14=2.13445613\\Version=AM64L-G03RevE.01\
State=2-A\HF=-612.0953256\S2=0.771206\S2-1=0.\S2A=0.750151\RMSD=6.057e
-09\RMSF=4.623e-06\Thermal=0.\Dipole=0.4150285,0.0000397,-0.3581584\PG
=C01 [X(C8H11O4)]\\@

Decarbonylation product 42 (n=2, R=CO_2Me)

HF/3-21G*

1\1\GINC-GOMBERG01\FOpt\UHF\3-21G*\C7H11O3(2)\HMAITKEN\24-Nov-2010\1\\
#HF/3-21G* opt=(grad)\\decarbonylation radical\\0,2\C\O,1,B1\C,2,B2,1,
A1\C,3,B3,2,A2,1,D1,0\H,4,B4,3,A3,2,D2,0\H,3,B5,2,A4,1,D3,0\H,1,B6,2,A
5,3,D4,0\H,1,B7,2,A6,3,D5,0\C,1,B8,2,A7,3,D6,0\H,9,B9,1,A8,2,D7,0\H,9,
B10,1,A9,2,D8,0\C,9,B11,1,A10,2,D9,0\H,12,B12,9,A11,1,D10,0\H,12,B13,9
,A12,1,D11,0\C,4,B14,3,A13,2,D12,0\O,15,B15,4,A14,3,D13,0\O,15,B16,4,A
15,3,D14,0\C,17,B17,15,A16,4,D15,0\H,18,B18,17,A17,15,D16,0\H,18,B19,1
7,A18,15,D17,0\H,18,B20,17,A19,15,D18,0\\B1=1.44916163\B2=1.34918083\B
3=1.32452304\B4=1.06766649\B5=1.06819998\B6=1.08210645\B7=1.08210414\B
8=1.53250419\B9=1.0826766\B10=1.08267223\B11=1.50705451\B12=1.07317788
\B13=1.07317404\B14=1.45613696\B15=1.20721897\B16=1.35915281\B17=1.450
46538\B18=1.07661601\B19=1.07928977\B20=1.07928978\A1=120.99207099\A2=
127.42355066\A3=123.67083209\A4=111.54385473\A5=109.60938415\A6=109.61
054796\A7=106.072568\A8=107.83869565\A9=107.84216071\A10=111.26240002\
A11=120.58141985\A12=120.58481137\A13=121.19796547\A14=125.71180442\A1
5=112.62729078\A16=117.7466045\A17=105.30477603\A18=110.39556297\A19=1
10.39539331\D1=0.00267104\D2=0.00003259\D3=-179.99766567\D4=-59.898874
43\D5=59.88429003\D6=179.99347176\D7=58.08203424\D8=-58.11750277\D9=17
9.98114645\D10=273.52141481\D11=86.55304521\D12=-180.0004829\D13=-180.
00090673\D14=0.0016757\D15=-180.00113995\D16=180.00091531\D17=-60.3198

232\D18=60.32175899\\Version=AM64L-G03RevE.01\State=2-A\HF=-493.254442
4\S2=0.763318\S2-1=0.\S2A=0.750128\RMSD=5.860e-09\RMSF=3.270e-06\Therm
al=0.\Dipole=-0.8090101,-0.0000829,-0.063432\PG=C01 [X(C7H11O3)]\\@

HF/6-31G*

1\1\GINC-GOMBERG07\FOpt\UHF\6-31G(d)\C7H11O3(2)\HMAITKEN\09-Nov-2010\1
\\#HF/6-31G* opt=(grad,readfc) geom=checkpoint guess=read\\decarbonyla
tion radical\\0,2\C\O,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\H,4,B4,3,A3,
2,D2,0\H,3,B5,2,A4,1,D3,0\H,1,B6,2,A5,3,D4,0\H,1,B7,2,A6,3,D5,0\C,1,B8
,2,A7,3,D6,0\H,9,B9,1,A8,2,D7,0\H,9,B10,1,A9,2,D8,0\C,9,B11,1,A10,2,D9
,0\H,12,B12,9,A11,1,D10,0\H,12,B13,9,A12,1,D11,0\C,4,B14,3,A13,2,D12,0
\O,15,B15,4,A14,3,D13,0\O,15,B16,4,A15,3,D14,0\C,17,B17,15,A16,4,D15,0
\H,18,B18,17,A17,15,D16,0\H,18,B19,17,A18,15,D17,0\H,18,B20,17,A19,15,
D18,0\\B1=1.41298002\B2=1.32453414\B3=1.33051056\B4=1.07122746\B5=1.07
208125\B6=1.08452659\B7=1.08452838\B8=1.52481515\B9=1.08530857\B10=1.0
8530621\B11=1.5007049\B12=1.07484629\B13=1.07484615\B14=1.46946994\B15
=1.19205693\B16=1.33128045\B17=1.41502199\B18=1.07916205\B19=1.0803543
3\B20=1.0803533\A1=119.67957197\A2=127.86463315\A3=123.27040322\A4=111
.01393554\A5=109.46956385\A6=109.47029508\A7=107.54323958\A8=108.24744
95\A9=108.24810329\A10=112.23793454\A11=120.76866619\A12=120.76872515\
A13=122.34653019\A14=123.42094033\A15=113.86510565\A16=116.72483268\A1
7=105.83670399\A18=110.61748076\A19=110.61775124\D1=-0.00803669\D2=0.0
0076463\D3=-180.00697655\D4=-59.32109802\D5=59.34946013\D6=180.0146858
3\D7=57.88320139\D8=-57.87921702\D9=180.00191756\D10=275.24358189\D11=
84.77260366\D12=-180.00149784\D13=-179.99831527\D14=0.0059834\D15=-179
.99900284\D16=180.00040217\D17=-60.56618121\D18=60.56656302\\Version=A
M64L-G03RevE.01\State=2-A\HF=-496.0107347\S2=0.762584\S2-1=0.\S2A=0.75
0104\RMSD=4.459e-09\RMSF=3.708e-06\Thermal=0.\Dipole=-0.9310388,0.0001
72,0.0443176\PG=C01 [X(C7H11O3)]\\@

HF/6-311G**

1\1\GINC-GOMBERG02\FOpt\UHF\6-311G(d,p)\C7H11O3(2)\HMAITKEN\10-Nov-201
0\1\\#HF/6-311G** opt=(grad,readfc) geom=checkpoint guess=read\\decarb
onylation radical\\0,2\C\O,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\H,4,B4,
3,A3,2,D2,0\H,3,B5,2,A4,1,D3,0\H,1,B6,2,A5,3,D4,0\H,1,B7,2,A6,3,D5,0\C
,1,B8,2,A7,3,D6,0\H,9,B9,1,A8,2,D7,0\H,9,B10,1,A9,2,D8,0\C,9,B11,1,A10
,2,D9,0\H,12,B12,9,A11,1,D10,0\H,12,B13,9,A12,1,D11,0\C,4,B14,3,A13,2,
D12,0\O,15,B15,4,A14,3,D13,0\O,15,B16,4,A15,3,D14,0\C,17,B17,15,A16,4,
D15,0\H,18,B18,17,A17,15,D16,0\H,18,B19,17,A18,15,D17,0\H,18,B20,17,A1
9,15,D18,0\\B1=1.41224009\B2=1.32205567\B3=1.32962197\B4=1.07127838\B5
=1.0728458\B6=1.08574566\B7=1.08574594\B8=1.52340121\B9=1.08572407\B10
=1.08573678\B11=1.50048558\B12=1.07559016\B13=1.07559881\B14=1.4703666
1\B15=1.18647549\B16=1.32887001\B17=1.41488417\B18=1.07965707\B19=1.08
168124\B20=1.08168501\A1=119.71780969\A2=127.91706862\A3=123.41193364\
A4=111.30312672\A5=109.50250745\A6=109.50190095\A7=107.60652235\A8=108
.22169651\A9=108.21757232\A10=112.27983417\A11=120.76330791\A12=120.75
884364\A13=122.27001725\A14=123.36076545\A15=113.84020216\A16=117.0146
2666\A17=105.84940119\A18=110.64075416\A19=110.64027481\D1=0.00272925\
D2=-0.00149352\D3=-179.99806206\D4=-59.39032522\D5=59.37962376\D6=179.
99390155\D7=57.93122777\D8=-57.9165838\D9=180.00967227\D10=274.7277648
2\D11=85.10583886\D12=-179.99709631\D13=-180.00946824\D14=-0.01019974\
D15=-180.00395959\D16=180.01475515\D17=-60.52813347\D18=60.55879743\\V
ersion=AM64L-G03RevE.01\State=2-A\HF=-496.1373092\S2=0.762745\S2-1=0.\

S2A=0.750105\RMSD=5.374e-09\RMSF=4.900e-06\Thermal=0.\Dipole=-0.921436
3,0.0000635,0.0691641\PG=C01 [X(C7H11O3)]\\@

BHandHLYP/6-311G**

1\1\GINC-GOMBERG01\FOpt\UBHandHLYP\6-311G(d,p)\C7H11O3(2)\HMAITKEN\10-
Nov-2010\1\\#BHandHLYP/6-311G** opt=(grad,readfc) geom=checkpoint gues
s=read\\decarbonylation radical\\0,2\C\O,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,
1,D1,0\H,4,B4,3,A3,2,D2,0\H,3,B5,2,A4,1,D3,0\H,1,B6,2,A5,3,D4,0\H,1,B7
,2,A6,3,D5,0\C,1,B8,2,A7,3,D6,0\H,9,B9,1,A8,2,D7,0\H,9,B10,1,A9,2,D8,0
\C,9,B11,1,A10,2,D9,0\H,12,B12,9,A11,1,D10,0\H,12,B13,9,A12,1,D11,0\C,
4,B14,3,A13,2,D12,0\O,15,B15,4,A14,3,D13,0\O,15,B16,4,A15,3,D14,0\C,17
,B17,15,A16,4,D15,0\H,18,B18,17,A17,15,D16,0\H,18,B19,17,A18,15,D17,0\
H,18,B20,17,A19,15,D18,0\\B1=1.41680672\B2=1.32559041\B3=1.33273223\B4
=1.07276334\B5=1.07515152\B6=1.0873778\B7=1.08839455\B8=1.51273367\B9=
1.08679308\B10=1.09376778\B11=1.48446525\B12=1.07442254\B13=1.07664004
\B14=1.46094388\B15=1.19633469\B16=1.33957218\B17=1.41873831\B18=1.080
55349\B19=1.08337658\B20=1.0833582\A1=118.69466614\A2=127.72830441\A3=
123.29227129\A4=111.39666878\A5=109.51487705\A6=109.34158807\A7=107.72
636121\A8=109.08492403\A9=107.74023626\A10=112.38234662\A11=120.721302
25\A12=120.74038744\A13=122.28446669\A14=123.88534501\A15=113.46482726
\A16=115.8774205\A17=105.8162595\A18=110.66788835\A19=110.67083672\D1=
-0.20133319\D2=0.05579272\D3=-180.15392012\D4=-58.81649763\D5=59.69567
145\D6=180.29079281\D7=59.76980588\D8=-54.81390858\D9=182.9875168\D10=
206.25773511\D11=36.51856906\D12=-179.94156832\D13=-180.08362641\D14=-
0.07474371\D15=-180.00824419\D16=179.90730085\D17=-60.47568385\D18=60.
28325911\\Version=AM64L-G03RevE.01\State=2-A\HF=-498.8045473\S2=0.7552
19\S2-1=0.\S2A=0.750017\RMSD=7.731e-09\RMSF=8.016e-06\Thermal=0.\Dipol
e=-0.9799571,-0.0297351,0.0475133\PG=C01 [X(C7H11O3)]\\@

BHandHLYP/6-311++G**

1\1\GINC-GOMBERG01\FOpt\UBHandHLYP\6-311++G(d,p)\C7H11O3(2)\HMAITKEN\1
0-Nov-2010\1\\#BHandHLYP/6-311++G(d,p) opt=(grad,readfc) geom=checkpoi
nt guess=read\\decarbonylation radical\\0,2\C\O,1,B1\C,2,B2,1,A1\C,3,B
3,2,A2,1,D1,0\H,4,B4,3,A3,2,D2,0\H,3,B5,2,A4,1,D3,0\H,1,B6,2,A5,3,D4,0
\H,1,B7,2,A6,3,D5,0\C,1,B8,2,A7,3,D6,0\H,9,B9,1,A8,2,D7,0\H,9,B10,1,A9
,2,D8,0\C,9,B11,1,A10,2,D9,0\H,12,B12,9,A11,1,D10,0\H,12,B13,9,A12,1,D
11,0\C,4,B14,3,A13,2,D12,0\O,15,B15,4,A14,3,D13,0\O,15,B16,4,A15,3,D14
,0\C,17,B17,15,A16,4,D15,0\H,18,B18,17,A17,15,D16,0\H,18,B19,17,A18,15
,D17,0\H,18,B20,17,A19,15,D18,0\\B1=1.41736328\B2=1.32565463\B3=1.3337
2268\B4=1.07286336\B5=1.07527392\B6=1.08727381\B7=1.08825329\B8=1.5127
8155\B9=1.086881\B10=1.09378227\B11=1.48455587\B12=1.07455904\B13=1.07
671026\B14=1.46055531\B15=1.19825306\B16=1.33869074\B17=1.41947593\B18
=1.08058502\B19=1.08318986\B20=1.08318344\A1=118.83410114\A2=127.54495
223\A3=123.23145136\A4=111.42294513\A5=109.39171037\A6=109.252363\A7=1
07.90221615\A8=109.25965291\A9=107.88625583\A10=112.29342066\A11=120.6
7298574\A12=120.81318736\A13=122.27712441\A14=123.76861053\A15=113.680
66822\A16=116.20698656\A17=105.7494156\A18=110.61835465\A19=110.619630
36\D1=-0.2261241\D2=0.05693004\D3=-180.17967967\D4=-58.90793153\D5=59.
58138526\D6=180.17793225\D7=60.21342019\D8=-54.5510311\D9=183.40696124
\D10=205.68998573\D11=35.61684045\D12=-179.94071245\D13=-180.07726134\
D14=-0.06897679\D15=-180.01038259\D16=179.9734661\D17=-60.47110928\D18
=60.41529611\\Version=AM64L-G03RevE.01\State=2-A\HF=-498.8146629\S2=0.
755263\S2-1=0.\S2A=0.750018\RMSD=7.187e-09\RMSF=3.597e-05\Thermal=0.\D

ipole=-1.0205469,-0.0325791,0.0608421\PG=C01 [X(C7H11O3)]\\@

Alkyl cyclization transition state 42 →43 (n=2, R=CO_2Me)

HF/3-21G*

1\1\GINC-GOMBERG06\FTS\UHF\3-21G*\C7H11O3(2)\HMAITKEN\13-Oct-2010\1\\#
HF/3-21G* opt=(grad,readfc,ts,noeigentest,nofreeze) geom=checkpoint gu
ess=read\\decarbonylated cyclic ts\\0,2\C\O,1,B1\C,2,B2,1,A1\C,1,B3,2,
A2,3,D1,0\H,1,B4,2,A3,3,D2,0\H,1,B5,2,A4,3,D3,0\H,3,B6,2,A5,1,D4,0\H,4
,B7,1,A6,2,D5,0\H,4,B8,1,A7,2,D6,0\C,3,B9,2,A8,1,D7,0\H,10,B10,3,A9,2,
D8,0\C,3,B11,1,A10,2,D9,0\H,12,B12,4,A11,1,D10,0\H,12,B13,4,A12,1,D11,
0\C,10,B14,3,A13,2,D12,0\O,15,B15,10,A14,3,D13,0\O,15,B16,10,A15,3,D14
,0\C,17,B17,15,A16,10,D15,0\H,18,B18,17,A17,15,D16,0\H,18,B19,17,A18,1
5,D17,0\H,18,B20,17,A19,15,D18,0\\B1=1.44287187\B2=1.3909403\B3=1.5384
0879\B4=1.0775915\B5=1.08464767\B6=1.07029778\B7=1.08546571\B8=1.08196
911\B10=1.06845244\B12=1.07315154\B13=1.07623619\B14=1.44282177\B15=1.
21577447\B16=1.36181526\B17=1.44940263\B18=1.07671441\B19=1.07963619\B
20=1.07961962\A1=113.25077954\A2=106.9291703\A3=106.67519147\A4=110.00
233413\A5=116.77018898\A6=109.72787176\A7=108.67509296\A8=117.67902815
\A9=120.70482741\A10=65.04655925\A11=118.68779713\A12=117.56759159\A13
=121.72348639\A14=125.52191777\A15=112.89131076\A16=117.72624466\A17=1
05.34360869\A18=110.51336172\A19=110.51573386\D1=53.8253143\D2=175.068
07692\D3=-65.97977792\D4=62.37329223\D5=-171.92020905\D6=69.42189587\D
7=-142.31351144\D8=12.11740518\D9=146.34415778\D10=135.48877361\D11=-7
7.34078771\D12=-170.38229405\D13=180.46572332\D14=0.2205888\D15=179.17
068028\D16=180.19921062\D17=-60.19087075\D18=60.55873594\B9=1.37501808
\B11=2.21569561\\Version=AM64L-G03RevE.01\State=2-A\HF=-493.2375203\S2
=1.062814\S2-1=0.\S2A=0.79324\RMSD=6.999e-09\RMSF=1.592e-05\Thermal=0.
\Dipole=0.4831126,0.4027437,-1.3709063\PG=C01 [X(C7H11O3)]\\@

HF/6-31G*

1\1\GINC-GOMBERG06\FTS\UHF\6-31G(d)\C7H11O3(2)\HMAITKEN\13-Oct-2010\1\
\#HF/6-31G* opt=(grad,readfc,ts,noeigentest,nofreeze) geom=checkpoint
guess=read\\decarbonylated cyclic ts\\0,2\C\O,1,B1\C,2,B2,1,A1\C,1,B3,
2,A2,3,D1,0\H,1,B4,2,A3,3,D2,0\H,1,B5,2,A4,3,D3,0\H,3,B6,2,A5,1,D4,0\H
,4,B7,1,A6,2,D5,0\H,4,B8,1,A7,2,D6,0\C,3,B9,2,A8,1,D7,0\H,10,B10,3,A9,
2,D8,0\C,3,B11,1,A10,2,D9,0\H,12,B12,4,A11,1,D10,0\H,12,B13,4,A12,1,D1
1,0\C,10,B14,3,A13,2,D12,0\O,15,B15,10,A14,3,D13,0\O,15,B16,10,A15,3,D
14,0\C,17,B17,15,A16,10,D15,0\H,18,B18,17,A17,15,D16,0\H,18,B19,17,A18
,15,D17,0\H,18,B20,17,A19,15,D18,0\\B1=1.4033215\B2=1.35851044\B3=1.52
780065\B4=1.08059454\B5=1.08848932\B6=1.07523133\B7=1.08770432\B8=1.08
428233\B10=1.07248021\B12=1.07570812\B13=1.07817193\B14=1.46171714\B15
=1.19433352\B16=1.33217669\B17=1.41483123\B18=1.07911329\B19=1.0804904
1\B20=1.08054093\A1=112.64136306\A2=107.59066908\A3=107.06238779\A4=10
9.93084053\A5=115.74386458\A6=110.13375417\A7=108.85817474\A8=117.5600
2315\A9=120.128634\A10=66.16186435\A11=118.40416844\A12=117.54423196\A
13=123.59727535\A14=123.5016152\A15=113.57157458\A16=116.7112211\A17=1
05.86306256\A18=110.61871537\A19=110.64009349\D1=55.35858902\D2=177.09
793168\D3=-65.22534446\D4=61.23355259\D5=-170.95470725\D6=71.09359901\
D7=-147.39589932\D8=15.47721845\D9=143.73537902\D10=134.90655863\D11=-
81.4250422\D12=-169.0803859\D13=181.35669196\D14=1.32614466\D15=179.44
093023\D16=180.06802218\D17=-60.51154051\D18=60.61827107\B9=1.38837794
\B11=2.18640485\\Version=AM64L-G03RevE.01\State=2-A\HF=-495.9901585\S2

=1.019656\S2-1=0.\S2A=0.769004\RMSD=9.887e-09\RMSF=4.140e-05\Thermal=0
.\Dipole=0.3884244,0.4338684,-1.4172184\PG=C01 [X(C7H11O3)]\\@

HF/6-311G****

1\1\GINC-GOMBERG03\FTS\UHF\6-311G(d,p)\C7H11O3(2)\HMAITKEN\14-Oct-2010
\1\\#HF/6-311G** opt=(grad,readfc,ts,noeigentest,nofreeze) geom=checkp
oint guess=read\\decarbonylated cyclic ts\\0,2\C\O,1,B1\C,2,B2,1,A1\C,
1,B3,2,A2,3,D1,0\H,1,B4,2,A3,3,D2,0\H,1,B5,2,A4,3,D3,0\H,3,B6,2,A5,1,D
4,0\H,4,B7,1,A6,2,D5,0\H,4,B8,1,A7,2,D6,0\C,3,B9,2,A8,1,D7,0\H,10,B10,
3,A9,2,D8,0\C,3,B11,1,A10,2,D9,0\H,12,B12,4,A11,1,D10,0\H,12,B13,4,A12
,1,D11,0\C,10,B14,3,A13,2,D12,0\O,15,B15,10,A14,3,D13,0\O,15,B16,10,A1
5,3,D14,0\C,17,B17,15,A16,10,D15,0\H,18,B18,17,A17,15,D16,0\H,18,B19,1
7,A18,15,D17,0\H,18,B20,17,A19,15,D18,0\\B1=1.40246431\B2=1.35669241\B
3=1.52655202\B4=1.08090828\B5=1.08977181\B6=1.0757228\B7=1.08798057\B8
=1.08480669\B10=1.07276264\B12=1.07641045\B13=1.07894125\B14=1.4617802
\B15=1.18883711\B16=1.33009511\B17=1.41459034\B18=1.0796329\B19=1.0818
2981\B20=1.08183623\A1=112.59396319\A2=107.46590034\A3=107.17536089\A4
=109.90683295\A5=115.92398475\A6=110.15023389\A7=108.90111038\A8=117.5
5238437\A9=120.22337392\A10=66.28565345\A11=118.39012587\A12=117.44929
886\A13=123.4855135\A14=123.51490735\A15=113.52079666\A16=116.99265548
\A17=105.8994266\A18=110.64427595\A19=110.65696134\D1=55.17377365\D2=1
76.93648724\D3=-65.29381911\D4=61.66236238\D5=-170.9432866\D6=70.96236
503\D7=-147.31026528\D8=15.30924587\D9=144.01226257\D10=135.52529518\D
11=-81.08737398\D12=-169.11417037\D13=181.13291905\D14=1.09359497\D15=
179.48243677\D16=180.05473069\D17=-60.49479163\D18=60.58154424\B9=1.38
809224\B11=2.17504055\\Version=AM64L-G03RevE.01\State=2-A\HF=-496.1146
84\S2=1.011839\S2-1=0.\S2A=0.768171\RMSD=8.242e-09\RMSF=2.265e-05\Ther
mal=0.\Dipole=0.3833955,0.4426216,-1.4126805\PG=C01 [X(C7H11O3)]\\@

BHandHLYP/6-311G****

1\1\GINC-GOMBERG05\FTS\UBHandHLYP\6-311G(d,p)\C7H11O3(2)\HMAITKEN\14-O
ct-2010\1\\#BHandHLYP/6-311G** opt=(grad,readfc,ts,noeigentest,nofreez
e) geom=checkpoint guess=read\\decarbonylated cyclic ts\\0,2\C\O,1,B1\
C,2,B2,1,A1\C,1,B3,2,A2,3,D1,0\H,1,B4,2,A3,3,D2,0\H,1,B5,2,A4,3,D3,0\H
,3,B6,2,A5,1,D4,0\H,4,B7,1,A6,2,D5,0\H,4,B8,1,A7,2,D6,0\C,3,B9,2,A8,1,
D7,0\H,10,B10,3,A9,2,D8,0\C,3,B11,1,A10,2,D9,0\H,12,B12,4,A11,1,D10,0\
H,12,B13,4,A12,1,D11,0\C,10,B14,3,A13,2,D12,0\O,15,B15,10,A14,3,D13,0\
O,15,B16,10,A15,3,D14,0\C,17,B17,15,A16,10,D15,0\H,18,B18,17,A17,15,D1
6,0\H,18,B19,17,A18,15,D17,0\H,18,B20,17,A19,15,D18,0\\B1=1.40826368\B
2=1.35028153\B3=1.52695006\B4=1.08180649\B5=1.09083379\B6=1.07839825\B
7=1.08936256\B8=1.08497648\B10=1.07392263\B12=1.07530394\B13=1.0781307
5\B14=1.45049327\B15=1.19865107\B16=1.34374856\B17=1.41807989\B18=1.08
072167\B19=1.0835439\B20=1.08346002\A1=112.03902295\A2=107.30865531\A3
=107.08510575\A4=109.90654127\A5=116.28754427\A6=109.45190779\A7=108.7
2835231\A8=119.23118232\A9=120.41367258\A10=65.67335172\A11=119.321235
35\A12=118.54325061\A13=123.16391012\A14=124.41344461\A15=113.09672028
\A16=115.75333989\A17=105.87767072\A18=110.70380368\A19=110.72220161\D
1=57.99623381\D2=179.62731311\D3=-62.32615337\D4=53.9858932\D5=-171.58
506725\D6=70.86890993\D7=-149.43948058\D8=12.68707362\D9=140.80434753\
D10=131.37902164\D11=-79.81740582\D12=-170.00224374\D13=179.84251132\D
14=-0.53456275\D15=179.55917074\D16=179.78764232\D17=-60.60828825\D18=
60.12016433\B9=1.36443197\B11=2.22326695\\Version=AM64L-G03RevE.01\Sta
te=2-A\HF=-498.7882167\S2=0.821957\S2-1=0.\S2A=0.751069\RMSD=6.405e-09

\RMSF=2.338e-05\Thermal=0.\Dipole=0.1839446,0.3763373,-1.6268685\PG=C0
1 [X(C7H11O3)]\\@

BHandHLYP/6-311++G**

1\1\GINC-GOMBERG05\FTS\UBHandHLYP\6-311++G(d,p)\C7H11O3(2)\HMAITKEN\14
-Oct-2010\1\\#BHandHLYP/6-311++G(d,p) opt=(grad,readfc,ts,noeigentest,
nofreeze) geom=checkpoint guess=read\\decarbonylated cyclic ts\\0,2\C\
O,1,B1\C,2,B2,1,A1\C,1,B3,2,A2,3,D1,0\H,1,B4,2,A3,3,D2,0\H,1,B5,2,A4,3
,D3,0\H,3,B6,2,A5,1,D4,0\H,4,B7,1,A6,2,D5,0\H,4,B8,1,A7,2,D6,0\C,3,B9,
2,A8,1,D7,0\H,10,B10,3,A9,2,D8,0\C,3,B11,1,A10,2,D9,0\H,12,B12,4,A11,1
,D10,0\H,12,B13,4,A12,1,D11,0\C,10,B14,3,A13,2,D12,0\O,15,B15,10,A14,3
,D13,0\O,15,B16,10,A15,3,D14,0\C,17,B17,15,A16,10,D15,0\H,18,B18,17,A1
7,15,D16,0\H,18,B19,17,A18,15,D17,0\H,18,B20,17,A19,15,D18,0\\B1=1.408
89283\B2=1.35078699\B3=1.52659712\B4=1.08195266\B5=1.09063073\B6=1.078
39506\B7=1.08939423\B8=1.08500739\B10=1.07419312\B12=1.07543415\B13=1.
07820386\B14=1.44993122\B15=1.20084162\B16=1.34272152\B17=1.41881005\B
18=1.08076511\B19=1.08335516\B20=1.08333868\A1=112.23025245\A2=107.327
34205\A3=107.068284\A4=109.80712771\A5=116.15985462\A6=109.33922911\A7
=108.8217275\A8=119.16812872\A9=120.36198462\A10=65.6061082\A11=119.36
364091\A12=118.59138917\A13=123.34756875\A14=124.24562866\A15=113.3688
7617\A16=116.09052686\A17=105.8174194\A18=110.64308786\A19=110.6879451
\D1=57.94501072\D2=179.56406671\D3=-62.46720949\D4=54.03160158\D5=-171
.11264323\D6=71.3832778\D7=-149.5140386\D8=13.3474017\D9=140.67910974\
D10=130.95072925\D11=-79.96841963\D12=-169.61272228\D13=181.27203895\D
14=0.97058529\D15=179.58622843\D16=179.98887909\D17=-60.4666324\D18=60
.37018832\B9=1.36474967\B11=2.22586362\\Version=AM64L-G03RevE.01\State
=2-A\HF=-498.7981621\S2=0.821361\S2-1=0.\S2A=0.751043\RMSD=4.272e-09\R
MSF=1.999e-05\Thermal=0.\Dipole=0.1972294,0.4065883,-1.7150807\PG=C01
[X(C7H11O3)]\\@

Alkyl cyclization product 43 (R=CO_2Me)

HF/3-21G*

1\1\GINC-GOMBERG05\FOpt\UHF\3-21G*\C7H11O3(2)\HMAITKEN\13-Oct-2010\1\\
#HF/3-21G* opt=grad\\5-exo decarbonylation product\\0,2\C\O,1,B1\C,2,B
2,1,A1\C,1,B3,2,A2,3,D1,0\H,1,B4,2,A3,3,D2,0\H,1,B5,2,A4,3,D3,0\H,3,B6
,2,A5,1,D4,0\H,4,B7,1,A6,2,D5,0\H,4,B8,1,A7,2,D6,0\C,3,B9,2,A8,1,D7,0\
H,10,B10,3,A9,2,D8,0\C,4,B11,1,A10,2,D9,0\H,12,B12,4,A11,1,D10,0\H,12,
B13,4,A12,1,D11,0\C,10,B14,3,A13,2,D12,0\O,15,B15,10,A14,3,D13,0\O,15,
B16,10,A15,3,D14,0\C,17,B17,15,A16,10,D15,0\H,18,B18,17,A17,15,D16,0\H
,18,B19,17,A18,15,D17,0\H,18,B20,17,A19,15,D18,0\\B1=1.45539598\B2=1.4
5046962\B3=1.53999525\B4=1.07890803\B5=1.08130392\B6=1.08059452\B7=1.0
8085408\B8=1.08288849\B9=1.49683808\B10=1.06754819\B11=1.54044238\B12=
1.07743762\B13=1.08323383\B14=1.42903507\B15=1.22720437\B16=1.35794861
\B17=1.44887799\B18=1.0799595\B19=1.07645711\B20=1.08005126\A1=110.620
06563\A2=105.49780577\A3=108.50873074\A4=108.97352553\A5=108.57661341\
A6=112.25280688\A7=110.45613115\A8=108.13727948\A9=120.37368352\A10=10
1.91209414\A11=114.40225857\A12=109.90962146\A13=120.11712213\A14=124.
5281279\A15=113.71728261\A16=117.85561758\A17=110.63702523\A18=105.255
90395\A19=110.64147707\D1=11.91284003\D2=133.61441782\D3=-107.17158212
\D4=132.02931732\D5=-152.35296548\D6=85.68714497\D7=-107.89847895\D8=0
.31656363\D9=-31.30042991\D10=158.59654559\D11=-78.18734355\D12=-175.8
8730762\D13=-2.39259943\D14=-181.92300859\D15=180.06158721\D16=60.1717

9073\D17=179.71935182\D18=-60.7202587\\Version=AM64L-G03RevE.01\State=
2-A\HF=-493.2828087\S2=0.847172\S2-1=0.\S2A=0.75236\RMSD=9.552e-09\RMS
F=3.703e-05\Thermal=0.\Dipole=0.3760019,-0.3931159,-0.5333552\PG=C01 [
X(C7H11O3)]\\@

HF/6-31G*

1\1\GINC-GOMBERG03\FOpt\UHF\6-31G(d)\C7H11O3(2)\HMAITKEN\13-Oct-2010\1
\\#HF/6-31G* opt=(grad,readfc) geom=checkpoint guess=read\\5-exo decar
bonylation product\\0,2\C\O,1,B1\C,2,B2,1,A1\C,1,B3,2,A2,3,D1,0\H,1,B4
,2,A3,3,D2,0\H,1,B5,2,A4,3,D3,0\H,3,B6,2,A5,1,D4,0\H,4,B7,1,A6,2,D5,0\
H,4,B8,1,A7,2,D6,0\C,3,B9,2,A8,1,D7,0\H,10,B10,3,A9,2,D8,0\C,4,B11,1,A
10,2,D9,0\H,12,B12,4,A11,1,D10,0\H,12,B13,4,A12,1,D11,0\C,10,B14,3,A13
,2,D12,0\O,15,B15,10,A14,3,D13,0\O,15,B16,10,A15,3,D14,0\C,17,B17,15,A
16,10,D15,0\H,18,B18,17,A17,15,D16,0\H,18,B19,17,A18,15,D17,0\H,18,B20
,17,A19,15,D18,0\\B1=1.40842283\B2=1.41163092\B3=1.52344527\B4=1.08210
95\B5=1.08755446\B6=1.08412167\B7=1.08359757\B8=1.08580251\B9=1.500857
64\B10=1.07244071\B11=1.52871572\B12=1.08127294\B13=1.0848099\B14=1.45
544535\B15=1.19838569\B16=1.32839059\B17=1.41473033\B18=1.08072145\B19
=1.07881759\B20=1.08082261\A1=111.4338748\A2=105.27501707\A3=108.24182
539\A4=109.87192013\A5=109.08262325\A6=113.01084133\A7=110.28602889\A8
=108.51055592\A9=119.89820552\A10=101.12375517\A11=114.22395216\A12=11
0.25125521\A13=120.4716909\A14=123.78383368\A15=112.88179437\A16=116.8
4694957\A17=110.64653149\A18=105.84470052\A19=110.66004394\D1=22.98577
979\D2=145.30519039\D3=-96.61155132\D4=118.53185811\D5=-157.22235071\D
6=81.54939104\D7=-123.11391066\D8=11.68328789\D9=-35.69050514\D10=156.
47437606\D11=-82.10315655\D12=-166.61057348\D13=-1.31779581\D14=-181.1
0050269\D15=180.16821898\D16=60.42662326\D17=179.84925682\D18=-60.7176
7056\\Version=AM64L-G03RevE.01\State=2-A\HF=-496.0379667\S2=0.782751\S
2-1=0.\S2A=0.750609\RMSD=6.178e-09\RMSF=1.312e-05\Thermal=0.\Dipole=0.
1380825,-0.5569758,-0.4235548\PG=C01 [X(C7H11O3)]\\@

HF/6-311G**

1\1\GINC-GOMBERG05\FOpt\UHF\6-311G(d,p)\C7H11O3(2)\HMAITKEN\13-Oct-201
0\1\\#HF/6-311G** opt=(grad,readfc) geom=checkpoint guess=read\\5-exo
decarbonylation product\\0,2\C\O,1,B1\C,2,B2,1,A1\C,1,B3,2,A2,3,D1,0\H
,1,B4,2,A3,3,D2,0\H,1,B5,2,A4,3,D3,0\H,3,B6,2,A5,1,D4,0\H,4,B7,1,A6,2,
D5,0\H,4,B8,1,A7,2,D6,0\C,3,B9,2,A8,1,D7,0\H,10,B10,3,A9,2,D8,0\C,4,B1
1,1,A10,2,D9,0\H,12,B12,4,A11,1,D10,0\H,12,B13,4,A12,1,D11,0\C,10,B14,
3,A13,2,D12,0\O,15,B15,10,A14,3,D13,0\O,15,B16,10,A15,3,D14,0\C,17,B17
,15,A16,10,D15,0\H,18,B18,17,A17,15,D16,0\H,18,B19,17,A18,15,D17,0\H,1
8,B20,17,A19,15,D18,0\\B1=1.40800166\B2=1.41082731\B3=1.52246214\B4=1.
0824663\B5=1.08864242\B6=1.08438853\B7=1.08383702\B8=1.08634492\B9=1.5
0000634\B10=1.07284814\B11=1.5285326\B12=1.08145094\B13=1.08530774\B14
=1.45613557\B15=1.19273915\B16=1.32624376\B17=1.41463032\B18=1.0820059
8\B19=1.07929777\B20=1.08211908\A1=111.41023581\A2=105.29010246\A3=108
.32573352\A4=109.88011315\A5=109.20008248\A6=112.94923865\A7=110.26380
652\A8=108.57470578\A9=119.98494414\A10=101.10650049\A11=114.27850288\
A12=110.23484116\A13=120.49515903\A14=123.8790635\A15=112.76104862\A16
=117.08528864\A17=110.66499631\A18=105.85082426\A19=110.68521926\D1=23
.02180685\D2=145.27512664\D3=-96.50333758\D4=118.52917976\D5=-157.2672
2176\D6=81.46869285\D7=-123.16041645\D8=12.96230368\D9=-35.74940041\D1
0=156.52879975\D11=-81.93257867\D12=-165.33467233\D13=-1.6148426\D14=-
181.44761413\D15=180.18962222\D16=60.41534214\D17=179.85967418\D18=-60

.68048138\\Version=AM64L-G03RevE.01\State=2-A\HF=-496.1611032\S2=0.781
321\S2-1=0.\S2A=0.750586\RMSD=6.340e-09\RMSF=2.352e-06\Thermal=0.\Dipo
le=0.1430577,-0.5483507,-0.4242547\PG=C01 [X(C7H11O3)]\\@

BHandHLYP/6-311G**

1\1\GINC-GOMBERG12\FOpt\UBHandHLYP\6-311G(d,p)\C7H11O3(2)\HMAITKEN\13-
Oct-2010\1\\#BHandHLYP/6-311G** opt=(grad,readfc) geom=checkpoint gues
s=read\\5-exo decarbonylation product\\0,2\C\O,1,B1\C,2,B2,1,A1\C,1,B3
,2,A2,3,D1,0\H,1,B4,2,A3,3,D2,0\H,1,B5,2,A4,3,D3,0\H,3,B6,2,A5,1,D4,0\
H,4,B7,1,A6,2,D5,0\H,4,B8,1,A7,2,D6,0\C,3,B9,2,A8,1,D7,0\H,10,B10,3,A9
,2,D8,0\C,4,B11,1,A10,2,D9,0\H,12,B12,4,A11,1,D10,0\H,12,B13,4,A12,1,D
11,0\C,10,B14,3,A13,2,D12,0\O,15,B15,10,A14,3,D13,0\O,15,B16,10,A15,3,
D14,0\C,17,B17,15,A16,10,D15,0\H,18,B18,17,A17,15,D16,0\H,18,B19,17,A1
8,15,D17,0\H,18,B20,17,A19,15,D18,0\\B1=1.41485787\B2=1.41762592\B3=1.
51732784\B4=1.0836302\B5=1.09057186\B6=1.08874077\B7=1.08412299\B8=1.0
8647915\B9=1.48431446\B10=1.07425387\B11=1.52374632\B12=1.08151618\B13
=1.08542554\B14=1.44244522\B15=1.2044358\B16=1.336881\B17=1.41866848\B
18=1.08364985\B19=1.08024626\B20=1.08375908\A1=110.56724506\A2=105.346
41652\A3=108.06175688\A4=110.01892183\A5=109.38577708\A6=112.95192502\
A7=110.25913175\A8=108.89959076\A9=119.76767508\A10=101.23650385\A11=1
14.4358215\A12=110.38145272\A13=120.27083351\A14=124.23772469\A15=112.
61102381\A16=115.8716518\A17=110.67348587\A18=105.81717136\A19=110.684
65361\D1=24.17510822\D2=146.40279128\D3=-95.39163708\D4=116.9289566\D5
=-158.08791647\D6=80.5312072\D7=-124.5450555\D8=9.47990858\D9=-36.7060
7734\D10=156.57154042\D11=-81.61489764\D12=-168.39031916\D13=-2.132463
34\D14=-181.87930795\D15=179.94511073\D16=60.25443223\D17=179.8918493\
D18=-60.45732971\\Version=AM64L-G03RevE.01\State=2-A\HF=-498.8317455\S
2=0.761195\S2-1=0.\S2A=0.750076\RMSD=7.553e-09\RMSF=2.330e-05\Thermal=
0.\Dipole=0.098172,-0.4873486,-0.4230136\PG=C01 [X(C7H11O3)]\\@

BHandHLYP/6-311++G**

1\1\GINC-GOMBERG02\FOpt\UBHandHLYP\6-311++G(d,p)\C7H11O3(2)\HMAITKEN\1
5-Oct-2010\0\\#BHandHLYP/6-311++G(d,p) opt=(readfc) geom=checkpoint gu
ess=read\\5-exo decarbonylation product\\0,2\C,0.001262448,-0.00499143
34,-0.001446404\O,-0.0010499963,0.0092452195,1.4192541593\C,1.32257128
88,0.0048402779,1.9203482094\C,1.4643935594,0.0370944575,-0.4332190036
\H,-0.4899353394,-0.9155619677,-0.335424921\H,-0.5693786675,0.84323795
04,-0.3651981921\H,1.6449481424,1.0261661003,2.1267301553\H,1.78698113
46,1.0620586835,-0.5913816266\H,1.6419649522,-0.5146459257,-1.34914551
08\C,1.3703439587,-0.776641817,3.1736449735\H,0.6114978103,-1.51206036
32,3.3693420294\C,2.1766592601,-0.5547933501,0.7762116593\H,2.11706499
95,-1.6399988808,0.7663046899\H,3.2157919987,-0.2647313832,0.867206691
1\C,2.4414040611,-0.5822046358,4.1189375485\O,3.344943714,0.2029789751
,3.9755648013\O,2.3305289812,-1.3790230681,5.1872971494\C,3.3432864083
,-1.2503619163,6.1727541078\H,3.3526336181,-0.2465445404,6.5809631878\
H,3.0971086971,-1.9677900413,6.9421125928\H,4.3171240977,-1.4676059571
,5.7501812801\\Version=AM64L-G03RevE.01\State=2-A\HF=-498.8423581\S2=0
.761351\S2-1=0.\S2A=0.750078\RMSD=5.494e-09\RMSF=7.308e-05\Thermal=0.\
Dipole=0.1334988,-0.4938475,-0.4016203\PG=C01 [X(C7H11O3)]\\@

6-Membered β-disubstituted system 48

Acyl radical 48

HF/3-21G*

1\1\GINC-GOMBERG04\FOpt\UHF\3-21G*\C12H21O5Si1(2)\HMAITKEN\26-Oct-2010
\1\\#HF/3-21G* opt=(grad)\\6 exo starting material\\0,2\C\C,1,B1\O,2,B
2,1,A1\C,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\H,5,B5,4,A4,3,D3,0\H,2,B6
,1,A5,3,D4,0\H,2,B7,1,A6,3,D5,0\H,1,B8,2,A7,3,D6,0\H,1,B9,2,A8,3,D7,0\
C,1,B10,2,A9,3,D8,0\H,11,B11,1,A10,2,D9,0\H,11,B12,1,A11,2,D10,0\C,11,
B13,1,A12,2,D11,0\O,14,B14,11,A13,1,D12,0\C,5,B15,4,A14,3,D13,0\O,16,B
16,5,A15,4,D14,0\O,16,B17,5,A16,4,D15,0\C,18,B18,16,A17,5,D16,0\H,19,B
19,18,A18,16,D17,0\H,19,B20,18,A19,16,D18,0\H,19,B21,18,A20,16,D19,0\C
,4,B22,3,A21,2,D20,0\H,23,B23,4,A22,3,D21,0\H,23,B24,4,A23,3,D22,0\O,2
3,B25,4,A24,3,D23,0\Si,26,B26,23,A25,4,D24,0\C,27,B27,26,A26,23,D25,0\
H,28,B28,27,A27,26,D26,0\H,28,B29,27,A28,26,D27,0\H,28,B30,27,A29,26,D
28,0\C,27,B31,26,A30,23,D29,0\H,32,B32,27,A31,26,D30,0\H,32,B33,27,A32
,26,D31,0\H,32,B34,27,A33,26,D32,0\C,27,B35,26,A34,23,D33,0\H,36,B36,2
7,A35,26,D34,0\H,36,B37,27,A36,26,D35,0\H,36,B38,27,A37,26,D36,0\\B1=1
.52241737\B2=1.44952341\B3=1.35550376\B4=1.33114034\B5=1.06695982\B6=1
.0824007\B7=1.08216596\B8=1.08120869\B9=1.08084921\B10=1.53930638\B11=
1.08494597\B12=1.08469093\B13=1.5147413\B14=1.18455589\B15=1.45206822\
B16=1.20804083\B17=1.35810092\B18=1.45353288\B19=1.07641338\B20=1.0788
9827\B21=1.07888154\B22=1.52788063\B23=1.07369021\B24=1.08107537\B25=1
.4128292\B26=1.64389521\B27=1.88176537\B28=1.08864538\B29=1.08904273\B
30=1.08564034\B31=1.88088212\B32=1.08896291\B33=1.08767428\B34=1.08841
111\B35=1.87254834\B36=1.08781389\B37=1.0887426\B38=1.08485235\A1=106.
54076483\A2=121.41264561\A3=122.61017913\A4=120.78470236\A5=111.299596
8\A6=111.17956236\A7=109.28820128\A8=109.06133278\A9=110.96250798\A10=
111.54002655\A11=111.53878344\A12=111.54205733\A13=130.45533295\A14=12
7.27620247\A15=124.66961599\A16=114.0557386\A17=117.6798039\A18=105.24
469092\A19=110.28023967\A20=110.22070042\A21=112.2395442\A22=108.80724
059\A23=107.88649059\A24=112.38370059\A25=138.28997268\A26=110.9175344
1\A27=110.64673913\A28=111.60510702\A29=111.29026411\A30=108.39709745\
A31=111.04318835\A32=111.25522225\A33=111.5594298\A34=108.99146901\A35
=110.71844944\A36=111.20987839\A37=111.60105924\D1=177.69908312\D2=2.7
6705995\D3=-1.23828178\D4=-119.24175304\D5=119.0304789\D6=58.43204898\
D7=-59.01764643\D8=-180.23394708\D9=-59.41149513\D10=60.5531873\D11=-1
79.35874902\D12=0.74999064\D13=-181.63785021\D14=-181.94282641\D15=-2.
61950045\D16=180.33281544\D17=-179.93631767\D18=-60.21499618\D19=60.35
132159\D20=-178.35297489\D21=-229.01688332\D22=-112.60993745\D23=10.96
383717\D24=-80.71677591\D25=10.63034998\D26=178.04315456\D27=-62.64933
505\D28=57.91016416\D29=-108.295575\D30=-177.93737126\D31=-58.06518238
\D32=62.11083755\D33=133.42091693\D34=57.86114104\D35=177.40188946\D36
=-62.10054541\\Version=AM64L-G03RevE.01\State=2-A\HF=-1123.830325\S2=0
.770878\S2-1=0.\S2A=0.750204\RMSD=7.558e-09\RMSF=1.586e-05\Thermal=0.\
Dipole=-0.2971429,-0.2863556,0.6897932\PG=C01 [X(C12H21O5Si1)]\\@

HF/6-31G*

1\1\GINC-GOMBERG05\FOpt\UHF\6-31G(d)\C12H21O5Si1(2)\HMAITKEN\26-Oct-20
10\1\\#HF/6-31G* opt=(grad,readfc) geom=checkpoint guess=read\\6 exo s
tarting material\\0,2\C\C,1,B1\O,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\C,4,B4,3
,A3,2,D2,0\H,5,B5,4,A4,3,D3,0\H,2,B6,1,A5,3,D4,0\H,2,B7,1,A6,3,D5,0\H,

1,B8,2,A7,3,D6,0\H,1,B9,2,A8,3,D7,0\C,1,B10,2,A9,3,D8,0\H,11,B11,1,A10
,2,D9,0\H,11,B12,1,A11,2,D10,0\C,11,B13,1,A12,2,D11,0\O,14,B14,11,A13,
1,D12,0\C,5,B15,4,A14,3,D13,0\O,16,B16,5,A15,4,D14,0\O,16,B17,5,A16,4,
D15,0\C,18,B18,16,A17,5,D16,0\H,19,B19,18,A18,16,D17,0\H,19,B20,18,A19
,16,D18,0\H,19,B21,18,A20,16,D19,0\C,4,B22,3,A21,2,D20,0\H,23,B23,4,A2
2,3,D21,0\H,23,B24,4,A23,3,D22,0\O,23,B25,4,A24,3,D23,0\Si,26,B26,23,A
25,4,D24,0\C,27,B27,26,A26,23,D25,0\H,28,B28,27,A27,26,D26,0\H,28,B29,
27,A28,26,D27,0\H,28,B30,27,A29,26,D28,0\C,27,B31,26,A30,23,D29,0\H,32
,B32,27,A31,26,D30,0\H,32,B33,27,A32,26,D31,0\H,32,B34,27,A33,26,D32,0
\C,27,B35,26,A34,23,D33,0\H,36,B36,27,A35,26,D34,0\H,36,B37,27,A36,26,
D35,0\H,36,B38,27,A37,26,D36,0\\B1=1.51863757\B2=1.40724782\B3=1.33593
595\B4=1.33597201\B5=1.07075934\B6=1.08552985\B7=1.08489022\B8=1.08368
332\B9=1.08357665\B10=1.53038142\B11=1.08650085\B12=1.08644632\B13=1.5
174259\B14=1.16481313\B15=1.47367689\B16=1.19301287\B17=1.3275791\B18=
1.41684705\B19=1.07902215\B20=1.07997\B21=1.08004852\B22=1.5112563\B23
=1.0733604\B24=1.08728718\B25=1.39527021\B26=1.6586135\B27=1.88579811\
B28=1.08787499\B29=1.08712262\B30=1.08610292\B31=1.88744588\B32=1.0877
203\B33=1.0869792\B34=1.08781952\B35=1.87745436\B36=1.08644221\B37=1.0
8742027\B38=1.08644714\A1=107.20897413\A2=121.60937278\A3=123.0456623\
A4=119.43716529\A5=110.91431736\A6=111.04986734\A7=109.28131171\A8=109
.18297831\A9=111.5296379\A10=111.84904793\A11=111.82533364\A12=113.108
9093\A13=129.18215611\A14=130.42361752\A15=121.23280356\A16=116.610633
27\A17=116.64568376\A18=105.73303275\A19=110.55393305\A20=110.54845241
\A21=108.48036221\A22=110.96763145\A23=106.55466421\A24=108.88564634\A
25=128.09308504\A26=110.6543054\A27=110.54097109\A28=112.490036\A29=11
1.30939167\A30=109.63442214\A31=111.22355604\A32=111.23000992\A33=111.
92426332\A34=105.29957528\A35=111.07302148\A36=111.53143997\A37=111.04
101131\D1=176.61389323\D2=5.051503\D3=-0.5483209\D4=-119.83862811\D5=1
19.75042581\D6=58.03478279\D7=-58.67852451\D8=-180.28468497\D9=-59.394
23055\D10=59.43679536\D11=-179.97146581\D12=0.10379545\D13=-179.472883
19\D14=-183.82033297\D15=-4.32745107\D16=179.27663043\D17=-179.5110328
2\D18=-60.10567054\D19=61.04516064\D20=-176.11091891\D21=-177.82355865
\D22=-59.65059831\D23=60.94865548\D24=-133.96178419\D25=54.73786923\D2
6=175.88402076\D27=-64.4694279\D28=56.23942533\D29=-66.04873919\D30=-1
78.40210909\D31=-58.51311563\D32=61.74780432\D33=174.68024028\D34=58.4
3862747\D35=178.63543095\D36=-61.20563486\\Version=AM64L-G03RevE.01\St
ate=2-A\HF=-1129.8902489\S2=0.761536\S2-1=0.\S2A=0.750099\RMSD=3.574e-
09\RMSF=7.684e-06\Thermal=0.\Dipole=0.402115,-0.3276869,0.293241\PG=C0
1 [X(C12H21O5Si1)]\\@

HF/6-311G*

1\1\GINC-GOMBERG05\FOpt\UHF\6-311G(d,p)\C12H21O5Si1(2)\HMAITKEN\27-Oct
-2010\1\\#HF/6-311G** opt=(grad,readfc) geom=checkpoint guess=read\\6
exo starting material\\0,2\C\C,1,B1\O,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\C,4
,B4,3,A3,2,D2,0\H,5,B5,4,A4,3,D3,0\H,2,B6,1,A5,3,D4,0\H,2,B7,1,A6,3,D5
,0\H,1,B8,2,A7,3,D6,0\H,1,B9,2,A8,3,D7,0\C,1,B10,2,A9,3,D8,0\H,11,B11,
1,A10,2,D9,0\H,11,B12,1,A11,2,D10,0\C,11,B13,1,A12,2,D11,0\O,14,B14,11
,A13,1,D12,0\C,5,B15,4,A14,3,D13,0\O,16,B16,5,A15,4,D14,0\O,16,B17,5,A
16,4,D15,0\C,18,B18,16,A17,5,D16,0\H,19,B19,18,A18,16,D17,0\H,19,B20,1
8,A19,16,D18,0\H,19,B21,18,A20,16,D19,0\C,4,B22,3,A21,2,D20,0\H,23,B23
,4,A22,3,D21,0\H,23,B24,4,A23,3,D22,0\O,23,B25,4,A24,3,D23,0\Si,26,B26
,23,A25,4,D24,0\C,27,B27,26,A26,23,D25,0\H,28,B28,27,A27,26,D26,0\H,28
,B29,27,A28,26,D27,0\H,28,B30,27,A29,26,D28,0\C,27,B31,26,A30,23,D29,0

\H,32,B32,27,A31,26,D30,0\H,32,B33,27,A32,26,D31,0\H,32,B34,27,A33,26,
D32,0\C,27,B35,26,A34,23,D33,0\H,36,B36,27,A35,26,D34,0\H,36,B37,27,A3
6,26,D35,0\H,36,B38,27,A37,26,D36,0\\B1=1.51706376\B2=1.40650212\B3=1.
33415808\B4=1.3351723\B5=1.07086556\B6=1.0867352\B7=1.0861683\B8=1.084
27151\B9=1.08409628\B10=1.52937102\B11=1.08675668\B12=1.08675992\B13=1
.51675613\B14=1.15751354\B15=1.47451174\B16=1.18748356\B17=1.32520246\
B18=1.41673616\B19=1.07962803\B20=1.08124612\B21=1.0813814\B22=1.50951
898\B23=1.07370717\B24=1.08848824\B25=1.39443507\B26=1.65321691\B27=1.
87944334\B28=1.08816663\B29=1.08737684\B30=1.08646344\B31=1.8811945\B3
2=1.08799737\B33=1.08729532\B34=1.08809926\B35=1.87094608\B36=1.086704
71\B37=1.08781989\B38=1.08670648\A1=107.33127877\A2=121.64109509\A3=12
3.08410862\A4=119.44283468\A5=110.78469658\A6=110.95041693\A7=109.2608
4026\A8=109.21707884\A9=111.51085686\A10=111.97240164\A11=111.94468748
\A12=113.31877941\A13=129.59397166\A14=130.47509697\A15=121.15288093\A
16=116.61790571\A17=116.89875814\A18=105.76166965\A19=110.56669815\A20
=110.5854112\A21=108.60786438\A22=110.76046335\A23=106.38670232\A24=10
8.78697254\A25=129.70238865\A26=110.3684673\A27=110.45848501\A28=112.1
9630817\A29=111.15791905\A30=109.58212388\A31=110.99222118\A32=111.090
19336\A33=111.75857976\A34=105.3801837\A35=110.93974209\A36=111.270485
43\A37=110.89693305\D1=176.91082232\D2=5.02565175\D3=-0.29880116\D4=-1
19.8613321\D5=119.78583911\D6=57.93397998\D7=-58.81449211\D8=-180.4080
1708\D9=-59.65149833\D10=59.45376995\D11=-180.11830642\D12=-0.13049688
\D13=-179.13571313\D14=-182.6432488\D15=-2.86535908\D16=179.07281621\D
17=-179.39906539\D18=-59.98624083\D19=61.12429203\D20=-175.9419681\D21
=-175.05379052\D22=-56.80611246\D23=63.60814152\D24=-136.06908627\D25=
57.04320458\D26=177.84583709\D27=-62.48269914\D28=58.14178815\D29=-63.
63760272\D30=-178.34426741\D31=-58.48195357\D32=61.86814258\D33=176.96
181497\D34=59.06017798\D35=179.22747622\D36=-60.66561529\\Version=AM64
L-G03RevE.01\State=2-A\HF=-1130.1287881\S2=0.761643\S2-1=0.\S2A=0.7500
98\RMSD=6.069e-09\RMSF=2.635e-05\Thermal=0.\Dipole=0.4806856,-0.280982
5,0.3262055\PG=C01 [X(C12H21O5Si1)]\\@

BHandHLYP/6-311G**

1\1\GINC-GOMBERG01\FOpt\UBHandHLYP\6-311G(d,p)\C12H21O5Si1(2)\HMAITKEN
\29-Oct-2010\1\\#BHandHLYP/6-311G** opt=(grad,readfc) geom=checkpoint
guess=read\\6 exo starting material\\0,2\C\C,1,B1\O,2,B2,1,A1\C,3,B3,2
,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\H,5,B5,4,A4,3,D3,0\H,2,B6,1,A5,3,D4,0\H,
2,B7,1,A6,3,D5,0\H,1,B8,2,A7,3,D6,0\H,1,B9,2,A8,3,D7,0\C,1,B10,2,A9,3,
D8,0\H,11,B11,1,A10,2,D9,0\H,11,B12,1,A11,2,D10,0\C,11,B13,1,A12,2,D11
,0\O,14,B14,11,A13,1,D12,0\C,5,B15,4,A14,3,D13,0\O,16,B16,5,A15,4,D14,
0\O,16,B17,5,A16,4,D15,0\C,18,B18,16,A17,5,D16,0\H,19,B19,18,A18,16,D1
7,0\H,19,B20,18,A19,16,D18,0\H,19,B21,18,A20,16,D19,0\C,4,B22,3,A21,2,
D20,0\H,23,B23,4,A22,3,D21,0\H,23,B24,4,A23,3,D22,0\O,23,B25,4,A24,3,D
23,0\Si,26,B26,23,A25,4,D24,0\C,27,B27,26,A26,23,D25,0\H,28,B28,27,A27
,26,D26,0\H,28,B29,27,A28,26,D27,0\H,28,B30,27,A29,26,D28,0\C,27,B31,2
6,A30,23,D29,0\H,32,B32,27,A31,26,D30,0\H,32,B33,27,A32,26,D31,0\H,32,
B34,27,A33,26,D32,0\C,27,B35,26,A34,23,D33,0\H,36,B36,27,A35,26,D34,0\
H,36,B37,27,A36,26,D35,0\H,36,B38,27,A37,26,D36,0\\B1=1.5105808\B2=1.4
1179354\B3=1.33760143\B4=1.33892016\B5=1.07284828\B6=1.08896004\B7=1.0
8828611\B8=1.0851844\B9=1.08507151\B10=1.52359805\B11=1.08782982\B12=1
.08790723\B13=1.5102158\B14=1.16678284\B15=1.46388083\B16=1.19756051\B
17=1.33681136\B18=1.42090831\B19=1.08050722\B20=1.0828849\B21=1.083020
86\B22=1.50236323\B23=1.07681011\B24=1.09142292\B25=1.39994958\B26=1.6

6035994\B27=1.86964071\B28=1.08762011\B29=1.0869006\B30=1.08572321\B31
=1.87159261\B32=1.08753045\B33=1.08668789\B34=1.08746453\B35=1.8610416
\B36=1.08618986\B37=1.08722363\B38=1.08616483\A1=107.51632593\A2=120.4
8905152\A3=122.99383206\A4=119.37293518\A5=110.94679719\A6=110.9884732
6\A7=109.35195275\A8=109.30407922\A9=111.52704722\A10=112.10060196\A11
=112.09652349\A12=113.52321828\A13=128.37144813\A14=130.45384842\A15=1
21.73640033\A16=116.27639021\A17=115.76044999\A18=105.72651839\A19=110
.59003281\A20=110.58150852\A21=109.0817388\A22=110.11107139\A23=106.63
715179\A24=109.53834794\A25=127.77046727\A26=110.47417812\A27=110.4542
6665\A28=112.0987632\A29=111.14974943\A30=109.51270815\A31=111.0271238
9\A32=111.10075475\A33=111.65088526\A34=105.04122966\A35=110.94196902\
A36=111.18287744\A37=110.90299191\D1=176.36430103\D2=4.16718001\D3=-0.
0900823\D4=-119.9205769\D5=119.80830049\D6=57.49313128\D7=-59.21019775
\D8=-180.83400471\D9=-59.61351965\D10=59.14049905\D11=-180.2690763\D12
=-0.27851842\D13=-179.27923043\D14=-183.3093291\D15=-3.66909589\D16=17
9.10400801\D17=-179.17934716\D18=-59.57353187\D19=61.19297471\D20=-176
.92019367\D21=-180.1252687\D22=-62.46812743\D23=58.59081799\D24=-127.8
0332163\D25=55.06430696\D26=179.80228418\D27=-60.54915883\D28=59.91414
486\D29=-65.54386764\D30=-178.85854108\D31=-58.90205005\D32=61.3957143
3\D33=175.11965355\D34=58.3413232\D35=178.46656167\D36=-61.45280385\\V
ersion=AM64L-G03RevE.01\State=2-A\HF=-1135.2774603\S2=0.754793\S2-1=0.
\S2A=0.750014\RMSD=6.610e-09\RMSF=2.797e-05\Thermal=0.\Dipole=0.448983
2,-0.3441425,0.2475059\PG=C01 [X(C12H21O5Si1)]\\@

BHandHLYP/6-311++G(d,p)

1\1\GINC-GOMBERG02\FOpt\UBHandHLYP\6-311++G(d,p)\C12H21O5Si1(2)\HMAITK
EN\03-Nov-2010\1\\#BHandHLYP/6-311++G(d,p) opt=(grad,readfc) geom=chec
kpoint guess=read\\6 exo starting material\\0,2\C\C,1,B1\O,2,B2,1,A1\C
,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\H,5,B5,4,A4,3,D3,0\H,2,B6,1,A5,3,
D4,0\H,2,B7,1,A6,3,D5,0\H,1,B8,2,A7,3,D6,0\H,1,B9,2,A8,3,D7,0\C,1,B10,
2,A9,3,D8,0\H,11,B11,1,A10,2,D9,0\H,11,B12,1,A11,2,D10,0\C,11,B13,1,A1
2,2,D11,0\O,14,B14,11,A13,1,D12,0\C,5,B15,4,A14,3,D13,0\O,16,B16,5,A15
,4,D14,0\O,16,B17,5,A16,4,D15,0\C,18,B18,16,A17,5,D16,0\H,19,B19,18,A1
8,16,D17,0\H,19,B20,18,A19,16,D18,0\H,19,B21,18,A20,16,D19,0\C,4,B22,3
,A21,2,D20,0\H,23,B23,4,A22,3,D21,0\H,23,B24,4,A23,3,D22,0\O,23,B25,4,
A24,3,D23,0\Si,26,B26,23,A25,4,D24,0\C,27,B27,26,A26,23,D25,0\H,28,B28
,27,A27,26,D26,0\H,28,B29,27,A28,26,D27,0\H,28,B30,27,A29,26,D28,0\C,2
7,B31,26,A30,23,D29,0\H,32,B32,27,A31,26,D30,0\H,32,B33,27,A32,26,D31,
0\H,32,B34,27,A33,26,D32,0\C,27,B35,26,A34,23,D33,0\H,36,B36,27,A35,26
,D34,0\H,36,B37,27,A36,26,D35,0\H,36,B38,27,A37,26,D36,0\\B1=1.5111452
9\B2=1.41171656\B3=1.33759828\B4=1.33974548\B5=1.07304314\B6=1.0889523
8\B7=1.08832897\B8=1.08531761\B9=1.08514464\B10=1.52385524\B11=1.08800
698\B12=1.08790871\B13=1.50804022\B14=1.16680141\B15=1.46363193\B16=1.
19966982\B17=1.33545101\B18=1.4215187\B19=1.0806029\B20=1.08282254\B21
=1.08285467\B22=1.50235959\B23=1.07731723\B24=1.09136738\B25=1.4000607
9\B26=1.66302755\B27=1.87019777\B28=1.08772669\B29=1.0871293\B30=1.086
13441\B31=1.87154808\B32=1.08767843\B33=1.08685759\B34=1.08759457\B35=
1.86124221\B36=1.08636679\B37=1.08730744\B38=1.08630668\A1=107.5086422
6\A2=120.68251353\A3=122.8609262\A4=119.31409166\A5=111.00343037\A6=11
0.92988379\A7=109.42762767\A8=109.27644898\A9=111.29661245\A10=112.128
91798\A11=112.10180601\A12=113.76978906\A13=129.004548\A14=130.3640779
4\A15=121.6355821\A16=116.41209205\A17=116.09464453\A18=105.66655402\A
19=110.53547449\A20=110.57238259\A21=108.99487507\A22=110.23281627\A23

=106.55125372\A24=109.34293824\A25=127.60466098\A26=109.98502936\A27=1
10.61793324\A28=112.06942569\A29=111.00412256\A30=109.5088524\A31=111.
07030662\A32=111.05364798\A33=111.62556918\A34=104.84393535\A35=110.86
73778\A36=111.26080526\A37=110.82330249\D1=175.78655033\D2=4.45341655\
D3=0.20059653\D4=-119.97688885\D5=119.68641891\D6=58.46883404\D7=-58.3
435554\D8=-179.88920495\D9=-59.17629807\D10=59.54897476\D11=-179.77770
863\D12=0.28213325\D13=-178.71531531\D14=-182.98165955\D15=-3.15348522
\D16=179.03992656\D17=-179.80963127\D18=-60.30139674\D19=60.59259628\D
20=-176.50701363\D21=-177.33513173\D22=-59.56320756\D23=61.28009314\D2
4=-131.80294419\D25=54.67192262\D26=177.71762327\D27=-62.5886078\D28=5
7.84517888\D29=-65.95726228\D30=-178.39293722\D31=-58.44735507\D32=61.
85474497\D33=174.63301527\D34=59.00091136\D35=179.15752784\D36=-60.695
83077\\Version=AM64L-G03RevE.01\State=2-A\HF=-1135.2922019\S2=0.754975
\S2-1=0.\S2A=0.750015\RMSD=2.947e-09\RMSF=5.236e-05\Thermal=0.\Dipole=
0.5643478,-0.2963378,0.2714779\PG=C01 [X(C12H21O5Si1)]\\@

Cyclization transition state 48 → 49

HF/3-21G*

1\1\GINC-GOMBERG02\FTS\UHF\3-21G*\C12H21O5Si1(2)\HMAITKEN\01-Nov-2010\
1\\#HF/3-21G* opt=(grad,readfc,ts,noeigentest,nofreeze) geom=checkpoin
t guess=read\\6 exo ts\\0,2\O\C,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\C,
4,B4,3,A3,2,D2,0\O,5,B5,4,A4,3,D3,0\C,2,B6,5,A5,4,D4,0\C,7,B7,6,A6,5,D
5,0\H,3,B8,2,A7,1,D6,0\H,3,B9,2,A8,1,D7,0\H,4,B10,3,A9,2,D8,0\H,4,B11,
3,A10,2,D9,0\H,5,B12,4,A11,3,D10,0\H,5,B13,4,A12,3,D11,0\H,8,B14,7,A13
,6,D12,0\C,8,B15,7,A14,6,D13,0\O,16,B16,8,A15,7,D14,0\O,16,B17,8,A16,7
,D15,0\C,18,B18,16,A17,8,D16,0\H,19,B19,18,A18,16,D17,0\H,19,B20,18,A1
9,16,D18,0\H,19,B21,18,A20,16,D19,0\C,7,B22,6,A21,5,D20,0\H,23,B23,7,A
22,6,D21,0\H,23,B24,7,A23,6,D22,0\O,23,B25,7,A24,6,D23,0\Si,26,B26,23,
A25,7,D24,0\C,27,B27,26,A26,23,D25,0\H,28,B28,27,A27,26,D26,0\H,28,B29
,27,A28,26,D27,0\H,28,B30,27,A29,26,D28,0\C,27,B31,26,A30,23,D29,0\H,3
2,B32,27,A31,26,D30,0\H,32,B33,27,A32,26,D31,0\H,32,B34,27,A33,26,D32,
0\C,27,B35,26,A34,23,D33,0\H,36,B36,27,A35,26,D34,0\H,36,B37,27,A36,26
,D35,0\H,36,B38,27,A37,26,D36,0\\B1=1.18850848\B2=1.51328709\B3=1.5424
5095\B4=1.52907079\B5=1.44786443\B8=1.08515101\B9=1.084306\B10=1.08267
135\B11=1.08408274\B12=1.07880862\B13=1.07837867\B14=1.06911843\B15=1.
44200005\B16=1.21693356\B17=1.36072523\B18=1.45222263\B19=1.07650212\B
20=1.07914068\B21=1.07896491\B22=1.52901078\B23=1.07230842\B24=1.07784
836\B25=1.43344311\B26=1.65179208\B27=1.8744507\B28=1.08768715\B29=1.0
8856118\B30=1.08734838\B31=1.88130828\B32=1.08769054\B33=1.08890413\B3
4=1.08885074\B35=1.87780617\B36=1.08630399\B37=1.08776756\B38=1.088665
78\A1=130.87787814\A2=110.96019748\A3=112.96633979\A4=110.9760943\A5=5
2.82286606\A6=112.94349903\A7=107.96629902\A8=108.75420262\A9=109.8777
0932\A10=108.54656742\A11=110.07656888\A12=111.98767869\A13=117.566443
79\A14=126.62775057\A15=123.93157015\A16=114.85708167\A17=117.53915486
\A18=105.24495872\A19=110.47329736\A20=110.09178194\A21=115.6490163\A2
2=108.97713091\A23=111.62341859\A24=109.42910199\A25=134.61080493\A26=
105.70086151\A27=111.10338336\A28=111.22635468\A29=111.22462804\A30=10
9.71264444\A31=111.56717522\A32=110.78495902\A33=111.65652\A34=111.470
14785\A35=110.43574007\A36=111.88595904\A37=110.91495236\D1=133.402731
23\D2=60.66572276\D3=-70.79061323\D4=-163.71860062\D5=-155.2251505\D6=
-106.64520112\D7=10.67327386\D8=-60.76152165\D9=181.2970757\D10=174.04
819314\D11=52.81212745\D12=7.98819535\D13=-182.26857808\D14=-176.84167

627\D15=2.36750739\D16=-173.74329077\D17=178.67013173\D18=-61.5970787\
D19=59.2566397\D20=50.3520289\D21=-202.47605443\D22=-82.71688018\D23=3
4.52652784\D24=75.08290983\D25=-174.32978297\D26=63.22716573\D27=-176.
90400151\D28=-56.79820468\D29=66.8560202\D30=59.80168069\D31=179.77091
549\D32=-60.7893455\D33=-54.4707198\D34=-41.34741557\D35=78.22619763\D
36=198.32101624\B6=2.24714299\B7=1.38086528\\Version=AM64L-G03RevE.01\
State=2-A\HF=-1123.8073661\S2=1.129021\S2-1=0.\S2A=0.83063\RMSD=8.814e
-09\RMSF=1.724e-06\Thermal=0.\Dipole=1.1480005,-0.7953014,0.9594963\PG
=C01 [X(C12H21O5Si1)]\\@

HF/6-31G*

1\1\GINC-GOMBERG02\FTS\UHF\6-31G(d)\C12H21O5Si1(2)\HMAITKEN\01-Nov-201
0\1\\#HF/6-31G* opt=(grad,readfc,ts,noeigentest,nofreeze) geom=checkpo
int guess=read\\6 exo ts\\0,2\O\C,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\
C,4,B4,3,A3,2,D2,0\O,5,B5,4,A4,3,D3,0\C,2,B6,5,A5,4,D4,0\C,7,B7,6,A6,5
,D5,0\H,3,B8,2,A7,1,D6,0\H,3,B9,2,A8,1,D7,0\H,4,B10,3,A9,2,D8,0\H,4,B1
1,3,A10,2,D9,0\H,5,B12,4,A11,3,D10,0\H,5,B13,4,A12,3,D11,0\H,8,B14,7,A
13,6,D12,0\C,8,B15,7,A14,6,D13,0\O,16,B16,8,A15,7,D14,0\O,16,B17,8,A16
,7,D15,0\C,18,B18,16,A17,8,D16,0\H,19,B19,18,A18,16,D17,0\H,19,B20,18,
A19,16,D18,0\H,19,B21,18,A20,16,D19,0\C,7,B22,6,A21,5,D20,0\H,23,B23,7
,A22,6,D21,0\H,23,B24,7,A23,6,D22,0\O,23,B25,7,A24,6,D23,0\Si,26,B26,2
3,A25,7,D24,0\C,27,B27,26,A26,23,D25,0\H,28,B28,27,A27,26,D26,0\H,28,B
29,27,A28,26,D27,0\H,28,B30,27,A29,26,D28,0\C,27,B31,26,A30,23,D29,0\H
,32,B32,27,A31,26,D30,0\H,32,B33,27,A32,26,D31,0\H,32,B34,27,A33,26,D3
2,0\C,27,B35,26,A34,23,D33,0\H,36,B36,27,A35,26,D34,0\H,36,B37,27,A36,
26,D35,0\H,36,B38,27,A37,26,D36,0\\B1=1.16833711\B2=1.5159898\B3=1.532
34068\B4=1.52369405\B5=1.406034\B8=1.08739997\B9=1.08542464\B10=1.0854
9346\B11=1.08628664\B12=1.08095249\B13=1.08348279\B14=1.07265561\B15=1
.46476618\B16=1.19469686\B17=1.32976587\B18=1.41681564\B19=1.07893224\
B20=1.0802154\B21=1.07989549\B22=1.52422778\B23=1.07655213\B24=1.08175
342\B25=1.3962936\B26=1.66045916\B27=1.87959967\B28=1.08669011\B29=1.0
8748013\B30=1.08657854\B31=1.88714475\B32=1.0872227\B33=1.08775092\B34
=1.08667323\B35=1.88390096\B36=1.08661737\B37=1.08602746\B38=1.0881399
5\A1=128.22340434\A2=112.6498809\A3=113.73103155\A4=111.83722019\A5=52
.25021535\A6=111.18171555\A7=106.45465733\A8=108.10479585\A9=109.78209
447\A10=108.67759452\A11=109.60783915\A12=111.67939275\A13=116.5412078
2\A14=129.71197294\A15=121.60964692\A16=115.86876536\A17=116.61509058\
A18=105.77019035\A19=110.62317337\A20=110.35780021\A21=115.47709881\A2
2=109.31600003\A23=110.52538325\A24=110.73114545\A25=131.06956051\A26=
104.82523866\A27=110.99713822\A28=111.50928474\A29=111.22223339\A30=10
9.85758555\A31=111.59864846\A32=110.51153486\A33=112.12028847\A34=111.
4954787\A35=111.11733689\A36=112.53610659\A37=110.54277805\D1=140.5729
2721\D2=54.12565743\D3=-68.4730607\D4=-162.53733574\D5=-157.78740093\D
6=-98.76641153\D7=16.49321037\D8=-67.52777934\D9=175.68380777\D10=175.
61909195\D11=56.66807399\D12=12.07193801\D13=-178.51858662\D14=-174.42
574703\D15=5.88029376\D16=-176.2691239\D17=178.87571617\D18=-61.623046
99\D19=59.6026662\D20=52.36701361\D21=-187.95194235\D22=-70.04030669\D
23=47.73183777\D24=93.25779615\D25=-197.0630695\D26=59.64121643\D27=-1
80.38534229\D28=-60.07217848\D29=43.83665315\D30=56.99619989\D31=176.4
8891739\D32=-63.95839284\D33=-78.06072215\D34=-51.7368348\D35=68.80092
887\D36=188.82777519\B6=2.19854261\B7=1.40210611\\Version=AM64L-G03Rev
E.01\State=2-A\HF=-1129.8600864\S2=1.052876\S2-1=0.\S2A=0.776914\RMSD=
4.878e-09\RMSF=2.651e-06\Thermal=0.\Dipole=0.974684,-0.9966325,0.99570

62\PG=C01 [X(C12H21O5Si1)]\\@

HF/6-311G*

1\1\GINC-GOMBERG02\FTS\UHF\6-311G(d,p)\C12H21O5Si1(2)\HMAITKEN\03-Nov-
2010\1\\#HF/6-311G** opt=(grad,readfc,ts,noeigentest,nofreeze) geom=ch
eckpoint guess=read\\6 exo ts\\0,2\O\C,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,1,
D1,0\C,4,B4,3,A3,2,D2,0\O,5,B5,4,A4,3,D3,0\C,2,B6,5,A5,4,D4,0\C,7,B7,6
,A6,5,D5,0\H,3,B8,2,A7,1,D6,0\H,3,B9,2,A8,1,D7,0\H,4,B10,3,A9,2,D8,0\H
,4,B11,3,A10,2,D9,0\H,5,B12,4,A11,3,D10,0\H,5,B13,4,A12,3,D11,0\H,8,B1
4,7,A13,6,D12,0\C,8,B15,7,A14,6,D13,0\O,16,B16,8,A15,7,D14,0\O,16,B17,
8,A16,7,D15,0\C,18,B18,16,A17,8,D16,0\H,19,B19,18,A18,16,D17,0\H,19,B2
0,18,A19,16,D18,0\H,19,B21,18,A20,16,D19,0\C,7,B22,6,A21,5,D20,0\H,23,
B23,7,A22,6,D21,0\H,23,B24,7,A23,6,D22,0\O,23,B25,7,A24,6,D23,0\Si,26,
B26,23,A25,7,D24,0\C,27,B27,26,A26,23,D25,0\H,28,B28,27,A27,26,D26,0\H
,28,B29,27,A28,26,D27,0\H,28,B30,27,A29,26,D28,0\C,27,B31,26,A30,23,D2
9,0\H,32,B32,27,A31,26,D30,0\H,32,B33,27,A32,26,D31,0\H,32,B34,27,A33,
26,D32,0\C,27,B35,26,A34,23,D33,0\H,36,B36,27,A35,26,D34,0\H,36,B37,27
,A36,26,D35,0\H,36,B38,27,A37,26,D36,0\\B1=1.16170874\B2=1.51506361\B3
=1.53147187\B4=1.52286013\B5=1.4053423\B8=1.08755931\B9=1.08574547\B10
=1.08614642\B11=1.08663268\B12=1.08127684\B13=1.08477082\B14=1.0730799
6\B15=1.46495634\B16=1.18937357\B17=1.3276595\B18=1.41631566\B19=1.079
58148\B20=1.0815101\B21=1.0812508\B22=1.52475779\B23=1.07734298\B24=1.
08214057\B25=1.39541193\B26=1.65506508\B27=1.87351145\B28=1.08698767\B
29=1.08787342\B30=1.08686981\B31=1.88103516\B32=1.08758287\B33=1.08798
045\B34=1.086855\B35=1.87739348\B36=1.08689276\B37=1.08622493\B38=1.08
841317\A1=128.51610013\A2=112.63884957\A3=113.80734505\A4=111.95961915
\A5=52.18958027\A6=111.19100692\A7=106.22601746\A8=107.95254248\A9=109
.71271541\A10=108.68605419\A11=109.52658512\A12=111.61742975\A13=116.5
619101\A14=129.73665127\A15=121.60122617\A16=115.8355622\A17=116.88520
548\A18=105.81953426\A19=110.68594675\A20=110.35640284\A21=115.5117718
2\A22=108.99182447\A23=110.59350647\A24=110.94726137\A25=133.05289952\
A26=104.98999267\A27=110.8561569\A28=111.25674642\A29=111.07601093\A30
=109.72087662\A31=111.43988573\A32=110.37063848\A33=111.87132595\A34=1
11.16427983\A35=110.89587974\A36=112.26689118\A37=110.41188235\D1=139.
98351929\D2=54.28221633\D3=-68.1045826\D4=-163.0383515\D5=-158.075187\
D6=-99.3645857\D7=15.8981295\D8=-67.41487015\D9=175.74685024\D10=175.8
8594489\D11=57.02062897\D12=12.02265752\D13=-178.60598725\D14=-174.784
2499\D15=5.38071935\D16=-175.74962479\D17=179.01568401\D18=-61.4052763
3\D19=59.77747759\D20=52.50687387\D21=-188.26212989\D22=-70.38822235\D
23=47.56109932\D24=89.89545673\D25=-198.57156101\D26=59.69340524\D27=-
180.38030339\D28=-60.11425941\D29=42.26489354\D30=58.02055681\D31=177.
54312139\D32=-62.90096332\D33=-79.52276269\D34=-52.60412155\D35=67.849
10111\D36=187.89499742\B6=2.19291049\B7=1.40123313\\Version=AM64L-G03R
evE.01\State=2-A\HF=-1130.0966337\S2=1.047651\S2-1=0.\S2A=0.775606\RMS
D=5.976e-09\RMSF=1.676e-05\Thermal=0.\Dipole=1.004668,-0.9754885,0.997
1199\PG=C01 [X(C12H21O5Si1)]\\@

BHandHLYP/6-311G**

1\1\GINC-GOMBERG01\FTS\UBHandHLYP\6-311G(d,p)\C12H21O5Si1(2)\HMAITKEN\
03-Nov-2010\1\\#BHandHLYP/6-311G** opt=(grad,readfc,ts,noeigentest,nof
reeze) geom=checkpoint guess=read\\6 exo ts\\0,2\O\C,1,B1\C,2,B2,1,A1\
C,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\O,5,B5,4,A4,3,D3,0\C,2,B6,5,A5,4
,D4,0\C,7,B7,6,A6,5,D5,0\H,3,B8,2,A7,1,D6,0\H,3,B9,2,A8,1,D7,0\H,4,B10

,3,A9,2,D8,0\H,4,B11,3,A10,2,D9,0\H,5,B12,4,A11,3,D10,0\H,5,B13,4,A12,
3,D11,0\H,8,B14,7,A13,6,D12,0\C,8,B15,7,A14,6,D13,0\O,16,B16,8,A15,7,D
14,0\O,16,B17,8,A16,7,D15,0\C,18,B18,16,A17,8,D16,0\H,19,B19,18,A18,16
,D17,0\H,19,B20,18,A19,16,D18,0\H,19,B21,18,A20,16,D19,0\C,7,B22,6,A21
,5,D20,0\H,23,B23,7,A22,6,D21,0\H,23,B24,7,A23,6,D22,0\O,23,B25,7,A24,
6,D23,0\Si,26,B26,23,A25,7,D24,0\C,27,B27,26,A26,23,D25,0\H,28,B28,27,
A27,26,D26,0\H,28,B29,27,A28,26,D27,0\H,28,B30,27,A29,26,D28,0\C,27,B3
1,26,A30,23,D29,0\H,32,B32,27,A31,26,D30,0\H,32,B33,27,A32,26,D31,0\H,
32,B34,27,A33,26,D32,0\C,27,B35,26,A34,23,D33,0\H,36,B36,27,A35,26,D34
,0\H,36,B37,27,A36,26,D35,0\H,36,B38,27,A37,26,D36,0\\B1=1.16512587\B2
=1.51000844\B3=1.52533409\B4=1.51657958\B5=1.41220231\B8=1.08863586\B9
=1.08746752\B10=1.08651128\B11=1.08712007\B12=1.08270548\B13=1.0860465
8\B14=1.07473752\B15=1.44983394\B16=1.19995534\B17=1.34395709\B18=1.41
962571\B19=1.08075305\B20=1.08313003\B21=1.08294711\B22=1.52154448\B23
=1.0798228\B24=1.0840301\B25=1.40034423\B26=1.66682979\B27=1.86390481\
B28=1.0865254\B29=1.08730867\B30=1.08626357\B31=1.87009434\B32=1.08704
112\B33=1.0873798\B34=1.08643365\B35=1.86665243\B36=1.08636562\B37=1.0
8567362\B38=1.08786918\A1=128.73657125\A2=113.49555076\A3=113.75821443
\A4=111.32835354\A5=52.17294482\A6=112.40410925\A7=105.52915984\A8=107
.78502863\A9=109.72381738\A10=108.67544833\A11=109.7379985\A12=112.140
00318\A13=116.44854453\A14=130.03193569\A15=122.67222535\A16=115.56123
267\A17=115.62898373\A18=105.80766454\A19=110.73901998\A20=110.4313107
8\A21=115.59288121\A22=108.55217575\A23=110.96940419\A24=110.78920121\
A25=129.97828364\A26=104.37959106\A27=110.86212298\A28=111.13738626\A2
9=111.13140615\A30=109.41038748\A31=111.42278741\A32=110.48798109\A33=
111.57564422\A34=111.00734056\A35=110.87396576\A36=111.92921403\A37=11
0.47543971\D1=142.36284187\D2=53.09879226\D3=-68.33314174\D4=-162.6264
4731\D5=-159.95824602\D6=-97.02379323\D7=17.60663008\D8=-68.42445416\D
9=174.82072401\D10=176.06581992\D11=56.63046101\D12=11.50588993\D13=-1
77.71946847\D14=-175.12666341\D15=4.6389479\D16=-176.59129721\D17=179.
36945354\D18=-60.87361018\D19=59.92196283\D20=47.35700966\D21=-188.814
02466\D22=-70.80283243\D23=47.09010395\D24=81.65429159\D25=-198.468296
46\D26=59.51972712\D27=-180.67229302\D28=-60.3995504\D29=42.37028859\D
30=60.79547461\D31=180.46507633\D32=-59.89676672\D33=-79.63259439\D34=
-52.90452971\D35=67.27596669\D36=187.47294317\B6=2.20328952\B7=1.37586
24\\Version=AM64L-G03RevE.01\State=2-A\HF=-1135.2527087\S2=0.819856\S2
-1=0.\S2A=0.751051\RMSD=7.961e-09\RMSF=4.059e-05\Thermal=0.\Dipole=1.2
741345,-0.9050981,1.0610721\PG=C01 [X(C12H21O5Si1)]\\@

BHandHLYP/6-311++G(d,p)

1\1\GINC-GOMBERG06\FTS\UBHandHLYP\6-311++G(d,p)\C12H21O5Si1(2)\HMAITKE
N\06-Nov-2010\1\\#BHandHLYP/6-311++G(d,p) opt=(grad,readfc,ts,noeigent
est,nofreeze) geom=checkpoint guess=read\\6 exo ts\\0,2\O\C,1,B1\C,2,B
2,1,A1\C,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\O,5,B5,4,A4,3,D3,0\C,2,B6
,5,A5,4,D4,0\C,7,B7,6,A6,5,D5,0\H,3,B8,2,A7,1,D6,0\H,3,B9,2,A8,1,D7,0\
H,4,B10,3,A9,2,D8,0\H,4,B11,3,A10,2,D9,0\H,5,B12,4,A11,3,D10,0\H,5,B13
,4,A12,3,D11,0\H,8,B14,7,A13,6,D12,0\C,8,B15,7,A14,6,D13,0\O,16,B16,8,
A15,7,D14,0\O,16,B17,8,A16,7,D15,0\C,18,B18,16,A17,8,D16,0\H,19,B19,18
,A18,16,D17,0\H,19,B20,18,A19,16,D18,0\H,19,B21,18,A20,16,D19,0\C,7,B2
2,6,A21,5,D20,0\H,23,B23,7,A22,6,D21,0\H,23,B24,7,A23,6,D22,0\O,23,B25
,7,A24,6,D23,0\Si,26,B26,23,A25,7,D24,0\C,27,B27,26,A26,23,D25,0\H,28,
B28,27,A27,26,D26,0\H,28,B29,27,A28,26,D27,0\H,28,B30,27,A29,26,D28,0\
C,27,B31,26,A30,23,D29,0\H,32,B32,27,A31,26,D30,0\H,32,B33,27,A32,26,D

31,0\H,32,B34,27,A33,26,D32,0\C,27,B35,26,A34,23,D33,0\H,36,B36,27,A35
,26,D34,0\H,36,B37,27,A36,26,D35,0\H,36,B38,27,A37,26,D36,0\\B1=1.1657
6983\B2=1.50916743\B3=1.52564154\B4=1.51598811\B5=1.41244676\B8=1.0886
3315\B9=1.08759516\B10=1.08669287\B11=1.08724646\B12=1.08304955\B13=1.
08605442\B14=1.07496975\B15=1.44929909\B16=1.20228291\B17=1.34244184\B
18=1.42025346\B19=1.08088347\B20=1.08318799\B21=1.08294262\B22=1.52160
285\B23=1.08006141\B24=1.08414867\B25=1.39991563\B26=1.66853002\B27=1.
86398756\B28=1.08664695\B29=1.08746955\B30=1.08644988\B31=1.87063931\B
32=1.08720674\B33=1.08760845\B34=1.08658122\B35=1.8667762\B36=1.086685
9\B37=1.08596907\B38=1.08802647\A1=128.65368555\A2=113.43667516\A3=113
.75362687\A4=111.41814873\A5=52.26017957\A6=112.2829148\A7=105.6386083
1\A8=107.80547454\A9=109.71290609\A10=108.64409297\A11=109.77820456\A1
2=112.15962045\A13=116.49746577\A14=130.08281683\A15=122.56854554\A16=
115.68769069\A17=115.94945709\A18=105.76370117\A19=110.7207251\A20=110
.45108685\A21=115.71583028\A22=108.57918226\A23=110.91366712\A24=110.7
429108\A25=130.34954959\A26=104.29246909\A27=110.81729421\A28=111.1568
4703\A29=111.11222119\A30=109.28492099\A31=111.30617834\A32=110.444554
94\A33=111.77286999\A34=110.88024232\A35=110.84160907\A36=111.95316892
\A37=110.56082056\D1=140.02383792\D2=53.20125232\D3=-67.25196245\D4=-1
64.1599119\D5=-161.16812892\D6=-99.26039644\D7=15.45891637\D8=-68.5775
9813\D9=174.76154201\D10=177.07569749\D11=57.67157012\D12=11.380854\D1
3=-176.99687098\D14=-176.77444344\D15=3.01924966\D16=-176.85095239\D17
=179.43989284\D18=-60.85761284\D19=60.0226609\D20=46.40665387\D21=-187
.96509754\D22=-70.02697512\D23=47.9062296\D24=86.44161519\D25=-198.728
24697\D26=58.98606096\D27=-181.19085998\D28=-60.91434417\D29=42.255866
94\D30=58.43842514\D31=177.94219354\D32=-62.42474401\D33=-79.76055307\
D34=-55.07470584\D35=65.15056172\D36=185.36611033\B6=2.19920329\B7=1.3
7733856\\Version=AM64L-G03RevE.01\State=2-A\HF=-1135.2664262\S2=0.8203
93\S2-1=0.\S2A=0.751049\RMSD=2.760e-09\RMSF=3.839e-05\Thermal=0.\Dipol
e=1.2941613,-0.9895145,1.2143318\PG=C01 [X(C12H21O5Si1)]\\@

Cyclization product 49

HF/3-21G*

1\1\GINC-GOMBERG02\FOpt\UHF\3-21G*\C12H21O5Si1(2)\HMAITKEN\26-Oct-2010
\1\\#HF/3-21G* opt=(grad)\\6 exo cyclic radical product\\0,2\C\C,1,B1\
C,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\H,1,B4,4,A3,3,D2,0\H,1,B5,4,A4,3,D3,0\H
,3,B6,2,A5,1,D4,0\H,3,B7,2,A6,1,D5,0\H,4,B8,3,A7,2,D6,0\H,4,B9,3,A8,2,
D7,0\O,3,B10,2,A9,1,D8,0\C,2,B11,1,A10,4,D9,0\H,12,B12,2,A11,1,D10,0\C
,1,B13,4,A12,3,D11,0\O,14,B14,1,A13,4,D12,0\C,12,B15,2,A14,1,D13,0\O,1
6,B16,12,A15,2,D14,0\O,16,B17,12,A16,2,D15,0\C,18,B18,16,A17,12,D16,0\
H,19,B19,18,A18,16,D17,0\H,19,B20,18,A19,16,D18,0\H,19,B21,18,A20,16,D
19,0\C,2,B22,1,A21,14,D20,0\H,23,B23,2,A22,1,D21,0\H,23,B24,2,A23,1,D2
2,0\O,23,B25,2,A24,1,D23,0\Si,26,B26,23,A25,2,D24,0\C,27,B27,26,A26,23
,D25,0\H,28,B28,27,A27,26,D26,0\H,28,B29,27,A28,26,D27,0\H,28,B30,27,A
29,26,D28,0\C,27,B31,26,A30,23,D29,0\H,32,B32,27,A31,26,D30,0\H,32,B33
,27,A32,26,D31,0\H,32,B34,27,A33,26,D32,0\C,27,B35,26,A34,23,D33,0\H,3
6,B36,27,A35,26,D34,0\H,36,B37,27,A36,26,D35,0\H,36,B38,27,A37,26,D36,
0\\B1=2.58775789\B2=2.46867662\B3=1.52683477\B4=1.08764592\B5=1.081099
33\B6=1.07851315\B7=1.08299071\B8=1.08295472\B9=1.08282471\B10=1.44183
451\B11=1.4935222\B12=1.06706085\B13=1.51222584\B14=1.20991329\B15=1.4
3506828\B16=1.22351084\B17=1.35377387\B18=1.45\B19=1.07988354\B20=1.07
624061\B21=1.07945183\B22=1.53960945\B23=1.07630363\B24=1.08089141\B25

=1.42033462\B26=1.64883572\B27=1.87856829\B28=1.0887887\B29=1.08811244
\B30=1.08755219\B31=1.87845034\B32=1.08667687\B33=1.08869654\B34=1.088
9725\B35=1.87648617\B36=1.08897687\B37=1.08749559\B38=1.08634039\A1=59
.28926566\A2=92.13027442\A3=109.13320332\A4=112.05887574\A5=136.142160
15\A6=95.24262896\A7=108.86000165\A8=110.32931665\A9=30.99346166\A10=1
36.9857692\A11=117.46293853\A12=110.99454026\A13=122.97158483\A14=123.
957827\A15=126.62711701\A16=111.85605573\A17=118.08738068\A18=110.5074
997\A19=105.16650132\A20=110.49474973\A21=100.55479231\A22=108.3402375
3\A23=109.24883437\A24=109.36924886\A25=135.93927773\A26=107.78084415\
A27=111.15309165\A28=111.28080686\A29=111.22064553\A30=110.36891298\A3
1=110.65310884\A32=112.21227875\A33=110.47702044\A34=109.75037244\A35=
110.83600567\A36=111.51252274\A37=111.01135465\D1=20.70299424\D2=-66.0
7022414\D3=174.26489637\D4=145.72850466\D5=-90.27467796\D6=87.05046704
\D7=-154.01449556\D8=146.54982809\D9=102.67810034\D10=-76.38341872\D11
=53.38112333\D12=137.20542454\D13=95.89519869\D14=13.82864296\D15=-168
.0386776\D16=180.64451123\D17=62.51290596\D18=-178.03145394\D19=-58.41
683501\D20=105.74637553\D21=-84.90294015\D22=34.06681963\D23=153.42101
316\D24=137.37947184\D25=124.65779715\D26=177.91127471\D27=-62.1488177
3\D28=57.89169683\D29=4.50600982\D30=-59.49315691\D31=61.40058509\D32=
181.10665704\D33=-116.33861111\D34=-171.05168731\D35=-51.10607419\D36=
69.35772871\\Version=AM64L-G03RevE.01\State=2-A\HF=-1123.8579042\S2=0.
826751\S2-1=0.\S2A=0.752171\RMSD=6.993e-09\RMSF=1.480e-05\Thermal=0.\D
ipole=0.5465215,-0.1253994,-0.7950025\PG=C01 [X(C12H21O5Si1)]\\@

HF/6-31G*

1\1\GINC-GOMBERG03\FOpt\UHF\6-31G(d)\C12H21O5Si1(2)\HMAITKEN\26-Oct-20
10\1\\#HF/6-31G* opt=(grad,readfc) geom=checkpoint guess=read\\6 exo c
yclic radical product\\0,2\C\C,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\H,1
,B4,4,A3,3,D2,0\H,1,B5,4,A4,3,D3,0\H,3,B6,2,A5,1,D4,0\H,3,B7,2,A6,1,D5
,0\H,4,B8,3,A7,2,D6,0\H,4,B9,3,A8,2,D7,0\O,3,B10,2,A9,1,D8,0\C,2,B11,1
,A10,4,D9,0\H,12,B12,2,A11,1,D10,0\C,1,B13,4,A12,3,D11,0\O,14,B14,1,A1
3,4,D12,0\C,12,B15,2,A14,1,D13,0\O,16,B16,12,A15,2,D14,0\O,16,B17,12,A
16,2,D15,0\C,18,B18,16,A17,12,D16,0\H,19,B19,18,A18,16,D17,0\H,19,B20,
18,A19,16,D18,0\H,19,B21,18,A20,16,D19,0\C,2,B22,1,A21,14,D20,0\H,23,B
23,2,A22,1,D21,0\H,23,B24,2,A23,1,D22,0\O,23,B25,2,A24,1,D23,0\Si,26,B
26,23,A25,2,D24,0\C,27,B27,26,A26,23,D25,0\H,28,B28,27,A27,26,D26,0\H,
28,B29,27,A28,26,D27,0\H,28,B30,27,A29,26,D28,0\C,27,B31,26,A30,23,D29
,0\H,32,B32,27,A31,26,D30,0\H,32,B33,27,A32,26,D31,0\H,32,B34,27,A33,2
6,D32,0\C,27,B35,26,A34,23,D33,0\H,36,B36,27,A35,26,D34,0\H,36,B37,27,
A36,26,D35,0\H,36,B38,27,A37,26,D36,0\\B1=2.60259281\B2=2.42093541\B3=
1.52029733\B4=1.0890253\B5=1.08238987\B6=1.08108875\B7=1.08640406\B8=1
.08582409\B9=1.08563184\B10=1.40358215\B11=1.50501259\B12=1.0715136\B1
3=1.51616389\B14=1.18998499\B15=1.45921947\B16=1.19641964\B17=1.328529
6\B18=1.41421368\B19=1.08091091\B20=1.07889171\B21=1.08051807\B22=1.53
911135\B23=1.08026729\B24=1.08606532\B25=1.38950092\B26=1.65981694\B27
=1.88837276\B28=1.08778148\B29=1.08780109\B30=1.08702876\B31=1.8843972
1\B32=1.08592816\B33=1.08729551\B34=1.08794024\B35=1.87785971\B36=1.08
747574\B37=1.0864621\B38=1.08646957\A1=59.544126\A2=94.10223969\A3=109
.63881608\A4=112.54191124\A5=136.22010634\A6=94.96543504\A7=108.828771
55\A8=110.49879392\A9=30.78528348\A10=137.28218653\A11=116.61925093\A1
2=111.62243257\A13=122.24963697\A14=125.33343551\A15=126.03264362\A16=
111.04310335\A17=116.83667915\A18=110.65331048\A19=105.81914377\A20=11
0.59996795\A21=101.58676994\A22=108.42484033\A23=109.30655341\A24=109.

02632122\A25=127.68413157\A26=109.4328543\A27=111.1205659\A28=111.9669
9564\A29=111.27596026\A30=110.50723481\A31=111.24962817\A32=112.224131
81\A33=110.65777339\A34=105.3342168\A35=111.57745163\A36=111.0248933\A
37=111.0112164\D1=18.56286282\D2=-70.48238088\D3=170.07856714\D4=145.3
3578164\D5=-92.89171576\D6=90.42291756\D7=-151.80409299\D8=143.2297167
6\D9=104.76064261\D10=-76.9272723\D11=48.503853\D12=138.69146941\D13=9
7.763272\D14=9.15454535\D15=-171.76476442\D16=179.97241279\D17=61.2121
095\D18=-179.40937512\D19=-59.97459775\D20=107.05752483\D21=-88.218156
47\D22=29.51656811\D23=150.11552476\D24=171.96807605\D25=73.80972309\D
26=178.07742598\D27=-62.20445464\D28=58.26234481\D29=-47.03998171\D30=
-51.35154239\D31=68.96296895\D32=188.59724274\D33=-167.33218177\D34=-1
77.12626427\D35=-56.89737278\D36=62.67492942\\Version=AM64L-G03RevE.01
\State=2-A\HF=-1129.9121826\S2=0.780755\S2-1=0.\S2A=0.750567\RMSD=5.52
4e-09\RMSF=9.766e-06\Thermal=0.\Dipole=0.8696787,-0.3427081,-0.4846607
\PG=C01 [X(C12H21O5Si1)]\\@

HF/6-311G*

1\1\GINC-GOMBERG03\FOpt\UHF\6-311G(d,p)\C12H21O5Si1(2)\HMAITKEN\27-Oct
-2010\1\\#HF/6-311G** opt=(grad,readfc) geom=checkpoint guess=read\\6
exo cyclic radical product\\0,2\C\C,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,1,D1,
0\H,1,B4,4,A3,3,D2,0\H,1,B5,4,A4,3,D3,0\H,3,B6,2,A5,1,D4,0\H,3,B7,2,A6
,1,D5,0\H,4,B8,3,A7,2,D6,0\H,4,B9,3,A8,2,D7,0\O,3,B10,2,A9,1,D8,0\C,2,
B11,1,A10,4,D9,0\H,12,B12,2,A11,1,D10,0\C,1,B13,4,A12,3,D11,0\O,14,B14
,1,A13,4,D12,0\C,12,B15,2,A14,1,D13,0\O,16,B16,12,A15,2,D14,0\O,16,B17
,12,A16,2,D15,0\C,18,B18,16,A17,12,D16,0\H,19,B19,18,A18,16,D17,0\H,19
,B20,18,A19,16,D18,0\H,19,B21,18,A20,16,D19,0\C,2,B22,1,A21,14,D20,0\H
,23,B23,2,A22,1,D21,0\H,23,B24,2,A23,1,D22,0\O,23,B25,2,A24,1,D23,0\Si
,26,B26,23,A25,2,D24,0\C,27,B27,26,A26,23,D25,0\H,28,B28,27,A27,26,D26
,0\H,28,B29,27,A28,26,D27,0\H,28,B30,27,A29,26,D28,0\C,27,B31,26,A30,2
3,D29,0\H,32,B32,27,A31,26,D30,0\H,32,B33,27,A32,26,D31,0\H,32,B34,27,
A33,26,D32,0\C,27,B35,26,A34,23,D33,0\H,36,B36,27,A35,26,D34,0\H,36,B3
7,27,A36,26,D35,0\H,36,B38,27,A37,26,D36,0\\B1=2.60094912\B2=2.4184903
7\B3=1.51936193\B4=1.089186\B5=1.08242328\B6=1.08137543\B7=1.08758362\
B8=1.08645281\B9=1.08592647\B10=1.40259455\B11=1.50451768\B12=1.071745
04\B13=1.51562687\B14=1.18449605\B15=1.4599636\B16=1.1907764\B17=1.326
41112\B18=1.41403309\B19=1.08222807\B20=1.07937667\B21=1.08179988\B22=
1.53826132\B23=1.08190752\B24=1.08725886\B25=1.38781912\B26=1.65434818
\B27=1.88221926\B28=1.08807877\B29=1.08814813\B30=1.08732924\B31=1.878
1316\B32=1.08618576\B33=1.0876561\B34=1.08820049\B35=1.87139517\B36=1.
08786578\B37=1.08672744\B38=1.08670404\A1=59.59890702\A2=94.09567358\A
3=109.72884239\A4=112.59651731\A5=136.32658339\A6=94.99002029\A7=108.8
1842988\A8=110.39498699\A9=30.80694751\A10=137.40487709\A11=116.560245
67\A12=111.61156739\A13=122.33635556\A14=125.51676188\A15=126.10617068
\A16=110.93176213\A17=117.09107254\A18=110.68527269\A19=105.8251691\A2
0=110.62219013\A21=101.19680705\A22=108.15307187\A23=109.38348134\A24=
109.18809767\A25=129.66163513\A26=109.32471955\A27=110.94526132\A28=11
1.73297454\A29=111.16169321\A30=110.31220235\A31=111.11663442\A32=111.
96605255\A33=110.4778983\A34=105.43903546\A35=111.32950065\A36=110.849
13592\A37=110.88254246\D1=18.46211145\D2=-70.22774952\D3=170.06173559\
D4=145.18518513\D5=-92.94446984\D6=90.53031184\D7=-151.67107671\D8=143
.26207042\D9=105.03587223\D10=-76.86572901\D11=48.52183285\D12=138.298
18863\D13=97.87002225\D14=9.45572231\D15=-171.43394625\D16=179.8704352
7\D17=61.54427988\D18=-179.06610728\D19=-59.6101264\D20=107.08942875\D

21=-88.38740714\D22=29.24701762\D23=150.04939774\D24=171.70116759\D25=
74.5422926\D26=178.57160168\D27=-61.78519642\D28=58.72371011\D29=-46.1
1324562\D30=-52.90066039\D31=67.39950907\D32=186.97677511\D33=-166.518
1584\D34=-177.46486943\D35=-57.28298581\D36=62.36096419\\Version=AM64L
-G03RevE.01\State=2-A\HF=-1130.1470865\S2=0.779183\S2-1=0.\S2A=0.75053
7\RMSD=9.070e-09\RMSF=1.148e-05\Thermal=0.\Dipole=0.8689106,-0.3563544
,-0.4810767\PG=C01 [X(C12H21O5Si1)]\\@

BHandHLYP/6-311G**

1\1\GINC-GOMBERG04\FOpt\UBHandHLYP\6-311G(d,p)\C12H21O5Si1(2)\HMAITKEN
\29-Oct-2010\1\\#BHandHLYP/6-311G** opt=(grad,readfc) geom=checkpoint
guess=read\\6 exo cyclic radical product\\0,2\C\C,1,B1\C,2,B2,1,A1\C,3
,B3,2,A2,1,D1,0\H,1,B4,4,A3,3,D2,0\H,1,B5,4,A4,3,D3,0\H,3,B6,2,A5,1,D4
,0\H,3,B7,2,A6,1,D5,0\H,4,B8,3,A7,2,D6,0\H,4,B9,3,A8,2,D7,0\O,3,B10,2,
A9,1,D8,0\C,2,B11,1,A10,4,D9,0\H,12,B12,2,A11,1,D10,0\C,1,B13,4,A12,3,
D11,0\O,14,B14,1,A13,4,D12,0\C,12,B15,2,A14,1,D13,0\O,16,B16,12,A15,2,
D14,0\O,16,B17,12,A16,2,D15,0\C,18,B18,16,A17,12,D16,0\H,19,B19,18,A18
,16,D17,0\H,19,B20,18,A19,16,D18,0\H,19,B21,18,A20,16,D19,0\C,2,B22,1,
A21,14,D20,0\H,23,B23,2,A22,1,D21,0\H,23,B24,2,A23,1,D22,0\O,23,B25,2,
A24,1,D23,0\Si,26,B26,23,A25,2,D24,0\C,27,B27,26,A26,23,D25,0\H,28,B28
,27,A27,26,D26,0\H,28,B29,27,A28,26,D27,0\H,28,B30,27,A29,26,D28,0\C,2
7,B31,26,A30,23,D29,0\H,32,B32,27,A31,26,D30,0\H,32,B33,27,A32,26,D31,
0\H,32,B34,27,A33,26,D32,0\C,27,B35,26,A34,23,D33,0\H,36,B36,27,A35,26
,D34,0\H,36,B37,27,A36,26,D35,0\H,36,B38,27,A37,26,D36,0\\B1=2.5912078
8\B2=2.4123332\B3=1.51410471\B4=1.09035035\B5=1.08355871\B6=1.08289235
\B7=1.0897048\B8=1.08685419\B9=1.08655606\B10=1.40742892\B11=1.4896127
6\B12=1.07342217\B13=1.50977459\B14=1.1932541\B15=1.44513389\B16=1.203
22819\B17=1.33675633\B18=1.41815719\B19=1.08389508\B20=1.080277\B21=1.
08337183\B22=1.53562334\B23=1.08475992\B24=1.08921763\B25=1.39251564\B
26=1.66307407\B27=1.87218537\B28=1.08764715\B29=1.08753371\B30=1.08673
066\B31=1.86779437\B32=1.08596417\B33=1.08711607\B34=1.08754604\B35=1.
86176812\B36=1.08724016\B37=1.08628958\B38=1.08617639\A1=59.60060335\A
2=94.15315892\A3=109.54744303\A4=112.79579085\A5=136.81622663\A6=94.17
778845\A7=108.77138608\A8=110.46914591\A9=31.52099803\A10=137.84314089
\A11=116.646623\A12=112.03845483\A13=122.59509992\A14=125.13203801\A15
=126.45532497\A16=110.85844843\A17=115.94041756\A18=110.6758045\A19=10
5.78033688\A20=110.60772026\A21=100.51225612\A22=107.63997128\A23=109.
3579215\A24=109.09291005\A25=127.5069955\A26=109.34790024\A27=110.9216
9297\A28=111.63036236\A29=111.21213078\A30=110.06397247\A31=110.944721
83\A32=111.93550451\A33=110.50473383\A34=105.00877299\A35=111.26080356
\A36=110.81251629\A37=110.92224984\D1=18.28453885\D2=-70.25399744\D3=1
70.17341114\D4=145.74523746\D5=-93.0661151\D6=90.81579111\D7=-151.4333
0867\D8=142.36503507\D9=106.76960949\D10=-79.61822348\D11=48.34950274\
D12=138.61401153\D13=96.46656988\D14=9.08242138\D15=-171.83725471\D16=
179.83464769\D17=62.26072822\D18=-178.20485413\D19=-58.5316828\D20=107
.51581195\D21=-88.96091939\D22=28.7462776\D23=149.58802493\D24=164.914
96391\D25=78.02265106\D26=179.14172059\D27=-61.2816661\D28=59.23525405
\D29=-42.83407484\D30=-49.01695025\D31=71.04383873\D32=190.6464603\D33
=-163.23540753\D34=-176.61137672\D35=-56.49999187\D36=63.1841799\\Vers
ion=AM64L-G03RevE.01\State=2-A\HF=-1135.2941059\S2=0.760948\S2-1=0.\S2
A=0.750073\RMSD=4.404e-09\RMSF=1.588e-05\Thermal=0.\Dipole=0.7742364,-
0.3407243,-0.4417368\PG=C01 [X(C12H21O5Si1)]\\@

BHandHLYP/6-311++G(d,p)

1\1\GINC-GOMBERG02\FOpt\UBHandHLYP\6-311++G(d,p)\C12H21O5Si1(2)\HMAITK
EN\04-Nov-2010\1\\#BHandHLYP/6-311++G(d,p) opt=(grad,readfc) geom=chec
kpoint guess=read\\6 exo cyclic radical product\\0,2\C\C,1,B1\C,2,B2,1
,A1\C,3,B3,2,A2,1,D1,0\H,1,B4,4,A3,3,D2,0\H,1,B5,4,A4,3,D3,0\H,3,B6,2,
A5,1,D4,0\H,3,B7,2,A6,1,D5,0\H,4,B8,3,A7,2,D6,0\H,4,B9,3,A8,2,D7,0\O,3
,B10,2,A9,1,D8,0\C,2,B11,1,A10,4,D9,0\H,12,B12,2,A11,1,D10,0\C,1,B13,4
,A12,3,D11,0\O,14,B14,1,A13,4,D12,0\C,12,B15,2,A14,1,D13,0\O,16,B16,12
,A15,2,D14,0\O,16,B17,12,A16,2,D15,0\C,18,B18,16,A17,12,D16,0\H,19,B19
,18,A18,16,D17,0\H,19,B20,18,A19,16,D18,0\H,19,B21,18,A20,16,D19,0\C,2
,B22,1,A21,14,D20,0\H,23,B23,2,A22,1,D21,0\H,23,B24,2,A23,1,D22,0\O,23
,B25,2,A24,1,D23,0\Si,26,B26,23,A25,2,D24,0\C,27,B27,26,A26,23,D25,0\H
,28,B28,27,A27,26,D26,0\H,28,B29,27,A28,26,D27,0\H,28,B30,27,A29,26,D2
8,0\C,27,B31,26,A30,23,D29,0\H,32,B32,27,A31,26,D30,0\H,32,B33,27,A32,
26,D31,0\H,32,B34,27,A33,26,D32,0\C,27,B35,26,A34,23,D33,0\H,36,B36,27
,A35,26,D34,0\H,36,B37,27,A36,26,D35,0\H,36,B38,27,A37,26,D36,0\\B1=2.
58938482\B2=2.41414878\B3=1.51418847\B4=1.09035881\B5=1.08362253\B6=1.
08315441\B7=1.08950395\B8=1.08695971\B9=1.08665989\B10=1.40841125\B11=
1.49009738\B12=1.07371945\B13=1.50917115\B14=1.19401101\B15=1.44503666
\B16=1.20360984\B17=1.33802602\B18=1.41836272\B19=1.08371267\B20=1.080
41063\B21=1.08337691\B22=1.5364131\B23=1.08535748\B24=1.08918555\B25=1
.39199738\B26=1.66580115\B27=1.87267557\B28=1.08776432\B29=1.08767445\
B30=1.08690205\B31=1.86808866\B32=1.08617109\B33=1.08721565\B34=1.0877
4962\B35=1.86161181\B36=1.08737765\B37=1.08644256\B38=1.08631913\A1=59
.69055346\A2=94.23170622\A3=109.63308484\A4=112.6574638\A5=136.7705063
2\A6=94.15142749\A7=108.90479903\A8=110.30732957\A9=31.51095639\A10=13
8.63221418\A11=116.66516745\A12=111.91791002\A13=122.62003581\A14=125.
19598926\A15=126.458123\A16=110.88328184\A17=116.15076991\A18=110.6438
9321\A19=105.76348039\A20=110.54841557\A21=99.74438629\A22=107.5722431
7\A23=109.34192405\A24=109.29339825\A25=127.16193362\A26=109.15148914\
A27=110.97942487\A28=111.64749564\A29=111.15535879\A30=109.90313991\A3
1=111.07435018\A32=111.89706548\A33=110.55780949\A34=104.90010475\A35=
111.24488783\A36=110.76509064\A37=110.92415321\D1=17.74479691\D2=-70.5
1344711\D3=169.9305486\D4=145.22411083\D5=-93.71525682\D6=91.87101767\
D7=-150.48644676\D8=142.01331637\D9=107.7427795\D10=-81.14476597\D11=4
8.10513092\D12=137.02214188\D13=95.64858592\D14=7.88118212\D15=-172.92
813399\D16=179.42999302\D17=61.46636549\D18=-179.00024161\D19=-59.4113
0542\D20=109.05797045\D21=-88.49295616\D22=29.0367212\D23=150.08501011
\D24=167.32694067\D25=75.42319588\D26=179.0084291\D27=-61.41613494\D28
=59.11654761\D29=-45.23892447\D30=-51.24914378\D31=68.87612443\D32=188
.42352153\D33=-165.75177199\D34=-176.76472485\D35=-56.66314987\D36=63.
01445434\\Version=AM64L-G03RevE.01\State=2-A\HF=-1135.3082433\S2=0.760
85\S2-1=0.\S2A=0.750073\RMSD=3.196e-09\RMSF=1.656e-05\Thermal=0.\Dipol
e=0.8755203,-0.4787114,-0.4490768\PG=C01 [X(C12H21O5Si1)]\\@

Decarbonylation transition state

HF/3-21G*

1\1\GINC-GOMBERG01\FTS\UHF\3-21G*\C12H21O5Si1(2)\HMAITKEN\03-Dec-2010\
1\\#HF/3-21G* opt=(grad,readfc,ts,noeigentest,nofreeze) geom=checkpoin
t guess=read\\decarbonylation ts\\0,2\C\C,1,B1\O,2,B2,1,A1\C,3,B3,2,A2
,1,D1,0\C,4,B4,3,A3,2,D2,0\H,5,B5,4,A4,3,D3,0\H,2,B6,1,A5,3,D4,0\H,2,B
7,1,A6,3,D5,0\H,1,B8,2,A7,3,D6,0\H,1,B9,2,A8,3,D7,0\C,1,B10,2,A9,3,D8,

0\H,11,B11,1,A10,2,D9,0\H,11,B12,1,A11,2,D10,0\C,11,B13,1,A12,2,D11,0\
O,14,B14,11,A13,1,D12,0\C,5,B15,4,A14,3,D13,0\O,16,B16,5,A15,4,D14,0\O
,16,B17,5,A16,4,D15,0\C,18,B18,16,A17,5,D16,0\H,19,B19,18,A18,16,D17,0
\H,19,B20,18,A19,16,D18,0\H,19,B21,18,A20,16,D19,0\C,4,B22,3,A21,2,D20
,0\H,23,B23,4,A22,3,D21,0\H,23,B24,4,A23,3,D22,0\O,23,B25,4,A24,3,D23,
0\Si,26,B26,23,A25,4,D24,0\C,27,B27,26,A26,23,D25,0\H,28,B28,27,A27,26
,D26,0\H,28,B29,27,A28,26,D27,0\H,28,B30,27,A29,26,D28,0\C,27,B31,26,A
30,23,D29,0\H,32,B32,27,A31,26,D30,0\H,32,B33,27,A32,26,D31,0\H,32,B34
,27,A33,26,D32,0\C,27,B35,26,A34,23,D33,0\H,36,B36,27,A35,26,D34,0\H,3
6,B37,27,A36,26,D35,0\H,36,B38,27,A37,26,D36,0\\B1=1.52748351\B2=1.451
27072\B3=1.35483035\B4=1.33130218\B5=1.06692399\B6=1.0819226\B7=1.0816
7833\B8=1.08144405\B9=1.08106687\B10=1.5137677\B11=1.07843115\B12=1.07
839338\B14=1.15097605\B15=1.4518241\B16=1.20804362\B17=1.35852014\B18=
1.45341164\B19=1.07644431\B20=1.07888457\B21=1.07890497\B22=1.52791968
\B23=1.07376528\B24=1.08087412\B25=1.41347272\B26=1.64312442\B27=1.881
65518\B28=1.08871847\B29=1.08902281\B30=1.08560247\B31=1.88085213\B32=
1.08898761\B33=1.08767202\B34=1.08839485\B35=1.87337187\B36=1.0877944\
B37=1.08884673\B38=1.08479809\A1=106.50586392\A2=121.39605301\A3=122.6
530769\A4=120.74945267\A5=111.28273574\A6=111.10651969\A7=108.76643119
\A8=108.55272651\A9=111.15085891\A10=116.81199042\A11=116.78902885\A12
=104.54239006\A13=119.68861207\A14=127.27252355\A15=124.71358283\A16=1
14.05111361\A17=117.66050187\A18=105.25157298\A19=110.28726623\A20=110
.2272545\A21=112.27753934\A22=108.83161216\A23=107.93133892\A24=112.43
92675\A25=138.28199793\A26=111.0144925\A27=110.66818745\A28=111.568511
87\A29=111.30221705\A30=108.41941663\A31=111.06682265\A32=111.26489037
\A33=111.53371427\A34=109.02220028\A35=110.69033027\A36=111.20311698\A
37=111.47197785\D1=177.44972427\D2=2.70786987\D3=-1.18199463\D4=-119.2
0063951\D5=118.98270224\D6=58.03275518\D7=-58.9942994\D8=-180.41429532
\D9=-69.82071967\D10=69.98820687\D11=-179.90746309\D12=180.05732267\D1
3=-181.54886652\D14=178.16622835\D15=-2.52580747\D16=180.29956128\D17=
-179.68890593\D18=-59.95881813\D19=60.60280407\D20=-178.38747548\D21=-
229.58528211\D22=-113.14048812\D23=10.4169393\D24=-79.89934641\D25=10.
04917867\D26=178.1041392\D27=-62.62633589\D28=57.90227658\D29=-108.938
74475\D30=-177.88604341\D31=-57.98386951\D32=62.16953712\D33=132.85221
05\D34=58.07969143\D35=177.61379221\D36=-61.78492906\B13=1.98545735\\V
ersion=AM64L-G03RevE.01\State=2-A\HF=-1123.8099799\S2=0.806686\S2-1=0.
\S2A=0.750854\RMSD=7.713e-09\RMSF=1.300e-05\Thermal=0.\Dipole=0.246095
4,-0.294251,0.356984\PG=C01 [X(C12H21O5Si1)]\\@

HF/6-31G*

1\1\GINC-GOMBERG01\FTS\UHF\6-31G(d)\C12H21O5Si1(2)\HMAITKEN\04-Dec-201
0\1\\#HF/6-31G* opt=(grad,readfc,ts,noeigentest,nofreeze) geom=checkpo
int guess=read\\decarbonylation ts\\0,2\C\C,1,B1\O,2,B2,1,A1\C,3,B3,2,
A2,1,D1,0\C,4,B4,3,A3,2,D2,0\H,5,B5,4,A4,3,D3,0\H,2,B6,1,A5,3,D4,0\H,2
,B7,1,A6,3,D5,0\H,1,B8,2,A7,3,D6,0\H,1,B9,2,A8,3,D7,0\C,1,B10,2,A9,3,D
8,0\H,11,B11,1,A10,2,D9,0\H,11,B12,1,A11,2,D10,0\C,11,B13,1,A12,2,D11,
0\O,14,B14,11,A13,1,D12,0\C,5,B15,4,A14,3,D13,0\O,16,B16,5,A15,4,D14,0
\O,16,B17,5,A16,4,D15,0\C,18,B18,16,A17,5,D16,0\H,19,B19,18,A18,16,D17
,0\H,19,B20,18,A19,16,D18,0\H,19,B21,18,A20,16,D19,0\C,4,B22,3,A21,2,D
20,0\H,23,B23,4,A22,3,D21,0\H,23,B24,4,A23,3,D22,0\O,23,B25,4,A24,3,D2
3,0\Si,26,B26,23,A25,4,D24,0\C,27,B27,26,A26,23,D25,0\H,28,B28,27,A27,
26,D26,0\H,28,B29,27,A28,26,D27,0\H,28,B30,27,A29,26,D28,0\C,27,B31,26
,A30,23,D29,0\H,32,B32,27,A31,26,D30,0\H,32,B33,27,A32,26,D31,0\H,32,B

34,27,A33,26,D32,0\C,27,B35,26,A34,23,D33,0\H,36,B36,27,A35,26,D34,0\H
,36,B37,27,A36,26,D35,0\H,36,B38,27,A37,26,D36,0\\B1=1.52209925\B2=1.4
0999877\B3=1.32733011\B4=1.34030808\B5=1.07003557\B6=1.08466463\B7=1.0
8428741\B8=1.08448403\B9=1.08417963\B10=1.50860652\B11=1.07972111\B12=
1.0796411\B14=1.13414028\B15=1.46653984\B16=1.19306645\B17=1.33155202\
B18=1.41649805\B19=1.07918929\B20=1.08006076\B21=1.08008483\B22=1.5279
5402\B23=1.07892751\B24=1.08428278\B25=1.38531458\B26=1.65768827\B27=1
.88721245\B28=1.0878028\B29=1.08752852\B30=1.0857883\B31=1.88682526\B3
2=1.08775498\B33=1.08688184\B34=1.08773652\B35=1.87720363\B36=1.086495
11\B37=1.08743816\B38=1.086329\A1=107.15843946\A2=121.30604147\A3=123.
04837593\A4=120.30259381\A5=111.07112936\A6=110.93813826\A7=108.910747
66\A8=108.71389059\A9=111.88386063\A10=116.70920008\A11=116.68794323\A
12=107.82794256\A13=117.12418461\A14=128.1222786\A15=122.63974825\A16=
115.16250838\A17=116.66929603\A18=105.80812717\A19=110.57315824\A20=11
0.5415064\A21=111.3275564\A22=108.54330875\A23=108.10259913\A24=112.30
158519\A25=128.87026426\A26=110.84851159\A27=110.4917172\A28=112.33590
87\A29=111.47922659\A30=109.28614982\A31=111.31415033\A32=111.17176823
\A33=111.85995713\A34=105.69765304\A35=110.98695427\A36=111.59078796\A
37=111.01149576\D1=178.00048264\D2=2.2410107\D3=-0.6284997\D4=-119.864
32392\D5=119.55190961\D6=58.916304\D7=-57.47058547\D8=-179.32280041\D9
=-68.48007949\D10=69.04280412\D11=-179.69268453\D12=180.47548472\D13=-
180.85343102\D14=177.79113614\D15=-2.6904385\D16=179.94650813\D17=-179
.71651743\D18=-60.25970122\D19=60.82667118\D20=-178.17454732\D21=-231.
48283801\D22=-116.02157253\D23=8.34304537\D24=-105.97833925\D25=44.230
83029\D26=179.03723989\D27=-61.55075117\D28=59.30759552\D29=-76.039800
42\D30=-178.45493137\D31=-58.51441012\D32=61.60563158\D33=164.76476444
\D34=58.0823248\D35=178.21236921\D36=-61.46227678\B13=1.98084264\\Vers
ion=AM64L-G03RevE.01\State=2-A\HF=-1129.8675236\S2=0.808987\S2-1=0.\S2
A=0.750961\RMSD=5.388e-09\RMSF=1.637e-05\Thermal=0.\Dipole=0.8049947,-
0.3748653,0.0208221\PG=C01 [X(C12H21O5Si1)]\\@

HF/6-311G**

1\1\GINC-GOMBERG01\FTS\UHF\6-311G(d,p)\C12H21O5Si1(2)\HMAITKEN\07-Dec-
2010\1\\#HF/6-311G** opt=(grad,readfc,ts,noeigentest,nofreeze) geom=ch
eckpoint guess=read\\decarbonylation ts\\0,2\C\C,1,B1\O,2,B2,1,A1\C,3,
B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\H,5,B5,4,A4,3,D3,0\H,2,B6,1,A5,3,D4,
0\H,2,B7,1,A6,3,D5,0\H,1,B8,2,A7,3,D6,0\H,1,B9,2,A8,3,D7,0\C,1,B10,2,A
9,3,D8,0\H,11,B11,1,A10,2,D9,0\H,11,B12,1,A11,2,D10,0\C,11,B13,1,A12,2
,D11,0\O,14,B14,11,A13,1,D12,0\C,5,B15,4,A14,3,D13,0\O,16,B16,5,A15,4,
D14,0\O,16,B17,5,A16,4,D15,0\C,18,B18,16,A17,5,D16,0\H,19,B19,18,A18,1
6,D17,0\H,19,B20,18,A19,16,D18,0\H,19,B21,18,A20,16,D19,0\C,4,B22,3,A2
1,2,D20,0\H,23,B23,4,A22,3,D21,0\H,23,B24,4,A23,3,D22,0\O,23,B25,4,A24
,3,D23,0\Si,26,B26,23,A25,4,D24,0\C,27,B27,26,A26,23,D25,0\H,28,B28,27
,A27,26,D26,0\H,28,B29,27,A28,26,D27,0\H,28,B30,27,A29,26,D28,0\C,27,B
31,26,A30,23,D29,0\H,32,B32,27,A31,26,D30,0\H,32,B33,27,A32,26,D31,0\H
,32,B34,27,A33,26,D32,0\C,27,B35,26,A34,23,D33,0\H,36,B36,27,A35,26,D3
4,0\H,36,B37,27,A36,26,D35,0\H,36,B38,27,A37,26,D36,0\\B1=1.52064966\B
2=1.40790786\B3=1.33363742\B4=1.33530632\B5=1.07084648\B6=1.08624978\B
7=1.08571065\B8=1.0849254\B9=1.08475119\B10=1.50811486\B11=1.08045659\
B12=1.08043759\B14=1.12649283\B15=1.47443731\B16=1.18744973\B17=1.3255
4139\B18=1.41655543\B19=1.07966956\B20=1.08126714\B21=1.0813995\B22=1.
50952933\B23=1.0736545\B24=1.08854084\B25=1.39472226\B26=1.6524877\B27
=1.87992226\B28=1.08817538\B29=1.08737522\B30=1.08646162\B31=1.8812494

3\B32=1.08798852\B33=1.08728463\B34=1.08808854\B35=1.87104823\B36=1.08
667895\B37=1.08783595\B38=1.08670726\A1=107.27849468\A2=121.64171006\A
3=123.11931732\A4=119.42972731\A5=110.75879158\A6=110.92006373\A7=108.
7989868\A8=108.75616495\A9=111.97550476\A10=116.64484115\A11=116.61786
832\A12=108.22714767\A13=117.21659432\A14=130.47410141\A15=121.1912089
2\A16=116.63549836\A17=116.88117217\A18=105.77439688\A19=110.5747016\A
20=110.59202565\A21=108.6327662\A22=110.780419\A23=106.3710918\A24=108
.83311699\A25=129.75519861\A26=110.35245737\A27=110.50407691\A28=112.1
4919142\A29=111.08800235\A30=109.63430644\A31=111.01432305\A32=111.081
33518\A33=111.74641857\A34=105.41121902\A35=110.92159218\A36=111.28482
026\A37=110.89830475\D1=177.02644287\D2=4.82993229\D3=-0.32465388\D4=-
119.82443342\D5=119.77322592\D6=57.71237118\D7=-58.73506945\D8=-180.48
107538\D9=-68.7909327\D10=68.68942375\D11=-180.05800837\D12=179.558988
95\D13=-179.07224276\D14=177.19757853\D15=-3.04433295\D16=179.06375124
\D17=-179.37326483\D18=-59.9574013\D19=61.14855218\D20=-176.15549842\D
21=-174.82411727\D22=-56.57453373\D23=63.80492491\D24=-136.50249611\D2
5=57.69470029\D26=177.78369052\D27=-62.50931089\D28=58.03106448\D29=-6
2.95698389\D30=-178.39246941\D31=-58.52223236\D32=61.80598952\D33=177.
58199878\D34=59.12650752\D35=179.29005191\D36=-60.56708166\B13=1.97308
603\\Version=AM64L-G03RevE.01\State=2-A\HF=-1130.1078229\S2=0.808108\S
2-1=0.\S2A=0.751004\RMSD=5.583e-09\RMSF=1.621e-05\Thermal=0.\Dipole=0.
9637605,-0.2777417,-0.0358083\PG=C01 [X(C12H21O5Si1)]\\@

BHandHLYP/6-311G**

1\1\GINC-GOMBERG01\FTS\UBHandHLYP\6-311G(d,p)\C12H21O5Si1(2)\HMAITKEN\
08-Dec-2010\1\\#BHandHLYP/6-311G** opt=(grad,readfc,ts,noeigentest,nof
reeze) geom=checkpoint guess=read\\decarbonylation ts\\0,2\C\C,1,B1\O,
2,B2,1,A1\C,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\H,5,B5,4,A4,3,D3,0\H,2
,B6,1,A5,3,D4,0\H,2,B7,1,A6,3,D5,0\H,1,B8,2,A7,3,D6,0\H,1,B9,2,A8,3,D7
,0\C,1,B10,2,A9,3,D8,0\H,11,B11,1,A10,2,D9,0\H,11,B12,1,A11,2,D10,0\C,
11,B13,1,A12,2,D11,0\O,14,B14,11,A13,1,D12,0\C,5,B15,4,A14,3,D13,0\O,1
6,B16,5,A15,4,D14,0\O,16,B17,5,A16,4,D15,0\C,18,B18,16,A17,5,D16,0\H,1
9,B19,18,A18,16,D17,0\H,19,B20,18,A19,16,D18,0\H,19,B21,18,A20,16,D19,
0\C,4,B22,3,A21,2,D20,0\H,23,B23,4,A22,3,D21,0\H,23,B24,4,A23,3,D22,0\
O,23,B25,4,A24,3,D23,0\Si,26,B26,23,A25,4,D24,0\C,27,B27,26,A26,23,D25
,0\H,28,B28,27,A27,26,D26,0\H,28,B29,27,A28,26,D27,0\H,28,B30,27,A29,2
6,D28,0\C,27,B31,26,A30,23,D29,0\H,32,B32,27,A31,26,D30,0\H,32,B33,27,
A32,26,D31,0\H,32,B34,27,A33,26,D32,0\C,27,B35,26,A34,23,D33,0\H,36,B3
6,27,A35,26,D34,0\H,36,B37,27,A36,26,D35,0\H,36,B38,27,A37,26,D36,0\\B
1=1.51759215\B2=1.41376788\B3=1.33646053\B4=1.33930177\B5=1.07277742\B
6=1.08808592\B7=1.08745994\B8=1.08595758\B9=1.08584285\B10=1.49296218\
B11=1.07919305\B12=1.07917604\B14=1.12920158\B15=1.46342861\B16=1.1975
908\B17=1.33742311\B18=1.42066907\B19=1.08055345\B20=1.08298841\B21=1.
08297672\B22=1.50324615\B23=1.07671969\B24=1.09153649\B25=1.39954605\B
26=1.65929615\B27=1.86997887\B28=1.08764823\B29=1.08691589\B30=1.08566
354\B31=1.87160001\B32=1.08755701\B33=1.08666684\B34=1.08746138\B35=1.
8613267\B36=1.08620976\B37=1.08722207\B38=1.08616944\A1=107.3030359\A2
=120.54411113\A3=123.01913557\A4=119.34659467\A5=110.95893489\A6=110.9
284813\A7=108.57819002\A8=108.48406687\A9=112.06838424\A10=118.2480529
6\A11=118.21633156\A12=106.00271716\A13=115.50243467\A14=130.45534044\
A15=121.80965564\A16=116.264237\A17=115.74199381\A18=105.73651993\A19=
110.60600481\A20=110.58410327\A21=109.17399841\A22=110.06188339\A23=10
6.69004165\A24=109.74934975\A25=128.16963313\A26=110.53726064\A27=110.

4425955\A28=112.09696713\A29=111.02195746\A30=109.57989814\A31=111.048
78009\A32=111.08015291\A33=111.6166257\A34=105.05116659\A35=110.920953
\A36=111.22250457\A37=110.87264868\D1=176.78357816\D2=3.66310328\D3=-0
.2858631\D4=-119.86561128\D5=119.70435852\D6=57.65030325\D7=-58.501964
68\D8=-180.37538391\D9=-72.7673659\D10=72.50162615\D11=-180.14942811\D
12=179.65915723\D13=-179.4613476\D14=175.86269552\D15=-4.65033314\D16=
179.24064348\D17=-179.90356325\D18=-60.30600479\D19=60.44958992\D20=-1
77.53916182\D21=-182.45509116\D22=-64.92993566\D23=56.31277301\D24=-12
5.17097011\D25=52.43329638\D26=178.02462001\D27=-62.32413285\D28=58.08
254035\D29=-68.23971593\D30=-178.73872732\D31=-58.75943689\D32=61.4939
0326\D33=172.4600006\D34=58.33195724\D35=178.46215584\D36=-61.39734332
\B13=2.12278367\\Version=AM64L-G03RevE.01\State=2-A\HF=-1135.2503428\S
2=0.77138\S2-1=0.\S2A=0.750148\RMSD=2.771e-09\RMSF=2.460e-05\Thermal=0
.\Dipole=0.6994681,-0.366526,-0.2268277\PG=C01 [X(C12H21O5Si1)]\\@

BHandHLYP/6-311++G(d,p)

1\1\GINC-GOMBERG01\FTS\UBHandHLYP\6-311++G(d,p)\C12H21O5Si1(2)\HMAITKE
N\10-Dec-2010\1\\#BHandHLYP/6-311++G(d,p) opt=(grad,readfc,ts,noeigent
est,nofreeze) geom=checkpoint guess=read\\decarbonylation ts\\0,2\C\C,
1,B1\O,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\H,5,B5,4,A4,3,D
3,0\H,2,B6,1,A5,3,D4,0\H,2,B7,1,A6,3,D5,0\H,1,B8,2,A7,3,D6,0\H,1,B9,2,
A8,3,D7,0\C,1,B10,2,A9,3,D8,0\H,11,B11,1,A10,2,D9,0\H,11,B12,1,A11,2,D
10,0\C,11,B13,1,A12,2,D11,0\O,14,B14,11,A13,1,D12,0\C,5,B15,4,A14,3,D1
3,0\O,16,B16,5,A15,4,D14,0\O,16,B17,5,A16,4,D15,0\C,18,B18,16,A17,5,D1
6,0\H,19,B19,18,A18,16,D17,0\H,19,B20,18,A19,16,D18,0\H,19,B21,18,A20,
16,D19,0\C,4,B22,3,A21,2,D20,0\H,23,B23,4,A22,3,D21,0\H,23,B24,4,A23,3
,D22,0\O,23,B25,4,A24,3,D23,0\Si,26,B26,23,A25,4,D24,0\C,27,B27,26,A26
,23,D25,0\H,28,B28,27,A27,26,D26,0\H,28,B29,27,A28,26,D27,0\H,28,B30,2
7,A29,26,D28,0\C,27,B31,26,A30,23,D29,0\H,32,B32,27,A31,26,D30,0\H,32,
B33,27,A32,26,D31,0\H,32,B34,27,A33,26,D32,0\C,27,B35,26,A34,23,D33,0\
H,36,B36,27,A35,26,D34,0\H,36,B37,27,A36,26,D35,0\H,36,B38,27,A37,26,D
36,0\\B1=1.51811515\B2=1.4138149\B3=1.33690901\B4=1.33986933\B5=1.0730
2587\B6=1.08807022\B7=1.08747819\B8=1.08604501\B9=1.08591834\B10=1.492
4718\B11=1.07910325\B12=1.07907685\B14=1.12960326\B15=1.46330228\B16=1
.19978966\B17=1.33570746\B18=1.42125742\B19=1.08063754\B20=1.08283307\
B21=1.08289\B22=1.5023417\B23=1.07731308\B24=1.09111528\B25=1.40105876
\B26=1.66231506\B27=1.87024735\B28=1.08775637\B29=1.08700637\B30=1.086
14879\B31=1.87191484\B32=1.08771524\B33=1.08687387\B34=1.08759087\B35=
1.86133526\B36=1.08636566\B37=1.08732912\B38=1.08635363\A1=107.2992848
3\A2=120.73326142\A3=122.94277257\A4=119.30311326\A5=110.89105891\A6=1
10.99508738\A7=108.61303378\A8=108.55023136\A9=111.93547673\A10=118.35
682594\A11=118.37474868\A12=105.90084464\A13=115.3964778\A14=130.31828
213\A15=121.67166296\A16=116.42766228\A17=116.08565472\A18=105.6682311
2\A19=110.5450882\A20=110.57848228\A21=108.95733945\A22=110.34063469\A
23=106.5965012\A24=109.23960593\A25=127.68038235\A26=110.10616626\A27=
110.72537389\A28=111.97618778\A29=110.92584673\A30=109.55807477\A31=11
0.9976\A32=111.0808326\A33=111.72335443\A34=104.79128392\A35=110.82421
009\A36=111.31387115\A37=110.8206349\D1=176.91349177\D2=4.20008992\D3=
-0.08602052\D4=-119.80734563\D5=119.67075501\D6=57.58628086\D7=-58.614
43416\D8=-180.49701035\D9=-73.01422448\D10=73.09770319\D11=-179.946677
63\D12=180.23270314\D13=-178.78446085\D14=176.65649872\D15=-3.56053199
\D16=179.02134693\D17=-179.66886895\D18=-60.15934857\D19=60.72745426\D
20=-176.48219552\D21=-174.74307001\D22=-56.7902155\D23=64.00354386\D24

=-131.93231731\D25=58.68902226\D26=178.15164847\D27=-62.05125929\D28=5
8.21175888\D29=-61.98386659\D30=-178.53352202\D31=-58.64863448\D32=61.
74108943\D33=178.58862197\D34=59.2239132\D35=179.41199036\D36=-60.4092
8067\B13=2.1368968\\Version=AM64L-G03RevE.01\State=2-A\HF=-1135.264110
3\S2=0.771132\S2-1=0.\S2A=0.75015\RMSD=5.351e-09\RMSF=2.750e-05\Therma
l=0.\Dipole=0.8383761,-0.2879617,-0.2608654\PG=C01 [X(C12H21O5Si1)]\\@

Decarbonylation product

HF/3-21G*

1\1\GINC-GOMBERG11\FOpt\UHF\3-21G*\C11H21O4Si1(2)\HMAITKEN\09-Nov-2010
\1\\#HF/3-21G* opt=(grad)\\decarbonylation\\0,2\C\O,1,B1\C,2,B2,1,A1\C
,3,B3,2,A2,1,D1,0\H,3,B4,2,A3,1,D2,0\H,1,B5,2,A4,3,D3,0\H,1,B6,2,A5,3,
D4,0\C,1,B7,2,A6,3,D5,0\H,8,B8,1,A7,2,D6,0\H,8,B9,1,A8,2,D7,0\C,8,B10,
1,A9,2,D8,0\H,11,B11,8,A10,1,D9,0\H,11,B12,8,A11,1,D10,0\C,4,B13,3,A12
,2,D11,0\O,14,B14,4,A13,3,D12,0\O,14,B15,4,A14,3,D13,0\C,16,B16,14,A15
,4,D14,0\H,17,B17,16,A16,14,D15,0\H,17,B18,16,A17,14,D16,0\H,17,B19,16
,A18,14,D17,0\C,4,B20,3,A19,2,D18,0\H,21,B21,4,A20,3,D19,0\H,21,B22,4,
A21,3,D20,0\O,21,B23,4,A22,3,D21,0\Si,24,B24,21,A23,4,D22,0\C,25,B25,2
4,A24,21,D23,0\H,26,B26,25,A25,24,D24,0\H,26,B27,25,A26,24,D25,0\H,26,
B28,25,A27,24,D26,0\C,25,B29,24,A28,21,D27,0\H,30,B30,25,A29,24,D28,0\
H,30,B31,25,A30,24,D29,0\H,30,B32,25,A31,24,D30,0\C,25,B33,24,A32,21,D
31,0\H,34,B34,25,A33,24,D32,0\H,34,B35,25,A34,24,D33,0\H,34,B36,25,A35
,24,D34,0\\B1=1.46312165\B2=1.34099482\B3=1.33231633\B4=1.06922347\B5=
1.07783979\B6=1.07967489\B7=1.52827603\B8=1.08718353\B9=1.08200285\B10
=1.5070197\B11=1.07227555\B12=1.07445301\B13=1.46218511\B14=1.21482813
\B15=1.35129498\B16=1.45316691\B17=1.07620973\B18=1.07875161\B19=1.079
08786\B20=1.50409931\B21=1.07899915\B22=1.07649849\B23=1.44612097\B24=
1.65627483\B25=1.8787313\B26=1.08567735\B27=1.08914962\B28=1.08789147\
B29=1.87686493\B30=1.08830462\B31=1.0889943\B32=1.08661915\B33=1.87759
366\B34=1.08773063\B35=1.0887019\B36=1.08753287\A1=125.22665091\A2=130
.67525045\A3=110.47794966\A4=109.60066946\A5=108.56775824\A6=105.77543
941\A7=107.74406669\A8=108.7193478\A9=111.02307273\A10=120.98315073\A1
1=119.96229753\A12=118.07826952\A13=124.51859738\A14=114.25935822\A15=
118.08383672\A16=105.15268905\A17=110.26520286\A18=110.24394286\A19=12
7.21105892\A20=108.20840099\A21=110.910501\A22=113.03390535\A23=131.33
720816\A24=111.44230393\A25=110.5963255\A26=110.58132179\A27=111.81319
2\A28=110.15952502\A29=111.96071941\A30=110.70344973\A31=110.30209969\
A32=105.85053493\A33=111.4120165\A34=111.06658126\A35=111.11463662\D1=
-16.34203161\D2=163.63637912\D3=-26.45766036\D4=93.71999691\D5=-147.42
719665\D6=58.40862009\D7=-57.67377694\D8=179.97985121\D9=-220.87470861
\D10=-50.73185255\D11=174.06775967\D12=-171.74508272\D13=7.48280742\D1
4=-178.31646601\D15=-179.57175066\D16=-59.87100722\D17=60.79176997\D18
=-2.56717171\D19=-154.34056005\D20=-35.91982431\D21=83.90806046\D22=86
.42414485\D23=-81.2984545\D24=69.54535713\D25=-171.23554878\D26=-51.33
455327\D27=40.0752885\D28=57.0047135\D29=176.95836824\D30=-63.84986047
\D31=159.6699751\D32=59.62318741\D33=179.57472472\D34=-60.5228823\\Ver
sion=AM64L-G03RevE.01\State=2-A\HF=-1011.7389369\S2=0.763226\S2-1=0.\S
2A=0.750127\RMSD=3.769e-09\RMSF=1.076e-06\Thermal=0.\Dipole=-0.6203316
,-0.026895,0.4215269\PG=C01 [X(C11H21O4Si1)]\\@

HF/6-31G*

1\1\GINC-GOMBERG07\FOpt\UHF\6-31G(d)\C11H21O4Si1(2)\HMAITKEN\09-Nov-20

10\1\\#HF/6-31G* opt=(grad,readfc) geom=checkpoint guess=read\\decarbo
nylation\\0,2\C\O,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\H,3,B4,2,A3,1,D2
,0\H,1,B5,2,A4,3,D3,0\H,1,B6,2,A5,3,D4,0\C,1,B7,2,A6,3,D5,0\H,8,B8,1,A
7,2,D6,0\H,8,B9,1,A8,2,D7,0\C,8,B10,1,A9,2,D8,0\H,11,B11,8,A10,1,D9,0\
H,11,B12,8,A11,1,D10,0\C,4,B13,3,A12,2,D11,0\O,14,B14,4,A13,3,D12,0\O,
14,B15,4,A14,3,D13,0\C,16,B16,14,A15,4,D14,0\H,17,B17,16,A16,14,D15,0\
H,17,B18,16,A17,14,D16,0\H,17,B19,16,A18,14,D17,0\C,4,B20,3,A19,2,D18,
0\H,21,B21,4,A20,3,D19,0\H,21,B22,4,A21,3,D20,0\O,21,B23,4,A22,3,D21,0
\Si,24,B24,21,A23,4,D22,0\C,25,B25,24,A24,21,D23,0\H,26,B26,25,A25,24,
D24,0\H,26,B27,25,A26,24,D25,0\H,26,B28,25,A27,24,D26,0\C,25,B29,24,A2
8,21,D27,0\H,30,B30,25,A29,24,D28,0\H,30,B31,25,A30,24,D29,0\H,30,B32,
25,A31,24,D30,0\C,25,B33,24,A32,21,D31,0\H,34,B34,25,A33,24,D32,0\H,34
,B35,25,A34,24,D33,0\H,34,B36,25,A35,24,D34,0\\B1=1.41998846\B2=1.3203
4116\B3=1.33959216\B4=1.07119451\B5=1.07994427\B6=1.08263675\B7=1.5204
2661\B8=1.09013924\B9=1.08518395\B10=1.500092\B11=1.07430213\B12=1.076
07777\B13=1.48106558\B14=1.19651163\B15=1.32876865\B16=1.41590985\B17=
1.07899245\B18=1.08008146\B19=1.08019238\B20=1.51292751\B21=1.07989186
\B22=1.07916931\B23=1.40492227\B24=1.66087684\B25=1.88474722\B26=1.085
2605\B27=1.08821742\B28=1.08732538\B29=1.8846288\B30=1.08750143\B31=1.
08802964\B32=1.08571984\B33=1.88329252\B34=1.08705288\B35=1.08766604\B
36=1.0868135\A1=124.59295108\A2=132.36672057\A3=109.09050677\A4=109.85
177047\A5=109.20266996\A6=106.97766615\A7=108.18941281\A8=109.10023462
\A9=111.79774682\A10=120.35121848\A11=120.32212698\A12=117.18199733\A1
3=123.32633075\A14=114.97808964\A15=116.92564544\A16=105.72148736\A17=
110.60152642\A18=110.60469664\A19=127.99311269\A20=108.02260674\A21=11
0.42923335\A22=113.47690736\A23=130.36258026\A24=111.12383431\A25=111.
50355006\A26=110.76516803\A27=111.28028951\A28=110.64438949\A29=111.73
9849\A30=110.3326003\A31=111.66930103\A32=104.80589592\A33=111.1797386
3\A34=111.46471643\A35=111.248216\D1=-7.87239106\D2=172.10764114\D3=-4
0.51372826\D4=79.14170819\D5=-161.44836276\D6=57.26355741\D7=-58.15918
839\D8=179.45807112\D9=-206.95450534\D10=-43.2533857\D11=176.88268547\
D12=-175.50923181\D13=4.55828768\D14=-179.50773882\D15=-180.08927928\D
16=-60.68155336\D17=60.52478681\D18=-1.4545967\D19=-154.83697908\D20=-
38.15302784\D21=82.20359162\D22=97.25734174\D23=-85.98584515\D24=67.45
907595\D25=-172.7244538\D26=-53.25661937\D27=36.6251164\D28=55.2174626
5\D29=174.55164689\D30=-65.97437104\D31=155.84915033\D32=58.82248279\D
33=178.77835505\D34=-61.00253407\\Version=AM64L-G03RevE.01\State=2-A\H
F=-1017.1526138\S2=0.762138\S2-1=0.\S2A=0.750098\RMSD=4.953e-09\RMSF=6
.354e-06\Thermal=0.\Dipole=-0.7040418,-0.0823308,0.2250406\PG=C01 [X(C
11H21O4Si1)]\\@

HF/6-311G**

1\1\GINC-GOMBERG04\FOpt\UHF\6-311G(d,p)\C11H21O4Si1(2)\HMAITKEN\10-Nov
-2010\1\\#HF/6-311G** opt=(grad,readfc) geom=checkpoint guess=read\\de
carbonylation\\0,2\C\O,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\H,3,B4,2,A3
,1,D2,0\H,1,B5,2,A4,3,D3,0\H,1,B6,2,A5,3,D4,0\C,1,B7,2,A6,3,D5,0\H,8,B
8,1,A7,2,D6,0\H,8,B9,1,A8,2,D7,0\C,8,B10,1,A9,2,D8,0\H,11,B11,8,A10,1,
D9,0\H,11,B12,8,A11,1,D10,0\C,4,B13,3,A12,2,D11,0\O,14,B14,4,A13,3,D12
,0\O,14,B15,4,A14,3,D13,0\C,16,B16,14,A15,4,D14,0\H,17,B17,16,A16,14,D
15,0\H,17,B18,16,A17,14,D16,0\H,17,B19,16,A18,14,D17,0\C,4,B20,3,A19,2
,D18,0\H,21,B21,4,A20,3,D19,0\H,21,B22,4,A21,3,D20,0\O,21,B23,4,A22,3,
D21,0\Si,24,B24,21,A23,4,D22,0\C,25,B25,24,A24,21,D23,0\H,26,B26,25,A2
5,24,D24,0\H,26,B27,25,A26,24,D25,0\H,26,B28,25,A27,24,D26,0\C,25,B29,

24,A28,21,D27,0\H,30,B30,25,A29,24,D28,0\H,30,B31,25,A30,24,D29,0\H,30
,B32,25,A31,24,D30,0\C,25,B33,24,A32,21,D31,0\H,34,B34,25,A33,24,D32,0
\H,34,B35,25,A34,24,D33,0\H,34,B36,25,A35,24,D34,0\\B1=1.4194548\B2=1.
318496\B3=1.33830141\B4=1.0718866\B5=1.08136096\B6=1.08378468\B7=1.518
41416\B8=1.09086053\B9=1.08579255\B10=1.49947111\B11=1.0749461\B12=1.0
7682765\B13=1.48171206\B14=1.19104583\B15=1.32638398\B16=1.41558832\B1
7=1.07953756\B18=1.08137317\B19=1.0815693\B20=1.51218105\B21=1.0809413
7\B22=1.07931742\B23=1.40403186\B24=1.65582076\B25=1.87809018\B26=1.08
559807\B27=1.08846499\B28=1.08760433\B29=1.87869913\B30=1.08781726\B31
=1.08828199\B32=1.08609024\B33=1.87711511\B34=1.08735271\B35=1.0880353
5\B36=1.08714058\A1=124.51727392\A2=132.3914623\A3=109.41365229\A4=109
.88374281\A5=109.24090573\A6=107.06642139\A7=108.20009372\A8=109.14486
223\A9=111.94090611\A10=120.23981048\A11=120.37900834\A12=117.21445697
\A13=123.18020199\A14=114.96787896\A15=117.22270632\A16=105.7474869\A1
7=110.63739211\A18=110.64123639\A19=128.05784733\A20=107.84958768\A21=
110.45307162\A22=113.29933192\A23=131.83773698\A24=110.81481523\A25=11
1.14990334\A26=110.6683783\A27=111.09967309\A28=110.43757056\A29=111.6
5399827\A30=110.15884526\A31=111.39203925\A32=105.0171663\A33=111.0001
8633\A34=111.26144794\A35=111.1017693\D1=-7.93959175\D2=171.86093648\D
3=-40.64084039\D4=79.1094147\D5=-161.51407552\D6=57.71718662\D7=-57.74
411165\D8=179.76627292\D9=-203.95893255\D10=-39.91143421\D11=176.24990
225\D12=-174.52051896\D13=5.40630424\D14=-179.48776754\D15=-179.432979
8\D16=-59.9969738\D17=61.18474129\D18=-1.80050543\D19=-153.75108803\D2
0=-37.08890393\D21=83.50500717\D22=100.11623423\D23=-88.44588\D24=66.6
4202198\D25=-173.56227797\D26=-54.00108155\D27=33.82245805\D28=56.1305
8983\D29=175.50674953\D30=-65.11332156\D31=153.18849305\D32=58.5643346
2\D33=178.47528676\D34=-61.33060328\\Version=AM64L-G03RevE.01\State=2-
A\HF=-1017.3628863\S2=0.762323\S2-1=0.\S2A=0.750101\RMSD=6.407e-09\RMS
F=1.107e-05\Thermal=0.\Dipole=-0.6743561,-0.0821008,0.2163922\PG=C01 [
X(C11H21O4Si1)]\\@

BHandHLYP/6-311G**

1\1\GINC-GOMBERG03\FOpt\UBHandHLYP\6-311G(d,p)\C11H21O4Si1(2)\HMAITKEN
\11-Nov-2010\1\\#BHandHLYP/6-311G** opt=(grad,readfc) geom=checkpoint
guess=read\\decarbonylation\\0,2\C\O,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,1,D1
,0\H,3,B4,2,A3,1,D2,0\H,1,B5,2,A4,3,D3,0\H,1,B6,2,A5,3,D4,0\C,1,B7,2,A
6,3,D5,0\H,8,B8,1,A7,2,D6,0\H,8,B9,1,A8,2,D7,0\C,8,B10,1,A9,2,D8,0\H,1
1,B11,8,A10,1,D9,0\H,11,B12,8,A11,1,D10,0\C,4,B13,3,A12,2,D11,0\O,14,B
14,4,A13,3,D12,0\O,14,B15,4,A14,3,D13,0\C,16,B16,14,A15,4,D14,0\H,17,B
17,16,A16,14,D15,0\H,17,B18,16,A17,14,D16,0\H,17,B19,16,A18,14,D17,0\C
,4,B20,3,A19,2,D18,0\H,21,B21,4,A20,3,D19,0\H,21,B22,4,A21,3,D20,0\O,2
1,B23,4,A22,3,D21,0\Si,24,B24,21,A23,4,D22,0\C,25,B25,24,A24,21,D23,0\
H,26,B26,25,A25,24,D24,0\H,26,B27,25,A26,24,D25,0\H,26,B28,25,A27,24,D
26,0\C,25,B29,24,A28,21,D27,0\H,30,B30,25,A29,24,D28,0\H,30,B31,25,A30
,24,D29,0\H,30,B32,25,A31,24,D30,0\C,25,B33,24,A32,21,D31,0\H,34,B34,2
5,A33,24,D32,0\H,34,B35,25,A34,24,D33,0\H,34,B36,25,A35,24,D34,0\\B1=1
.42585345\B2=1.32028068\B3=1.34229059\B4=1.07492213\B5=1.08410899\B6=1
.08562721\B7=1.51331337\B8=1.09391111\B9=1.08713407\B10=1.48467087\B11
=1.07461005\B12=1.07653796\B13=1.47167675\B14=1.20156528\B15=1.3361640
6\B16=1.41953025\B17=1.08043935\B18=1.08294847\B19=1.08330451\B20=1.50
418476\B21=1.083613\B22=1.08164514\B23=1.4113073\B24=1.66606173\B25=1.
86835866\B26=1.08550396\B27=1.08786747\B28=1.08681357\B29=1.86826451\B
30=1.08705786\B31=1.08769606\B32=1.08604298\B33=1.86652739\B34=1.08671

478\B35=1.08737907\B36=1.08643062\A1=123.4727984\A2=132.17426875\A3=10
9.56544316\A4=109.87843876\A5=109.06448349\A6=107.01389034\A7=107.7834
2071\A8=109.31411357\A9=112.17073916\A10=120.69721568\A11=120.65447405
\A12=117.31333209\A13=123.55290625\A14=114.71348449\A15=116.14481216\A
16=105.70859529\A17=110.64137908\A18=110.67736593\A19=127.8336643\A20=
107.71315363\A21=110.57574201\A22=113.48141839\A23=128.90767329\A24=11
0.94694405\A25=110.68227285\A26=110.65620462\A27=111.3588246\A28=110.1
0230799\A29=111.80967329\A30=110.26480436\A31=110.86701322\A32=104.432
34147\A33=111.01937686\A34=111.13524512\A35=111.06567549\D1=-4.5219620
8\D2=174.8356993\D3=-41.88089673\D4=77.79905971\D5=-162.81936655\D6=56
.92060045\D7=-57.78642314\D8=178.95291315\D9=-205.17538871\D10=-35.550
60616\D11=175.44564964\D12=-171.98423725\D13=7.78263919\D14=-179.04456
601\D15=-178.84285697\D16=-59.23170266\D17=61.64334868\D18=-1.25775626
\D19=-157.64070092\D20=-40.7920903\D21=79.67365799\D22=94.50711086\D23
=-83.85159283\D24=67.42234143\D25=-173.09730688\D26=-53.29016224\D27=3
8.01408\D28=56.03496418\D29=175.69125777\D30=-65.19820709\D31=157.5539
3648\D32=58.37692839\D33=178.24754948\D34=-61.59684832\\Version=AM64L-
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\RMSD=4.849e-09\RMSF=1.481e-05\Thermal=0.\Dipole=-0.6009889,-0.1153588
,0.2096549\PG=C01 [X(C11H21O4Si1)]\\@

BHandHLYP/6-311++G(d,p)

1\1\GINC-GOMBERG03\FOpt\UBHandHLYP\6-311++G(d,p)\C11H21O4Si1(2)\HMAITK
EN\25-Nov-2010\0\\#BHandHLYP/6-311++G(d,p) opt=(readfc) geom=checkpoin
t guess=read\\decarbonylation\\0,2\C,0.0048302404,0.0129463379,0.00086
825\O,0.0056311316,0.0667176182,1.4258371978\C,1.1044562132,0.04702725
95,2.1585272188\C,2.4028497636,-0.061754942,1.8321370694\H,0.846141385
2,0.1532942858,3.1965632682\H,0.7656041982,0.6777295866,-0.3924107981\
H,0.2198400129,-1.0036701121,-0.3135109268\C,-1.3760362136,0.427170688
,-0.4597622862\H,-1.584389509,1.4189419978,-0.0477640279\H,-2.11790225
44,-0.2385689633,-0.0258214529\C,-1.489377458,0.4452923134,-1.94005834
25\H,-2.4432320954,0.3180843327,-2.4186803822\H,-0.65502872,0.74258741
96,-2.5521663418\C,3.3839944275,0.0406423597,2.9250035584\O,4.57298742
36,0.0672255767,2.749008535\O,2.8542385702,0.1072684293,4.1503820196\C
,3.7720784655,0.2158386917,5.2283199374\H,3.167844133,0.2546510779,6.1
233197554\H,4.4321533003,-0.6423447406,5.2549034452\H,4.3665441397,1.1
163442685,5.1346841276\C,2.9977627241,-0.2162397772,0.4585351832\H,3.9
879977622,-0.6414636448,0.5720729208\H,2.4170213789,-0.9114873948,-0.1
323836663\O,3.0567313273,0.9951500684,-0.263236285\Si,4.3147012015,2.0
81524768,-0.3951530511\C,4.3463467057,3.2365454276,1.0737133335\H,4.58
41913007,2.6966636432,1.9852760114\H,5.1003953499,4.0092988069,0.93931
16482\H,3.3870702187,3.7298849024,1.2076376339\C,5.9379989346,1.165069
0305,-0.5237479404\H,5.9403243477,0.4663517354,-1.3566998748\H,6.75568
52922,1.8653768333,-0.6798036436\H,6.1480427155,0.6133343796,0.3882124
182\C,3.9423033708,3.0331724741,-1.9567420596\H,2.9755576104,3.5254272
837,-1.8906498485\H,4.6924893992,3.7993987254,-2.1378872803\H,3.921950
2017,2.3741017134,-2.820344061\\Version=AM64L-G03RevE.01\State=2-A\HF=
-1021.9815127\S2=0.755262\S2-1=0.\S2A=0.750018\RMSD=5.879e-09\RMSF=2.2
09e-06\Thermal=0.\Dipole=-0.5892072,-0.0524017,0.1435386\PG=C01 [X(C11
H21O4Si1)]\\@