Catalytic Kinetic Resolution of a Dynamic Racemate: Highly Stereoselective β-Lactone Formation by *N*-Heterocyclic Carbene Catalysis

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Supporting Information

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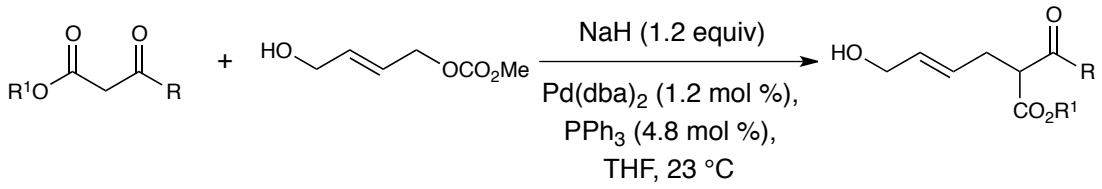
General Information

All reactions were carried out under a nitrogen atmosphere in oven-dried glassware with magnetic stirring. THF, toluene, and DMF were purified by passage through a bed of activated alumina.[1] Reagents were purified prior to use unless otherwise stated following the guidelines of Perrin and Armarego.[2] 1,2-Dichloroethane (DCE) was distilled from CaH_2 and carefully degassed (3 freeze/pump thaw cycles). Purification of reaction products was carried out by flash chromatography using EM Reagent silica gel 60 (230-400 mesh). Analytical thin layer chromatography was performed on EM Reagent 0.25 mm silica gel 60-F plates. Visualization was accomplished with UV light and ceric ammonium nitrate stain or potassium permangenate stain followed by heating. Infrared spectra were recorded on a Bruker Tensor 37 FT-IR spectrometer. ^{1}H NMR spectra were recorded on AVANCE III 500 MHz w/ direct cryoprobe (500 MHz) spectrometer, INOVA 500 MHz (funded by NSF CHE-9871268) spectrometer, 500 MHz DRR2 (variable temperature experiment) and are reported in ppm using solvent as an internal standard ($CDCl_3$ at 7.26 ppm and CD_2Cl_2 at 5.32 ppm). Data are reported as (ap = apparent, s = singlet, d = doublet, t = apparent triplet, q = quartet, m = multiplet, b = broad; coupling constant(s) in Hz; integration.) Proton-decoupled ^{13}C NMR spectra were recorded on an AVANCE III 500 MHz w/ direct cryoprobe (125 MHz) spectrometer and are reported in ppm using solvent as an internal standard ($CDCl_3$ at 77.0 ppm). Mass spectra were obtained on a WATERS Acquity-H UPLC-MS with a single quad detector (ESI) or on a Varian 1200 Quadrupole Mass Spectrometer and Micromass Quadro II Spectrometer (ESI). Ethyl benzoyl acetate was purchased from VWR and was used as is.

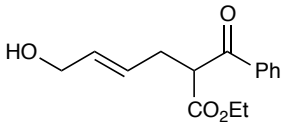
General Procedure for the Tsuji-Trost Allylation of β-Ketoesters



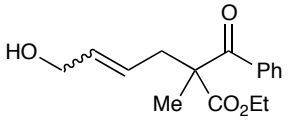
The allylic alcohols were prepared according to the reported procedure.[3] In a flame dried 50 mL round-bottomed flask was added $Pd(dba)_2$ (0.012 equiv) and triphenylphosphine (0.048 equiv). The flask was purged and diluted with THF (11 mL).In a flame dried 100 mL round-bottomed flask was added sodium hydride (60% in mineral oil) (1.2 equiv) and THF (33 mL) under nitrogen. Ethyl benzoylacetate (1.2 equiv) was slowly added to the NaH suspension at 23 °C causing a vigorous reaction. At the end of this addition, the solution becomes homogeneous and slightly yellow. At this time, THF (22 mL) and 4-hydroxybut-2-en-1-yl methyl carbonate (13.01 mmol) was added to the palladium catalyst and after 5 min of stirring; the catalyst solution was

[1] Pangborn, A. B.; Giardello, M. A.; Grubbs, R. H.; Rosen, R. K.; Timmers F. J., *Organometallics* **1996**, *15*, 1518-1520.
[2] Perrin, D. D.; Armarego, W. L. *Purification of Laboratory Chemicals;* 3rd Ed., Pergamon Press, Oxford. 1988.
[3] Cohen, D. T.; Eichman, C. C.; Phillips, E. M.; Zarefsky, E. R.; Scheidt, K. A. "*Angew. Chem. Int. Ed.* **2012**, *51,* 7309–7313.

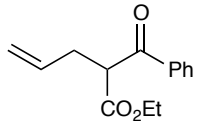
added to the sodium ketoester solution, which turns solution heterogeneous and yellow. The reaction mixture was stirred at 23 °C until completion (3-12 hrs). The reaction mixture was quenched by the addition of saturated NH_4Cl (30 mL) and EtOAc (20 mL). The layers were separated and the aqueous layer was back extracted with EtOAc (40 mL). The combined organic was washed with brine, dried over $MgSO_4$, filtered, and concentrated *in-vacuo*. The material was purified by flash chromatography EtOAc/hexanes (4:6) to afford 3.14 g (92% yield) of ethyl 2-benzoyl-6-hydroxyhex-4-enoate.



***(E)*-ethyl 2-benzoyl-6-hydroxyhex-4-enoate:** Prepared according to the general procedure using ethyl 3-oxo-3-phenylpropanoate (3.00 g, 15.31 mmol) and purified by flash chromatography using 40% EtOAc/hexanes to afford 3.14 g (92% yield) of product as a yellowish oil. Analytical data: ^{1}H NMR (500 MHz; $CDCl_3$): δ 7.99-7.97 (m, 2H), 7.59 (dddd, *J* = 7.4,7.4, 1.5, 1.5 Hz, 1H), 7.49-7.46 (m, 2H), 5.76-5.66 (m, 2H), 4.38 (ap t, *J* = 7.2 Hz, 1H), 4.18-4.09 (m, 2H), 4.05 (ap t, *J* = 4.4 Hz, 2H), 2.76-2.73 (m, 2H), 1.49 (bs, 1H), 1.16 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (125 MHz; $CDCl_3$): δ 194.6, 169.5, 136.2, 133.8, 132.2, 128.89(2C), 128.75(2C), 128.3, 63.4, 61.7, 54.2, 31.6, 14.1; IR (film) 3412, 3062, 2982, 2927, 2869, 1734, 1686, 1597, 1581, 1448, 1391, 1369, 1296, 1266, 1232, 1183, 1159, 1096, 1052, 1001, 973, 944, 889, 856, 777, 736, 689 cm^{-1}; LRMS (ESI): Mass calcd for $C_{15}H_{17}O_4$ $[M–H]^-$: 261; found 261.

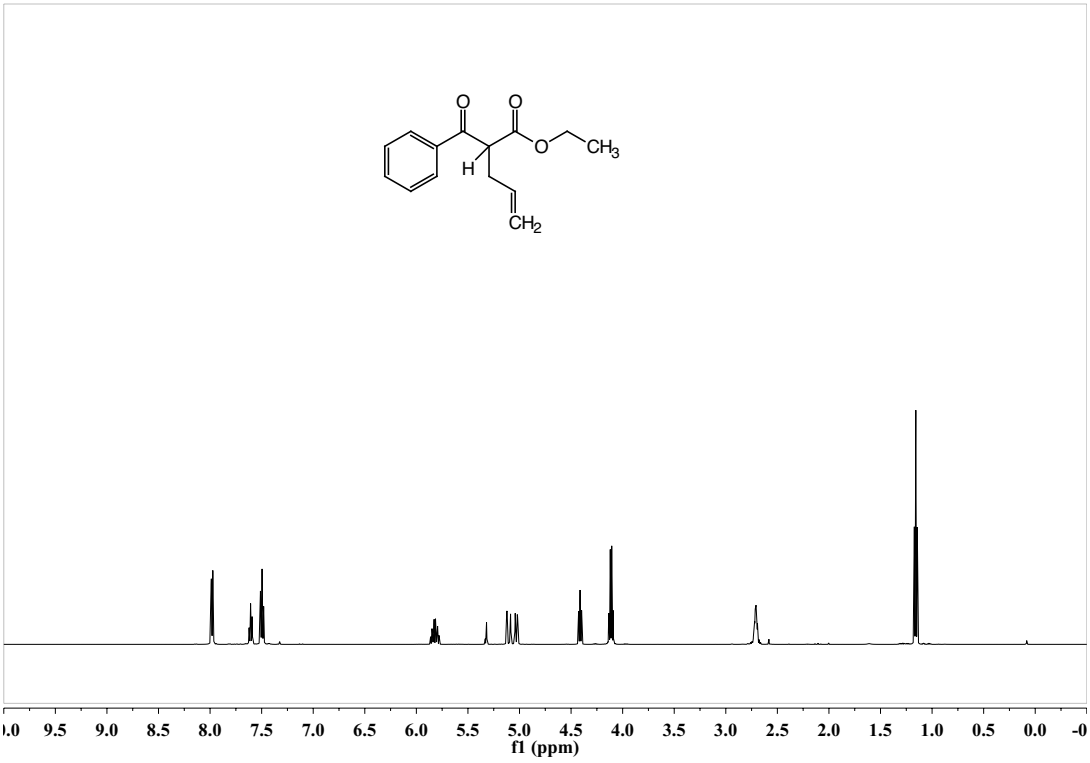


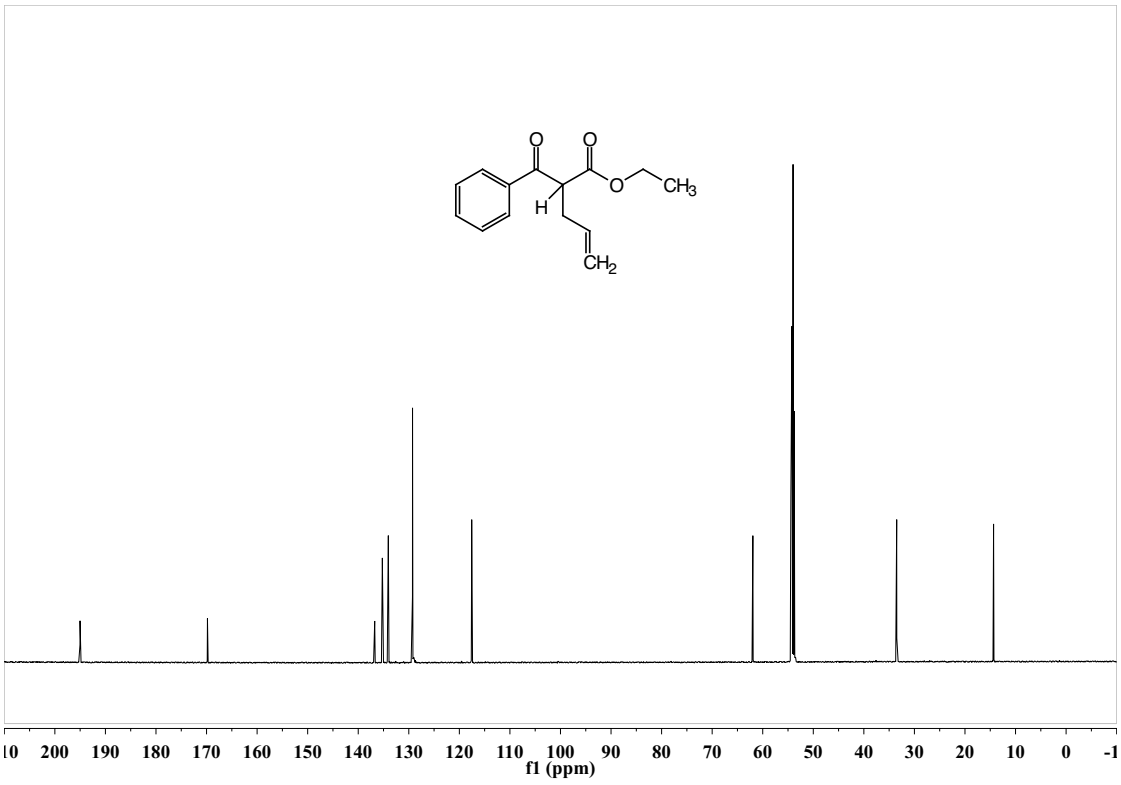
Ethyl 2-benzoyl-6-hydroxy-2-methylhex-4-enoate: Prepared according to the general procedure using ethyl 2-methyl-3-oxo-3-phenylpropanoate (0.573 g, 2.78 mmol) to afford 0.570 g (85% yield) of a mixture of *E* and *Z* isomers of ethyl 2-benzoyl-6-hydroxy-2-methylhex-4-enoate as a clear oil. Analytical data: ^{1}H NMR (500 MHz; $CDCl_3$): δ 7.84-7.82 (m, 4H), 7.54-7.51 (m, 2H), 7.44-7.40 (m, 4H), 5.74 (dtt, *J* = 11.0, 6.9, 1.5 Hz, 1H), 5.68-5.53 (m, 2H), 5.45 (dtt, *J* = 11.0, 8.0, 1.4 Hz, 1H), 4.14-4.05 (m, 8H), 2.81-2.75 (m, 4H), 1.59 (bs, 2H), 1.54 (s, 3H), 1.51 (s, 3H), 1.06 (t, *J* = 7.1 Hz, 3H), 1.06 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (125 MHz; $CDCl_3$): 197.3, 197.3, 174.0, 173.9, 135.6, 135.5, 133.9, 133.0, 132.9, 132.4, 128.7(4C), 128.7(4C), 126.4, 126.1, 63.5, 61.7, 61.6, 58.4, 57.1, 57.1, 39.5, 34.4, 21.2, 21.2, 14.0, 13.9; IR (film) 3401, 2983, 2936, 2872, 1734, 1682, 1597, 1580, 1447, 1378, 1240, 1196, 1115, 1017, 975, 704 cm^{-1}; LRMS (ESI): Mass calcd for $C_{16}H_{20}NaO_4$ $[M+Na]^+$: 299; found 299.



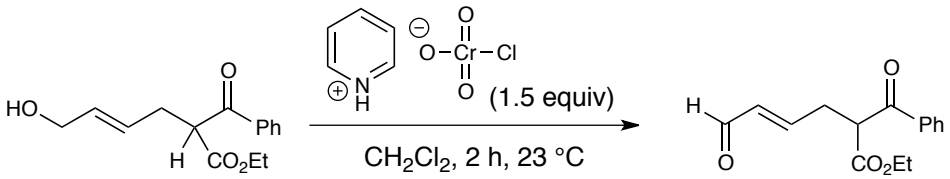
Ethyl 2-benzoylpent-4-enoate (24): In a flame dried 100 mL round-bottomed flask was added $Pd(dba)_2$ (0.012 equiv) and triphenylphosphine (0.048 equiv). The flask was purged and diluted with THF (9 mL). In a flame dried 100 mL round-bottomed flask was added sodium hydride

(60% in mineral oil) (1.1 equiv) and THF (30 mL) under nitrogen. Ethyl benzoylacetate (11.45 mmol) was slowly added to the NaH suspension at 23 °C causing a vigorous reaction. At the end of this addition, the solution becomes homogeneous and slightly yellow. At this time, THF (20 mL) and allyl methyl carbonate (1.1 equiv) was added to the palladium catalyst and after 5 min of stirring; the catalyst solution was added to the sodium ketoester solution, which turns solution heterogeneous and yellow. The reaction mixture was stirred at 23 °C until completion (24 hrs). The reaction mixture was quenched by the addition of saturated NH_4Cl (30 mL) and Et_2O (20 mL). The layers were separated and the aqueous layer was back extracted with Et_2O (40 mL). The combined organic was washed with brine, dried over $MgSO_4$, filtered, and concentrated *in-vacuo*. The material was purified by flash chromatography EtOAc/hexanes (5:95) to afford 0.99 g (37% yield) of ethyl 2-benzoylpent-4-enoate as a yellow oil. Analytical data for **24**: ^{1}H NMR (500 MHz; CD_2Cl_2): δ 8.02 – 7.95 (m, 2H), 7.63 – 7.56 (m, 1H), 7.52 – 7.46 (m, 2H), 5.82 (ap ddt, J = 17.1, 10.2, 6.9 Hz, 1H), 5.14 – 5.00 (m, 2H), 4.41 (t, J = 7.2 Hz, 1H), 4.11 (q, J = 7.1 Hz, 2H), 2.79 – 2.64 (m, 2H), 1.16 (t, J = 7.1 Hz, 3H); ^{13}C NMR (125 MHz; CD_2Cl_2): δ 195.0, 169.8, 136.7, 135.2, 134.1, 129.3(2C), 129.1(2C), 117.6, 62.0, 54.2, 33.5, 14.3; LRMS (ESI): Mass calcd for $C_{14}H_{17}O_3$ $[M+H]^+$: 233; found 233.

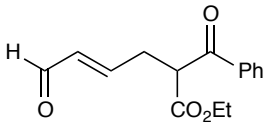




General Procedure for the Synthesis of Enal β-Ketoesters

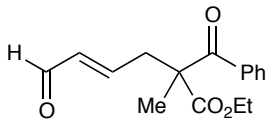


The enal β-ketoesters were prepared according to the reported procedure.[3] In a flame dried 250 mL RBF with a stirbar was added PCC (1.5 equiv), Celite (~ 10 g), and CH_2Cl_2 (85 mL). To this RBF was added ethyl 2-benzoyl-6-hydroxyhex-4-enoate (11.82 mmol) dissolved in CH_2Cl_2 (9 mL). The resulting solution was stirred at 23 °C for 2 hrs. The reaction mixture was then filtered through a SiO_2 plug washed with Et_2O and concentrated to afford 2.70 g (88% yield) of *(E)*-ethyl 2-benzoyl-6-oxohex-4-enoate. The corresponding enal was carried on the NHC reaction without further purification.



(*E*)-ethyl 2-benzoyl-6-oxohex-4-enoate: Prepared according to the general procedure using *(E)*-

ethyl 2-benzoyl-6-hydroxyhex-4-enoate (3.10 g, 15.31 mmol) to afford 2.70 g (88% yield) of product as a yellowish oil. Analytical data: ^{1}H NMR (500 MHz; $CDCl_3$): δ 9.49 (d, *J* = 7.8 Hz, 1H), 8.01-7.99 (m, 2H), 7.64-7.60 (m, 1H), 7.52-7.48 (m, 2H), 6.89 (ap dt, *J* = 15.7, 6.9 Hz, 1H), 6.18 (ap ddt, *J* = 15.7, 7.8, 1.4 Hz, 1H), 4.50 (ap t, *J* = 7.0 Hz, 1H), 4.19-4.13 (m, 2H), 3.04-3.01 (m, 2H), 1.16 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (125 MHz; $CDCl_3$): δ 193.7, 193.5, 168.8, 153.6, 135.7, 134.7, 134.1, 129.0(2C), 128.8(2C), 62.1, 52.8, 31.6, 14.1; IR (film) 2982, 2924, 2850, 2739, 1735, 1688, 1597, 1448, 1254, 1229, 1177, 1129, 1094, 1028, 978, 739, 691 cm^{-1}; LRMS (ESI): Mass calcd for $C_{15}H_{17}O_4$ $[M+H]^+$: 261; found 261.

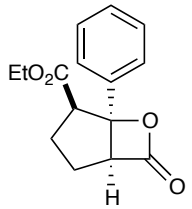


(*E*)-ethyl 2-benzoyl-2-methyl-6-oxohex-4-enoate (22): Prepared according to the general procedure using ethyl 2-benzoyl-6-hydroxy-2-methylhex-4-enoate (0.558 g, 2.02 mmol) to afford 0.503 g (91% yield) of (*E*)-ethyl 2-benzoyl-2-methyl-6-oxohex-4-enoate as a clear oil. Analytical data: ^{1}H NMR (500 MHz; $CDCl_3$): δ 9.50 (d, *J* = 7.9 Hz, 1H), 7.84 (dd, *J* = 8.5, 1.2 Hz, 2H), 7.57-7.54 (m, 1H), 7.46-7.43 (m, 2H), 6.78 (dt, *J* = 15.5, 7.7 Hz, 1H), 6.11 (dd, *J* = 15.5, 7.9 Hz, 1H), 4.13 (q, *J* = 7.1 Hz, 2H), 3.07-2.92 (m, 2H), 1.58 (s, 3H), 1.06 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (125 MHz; $CDCl_3$): 196.4, 193.6, 173.1, 152.3, 136.1, 134.9, 133.3, 128.8(2C), 128.7(2C), 62.0, 56.8, 40.0, 21.5, 14.0; IR (film) 2983, 2938, 2819, 2744, 1734, 1687, 1597, 1580, 1447, 1380, 1287, 1255, 1234, 1194, 1145, 1093, 1016, 976, 705 cm^{-1}; LRMS (ESI): Mass calcd for $C_{16}H_{19}O_4$ $[M+H]^+$: 275; found 275.

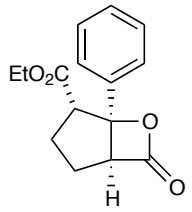
General Procedure for the Synthesis of β-lactones

The racemic and enantioenriched β-lactones were prepared according to the reported procedure.[3] In a nitrogen filled dry box a screw-capped vial equipped with a magnetic stirbar was charged with the corresponding enal β-ketoester **4** (0.400 mmol), azolium precatalyst **F** (0.07 equiv), and cesium carbonate (0.30 equiv). The vial was capped with a septum cap, removed from the drybox and put under positive N_2 pressure. The heterogeneous mixture was then diluted with degassed 1,2-dichloroethane (12 mL, 0.033 M) and stirred for 12 hours under static nitrogen pressure. Upon consumption of the aldehyde (all reactions were completed within 12 hours) the reaction mixture was diluted with dichloromethane (5 mL) washed with brine (10 mL) and separated. The aqueous phase was back extracted with dichloromethane (5 mL). The combined organic layers were filtered through a Biotage ISOLUTE® phase separator, and the organic filtrate was concentrated. The material was purified by flash chromatography with EtOAc/hexanes to afford the corresponding β-lactone.

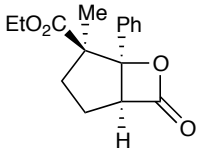
The corresponding racemic compounds were prepared by employing the same protocol but with achiral azolium precatalyst **E** (10 mol%).



(1*S*,4*R*,5*S*)-ethyl 7-oxo-5-phenyl-6-oxabicyclo[3.2.0]heptane-4-carboxylate (4): Prepared according to the general procedure using *(E)*-ethyl 2-benzoyl-6-oxohex-4-enoate (0.104 g, 0.400 mmol) and purified by flash chromatography using 20% EtOAc/hexanes to afford 77 mg (74% yield) of **4** as a white solid and 12 mg (12%) of **4b** as a light yellow solid. Analytical data for **4**: ^{1}H NMR (500 MHz; $CDCl_3$): δ 7.43-7.33 (m, 5H), 4.13 (dq, *J* = 10.8, 7.1 Hz, 1H), 4.01 (dq, *J* = 10.8, 7.1 Hz, 1H), 3.82 (d, *J* = 8.0 Hz, 1H), 3.17 (dd, *J* = 11.0, 8.0 Hz, 1H), 2.41-2.28 (m, 3H), 2.05-1.95 (m, 1H), 1.11 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (125 MHz; $CDCl_3$): δ 169.8, 169.2, 138.2, 128.5(2C), 128.3, 125.2(2C), 87.5, 63.9, 61.1, 53.8, 27.1, 25.4, 14.1; IR (film) 2925, 2853, 1829, 1738, 1465, 1449, 1370, 1323, 1292, 1261, 1229, 1168, 1116, 1071, 1041, 957, 928, 886, 808, 758, 699 cm^{-1}; LRMS (ESI): Mass calcd for $C_{15}H_{17}O_4$ $[M+H]^+$: 261; found 261; $[\alpha]_D^{25}$ = +61.0 ($CHCl_3$, c = 1.0). Enantiomeric ratio was measured by chiral phase HPLC (Chiralcel OJ, 15% *i*-PrOH/Hexanes, 1.0 mL/min, 210 nm), Rt (major) = 21.1 min, Rt (minor) = 29.0 min; ee = 98%.

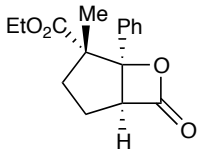


(1*S*,4*S*,5*S*)-ethyl 7-oxo-5-phenyl-6-oxabicyclo[3.2.0]heptane-4-carboxylate (4b):
Analytical data for **4b**: ^{1}H NMR (500 MHz; $CDCl_3$): δ 7.38-7.35 (m, 5H), 4.11 (d, *J* = 8.0 Hz, 1H), 3.76 (dq, *J* = 10.8, 7.1 Hz, 1H), 3.69 (dq, *J* = 10.8, 7.1 Hz, 1H), 3.47 (d, *J* = 6.2 Hz, 1H), 2.70-2.61 (m, 1H), 2.37-2.26 (m, 3H), 0.81 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (125 MHz; $CDCl_3$): δ 171.6, 170.3, 135.5, 129.0, 128.4(2C), 126.5(2C), 90.8, 60.8, 60.5, 54.0, 28.9, 27.5, 13.7; IR (film) 3059, 3033, 2980, 2943, 2873, 2851, 1832, 1730, 1688, 1496, 1448, 1392, 1371, 1344, 1309, 1269, 1248, 1214, 1186, 1112, 1076, 1042, 1003, 895, 847, 802, 758, 697 cm^{-1}; LRMS (ESI): Mass calcd for $C_{15}H_{17}O_4$ $[M+H]^+$: 261; found 261; $[\alpha]_D^{25}$ = +18.2 ($CHCl_3$, c = 1.0). Enantiomeric ratio was measured by chiral phase HPLC (Chiralcel OJ, 10% *i*-PrOH/Hexanes, 1.0 mL/min, 210 nm), Rt (major) = 14.3 min, Rt (minor) = 9.8 min; ee = 95%.



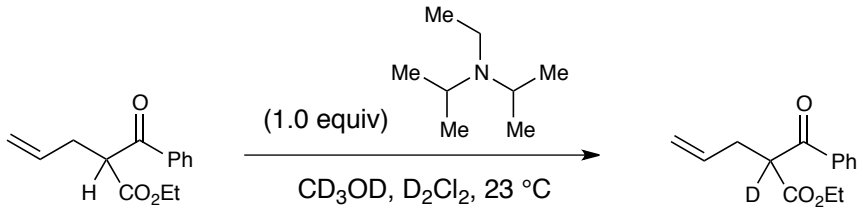
(1*S*,4*R*,5*R*)-ethyl 4-methyl-7-oxo-5-phenyl-6-oxabicyclo[3.2.0]heptane-4-carboxylate (22): Prepared according to the general procedure using (*E*)-ethyl 2-benzoyl-2-methyl-6-oxohex-4-enoate (0.109 g, 0.400 mmol) and purified by flash chromatography using 20% EtOAc/hexanes to afford 48 mg (44% yield) of **22** as a light yellow oil and 46 mg (42% yield) of **23** as a light yellow solid. Analytical data for **22**: ^{1}H NMR (500 MHz; $CDCl_3$): δ 7.38-7.35 (m, 5H), 4.24-4.11 (m, 2H), 3.91 (d, *J* = 7.3 Hz, 1H), 2.74 (ap td, *J* = 13.1, 6.9 Hz, 1H), 2.24 (dd, *J* = 13.5, 6.8 Hz, 1H), 2.16-2.03 (m, 2H), 1.25 (t, *J* = 7.1 Hz, 3H), 1.06 (s, 3H); ^{13}C NMR (125 MHz; $CDCl_3$):

172.7, 170.1, 135.5, 128.4, 127.6(4C), 90.3, 62.8, 61.3, 54.7, 34.1, 23.6, 21.4, 14.2. IR (film) 3061, 3031, 2978, 2882, 1828, 1730, 1498, 1466, 1450, 1379, 1366, 1312, 1276, 1254, 1172, 1148, 1132, 1095, 1027, 979, 942, 897, 865, 832, 789, 754, 701, 663 cm^{-1}; LRMS (ESI): Mass calcd for $C_{16}H_{19}O_2$ $[M+H]^+$: 275; found 275; $[\alpha]_D^{25}$ = +60.1 ($CHCl_3$, c = 1.0). Enantiomeric ratio was measured by chiral phase HPLC (OJ, 10% *i*-PrOH/Hexanes, 1.0 mL/min, 210 nm), Rt (major) = 15.1 min, Rt (minor) = 47.3 min; ee = 99%.

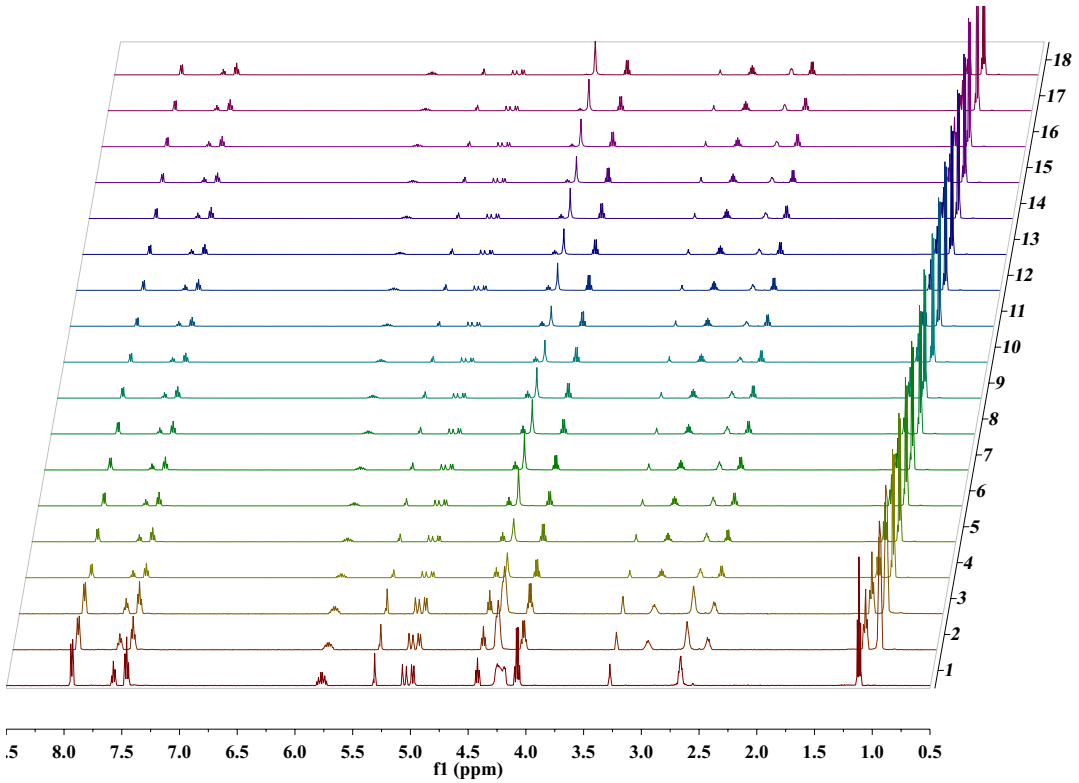


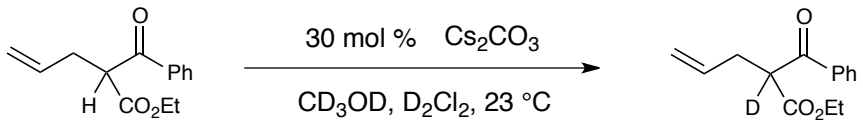
(1*S*,4*S*,5*R*)-ethyl 4-methyl-7-oxo-5-phenyl-6-oxabicyclo[3.2.0]heptane-4-carboxylate (23): Analytical data for **23**: ^{1}H NMR (500 MHz; $CDCl_3$): δ 7.40-7.31 (m, 5H), 4.09 (d, *J* = 8.4 Hz, 1H), 3.88-3.76 (m, 2H), 2.76-2.68 (m, 1H), 2.41 (dd, *J* = 13.7, 7.2 Hz, 1H), 2.24 (dd, *J* = 13.3, 7.2 Hz, 1H), 2.07 (td, *J* = 13.3, 7.2 Hz, 1H), 1.46 (s, 3H), 0.96 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (125 MHz; $CDCl_3$): 173.3, 171.0, 135.5, 128.6, 128.1(2C), 126.8(2C), 91.4, 61.5, 61.0, 56.8, 37.4, 26.2, 16.6, 13.8. IR (film) 2979, 2934, 2850, 1833, 1722, 1600, 1463, 1379, 1327, 1303, 1279, 1242, 1172, 1154, 1095, 1025, 979, 892, 800, 753 cm^{-1}; LRMS (ESI): Mass calcd for $C_{16}H_{19}O_2$ $[M+H]^+$: 275; found 275; $[\alpha]_D^{25}$ = +36.1 ($CHCl_3$, c = 1.0). Enantiomeric ratio was measured by chiral phase HPLC (OJ, 10% *i*-PrOH/Hexanes, 1.0 mL/min, 210 nm), Rt (major) = 9.0 min, Rt (minor) = 22.4 min; ee = 99%.

^{1}H NMR Deuterium Exchange Experiments



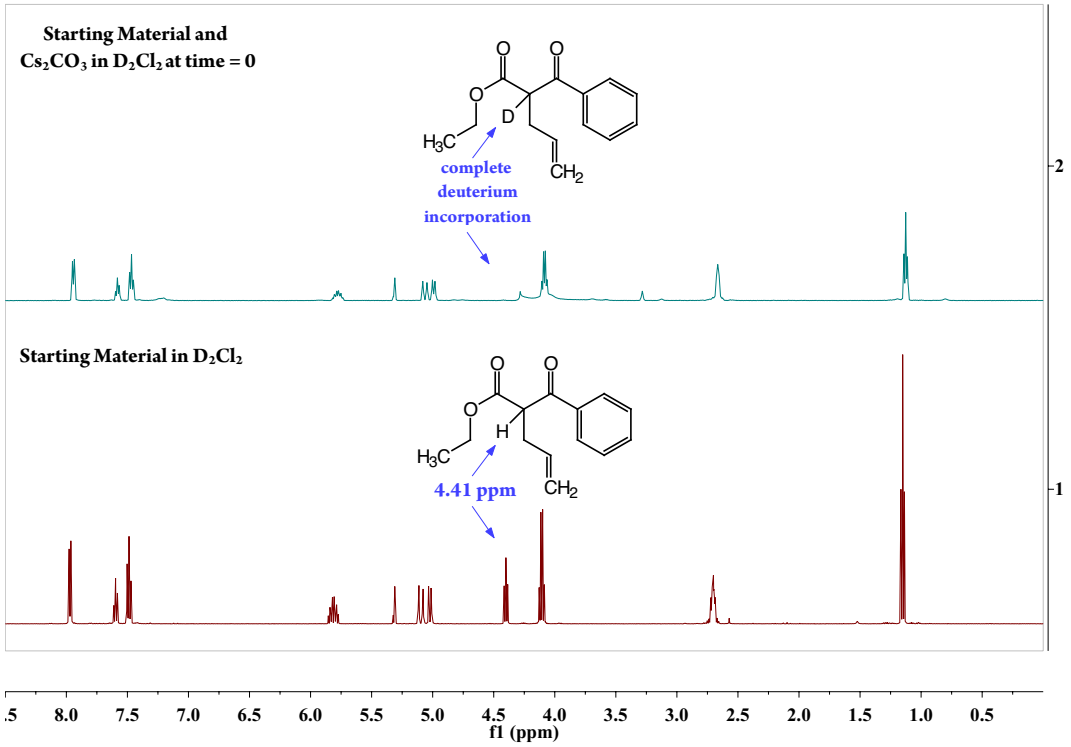
In a NMR tube was placed ethyl 2-benzoylpent-4-enoate (10 mg, 0.043 mmol), deutrated dichloromethane (0.75 mL) and deutrated methanol (0.55 mL) (0.033 M). The mixture was shaken vigorously. *N*-ethyl-*N*-isopropylpropan-2-amine (7.5 μL, 0.043 mmol) was added via a syringe. The mixture was shaken and the reaction was monitored by ^{1}H NMR over 25 hrs for the disappearance of chemical shift at 4.41 ppm. ^{1}H NMRs were taken at the time intervals of t = 0 min, 5 min, 10 min, 15 min, 30 min, 45 min, 1 hr, 1.5 h, 3 h, 4 h, 5 h, 6 h, 7 h, 8 h, 10 h, 12 h, 24.5 h). After 24.5 hours there was 90% conversion to ethyl 2-benzoyl-2-deuteriopent-4-enoate.

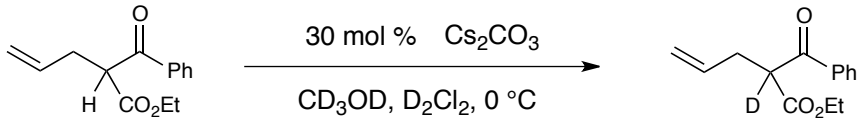




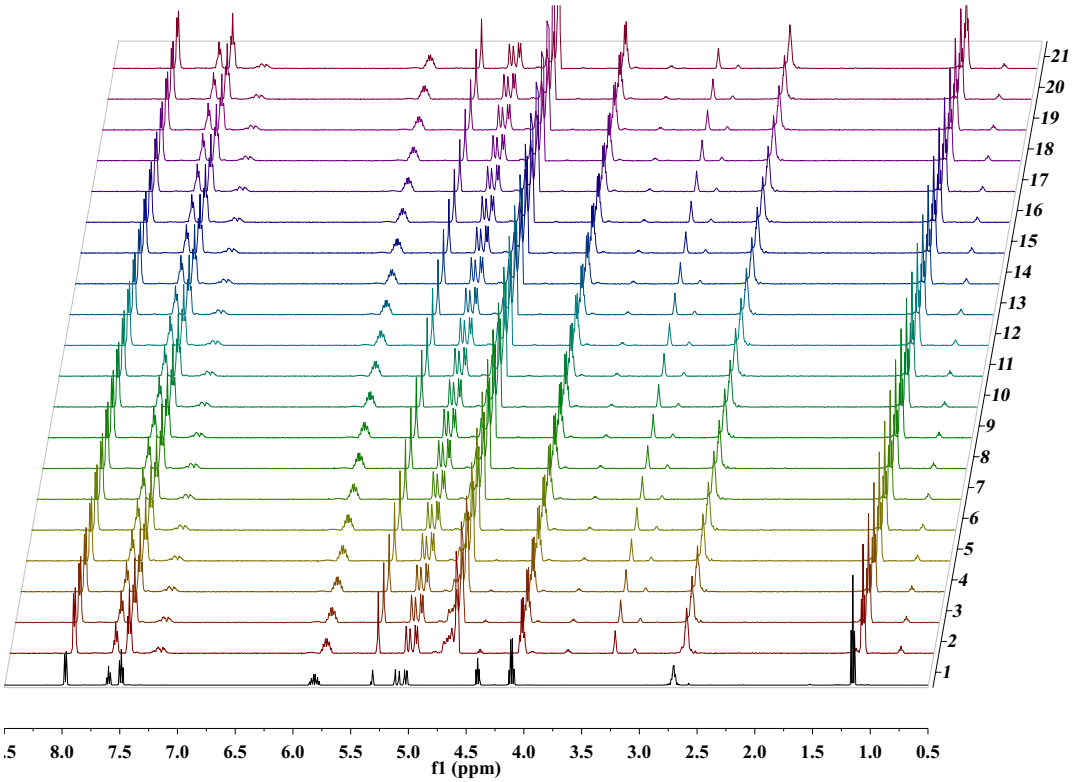
In a NMR tube was placed ethyl 2-benzoylpent-4-enoate (10 mg, 0.043 mmol) and deutrated dichloromethane (0.75 mL). Cesium Carbonate (4.2 mg, 0.013 mmol) was dissolved in deutrated methanol (0.55 mL) and the mixture was added to the NMR tube. The mixture was

shaken and a ^{1}H NMR was taken immediately (t = 0 min). At time = 0 there was complete conversion to ethyl 2-benzoyl-2-deuteriopent-4-enoate.

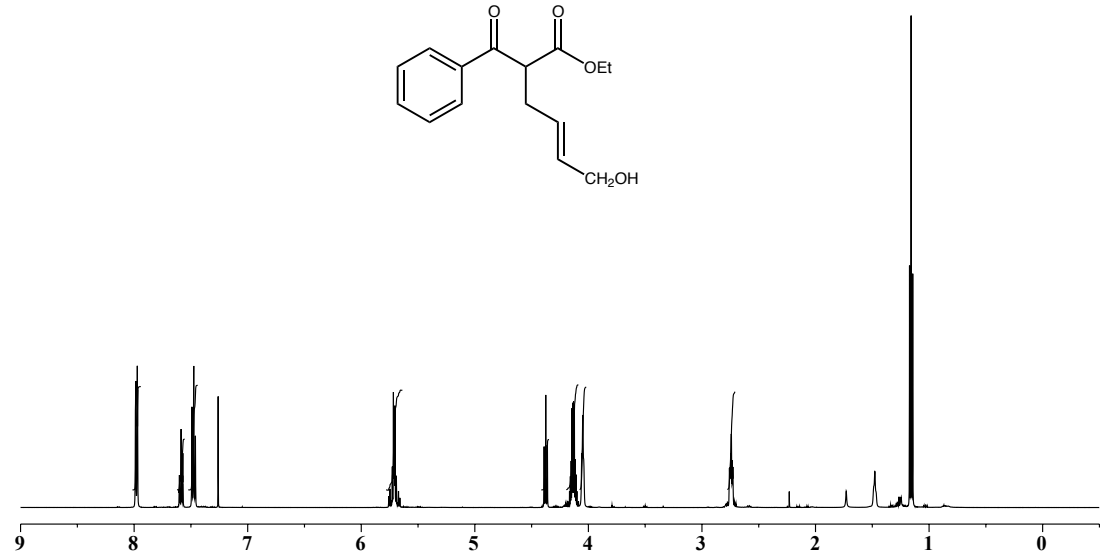


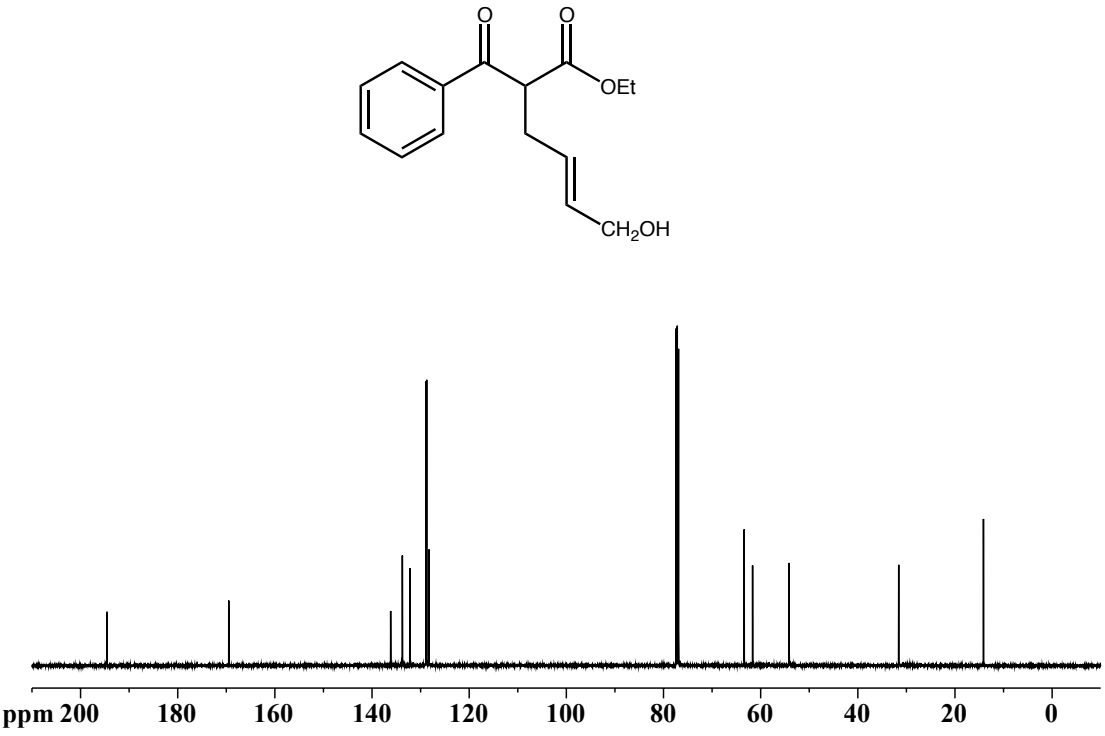


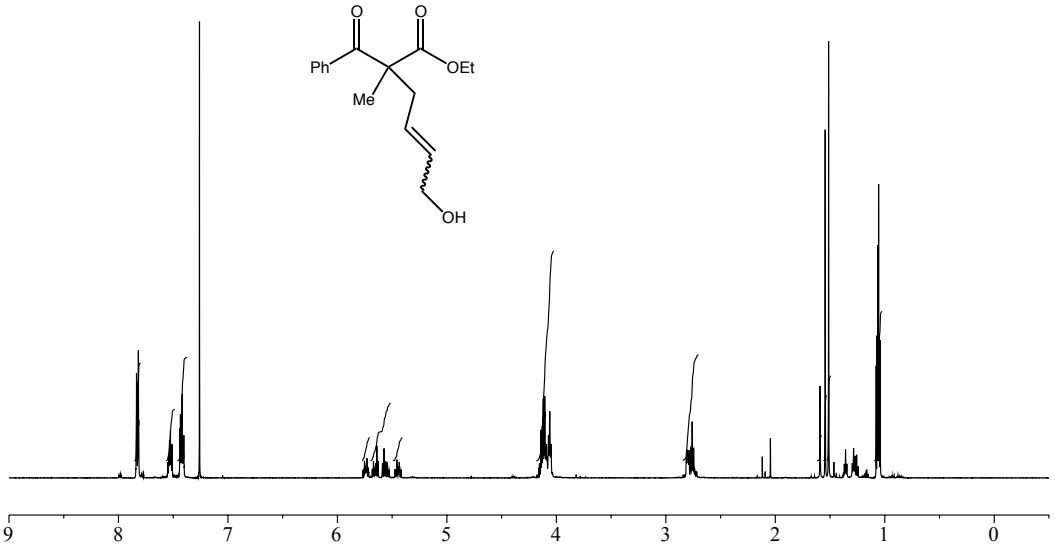
In a NMR tube was placed ethyl 2-benzoylpent-4-enoate (10 mg, 0.043 mmol) and deutrated dichloromethane (0.75 mL), the mixture was cooled to 0 °C. Cesium carbonate (4.2 mg, 0.013 mmol) was dissolved in deutrated methanol (0.55 mL) and homogenous mixture was cooled to 0 °C. The NMR probe was cooled to –10 °C. The cesium carbonate mixture was added to the NMR tube, the combined mixture was shaken, and 20 minute array of ^{1}H NMR specta were taken (one every minute). After 20 minutes there was nearly complete conversion to ethyl 2-benzoyl-2-deuteriopent-4-enoate.


21
20
19
18
17
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

Selected NMR Spectra



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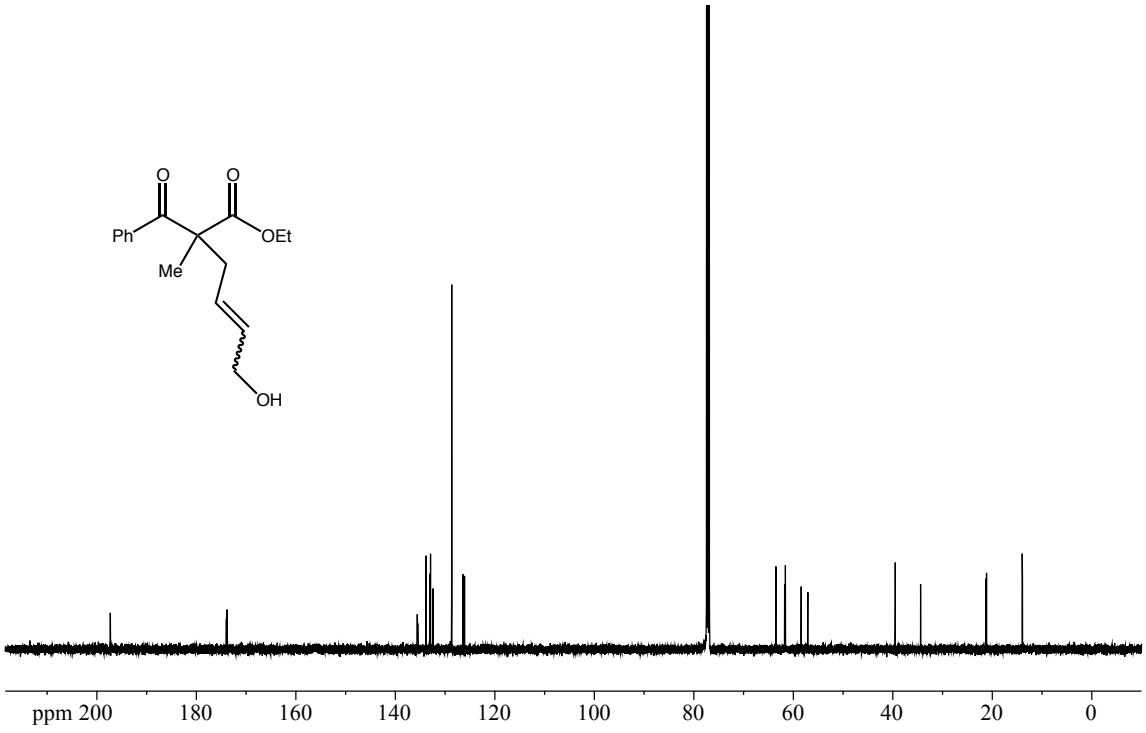
O
Ph
OEt
Me
OH
9
8
7
6
5
4
3
2
1
0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O
Ph
OEt
Me
OH
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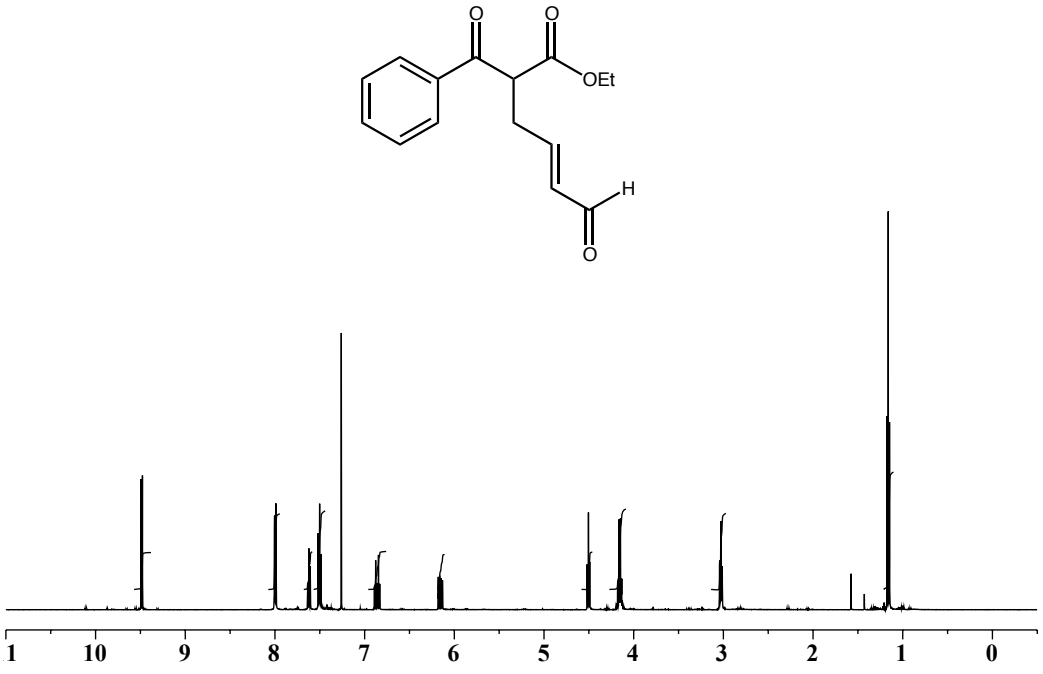
140
120
100
80
60
40
20
0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O
OEt
H
O
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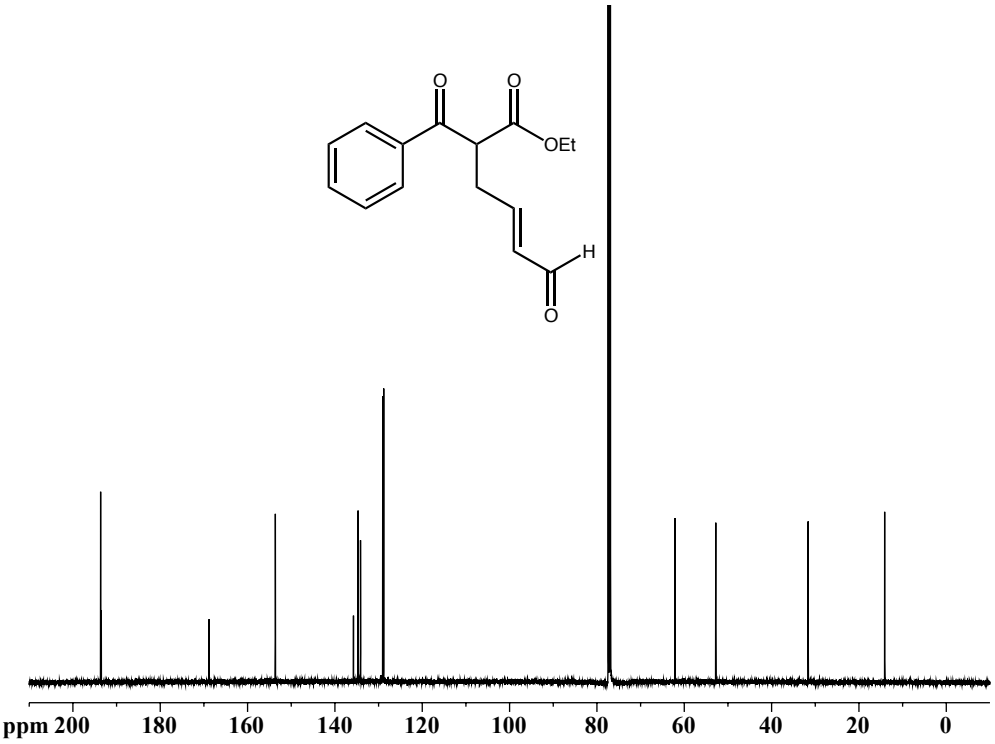
7
6
5
4
3
2
1
0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O
OEt
H
O
ppm 200
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140
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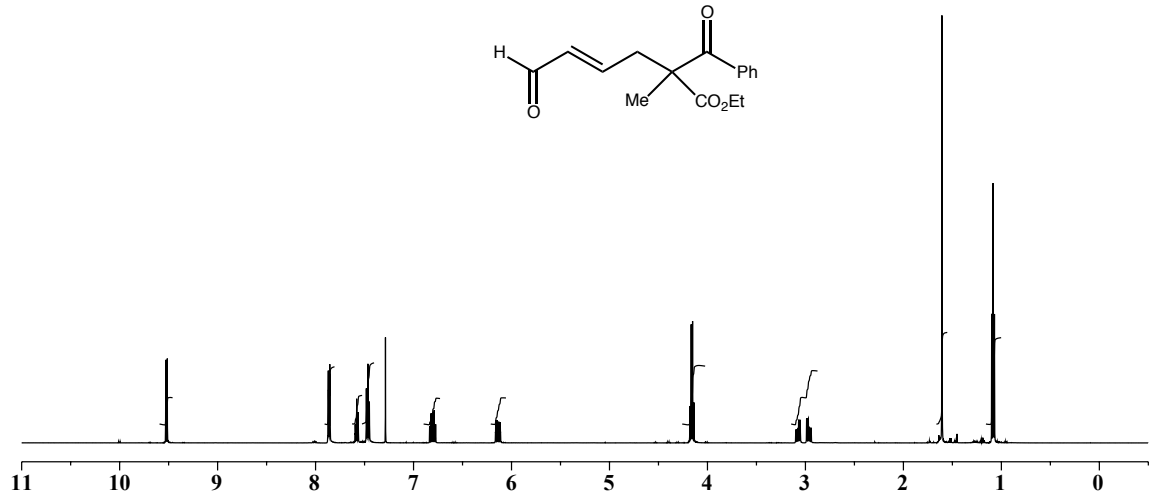
100
80
60
40
20
0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Ph
Me
CO2Et
O
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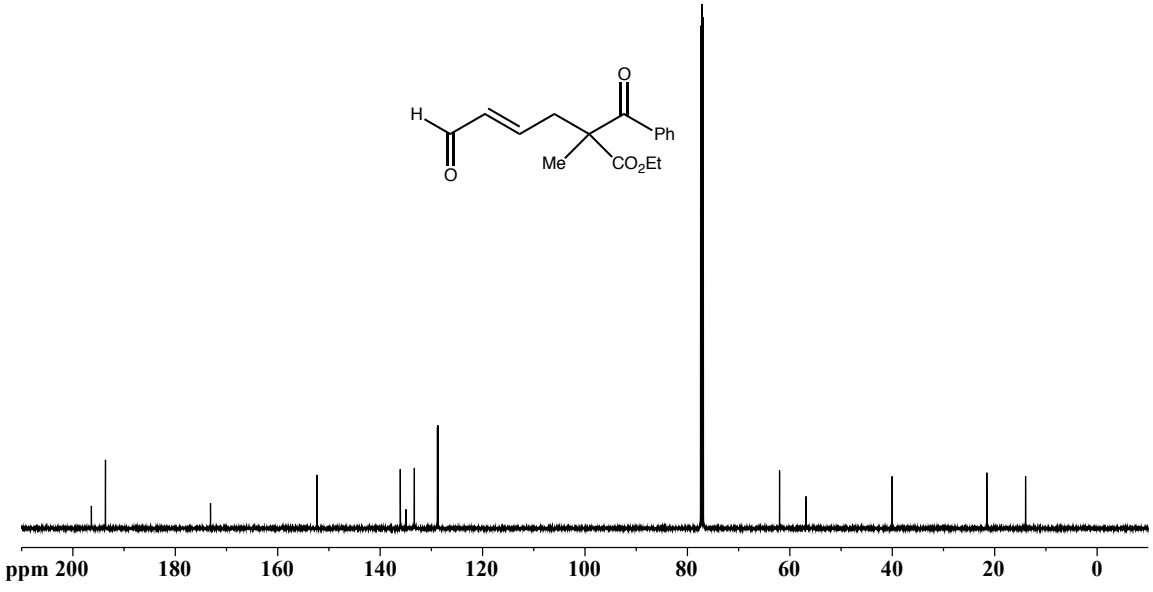
10
9
8
7
6
5
4
3
2
1
0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H
Ph
Me
CO2Et
O
ppm 200
180
160
140
120
100
80
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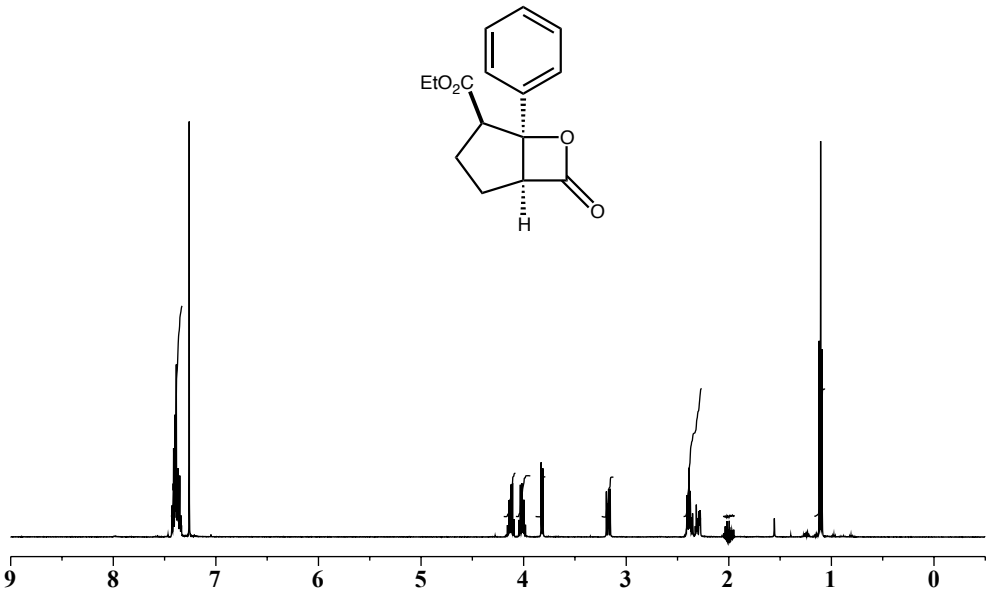
40
20
0


EtO2C
O
O
H
9
8
7
6
5
4
3
2
1
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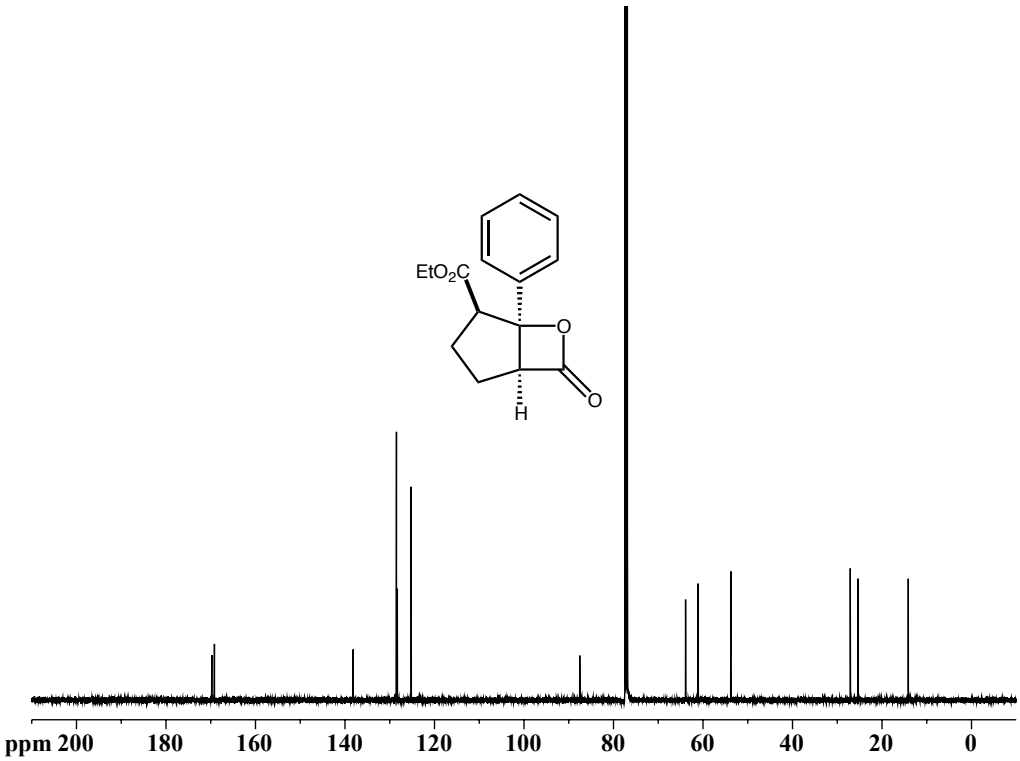
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O
O
H
ppm 200
180
160
140
120
100
80
60
40
20
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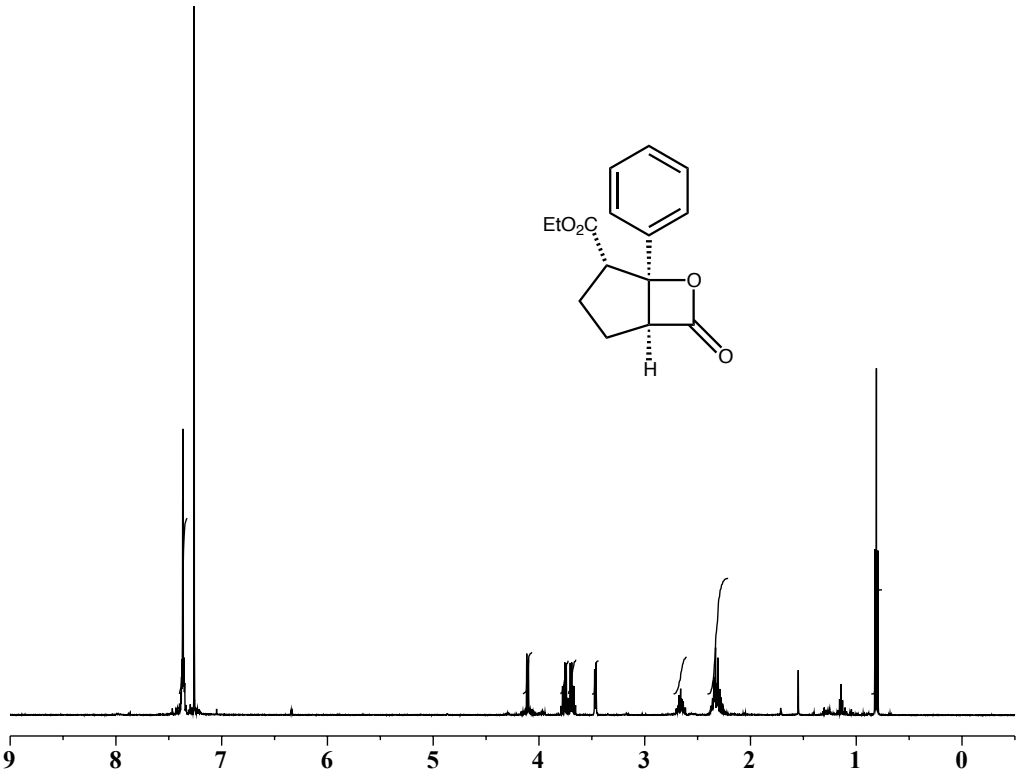
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O
H
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6
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3
2
1
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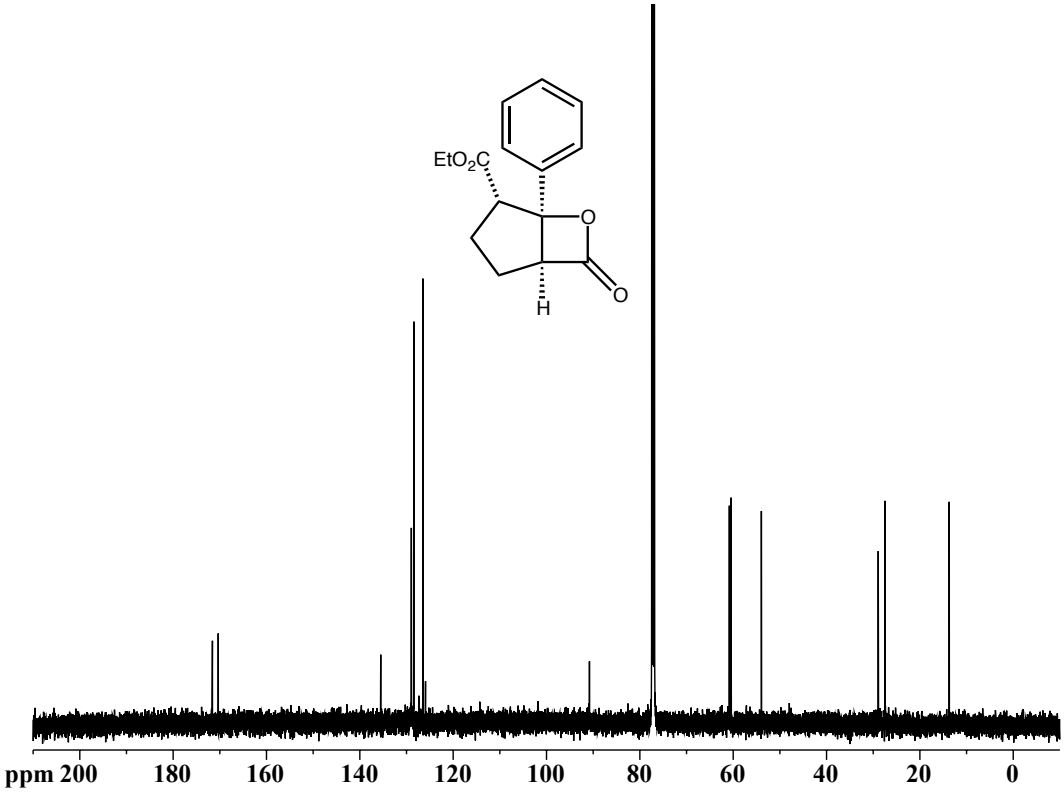
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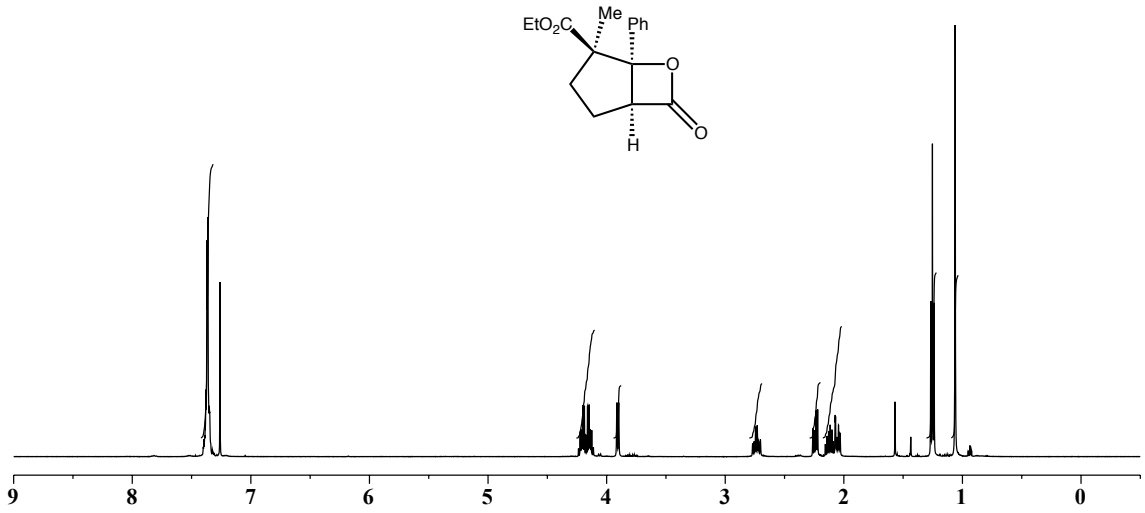
O
H
ppm 200
180
160
140
120
100
80
60
40
20
0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Me
Ph
O
O
H
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3
2
1
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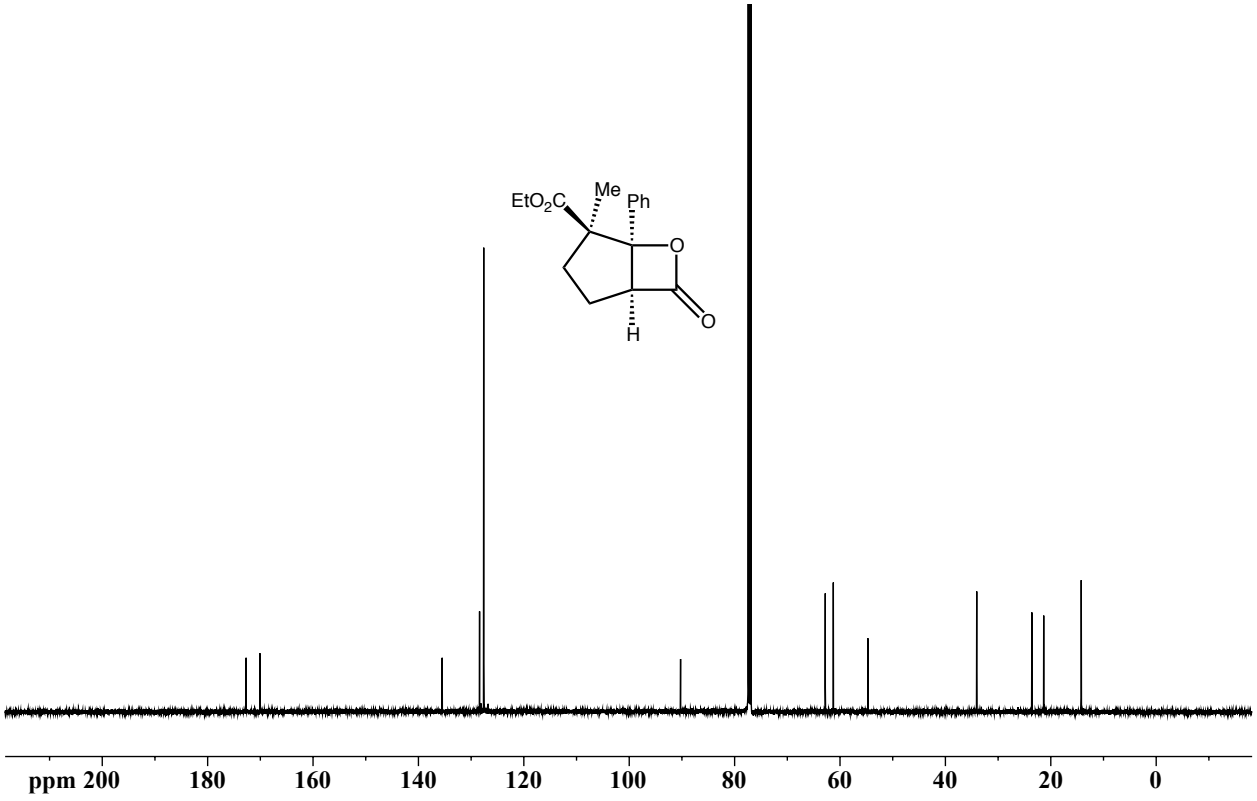
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Me
Ph
O
O
H
ppm 200
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20
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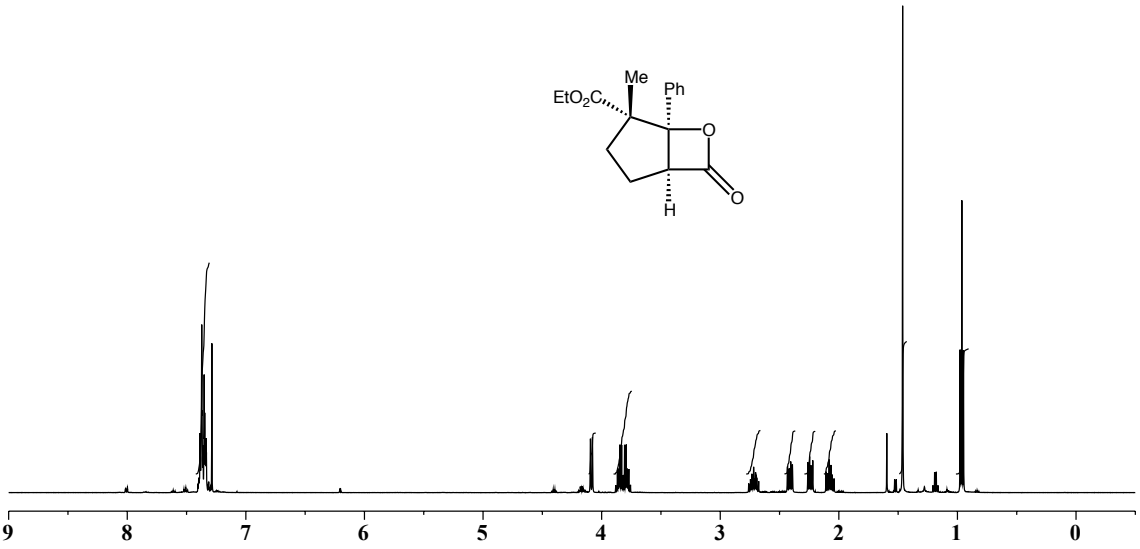
Me
Ph
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O
O
H
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3
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1
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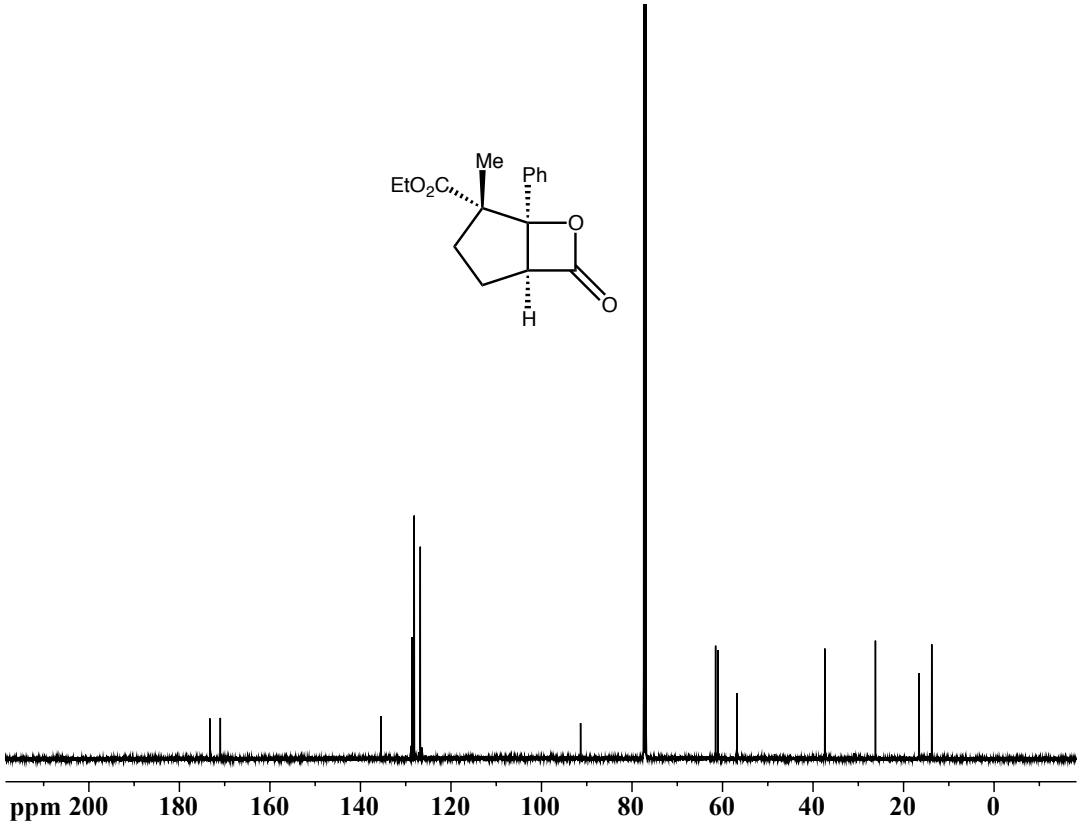
Me
Ph
EtO2C
O
O
H
ppm 200
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40
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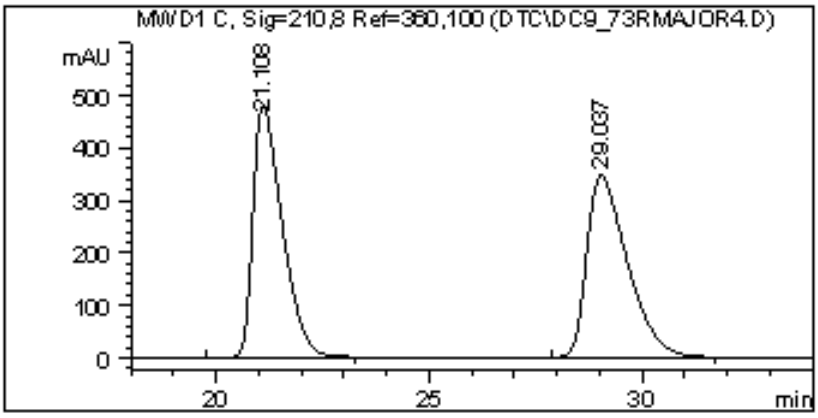
0

HPLC Traces of Racemic and Enantioenriched Compounds

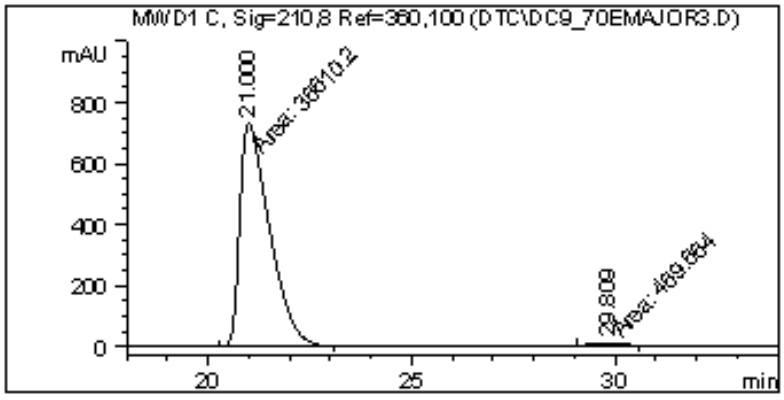
Racemic 4



Signal 1: MWD1 C, Sig=210,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.108	BB	0.7110	2.28276e4	479.88498	50.0078
2	29.037	VB	0.9721	2.28205e4	345.70071	49.9922
Totals :				4.56481e4	825.58569	

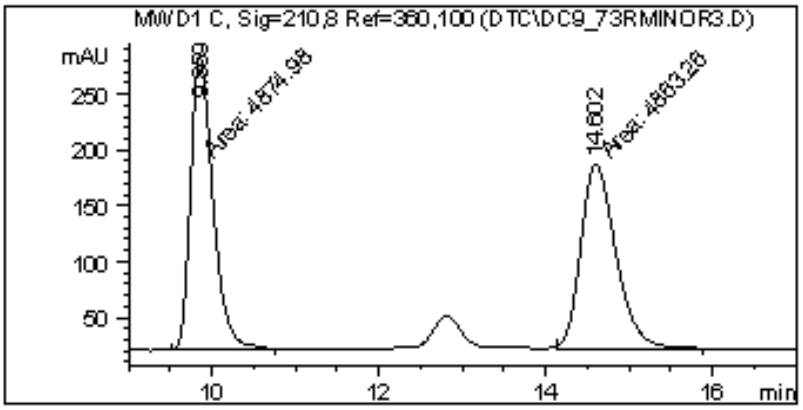
Enatioenriched 4



Signal 1: MWD1 C, Sig=210,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.000	MM	0.8394	3.66102e4	726.87646	98.7334
2	29.809	MM	0.8107	469.66406	9.65508	1.2666
Totals :				3.70799e4	736.53155	

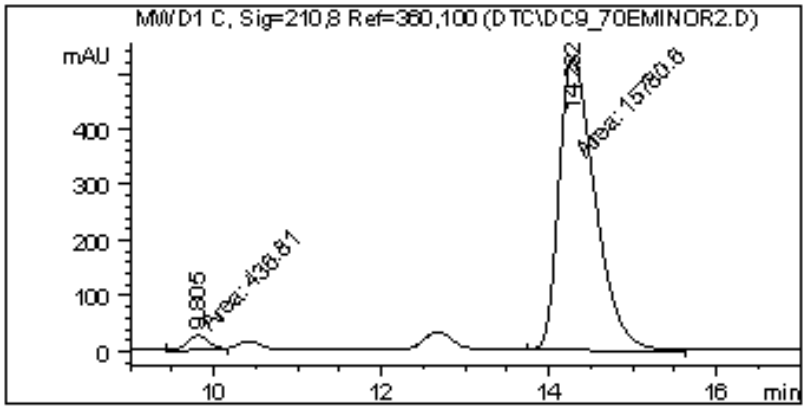
Racemic 4b



Signal 1: MWD1 C, Sig=210,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.859	MM	0.3107	4874.97803	261.53812	50.0602
2	14.602	MM	0.4905	4863.25635	165.25510	49.9398
Totals :				9738.23438	426.79321	

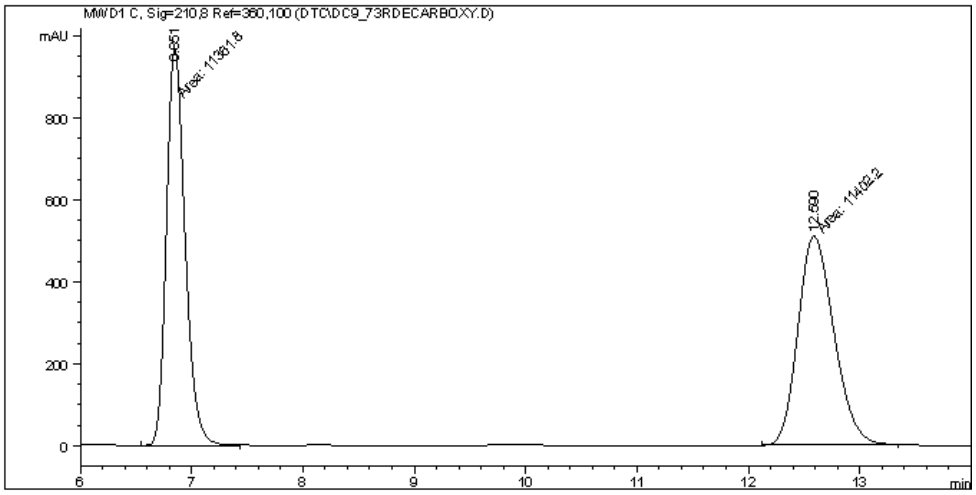
Enatioenriched 4b



Signal 1: MWD1 C, Sig=210,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.805	MM	0.2929	436.80957	24.85591	2.6935
2	14.282	MM	0.4987	1.57806e4	527.37256	97.3065
Totals :				1.62174e4	552.22847	

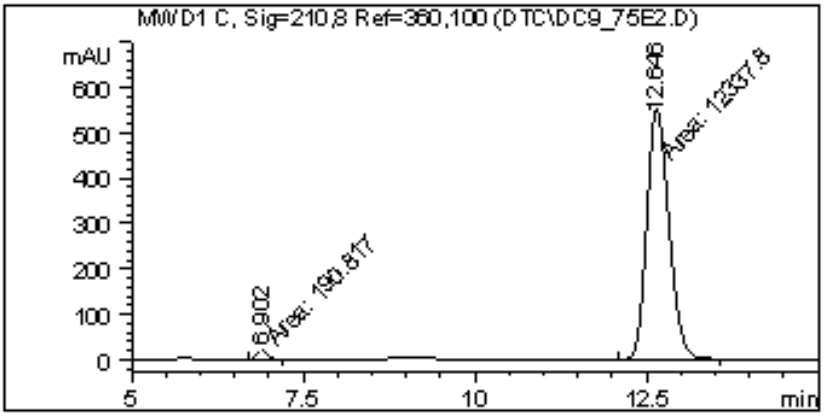
Racemic Ethyl 2-phenylcyclopent-2-enecarboxylate



Signal 1: MWD1 C, Sig=210,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.851	MM	0.1948	1.13618e4	972.31543	49.9114
2	12.590	MM	0.3737	1.14022e4	508.58969	50.0886
Totals :				2.27640e4	1480.90512	

Enantioenriched (*R*)-ethyl 2-phenylcyclopent-2-enecarboxylate

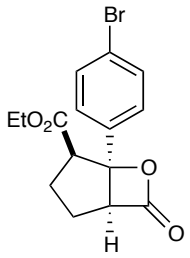


Signal 1: MWD1 C, Sig=210,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.902	MM	0.1727	190.81721	18.41193	1.5230
2	12.646	MM	0.3721	1.23378e4	552.63043	98.4770
Totals :				1.25287e4	571.04237	

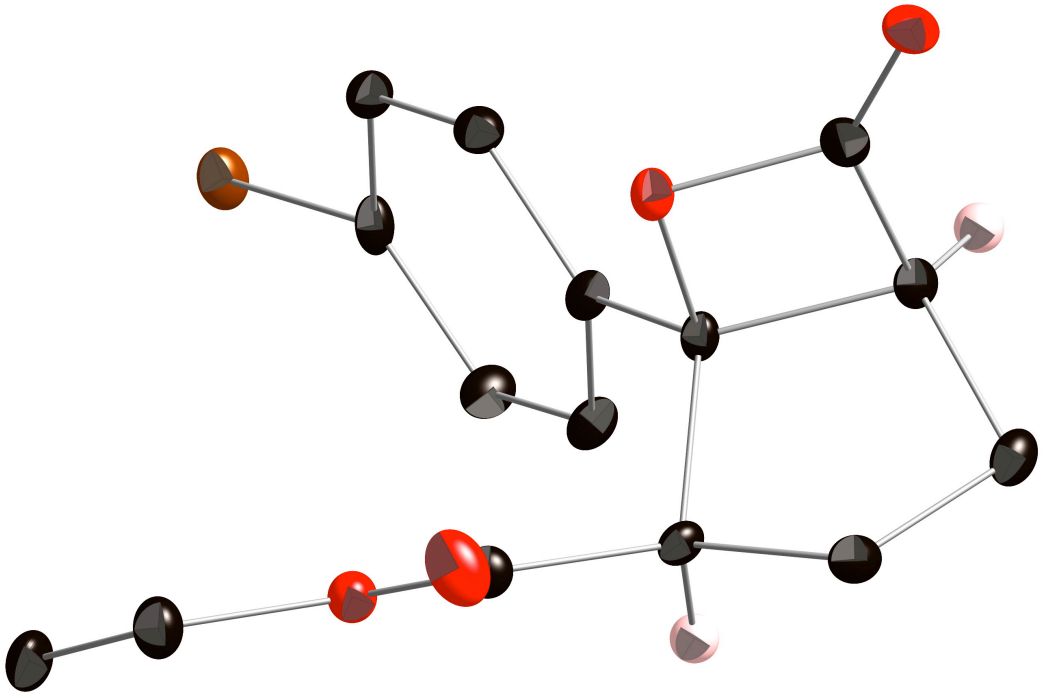
Determination of Absolute Stereochemistry of 5

The absolute stereochemistry of **5** was determined by the X-ray diffraction. Recrystallized from hexanes.



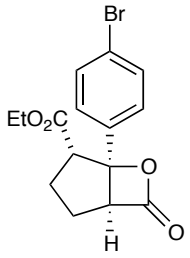
X-ray crystal structure of (1*S*,4*R*,5*S*)-ethyl 5-(4-bromophenyl)-7-oxo-6-oxabicyclo[3.2.0]heptane-4-carboxylate:

X-ray diffraction was performed at –120 ˚C and raw frame data were processed using SAINT. Molecular structure was solved using direct methods and refined by F2 by full-matrix least-squares techniques. The GOF = 0.93 for 363 variables refined to R1 = 0.056 for 3499 reflections with I>2α(I). A multi-scan adsorption correction was preformed. The flack parameter was 0.01. Further information is contained in the CCDC file 879780.



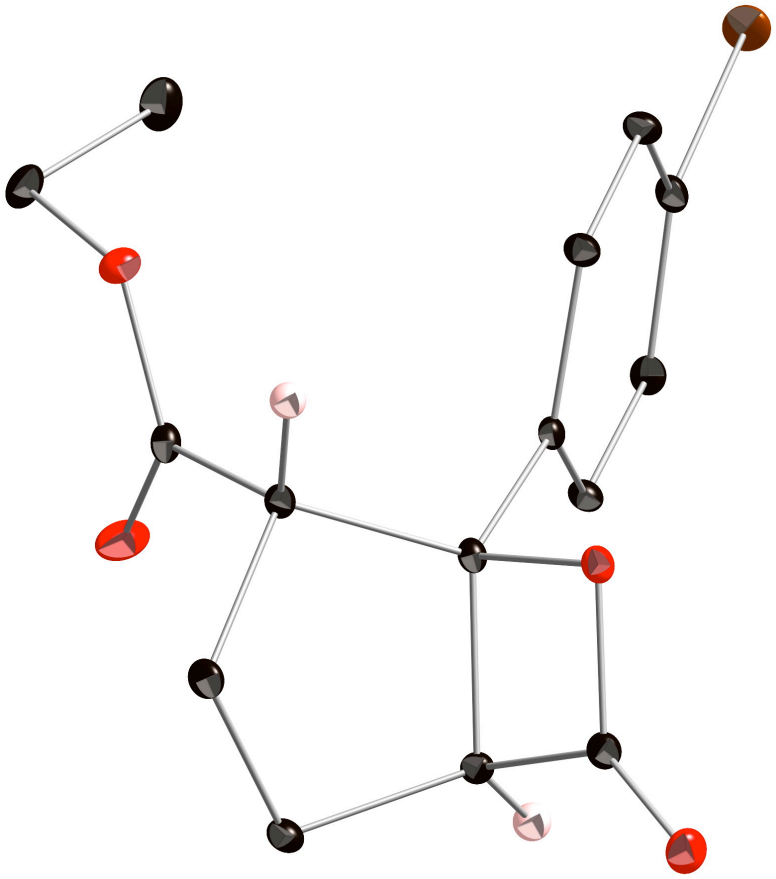
Determination of Absolute Stereochemistry of 5b

The absolute stereochemistry of **5b** was determined by the X-ray diffraction. Recrystallized from hexanes.



X-ray crystal structure of (1*S*,4*S*,5*S*)-ethyl 5-(4-bromophenyl)-7-oxo-6-oxabicyclo[3.2.0]heptane-4-carboxylate**:**

X-ray diffraction was performed at –120 ˚C and raw frame data were processed using SAINT. Molecular structure was solved using direct methods and refined by F2 by full-matrix least-squares techniques. The GOF = 0.58 for 182 variables refined to R1 = 0.034 for 3204 reflections with I>2α(I). A multi-scan absorption correction was preformed. The flack parameter was –0.004. Further information is contained in the CCDC file 879781.



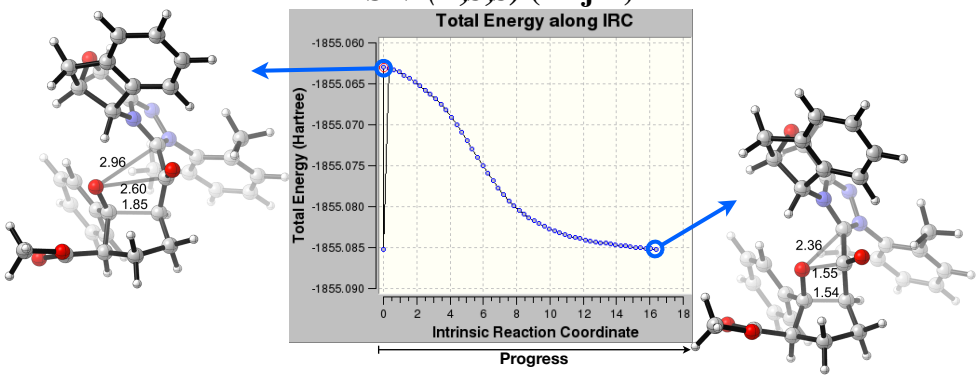
General Computational Methodology

The mechanism and origins of stereoselectivity of this reaction were studied using M06-2X[4]/6-31+G**[5,6]/PCM(DCE)[7]//M06-2X/6-31G* as implemented in the Gaussian 09 suite of programs.[8] Ethyl groups were modeled as methyl in order to reduce the degrees of freedom. Manual, exhaustive conformational searches were performed to ensure all relevant intermediates and transition structures were located. Intrinsic reaction coordinates (IRCs) were computed for all transition structures to verify reaction pathways.

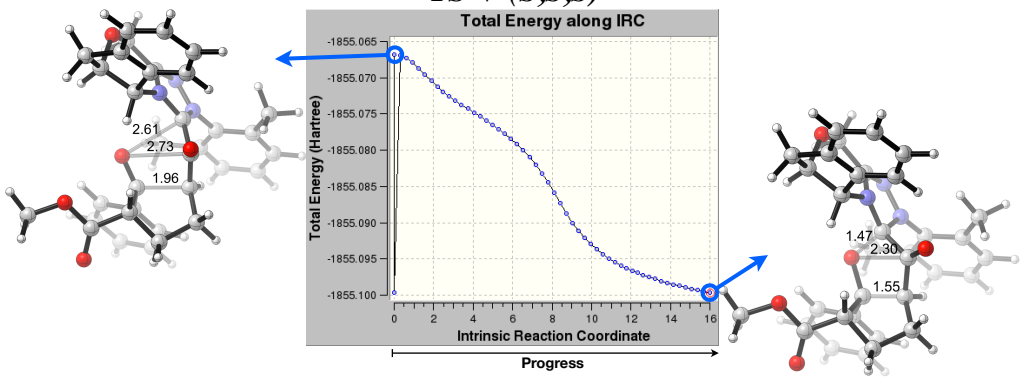
[4] Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.*, 2008, **120**, 215–241.
[5] W. J. Hehre, R. Ditchfield, and J. A. Pople, *J. Chem. Phys.*, 1972, **56**, 2257.
[6] P. C. Hariharan and J. A. Pople, *Theor. Chim. Acta*, 1973, **28**, 213–222.
[7] S. Miertuš, E. Scrocco, and J. Tomasi, *Chem. Phys.*, 1981, **55**, 117–129.
[8] Gaussian 09, Revision C.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

Intrinsic Reaction Coordinates for TS-V

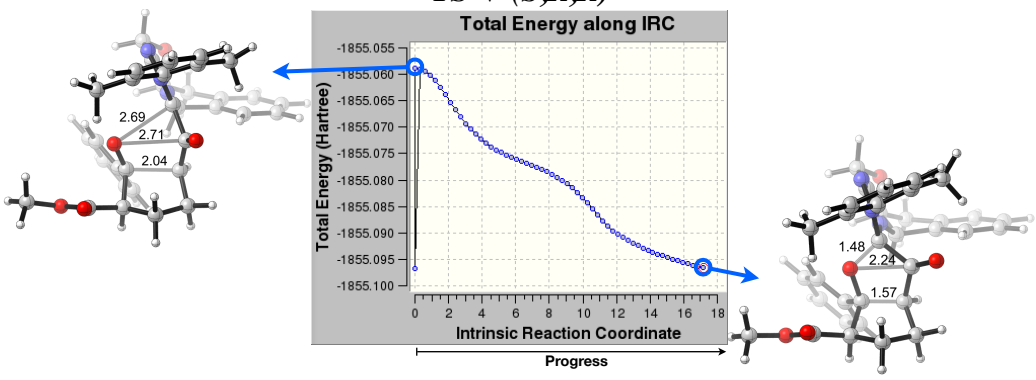
TS-V-*(R,S,S)* (major)



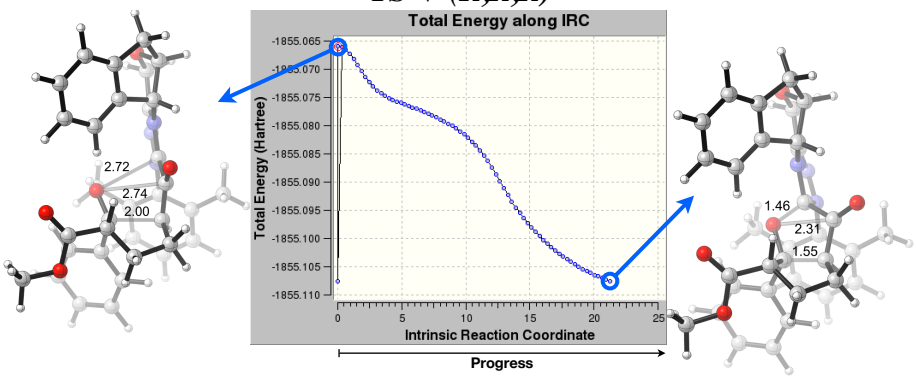
TS-V-*(S,S,S)*



TS-V-*(S,R,R)*



TS-V-*(R,R,R)*



Geometries and Thermodynamic Corrections for All Reported Structures

Gaussian input file parameters, XYZ coordinates for optimized structures, and thermodynamic corrections at M06-2X/6-31G*; single-point corrections at M06-2X/6-31+G(d,p)/PCM in dichloroethane with UFF radii. All geometries listed here are the lowest energy structures. All energies are in Hartrees.

—Parent Substrate—

I-Substrate

Supporting Information: 0000-a-sub_B-keto_ester-R-0003.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

==========

# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RM062X/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C14H14O4 C1[X(C14H14O4)] #Atoms= 32
Charge = 0 Multiplicity = 1

SCF Energy= -842.443339224 Predicted Change= -1.590531D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00164	0.00180	[YES]	0.00164	0.00180	[YES]

Atomic Type	X	Y	Z
C	-4.818885	-0.020201	-0.438658
H	-4.886439	0.022643	-1.547590
C	-3.602516	-0.671674	0.080835
H	-3.502958	-0.757426	1.161135
C	-2.660192	-1.113578	-0.758138
H	-2.814194	-0.979795	-1.831337
C	-1.358463	-1.717346	-0.328441
H	-1.111068	-2.599932	-0.925707
H	-1.400343	-2.027528	0.718971
C	-0.216707	-0.693164	-0.472622
H	-0.124576	-0.358833	-1.512218
C	-0.570005	0.500787	0.397471
O	-0.621392	0.457928	1.600089
O	-0.885057	1.581703	-0.330121
C	-1.349684	2.698888	0.433923
H	-0.587162	3.010614	1.150590
H	-2.260270	2.427909	0.973126
H	-1.549452	3.487774	-0.288868
C	1.112741	-1.309720	-0.015738
O	1.144816	-2.451871	0.384470
C	2.353103	-0.477519	-0.096705
O	-5.689315	0.448372	0.256646
C	3.537628	-1.027197	0.404497
H	3.501468	-2.022409	0.835625
C	4.721681	-0.305286	0.345738
H	5.638510	-0.733334	0.738558
C	4.731648	0.970503	-0.217760
H	5.657770	1.535423	-0.263968
C	3.556506	1.521825	-0.720441
H	3.564877	2.514090	-1.160216
C	2.367011	0.801264	-0.660824
H	1.458220	1.246251	-1.055591

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -842.443339224 Predicted Change= -1.590531D-08
Zero-point correction (ZPE)= -842.1864 0.25693
Internal Energy (U)= -842.1689 0.27437
Enthalpy (H)= -842.1680 0.27532
Gibbs Free Energy (G)= -842.2345 0.20877

Frequencies -- 21.7893 24.2763 42.8717
M06-2X/6-31+G(d,p)/PCM(DCE) SP: -842.5005031

I-NHC

Supporting Information: 0000-AzF-carbene.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

==========

# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RM062X/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C20H19N3O C1[X(C20H19N3O)] #Atoms= 43
Charge = 0 Multiplicity = 1

SCF Energy= -1012.58880870 Predicted Change= -1.292471D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00146	0.00180	[YES]	0.00146	0.00180	[YES]

Atomic Type	X	Y	Z
N	0.488187	-0.738820	-0.365817
C	-0.562768	-0.011023	-0.864456
N	-1.525512	-0.382301	0.006849
C	-2.879591	0.080751	-0.015513
N	-1.147649	-1.270519	0.997016
C	0.105901	-1.463152	0.734138
C	1.087586	-2.353729	1.428384
O	2.396922	-1.879975	1.202438
C	2.719068	-1.796012	-0.175758
C	1.850334	-0.716499	-0.871603
C	4.146080	-1.241662	-0.260550
C	3.932821	0.255856	-0.260846
C	2.613827	0.560020	-0.594636
C	4.836576	1.275466	0.008751
C	4.396118	2.597443	-0.058507
C	3.073872	2.893162	-0.391924
C	2.165526	1.871181	-0.667514
C	-3.702974	-0.298946	-1.079732
C	-3.183788	-1.177697	-2.186512
C	-5.017947	0.166698	-1.078976
C	-5.488999	0.972758	-0.048629
C	-4.646533	1.332627	0.997628
C	-3.322984	0.893964	1.031498
C	-2.391145	1.290541	2.145753
H	0.983330	-3.387075	1.061717
H	0.915380	-2.347960	2.505737
H	2.600043	-2.784550	-0.642792
H	1.805700	-0.908993	-1.949916
H	4.628267	-1.572986	-1.188430
H	4.742544	-1.604600	0.580918
H	5.864967	1.049919	0.277550
H	5.089190	3.405247	0.156599
H	2.749043	3.928226	-0.434670
H	1.130958	2.079322	-0.926925
H	-2.395336	-0.668319	-2.747692
H	-3.990817	-1.449227	-2.871133
H	-2.748027	-2.097458	-1.782003
H	-5.676574	-0.114383	-1.896034
H	-6.516278	1.324192	-0.062512
H	-5.012098	1.968840	1.799018
H	-2.849856	2.055366	2.776760
H	-1.452332	1.687139	1.744131
H	-2.134539	0.428091	2.767860

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1012.58880870 Predicted Change= -1.292471D-08
Zero-point correction (ZPE)= -1012.2309 0.35785
Internal Energy (U)= -1012.2121 0.37668
Enthalpy (H)= -1012.2111 0.37763
Gibbs Free Energy (G)= -1012.2788 0.31000

Frequencies -- 21.4932 28.0260 64.7719
M06-2X/6-31+G(d,p)/PCM(DCE) SP: -1012.650771

(R)-II

Supporting Information: 0100-AzF_tetrahedral-int-R-0001.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

```
================================================================================
==========
 # M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
 opt=(maxcycle=250) freq=noraman
 #N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RM062X/6-31G(d) Freq
 --------------------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C34H33N3O5   C1[X(C34H33N3O5)]  #Atoms= 75
 Charge = 0     Multiplicity = 1
 --------------------------------------------------------------------------------
 SCF Energy= -1855.05314400                  Predicted Change= -3.723794D-08
================================================================================
==========
 Optimization completed.           {Found       1       times}
 Item     Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00003 ||  0.00045   [ YES ]      0.00000 ||  0.00030   [ YES ]
 Displ      0.00600 ||  0.00180   [ NO ]       0.00600 ||  0.00180   [ NO ]
 --------------------------------------------------------------------------------
      Atomic          Coordinates (Angstroms)
       Type          X                 Y                 Z
 --------------------------------------------------------------------------------
      N       1.076587     0.613188    -0.741227
      C       2.003138     0.018903     0.029297
      N       2.897589    -0.476707    -0.821592
      C       4.156549    -1.071540    -0.474931
      N       2.549996    -0.267980    -2.130552
      C       1.423903     0.379981    -2.044053
      C       0.454365     0.693824    -3.143549
      H      -0.019952    -0.252511    -3.449125
      H       0.973524     1.117311    -4.005712
      O      -0.499589     1.624253    -2.715792
      C      -1.155882     1.285453    -1.491156
      H      -1.653330     0.309504    -1.576499
      C      -0.138164     1.332544    -0.330160
      H      -0.514882     0.825982     0.556618
      C      -2.085078     2.461219    -1.196994
      H      -2.861322     2.147133    -0.491410
      H      -2.558107     2.815996    -2.116617
      C      -1.140854     3.460491    -0.565657
      C      -0.000996     2.820306    -0.073932
      C      -1.289079     4.832825    -0.420801
      H      -2.171487     5.337764    -0.804718
      C      -0.278924     5.553264     0.217077
      H      -0.375353     6.629479     0.329149
      C       0.848270     4.903329     0.718415
      H       1.616628     5.476984     1.228156
      C       0.995678     3.521300     0.590577
      H       1.822694     2.978584     1.039011
      C       4.345396    -2.428418    -0.740242
      C       3.244487    -3.255518    -1.348134
      H       3.008851    -2.915440    -2.360945
      H       2.327581    -3.175160    -0.752975
      H       3.534494    -4.307451    -1.391456
      C       5.581580    -2.975407    -0.398379
      H       5.764484    -4.028623    -0.590496
      C       6.566711    -2.189821     0.191028
      H       7.522398    -2.632785     0.454275
      C       6.336851    -0.842147     0.449821
      H       7.109830    -0.236192     0.913269
      C       5.119256    -0.248111     0.118345
      C       4.843749     1.209432     0.390634
      H       5.755633     1.708812     0.724981
      H       4.074547     1.349292     1.162427
      H       4.491141     1.715936    -0.515120
      C       1.942073    -0.084311     1.555040
      H       2.944168    -0.492073     1.842808
      C       0.924553    -1.178477     1.895287
      H       0.808566    -1.279191     2.975693
      C       0.119726    -1.870308     1.085308
      H       0.181169    -1.772853     0.000973
      C      -0.996069    -2.746947     1.594137
      H      -0.841054    -2.954613     2.656297
      H      -1.022083    -3.700626     1.057110
      C      -2.381596    -2.075057     1.439630
      H      -3.111866    -2.605557     2.063636
      C      -2.295458    -0.629273     1.913952
      O      -2.577908     0.320770     1.215298
      O      -1.827227    -0.539160     3.150474
      C      -1.382731     0.774571     3.557112
      H      -1.229534     0.700662     4.632820
      H      -2.148822     1.515455     3.324745
      H      -0.436269     1.008227     3.047916
      C      -2.858090    -2.071120    -0.014347
      O      -2.073173    -2.310925    -0.911562
      C      -4.296432    -1.793326    -0.316380
      O       1.613975     1.094251     2.082733
      C      -4.719311    -1.940135    -1.640743
      H      -3.988564    -2.240940    -2.384614
      C      -6.044773    -1.708600    -1.983426
      H      -6.368706    -1.827133    -3.012644
      C      -6.958067    -1.322739    -1.003374
      H      -7.994818    -1.139057    -1.268924
      C      -6.542811    -1.168847     0.316824
      H      -7.251548    -0.860355     1.078747
      C      -5.215841    -1.404495     0.661341
      H      -4.902598    -1.266661     1.691609
 --------------------------------------------------------------------------------
 Statistical Thermodynamic Analysis
 Temperature= 298.150 Kelvin       Pressure= 1.00000 Atm
================================================================================
==========
 SCF Energy=     -1855.05314400              Predicted Change= -3.723794D-08
 Zero-point correction (ZPE)=                 -1854.4342  0.61891
 Internal Energy (U)=                         -1854.3981  0.65501
 Enthalpy (H)=                                            -1854.3971   0.65595
 Gibbs Free Energy (G)=                      -1854.5040   0.54906
 --------------------------------------------------------------------------------
 Frequencies --    10.9425              17.4096              23.5868
 M06-2X/6-31+G(d,p)/PCM(DCE) SP:  -1855.164611
```

(S)-II

```
 Supporting Information: 0100-AzF_tetrahedral-int-S-0001.log
 --------------------------------------------------------------------------------
 Using  Gaussian 09:  AM64L-G09RevC.01 23-Sep-2011
================================================================================
==========
 # M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
 opt=(maxcycle=250) freq=noraman
 #N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RM062X/6-31G(d) Freq
 --------------------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C34H33N3O5   C1[X(C34H33N3O5)]  #Atoms= 75
 Charge = 0     Multiplicity = 1
 --------------------------------------------------------------------------------
 SCF Energy= -1855.04958441                  Predicted Change= -2.790432D-08
================================================================================
==========
 Optimization completed.           {Found       1       times}
 Item     Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00003 ||  0.00045   [ YES ]      0.00000 ||  0.00030   [ YES ]
 Displ      0.00363 ||  0.00180   [ NO ]       0.00363 ||  0.00180   [ YES ]
 --------------------------------------------------------------------------------
      Atomic          Coordinates (Angstroms)
       Type          X                 Y                 Z
 --------------------------------------------------------------------------------
      N       0.915290     1.147845    -0.452581
      C       1.674683     0.137919     0.008201
      N       2.847643     0.280107    -0.603739
      C       4.046792    -0.457021    -0.324120
      N       2.856342     1.324860    -1.490671
      C       1.656060     1.817899    -1.387863
      C       1.006343     2.846191    -2.264460
      H       0.828150     2.382997    -3.247821
      H       1.665503     3.706081    -2.399980
      O      -0.187412     3.304989    -1.695418
      C      -1.089695     2.273849    -1.287162
      H      -1.346824     1.624291    -2.134961
      C      -0.472082     1.490728    -0.107615
      H      -0.991242     0.547522     0.059101
      C      -2.267379     3.006419    -0.647694
      H      -3.137774     2.343013    -0.608146
      H      -2.520773     3.902163    -1.221269
      C      -1.741421     3.295600     0.740545
      C      -0.684869     2.438273     1.058295
      C      -2.175587     4.242434     1.657186
      H      -2.995226     4.913117     1.413868
      C      -1.532931     4.323627     2.892503
      H      -1.855368     5.065307     3.617759
      C      -0.485361     3.458614     3.205306
      H      -0.004804     3.528572     4.176696
      C      -0.053880     2.492860     2.293979
      H       0.711240     1.760460     2.535667
      C       4.537434    -1.323697    -1.301067
      C       3.804674    -1.508430    -2.603052
      H       3.814533    -0.588151    -3.194881
      H       2.756076    -1.771302    -2.422328
      H       4.262841    -2.306074    -3.191563
      C       5.712748    -2.013736    -1.005239
      H       6.123583    -2.698419    -1.741469
      C       6.347828    -1.839449     0.220154
      H       7.260252    -2.386665     0.436315
      C       5.820198    -0.975200     1.174693
      H       6.317982    -0.848902     2.131542
      C       4.650324    -0.258871     0.922266
      C       4.052543     0.678025     1.941258
      H       3.081945     0.322272     2.315610
      H       3.888354     1.671079     1.507099
      H       4.728709     0.788402     2.791845
      C       1.238287    -0.913048     1.032679
      H       2.178915    -1.483223     1.243794
      C       0.300150    -1.904851     0.337531
      H      -0.026350    -2.682096     1.030534
      C      -0.234353    -1.852871    -0.884861
      H       0.038779    -1.068804    -1.592118
      C      -1.319291    -2.793049    -1.347580
      H      -1.382815    -3.641331    -0.658936
      H      -1.097296    -3.188107    -2.345249
```

C	-2.711422	-2.116031	-1.403940
H	-3.495061	-2.874754	-1.515805
C	-2.830209	-1.138122	-2.553572
O	-1.902741	-0.616670	-3.127431
O	-4.111500	-0.891733	-2.842476
C	-4.326845	0.145661	-3.798252
H	-3.928836	1.089604	-3.417105
H	-5.405701	0.210979	-3.928146
H	-3.835869	-0.095694	-4.743277
C	-2.959671	-1.313933	-0.118094
O	-3.084313	-0.105012	-0.169994
C	-2.905044	-2.038985	1.180056
O	0.673420	-0.309862	2.077685
C	-3.404591	-3.336439	1.330007
H	-3.902053	-3.833167	0.500507
C	-3.281834	-3.987626	2.552115
H	-3.687513	-4.986666	2.677115
C	-2.623675	-3.359622	3.609854
H	-2.505891	-3.880053	4.555794
C	-2.099477	-2.078837	3.450861
H	-1.544890	-1.602666	4.252333
C	-2.255020	-1.406180	2.244373
H	-1.787703	-0.435744	2.103731

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1855.04958441 Predicted Change= -2.790432D-08
Zero-point correction (ZPE)= -1854.4307 0.61887
Internal Energy (U)= -1854.3943 0.65520
Enthalpy (H)= -1854.3934 0.65614
Gibbs Free Energy (G)= -1854.4999 0.54967

Frequencies -- 16.8224 22.6388 31.5047
M06-2X/6-31+G(d,p)/PCM(DCE) SP: -1855.162748

(R)-III

Supporting Information: 0200-Breslow-R-E-0001.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

==========

# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RM062X/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C34H33N3O5 C1[X(C34H33N3O5)] #Atoms= 75
Charge = 0 Multiplicity = 1

SCF Energy= -1855.06666709 Predicted Change= -1.701788D-08

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00183	0.00180	[NO]	0.00183	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	3.053538	-1.191853	-0.570643
C	1.681179	-0.935205	-0.641757
N	1.144483	-1.828220	0.283250
C	-0.143659	-1.818597	0.885740
N	2.128875	-2.632383	0.853217
C	3.226085	-2.218597	0.329741
C	4.594939	-2.783131	0.539691
H	4.768345	-3.601700	-0.177229
H	4.687276	-3.177199	1.552462
O	5.562122	-1.773658	0.373408
C	5.499577	-1.169184	-0.907377
H	5.647170	-1.933113	-1.684644
C	4.163903	-0.404684	-1.092199
H	3.986402	-0.228353	-2.156899
C	6.557304	-0.062348	-0.910791
H	6.869557	0.161953	-1.938282
H	7.438738	-0.377560	-0.346039
C	5.818585	1.104782	-0.295958
C	4.439843	0.908036	-0.382770
C	6.330998	2.251741	0.294841
H	7.404136	2.405184	0.369870
C	5.442415	3.197840	0.805706
H	5.826832	4.097032	1.277695
C	4.065267	2.997149	0.718305
H	3.385535	3.743029	1.118603
C	3.549104	1.850208	0.115066
H	2.477145	1.704188	0.027443
C	-0.932914	-2.971831	0.751132
C	-0.416577	-4.157454	-0.018224
H	-0.066229	-3.852388	-1.010200
H	-1.197926	-4.911581	-0.138584
H	0.437436	-4.611535	0.493282
C	-2.197908	-2.978444	1.335951
H	-2.820147	-3.864833	1.241319
C	-2.670533	-1.864426	2.024546
H	-3.667031	-1.875200	2.455980
C	-1.868533	-0.736028	2.153713
H	-2.234570	0.138566	2.685200
C	-0.585187	-0.695284	1.600855
C	0.267424	0.534888	1.759348
H	0.160297	1.198922	0.891044
H	1.327612	0.277390	1.849982
H	-0.035252	1.090587	2.650765
C	1.038586	-0.049380	-1.453914
C	-0.392031	0.124042	-1.520092
H	-1.001341	-0.712975	-1.179691
C	-1.007617	1.230427	-1.972446
H	-0.421824	2.100759	-2.256287
C	-2.507461	1.379154	-1.926613
H	-3.007648	0.535219	-2.416517
H	-2.823761	2.292779	-2.437220
C	-2.990269	1.455009	-0.461497
H	-2.630458	0.577349	0.085983
C	-2.408560	2.674900	0.222121
O	-1.913081	3.623409	-0.328405
O	-2.501896	2.557242	1.559641
C	-2.007914	3.678141	2.290450
H	-0.948069	3.834290	2.074118
H	-2.154483	3.436255	3.342450
H	-2.563106	4.579064	2.021287
C	-4.511326	1.516536	-0.376292
O	-5.077757	2.579343	-0.223859
C	-5.286008	0.242216	-0.524623
O	1.832487	0.859998	-2.153109
H	1.462432	0.919106	-3.048334
C	-6.681835	0.330953	-0.542060
H	-7.134249	1.313951	-0.459576
C	-7.455646	-0.815768	-0.655922
H	-8.538524	-0.740796	-0.669119
C	-6.840273	-2.064417	-0.749206
H	-7.444963	-2.962567	-0.833456
C	-5.451780	-2.160621	-0.732061
H	-4.968427	-3.130381	-0.802255
C	-4.674397	-1.010915	-0.623543
H	-3.592867	-1.107166	-0.604494

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1855.06666709 Predicted Change= -1.701788D-08
Zero-point correction (ZPE)= -1854.4486 0.61800
Internal Energy (U)= -1854.4116 0.65496
Enthalpy (H)= -1854.4107 0.65591
Gibbs Free Energy (G)= -1854.5199 0.54668

Frequencies -- 12.6911 17.1596 22.5587
M06-2X/6-31+G(d,p)/PCM(DCE) SP: -1855.179363

(S)-III

Supporting Information: 0200-Breslow-S-E-0007.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

==========

# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RM062X/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C34H33N3O5 C1[X(C34H33N3O5)] #Atoms= 75
Charge = 0 Multiplicity = 1

SCF Energy= -1855.06813784 Predicted Change= -3.441642D-08

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.01598	0.00180	[NO]	0.01598	0.00180	[NO]

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	2.902695	-0.763630	-0.467806
C	1.613374	-0.498717	-0.007551
N	1.374212	-1.549665	0.858437
C	0.171349	-1.809910	1.571654
N	2.471536	-2.384420	0.991796
C	3.349011	-1.886250	0.194592
C	4.706216	-2.429190	-0.119296
H	4.634778	-3.147695	-0.951510
H	5.115282	-2.941021	0.752652
O	5.581609	-1.376859	-0.458154

C	5.111668	-0.622606	-1.561591
H	4.990553	-1.279909	-2.435087
C	3.796705	0.114263	-1.208065
H	3.289328	0.419577	-2.127073
C	6.117070	0.513336	-1.775871
H	6.081347	0.860611	-2.815781
H	7.132603	0.167369	-1.565469
C	5.625956	1.580090	-0.822703
C	4.298592	1.337647	-0.464108
C	6.307522	2.672107	-0.303180
H	7.342981	2.859783	-0.574141
C	5.647411	3.514502	0.591530
H	6.170123	4.366931	1.014680
C	4.327672	3.260837	0.961521
H	3.832791	3.914979	1.672810
C	3.638025	2.168863	0.432644
H	2.619301	1.955151	0.747068
C	-0.934128	-2.296008	0.864245
C	-0.815719	-2.626728	-0.597960
H	-0.008219	-3.347683	-0.766179
H	-0.584314	-1.729267	-1.183169
H	-1.750674	-3.046375	-0.978079
C	-2.137150	-2.427868	1.555415
H	-3.019049	-2.770914	1.022701
C	-2.219468	-2.107337	2.906887
H	-3.170854	-2.196083	3.421793
C	-1.094296	-1.664102	3.595235
H	-1.162030	-1.417552	4.651320
C	0.123205	-1.500324	2.934629
C	1.346060	-0.964994	3.630428
H	2.163292	-1.692361	3.604450
H	1.124817	-0.721548	4.672129
H	1.709777	-0.057979	3.132910
C	0.797632	0.539455	-0.382110
C	-0.435342	0.932873	0.250860
H	-0.716826	0.426580	1.171396
C	-1.227659	1.929008	-0.190813
H	-0.983040	2.435507	-1.124783
C	-2.498337	2.340165	0.491997
H	-2.576425	3.429584	0.575916
H	-2.546303	1.937781	1.510054
C	-3.741305	1.841247	-0.266309
H	-3.662901	2.080966	-1.333111
C	-5.002227	2.517346	0.248698
O	-5.044013	3.394471	1.071473
O	-6.090957	2.017343	-0.360441
C	-7.330304	2.575342	0.073586
H	-8.103317	2.060647	-0.494862
H	-7.355013	3.649048	-0.126049
H	-7.464234	2.409976	1.144731
C	-3.924990	0.330407	-0.075263
O	-4.274513	-0.084703	1.010563
C	-3.726039	-0.605532	-1.223987
O	1.242109	1.312378	-1.457310
H	1.350198	2.224787	-1.135707
C	-2.883183	-0.317022	-2.299349
H	-2.309015	0.604960	-2.310716
C	-2.736278	-1.238122	-3.333612
H	-2.065380	-1.018860	-4.158274
C	-3.446317	-2.435672	-3.309543
H	-3.338899	-3.146431	-4.123449
C	-4.294817	-2.724796	-2.240200
H	-4.852506	-3.656127	-2.223358
C	-4.424216	-1.817594	-1.196235
H	-5.075304	-2.019752	-0.350877

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1855.06813784 Predicted Change= -3.441642D-08
Zero-point correction (ZPE)= -1854.4506 0.61745
Internal Energy (U)= -1854.4133 0.65476
Enthalpy (H)= -1854.4124 0.65570
Gibbs Free Energy (G)= -1854.5231 0.54500

Frequencies -- 10.6442 19.1011 22.6568
M06-2X/6-31+G(d,p)/PCM(DCE) SP: -1855.181545

(R)-IV

Supporting Information: 0300-AzF-enolate-R-0002.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

==========

# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RM062X/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C34H33N3O5 C1[X(C34H33N3O5)] #Atoms= 75
Charge = 0 Multiplicity = 1

SCF Energy= -1855.08800097 Predicted Change= -3.300837D-08

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00004	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00182	0.00180	[NO]	0.00182	0.00180	[YES]

Atomic Type	X	Y	Z
N	1.260017	1.625304	-0.518219
C	1.863943	0.446722	-0.267829
C	1.149116	-0.877089	-0.249920
C	1.391732	-1.647632	0.847495
H	2.106131	-1.271497	1.577359
C	0.697700	-2.953470	1.138811
H	0.644977	-3.565698	0.229636
C	-0.733311	-2.770683	1.682971
H	-0.744854	-1.995334	2.456693
H	-1.092362	-3.695053	2.144584
C	-1.678271	-2.366538	0.545719
H	-1.102413	-1.802625	-0.201653
C	-2.161821	-3.604013	-0.191920
O	-1.760391	-4.726404	-0.013497
O	-3.098346	-3.300978	-1.109484
C	-3.580867	-4.409100	-1.865572
H	-2.762327	-4.878463	-2.415808
H	-4.321451	-3.999823	-2.551089
H	-4.034032	-5.151574	-1.204950
C	-2.865003	-1.517512	0.993678
O	-3.313979	-1.629800	2.116641
C	-3.448253	-0.515871	0.034554
H	1.289759	-3.521555	1.863964
O	0.389144	-1.020352	-1.273068
N	3.165079	0.733395	-0.210924
C	4.245900	-0.205465	-0.086993
N	3.416900	2.065585	-0.410104
C	2.235924	2.578750	-0.594462
C	1.864936	3.991782	-0.930005
H	2.063892	4.172307	-1.997768
H	2.462306	4.689876	-0.341118
O	0.512593	4.214273	-0.622162
C	-0.370601	3.304340	-1.268906
H	-0.214188	3.347091	-2.355966
C	-0.172678	1.879244	-0.700567
H	-0.529184	1.100607	-1.385120
C	-1.786401	3.679332	-0.824839
H	-2.517709	3.333005	-1.564951
H	-1.877810	4.764213	-0.723013
C	-1.945178	2.921396	0.472231
C	-0.996993	1.902501	0.568594
C	-2.874750	3.108708	1.485503
H	-3.617974	3.898192	1.413686
C	-2.841650	2.263935	2.594916
H	-3.567472	2.394173	3.391843
C	-1.890936	1.248689	2.687021
H	-1.892315	0.582549	3.544000
C	-0.954566	1.057734	1.669951
H	-0.219948	0.258178	1.733789
C	4.500437	-1.050927	-1.170251
C	3.686239	-0.972652	-2.435814
H	3.689561	0.049113	-2.833120
H	2.640152	-1.260136	-2.276372
H	4.109775	-1.631523	-3.196759
C	5.551724	-1.955797	-1.027131
H	5.778687	-2.631886	-1.846094
C	6.305692	-1.996021	0.141462
H	7.118954	-2.709266	0.232848
C	6.026383	-1.129474	1.192898
H	6.618479	-1.164461	2.102678
C	4.981013	-0.211536	1.098707
C	4.646369	0.734028	2.221427
H	3.585556	0.671031	2.489334
H	4.848239	1.771076	1.935309
H	5.236260	0.498320	3.109520
C	-4.562067	0.212709	0.457877
H	-4.952994	0.019598	1.452082
C	-5.144878	1.160891	-0.376047
H	-6.013288	1.719785	-0.039742
C	-4.613215	1.391626	-1.642826
H	-5.070548	2.126262	-2.300421
C	-3.494045	0.675607	-2.067435
H	-3.078662	0.849598	-3.056726
C	-2.910468	-0.275887	-1.235978
H	-2.036263	-0.819949	-1.583278

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1855.08800097 Predicted Change= -3.300837D-08
Zero-point correction (ZPE)= -1854.4682 0.61970

Internal Energy (U)= -1854.4320 0.65590
Enthalpy (H)= -1854.4311 0.65684
Gibbs Free Energy (G)= -1854.5364 0.55154

Frequencies -- 22.3405 28.7232 35.1065
M06-2X/6-31+G(d,p)/PCM(DCE) SP: -1855.200359

(S)-IV

Supporting Information: 0300-AzF-enolate-S-0004.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011
==========
# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RM062X/6-31G(d) Freq
---
Pointgroup= C1 Stoichiometry= C34H33N3O5 C1[X(C34H33N3O5)] #Atoms= 75
Charge = 0 Multiplicity = 1

SCF Energy= -1855.08905003 Predicted Change= -2.839271D-09
==========
Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00264	0.00180	[NO]	0.00264	0.00180	[YES]

Atomic Type	X	Y	Z
N	-1.250019	1.643255	0.255592
C	-1.790649	0.410615	0.173382
C	-1.023328	-0.854843	0.436681
C	-1.330958	-1.949728	-0.316042
H	-2.106088	-1.894151	-1.075213
C	-0.633187	-3.246309	-0.016070
H	-0.471244	-3.311339	1.065938
C	0.733001	-3.414129	-0.704849
H	0.595879	-3.463746	-1.791699
H	1.199040	-4.348945	-0.374196
C	1.693849	-2.251977	-0.409622
H	1.199858	-1.311619	-0.662742
C	2.888808	-2.359056	-1.332336
O	2.919108	-1.951483	-2.470425
O	3.918029	-3.002002	-0.758542
C	5.069840	-3.156620	-1.583604
H	5.802448	-3.683763	-0.974641
H	5.451724	-2.179047	-1.887611
H	4.822094	-3.733415	-2.477387
C	2.107288	-2.191814	1.059278
O	1.938448	-3.131573	1.803605
C	2.758984	-0.928369	1.548637
H	-1.265221	-4.092817	-0.307281
O	-0.164375	-0.715797	1.371012
N	-3.100855	0.624583	0.023661
C	-4.143984	-0.363345	-0.005342
N	-3.415042	1.957612	0.001867
C	-2.265246	2.549202	0.146030
C	-1.971800	4.012362	0.292837
H	-2.223399	4.322971	1.318940
H	-2.577613	4.593312	-0.404618
O	-0.620255	4.265548	0.005455
C	0.281215	3.489496	0.789375
H	0.095741	3.669899	1.857012
C	0.161819	1.998126	0.411704
H	0.562771	1.326349	1.181392
C	1.693647	3.857360	0.328586
H	2.413033	3.620482	1.122905
H	1.759181	4.925025	0.102329
C	1.900290	2.957725	-0.868575
C	0.981233	1.907949	-0.855374
C	2.847170	3.041717	-1.879679
H	3.566862	3.856034	-1.899490
C	2.856145	2.063726	-2.876146
H	3.595816	2.113038	-3.669428
C	1.921338	1.028835	-2.870278
H	1.951573	0.263046	-3.637301
C	0.964958	0.946461	-1.855872
H	0.240830	0.133953	-1.846859
C	-4.446764	-1.030596	1.184197
C	-3.706739	-0.729912	2.461015
H	-3.715336	0.345206	2.672789
H	-2.658671	-1.047806	2.408972
H	-4.178134	-1.243929	3.301265
C	-5.463649	-1.983144	1.128640
H	-5.726649	-2.525571	2.031883
C	-6.136948	-2.240728	-0.061385
H	-6.925570	-2.986657	-0.083353
C	-5.807941	-1.550839	-1.223639
H	-6.334455	-1.758120	-2.150652
C	-4.794952	-0.592896	-1.217813
C	-4.396678	0.157886	-2.460778
H	-4.940845	-0.219750	-3.328876
H	-3.323520	0.050130	-2.656650
H	-4.604167	1.227726	-2.358925
C	3.281138	0.039852	0.688377
H	3.215624	-0.071461	-0.391999
C	3.896642	1.177819	1.209431
H	4.313284	1.916178	0.529629
C	3.972114	1.364223	2.587115
H	4.449083	2.253213	2.990996
C	3.441557	0.402187	3.448315
H	3.497215	0.545744	4.523361
C	2.848371	-0.740974	2.930215
H	2.433133	-1.507425	3.576351

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
==========
SCF Energy= -1855.08905003 Predicted Change= -2.839271D-09
Zero-point correction (ZPE)= -1854.4701 0.61885
Internal Energy (U)= -1854.4337 0.65532
Enthalpy (H)= -1854.4327 0.65626
Gibbs Free Energy (G)= -1854.5405 0.54847

Frequencies -- 9.0908 22.3435 24.5945
M06-2X/6-31+G(d,p)/PCM(DCE) SP: -1855.202534

TS-V-*(S,R,R)*

Supporting Information: 0305-AzF-Re-aldol-R_ent-6.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011
==========
# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest,gdiis) iop(1/8=18) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31G(d) Freq
---
Pointgroup= C1 Stoichiometry= C34H33N3O5 C1[X(C34H33N3O5)] #Atoms= 75
Charge = 0 Multiplicity = 1

SCF Energy= -1855.05887507 Predicted Change= -3.140712D-08
==========
Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00004	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.01051	0.00180	[NO]	0.01051	0.00180	[NO]

Atomic Type	X	Y	Z
N	-1.084284	-0.613722	-0.734291
C	-0.026007	-1.068438	-0.027975
C	0.476218	-0.716844	1.371815
C	0.156618	0.585795	1.866408
H	-0.881953	0.889986	1.778281
C	0.888670	0.950989	3.140884
H	0.378186	1.785059	3.637993
C	2.298279	1.376838	2.717472
H	2.862422	0.508045	2.364452
H	2.865911	1.836546	3.532532
C	2.101452	2.334896	1.552864
H	1.660400	3.277508	1.899354
C	3.383689	2.651000	0.821704
O	4.443213	2.097006	0.972677
O	3.189048	3.638809	-0.073771
C	4.301159	3.894270	-0.923170
H	3.992812	4.702896	-1.585123
H	4.547026	2.998314	-1.498871
H	5.175522	4.188660	-0.337803
C	1.170979	1.678669	0.480417
O	1.729235	0.934972	-0.379382
C	0.065980	2.591012	-0.049146
H	0.928349	0.113247	3.846252
O	1.283403	-1.511058	1.836416
N	0.634282	-1.877280	-0.855277
C	1.758235	-2.755322	-0.604385
N	0.048454	-1.940668	-2.079495
C	-0.988419	-1.163566	-1.982853
C	-2.011345	-0.860630	-3.032043
H	-2.141426	-1.727112	-3.681981
H	-1.675249	-0.004888	-3.637688
O	-3.242321	-0.584106	-2.411154
C	-3.141515	0.526983	-1.535641
H	-2.760754	1.398571	-2.080403
C	-2.243787	0.191299	-0.316650
H	-1.871703	1.130413	0.098588
C	-4.520349	0.743621	-0.908843
H	-5.308008	0.520331	-1.633159
H	-4.620472	1.791533	-0.599475
C	-4.504319	-0.177861	0.288587

C	-3.192963	-0.517571	0.626390
C	-5.568140	-0.674567	1.028588
H	-6.591209	-0.419536	0.767054
C	-5.302803	-1.521005	2.105167
H	-6.125592	-1.924937	2.686958
C	-3.992011	-1.860196	2.436738
H	-3.800342	-2.522553	3.274781
C	-2.920704	-1.355393	1.699620
H	-1.901562	-1.618521	1.970124
C	3.010520	-2.418121	-1.114953
C	3.279481	-1.115440	-1.814149
H	3.379889	-0.307355	-1.083430
H	2.453974	-0.832856	-2.472606
H	4.193759	-1.193265	-2.407444
C	4.035283	-3.348196	-0.913429
H	5.026813	-3.117654	-1.292115
C	3.804779	-4.543012	-0.246312
H	4.617197	-5.249199	-0.104760
C	2.534285	-4.844988	0.235635
H	2.352626	-5.782286	0.753321
C	1.481494	-3.952519	0.062355
C	0.108661	-4.247477	0.602501
H	0.032132	-5.294549	0.903551
H	-0.674479	-4.049866	-0.138043
H	-0.085266	-3.624028	1.482396
C	-0.113222	2.638285	-1.432570
H	0.564097	2.046060	-2.041234
C	-1.117252	3.427854	-1.992121
H	-1.236607	3.469274	-3.072341
C	-1.970334	4.162976	-1.171799
H	-2.757707	4.772979	-1.605071
C	-1.790905	4.129020	0.212594
H	-2.441657	4.711243	0.858748
C	-0.772306	3.359672	0.765643
H	-0.643315	3.332460	1.846251

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -1855.05887507 Predicted Change= -3.140712D-08
Zero-point correction (ZPE)= -1854.4403 0.61848
Internal Energy (U)= -1854.4050 0.65385
Enthalpy (H)= -1854.4040 0.65479
Gibbs Free Energy (G)= -1854.5093 0.54949

Frequencies -- -270.7563 7.2320 15.8405
M06-2X/6-31+G(d,p)/PCM(DCE) SP: -1855.170435

TS-V-*(R,S,S)*

Supporting Information: 0305-AzF-Re-aldol-R-3.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RM062X/6-31G(d) Freq

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Pointgroup= C1 Stoichiometry= C34H33N3O5 C1[X(C34H33N3O5)] #Atoms= 75
Charge = 0 Multiplicity = 1

SCF Energy= -1855.06294493 Predicted Change= -5.451023D-10

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 ||	0.00045	[YES]	0.00000 ||	0.00030	[YES]
Displ	0.00037 ||	0.00180	[YES]	0.00037 ||	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	-1.176830	-0.770375	0.663074
C	-0.198478	-1.065344	-0.203757
C	0.054475	-0.321002	-1.508161
C	1.360086	0.284957	-1.619819
H	2.162251	-0.335821	-1.219959
C	1.627677	0.962048	-2.959254
H	2.700479	0.912886	-3.179226
C	1.194730	2.423424	-2.795361
H	0.103391	2.493335	-2.791442
H	1.583579	3.072449	-3.585702
C	1.706171	2.791490	-1.410933
H	2.801828	2.783647	-1.389826
C	1.265609	4.115270	-0.840180
O	1.761686	4.633126	0.131532
O	0.238412	4.659577	-1.514577
C	-0.283285	5.847448	-0.932467
H	-0.664113	5.639033	0.070354
H	-1.089706	6.173712	-1.588655
H	0.490958	6.615343	-0.861043
C	1.116210	1.696289	-0.451718
O	-0.126277	1.892926	-0.163520
C	2.022074	1.383719	0.747844
H	1.093402	0.469129	-3.777864
O	-0.921567	-0.128085	-2.209949
N	0.517207	-2.032770	0.367062
C	1.575044	-2.796476	-0.235999
N	0.055667	-2.336243	1.612260
C	-0.958299	-1.533400	1.774622
C	-1.740436	-1.271002	3.025866
H	-1.115782	-0.644664	3.682703
H	-1.963018	-2.206574	3.542127
O	-2.954141	-0.641910	2.723405
C	-2.816620	0.539590	1.934745
H	-2.177038	1.269270	2.448610
C	-2.290591	0.186120	0.527874
H	-1.862701	1.060472	0.021228
C	-4.244880	1.013643	1.662565
H	-4.241869	2.072904	1.379902
H	-4.867053	0.892740	2.553146
C	-4.655112	0.135532	0.500720
C	-3.526369	-0.371328	-0.147356
C	-5.927227	-0.192703	0.055231
H	-6.808031	0.196055	0.558709
C	-6.056163	-1.045952	-1.041092
H	-7.044898	-1.321516	-1.395079
C	-4.926984	-1.551013	-1.682883
H	-5.043100	-2.212132	-2.536152
C	-3.646360	-1.210326	-1.245413
H	-2.764683	-1.570537	-1.765695
C	1.302544	-3.482460	-1.426497
C	-0.063530	-3.507149	-2.066793
H	-0.235288	-2.636062	-2.707840
H	-0.862369	-3.531732	-1.318128
H	-0.161039	-4.399891	-2.688584
C	2.358457	-4.188133	-2.004327
H	2.182255	-4.728628	-2.929654
C	3.612937	-4.215477	-1.407711
H	4.421294	-4.767903	-1.876529
C	3.833466	-3.550872	-0.206400
H	4.810990	-3.585091	0.265620
C	2.814146	-2.828567	0.413036
C	3.037899	-2.130561	1.725080
H	4.101356	-1.935407	1.876021
H	2.675380	-2.749175	2.552690
H	2.507457	-1.176517	1.771087
C	1.431154	1.346372	2.011168
H	0.361133	1.528838	2.059204
C	2.200816	1.151195	3.157489
H	1.726474	1.141159	4.135691
C	3.580995	1.002593	3.054739
H	4.186600	0.870400	3.946596
C	4.181313	1.030430	1.795876
H	5.258051	0.915235	1.705015
C	3.406456	1.205852	0.654564
H	3.889050	1.220434	-0.321011

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -1855.06294493 Predicted Change= -5.451023D-10
Zero-point correction (ZPE)= -1854.4443 0.61856
Internal Energy (U)= -1854.4093 0.65358
Enthalpy (H)= -1854.4084 0.65453
Gibbs Free Energy (G)= -1854.5111 0.55183

Frequencies -- -214.2364 21.6359 21.9340
M06-2X/6-31+G(d,p)/PCM(DCE) SP: -1855.177494

TS-V-*(R,R,R)*

Supporting Information: 0305-AzF-Re-aldol-S_ent-3.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,modredundant)
Modredundant Input: B 4 20 F
# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest,nofreeze,gdiis) iop(1/8=18)
freq=noraman geom=allcheck guess=read
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C34H33N3O5 C1[X(C34H33N3O5)] #Atoms= 75
Charge = 0 Multiplicity = 1

SCF Energy= -1855.06596657 Predicted Change= -5.484592D-10

Optimization completed. {Found 3 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?

Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]	
Displ	0.00078	0.00180	[YES]	0.00078	0.00180	[YES]	

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	2.213732	1.338826	-0.183190
C	0.915325	1.314927	-0.562908
C	0.392381	0.410106	-1.677865
C	-1.006010	0.211428	-1.810673
H	-1.655376	1.026725	-1.523237
C	-1.431817	-0.699458	-2.948312
H	-2.282271	-0.278193	-3.494943
C	-1.777640	-2.100749	-2.384261
H	-1.527290	-2.890987	-3.098298
H	-2.844607	-2.190314	-2.161407
C	-0.973832	-2.232175	-1.100668
H	0.098482	-2.253285	-1.323093
C	-1.247852	-3.434312	-0.236752
O	-0.430009	-3.978758	0.466692
O	-2.541117	-3.808406	-0.275339
C	-2.892711	-4.839876	0.640433
H	-2.697478	-4.517130	1.666302
H	-2.316104	-5.745775	0.439135
H	-3.956842	-5.019407	0.492394
C	-1.192650	-0.967394	-0.205643
O	-0.329070	-0.745348	0.694093
C	-2.649012	-0.733001	0.229483
H	-0.600922	-0.790717	-3.654463
O	1.284201	-0.209533	-2.263566
N	0.316303	2.245301	0.185095
C	-1.068788	2.649177	0.212425
N	1.183828	2.862357	1.029459
C	2.327317	2.289999	0.788811
C	3.657856	2.652923	1.378532
H	3.558780	2.787536	2.457185
H	3.989109	3.605838	0.936294
O	4.596133	1.637012	1.154534
C	4.684319	1.252860	-0.209914
H	4.930008	2.128529	-0.828427
C	3.378019	0.558710	-0.653554
H	3.305190	0.518281	-1.740907
C	5.716052	0.123477	-0.282429
H	6.542110	0.321274	0.406103
H	6.124623	0.053488	-1.298105
C	4.894431	-1.094974	0.078209
C	3.532011	-0.832901	-0.076024
C	5.318234	-2.337450	0.528080
H	6.376247	-2.548929	0.657790
C	4.356987	-3.303542	0.830824
H	4.674403	-4.278759	1.188247
C	2.997530	-3.022208	0.701465
H	2.248359	-3.766333	0.954460
C	2.566749	-1.775340	0.244578
H	1.504591	-1.544098	0.207021
C	-1.561207	3.383987	-0.870500
C	-0.679692	3.773568	-2.028581
H	-1.163460	4.547909	-2.627834
H	-0.482013	2.916479	-2.683515
H	0.284014	4.162977	-1.684456
C	-2.915428	3.712672	-0.849720
H	-3.336151	4.268863	-1.682514
C	-3.721048	3.333643	0.220397
H	-4.778780	3.578766	0.212345
C	-3.179137	2.656463	1.305379
H	-3.809459	2.368304	2.141171
C	-1.827230	2.309894	1.337455
C	-1.217720	1.624371	2.527965
H	-2.002904	1.327233	3.226863
H	-0.527164	2.300047	3.043586
H	-0.675014	0.729297	2.205791
C	-2.909320	-1.023063	1.575175
H	-2.081461	-1.367302	2.188246
C	-4.180428	-0.858528	2.115350
H	-4.356744	-1.091908	3.161998
C	-5.224004	-0.392342	1.317504
H	-6.217318	-0.257367	1.735801
C	-4.980279	-0.104512	-0.021538
H	-5.783023	0.263095	-0.654688
C	-3.706510	-0.276650	-0.561025
H	-3.549041	-0.027624	-1.605894

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -1855.06596657 Predicted Change= -5.484592D-10
Zero-point correction (ZPE)= -1854.4459 0.61997
Internal Energy (U)= -1854.4112 0.65471
Enthalpy (H)= -1854.4103 0.65565
Gibbs Free Energy (G)= -1854.5111 0.55481

Frequencies -- -272.1313 26.4501 35.2386

M06-2X/6-31+G(d,p)/PCM(DCE) SP: -1855.173254

TS-V-*(S,S,S)*

Supporting Information: 0305-AzF-Re-aldol-S-2.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250,calcfc,ts,noeigentest,gdiis) iop(1/8=18) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31G(d) Freq

Pointgroup= C1 Stoichiometry= C34H33N3O5 C1[X(C34H33N3O5)] #Atoms= 75
Charge = 0 Multiplicity = 1

SCF Energy= -1855.06679073 Predicted Change= -7.514585D-10

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00085	0.00180	[YES]	0.00085	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	1.661874	-0.777219	-0.649049
C	0.635808	-1.209106	0.102553
C	0.262495	-0.592191	1.439432
C	-1.120451	-0.305180	1.625493
H	-1.811058	-1.023092	1.198093
C	-1.480540	0.352349	2.945348
H	-2.349214	-0.130020	3.405568
C	-1.745774	1.853661	2.699009
H	-1.452183	2.464713	3.557326
H	-2.806401	2.051055	2.516326
C	-0.961686	2.226123	1.452265
H	0.119908	2.197494	1.632141
C	-1.334080	3.586735	0.921617
O	-2.338850	4.196726	1.200635
O	-0.421665	4.049447	0.045275
C	-0.768165	5.289847	-0.561430
H	-1.710304	5.196035	-1.107766
H	0.048468	5.528605	-1.242097
H	-0.880194	6.070914	0.194528
C	-1.222626	1.163061	0.330545
O	-0.372945	1.087342	-0.617883
C	-2.690041	1.136273	-0.135342
H	-0.638551	0.238004	3.635539
O	1.215566	-0.191035	2.106777
N	0.012085	-2.125880	-0.629780
C	-1.176671	-2.858211	-0.288936
N	0.577465	-2.269502	-1.858257
C	1.562471	-1.416048	-1.849742
C	2.420114	-1.013003	-3.010995
H	1.776607	-0.498848	-3.740899
H	2.857620	-1.892113	-3.488737
O	3.470357	-0.189430	-2.585351
C	3.044255	0.902628	-1.774938
H	2.274727	1.489970	-2.292292
C	2.543441	0.375842	-0.412644
H	1.914366	1.125587	0.076669
C	4.316130	1.669062	-1.409419
H	4.065748	2.693691	-1.109797
H	4.995757	1.714498	-2.264314
C	4.850018	0.867857	-0.242846
C	3.834689	0.096389	0.326880
C	6.138539	0.824135	0.270535
H	6.931638	1.420027	-0.172624
C	6.401104	-0.013832	1.354013
H	7.406109	-0.068130	1.761481
C	5.385677	-0.786802	1.915160
H	5.606497	-1.433026	2.759078
C	4.086440	-0.733602	1.410073
H	3.284851	-1.305976	1.863553
C	-1.107741	-3.803323	0.737220
C	0.180335	-4.096789	1.462727
H	0.104357	-5.045768	1.997923
H	0.407252	-3.317406	2.200170
H	1.027795	-4.161071	0.773332
C	-2.295981	-4.444096	1.085281
H	-2.282040	-5.185651	1.878818
C	-3.487499	-4.134043	0.436989
H	-4.405021	-4.634582	0.730818
C	-3.513102	-3.185704	-0.579802
H	-4.447754	-2.934533	-1.072722
C	-2.348799	-2.525859	-0.975613
C	-2.363648	-1.489743	-2.066800
H	-2.075464	-1.941813	-3.022544
H	-1.669209	-0.669056	-1.855848
H	-3.365964	-1.063572	-2.165549
C	-2.926717	1.797662	-1.347562

H	-2.077137	2.253662	-1.847650
C	-4.196724	1.836623	-1.910139
H	-4.355815	2.354914	-2.851592
C	-5.262254	1.199158	-1.275642
H	-6.254642	1.217272	-1.716551
C	-5.042568	0.544454	-0.068011
H	-5.864374	0.046943	0.439316
C	-3.770000	0.522475	0.502540
H	-3.634733	0.004269	1.447362

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -1855.06679073 Predicted Change= -7.514585D-10
Zero-point correction (ZPE)= -1854.4470 0.61972
Internal Energy (U)= -1854.4121 0.65462
Enthalpy (H)= -1854.4112 0.65556
Gibbs Free Energy (G)= -1854.5132 0.55349

Frequencies -- -267.0310 23.5290 28.7963
M06-2X/6-31+G(d,p)/PCM(DCE) SP: -1855.175582

VIb-*(R,R,R)*

Supporting Information: 0410-AzF-spiro-R_ent-R-1.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RM062X/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C34H33N3O5 C1[X(C34H33N3O5)] #Atoms= 75
Charge = 0 Multiplicity = 1

SCF Energy= -1855.11021853 Predicted Change= -3.634295D-08

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00004	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00408	0.00180	[NO]	0.00408	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	1.352104	1.376452	0.387100
C	0.004093	1.160243	-0.072469
C	-0.107280	0.837683	-1.579417
C	-0.585578	-0.584905	-1.768001
H	0.241752	-1.148949	-2.213320
C	-1.876468	-0.648496	-2.599579
H	-1.863229	0.096379	-3.400811
C	-2.979702	-0.419225	-1.559757
H	-3.956440	-0.763722	-1.906834
H	-3.062006	0.643688	-1.309379
C	-2.503802	-1.194358	-0.324087
H	-2.864213	-0.777090	0.620337
C	-2.915417	-2.648688	-0.399312
O	-3.133617	-3.260084	-1.419275
O	-2.968278	-3.202699	0.818471
C	-3.156736	-4.617317	0.829898
H	-4.094464	-4.882394	0.337016
H	-3.175782	-4.905195	1.879754
H	-2.325841	-5.103990	0.312179
C	-0.935321	-1.057044	-0.335324
O	-0.588413	0.016875	0.549094
C	-0.214253	-2.317020	0.117627
H	-1.987089	-1.641406	-3.043597
O	0.166729	1.616521	-2.452591
N	-0.590087	2.411890	0.328512
C	-2.013407	2.552990	0.358373
N	0.140993	2.957512	1.402760
C	1.260165	2.340588	1.383723
C	2.382154	2.513540	2.370000
H	1.998191	2.286484	3.376455
H	2.746347	3.542975	2.365266
O	3.480371	1.686201	2.059944
C	3.110271	0.348050	1.780491
H	2.523454	-0.067574	2.614085
C	2.333688	0.308747	0.447505
H	1.803123	-0.651850	0.383118
C	4.400055	-0.420371	1.480124
H	4.242333	-1.493419	1.647716
H	5.211827	-0.085268	2.131428
C	4.630204	-0.118409	0.014932
C	3.453606	0.347275	-0.574608
C	5.795176	-0.225468	-0.731498
H	6.716602	-0.577868	-0.275674
C	5.769422	0.150011	-2.075385
H	6.675045	0.081484	-2.670628
C	4.597751	0.634907	-2.654096
H	4.599101	0.943936	-3.694932
C	3.424626	0.740215	-1.904815
H	2.521095	1.148817	-2.347824
C	-2.635352	3.157474	-0.746172
C	-1.857473	3.739208	-1.898680
H	-1.871009	3.070330	-2.766178
H	-0.813359	3.901817	-1.632691
H	-2.309091	4.687216	-2.205846
C	-4.032732	3.230306	-0.768463
H	-4.519563	3.691287	-1.624115
C	-4.790298	2.737295	0.282200
H	-5.874223	2.795702	0.249331
C	-4.154874	2.195997	1.396547
H	-4.744753	1.843983	2.238835
C	-2.765555	2.105149	1.464464
C	-2.120055	1.589335	2.725648
H	-1.361088	0.835046	2.510890
H	-2.876763	1.149533	3.381089
H	-1.628768	2.407443	3.260348
C	0.208788	-2.453430	1.441967
H	0.048733	-1.633110	2.134679
C	0.830548	-3.623969	1.866485
H	1.158160	-3.714836	2.897920
C	1.028794	-4.677063	0.976257
H	1.515923	-5.588958	1.307694
C	0.598155	-4.552849	-0.341639
H	0.746598	-5.366366	-1.045118
C	-0.020856	-3.379969	-0.767968
H	-0.370020	-3.302209	-1.794776

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -1855.11021853 Predicted Change= -3.634295D-08
Zero-point correction (ZPE)= -1854.4885 0.62164
Internal Energy (U)= -1854.4540 0.65615
Enthalpy (H)= -1854.4531 0.65709
Gibbs Free Energy (G)= -1854.5547 0.55544

Frequencies -- 15.4073 19.1539 29.8746
M06-2X/6-31+G(d,p)/PCM(DCE) SP: -1855.210665

VIb-*(R,S,S)*

Supporting Information: 0410-AzF-spiro-R-R-1.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RM062X/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C34H33N3O5 C1[X(C34H33N3O5)] #Atoms= 75
Charge = 0 Multiplicity = 1

SCF Energy= -1855.11290152 Predicted Change= -3.668496D-08

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00560	0.00180	[NO]	0.00560	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	-1.276898	-1.280914	-0.029714
C	-0.025600	-0.679184	-0.403615
C	0.039943	0.186374	-1.687739
C	1.141373	1.201391	-1.469493
H	2.055792	0.722389	-1.835884
C	0.933123	2.602323	-2.065143
H	1.703438	2.852309	-2.799007
C	0.982184	3.552445	-0.849602
H	0.381805	4.455761	-0.989852
H	2.012323	3.866491	-0.651059
C	0.501030	2.701166	0.343333
H	0.791664	3.114023	1.311080
C	-0.999807	2.581290	0.275156
O	-1.600407	2.149562	-0.684083
O	-1.611093	3.035831	1.373853
C	-3.042465	3.058821	1.303580
H	-3.438831	2.063284	1.091243
H	-3.365646	3.735731	0.509456
H	-3.377849	3.416514	2.275564
C	1.187173	1.328838	0.067768
O	0.438067	0.231600	0.615476
C	2.578571	1.346003	0.680569
H	-0.036791	2.641004	-2.566142
O	-0.612338	0.008282	-2.678818

N	0.781172	-1.880766	-0.588835
C	2.209307	-1.818027	-0.592669
N	0.196253	-2.970769	0.070416
C	-0.987211	-2.588679	0.354652
C	-1.993719	-3.421841	1.097860
H	-1.535345	-3.756967	2.040671
H	-2.262924	-4.305458	0.514663
O	-3.184685	-2.714538	1.344274
C	-2.953917	-1.392090	1.791164
H	-2.304583	-1.397037	2.679821
C	-2.355977	-0.559642	0.633620
H	-1.931679	0.357694	1.059751
C	-4.329822	-0.763870	2.023465
H	-4.244955	0.085702	2.714338
H	-5.018227	-1.491993	2.460700
C	-4.719463	-0.316603	0.631533
C	-3.590646	-0.240522	-0.187360
C	-5.978447	-0.018075	0.127614
H	-6.860005	-0.083302	0.759947
C	-6.093518	0.342196	-1.215066
H	-7.071740	0.567366	-1.629843
C	-4.965332	0.397000	-2.033602
H	-5.073969	0.664993	-3.080189
C	-3.698680	0.107425	-1.525992
H	-2.817301	0.141140	-2.157797
C	2.860514	-1.710977	-1.831737
C	2.105053	-1.759719	-3.137665
H	1.136986	-2.247567	-3.013178
H	2.689424	-2.305743	-3.883630
H	1.913454	-0.760079	-3.546612
C	4.252532	-1.577289	-1.842613
H	4.764438	-1.484078	-2.797279
C	4.977967	-1.591344	-0.659592
H	6.058592	-1.482303	-0.681102
C	4.321369	-1.762323	0.554852
H	4.889106	-1.781654	1.481450
C	2.934644	-1.883524	0.612392
C	2.254506	-2.100694	1.938877
H	1.943802	-3.144617	2.043286
H	1.360004	-1.479629	2.028596
H	2.937380	-1.850944	2.755778
C	2.702318	1.127121	2.056899
H	1.810272	0.911749	2.639072
C	3.948570	1.152680	2.668693
H	4.029483	0.967913	3.735962
C	5.092875	1.416564	1.915232
H	6.067986	1.438383	2.392444
C	4.976093	1.654898	0.551803
H	5.859855	1.860841	-0.044598
C	3.724654	1.619565	-0.062785
H	3.658813	1.799142	-1.132658

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1855.11290152 Predicted Change= -3.668496D-08
Zero-point correction (ZPE)= -1854.4911 0.62178
Internal Energy (U)= -1854.4568 0.65600
Enthalpy (H)= -1854.4559 0.65695
Gibbs Free Energy (G)= -1854.5542 0.55867

Frequencies -- 25.6683 37.9163 47.0323
M06-2X/6-31+G(d,p)/PCM(DCE) SP: -1855.212559

VIb-*(S,R,R)*

Supporting Information: 0410-AzF-spiro-S_ent-R-1.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

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# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RM062X/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C34H33N3O5 C1[X(C34H33N3O5)] #Atoms= 75
Charge = 0 Multiplicity = 1

SCF Energy= -1855.10369860 Predicted Change= -6.528203D-08

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Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00003	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00576	0.00180	[NO]	0.00576	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	0.881110	0.671946	0.817809
C	-0.409914	0.526560	0.206423
C	-0.408273	0.704990	-1.325754
C	-0.315916	-0.658588	-1.978136
H	0.702799	-0.773842	-2.367250
C	-1.401999	-0.823033	-3.055140
H	-1.567337	0.117935	-3.586237
C	-2.608059	-1.306223	-2.248450
H	-3.404159	-1.746080	-2.851859
H	-3.042361	-0.477581	-1.673336
C	-1.973377	-2.311309	-1.287519
H	-1.696979	-3.217881	-1.844638
C	-2.900364	-2.745638	-0.175367
O	-4.097958	-2.601118	-0.196703
O	-2.245839	-3.354235	0.820686
C	-3.064563	-3.780325	1.909315
H	-3.810957	-4.499654	1.565463
H	-3.573681	-2.922927	2.355695
H	-2.385495	-4.240691	2.625377
C	-0.656598	-1.639115	-0.813418
O	-0.954209	-0.815803	0.315590
C	0.433950	-2.642828	-0.474673
H	-1.098599	-1.583484	-3.783669
O	-0.501378	1.757422	-1.899717
N	-1.176695	1.427634	1.004997
C	-2.264131	2.227147	0.542650
N	-0.476013	1.839102	2.146842
C	0.698109	1.349357	2.010179
C	1.769494	1.281987	3.057049
H	1.507785	0.485643	3.772431
H	1.836857	2.226814	3.598786
O	3.033530	1.022765	2.488582
C	3.046878	-0.118998	1.648341
H	2.715619	-1.009199	2.203204
C	2.164530	0.142493	0.405668
H	2.006055	-0.815751	-0.103754
C	4.458778	-0.221656	1.071710
H	4.644331	-1.246058	0.723378
H	5.208672	0.029311	1.826696
C	4.406644	0.756456	-0.081354
C	3.080605	1.017682	-0.440359
C	5.453594	1.385877	-0.738220
H	6.483594	1.190673	-0.451788
C	5.161471	2.293262	-1.757652
H	5.969706	2.801477	-2.274764
C	3.839914	2.566699	-2.101257
H	3.624724	3.288987	-2.882729
C	2.784524	1.929351	-1.444077
H	1.759978	2.167726	-1.710336
C	-3.559165	1.694427	0.543762
C	-3.882467	0.334253	1.107165
H	-2.981881	-0.205241	1.401810
H	-4.429829	-0.277769	0.384393
H	-4.524697	0.447755	1.988076
C	-4.600063	2.490533	0.051068
H	-5.608229	2.083658	0.036816
C	-4.364070	3.783037	-0.390078
H	-5.184073	4.388161	-0.765795
C	-3.075743	4.311132	-0.338843
H	-2.890622	5.328745	-0.672452
C	-2.009646	3.547220	0.125194
C	-0.623724	4.129861	0.201713
H	-0.558205	5.039804	-0.400206
H	0.122987	3.418703	-0.162152
H	-0.366197	4.376672	1.236544
C	1.109675	-3.318924	-1.492273
H	0.844418	-3.137568	-2.532766
C	2.131428	-4.216208	-1.192264
H	2.653309	-4.727162	-1.995491
C	2.486371	-4.449353	0.133571
H	3.286463	-5.144122	0.369671
C	1.804527	-3.789791	1.154574
H	2.069442	-3.974625	2.191850
C	0.781802	-2.894751	0.853841
H	0.249239	-2.368978	1.639668

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1855.10369860 Predicted Change= -6.528203D-08
Zero-point correction (ZPE)= -1854.4827 0.62092
Internal Energy (U)= -1854.4479 0.65575
Enthalpy (H)= -1854.4469 0.65670
Gibbs Free Energy (G)= -1854.5492 0.55441

Frequencies -- 14.3875 22.4667 31.2596
M06-2X/6-31+G(d,p)/PCM(DCE) SP: -1855.205426

VIb-*(S,S,S)*

Supporting Information: 0410-AzF-spiro-S-R-1.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

==========

# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RM062X/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C34H33N3O5 C1[X(C34H33N3O5)] #Atoms= 75
Charge = 0 Multiplicity = 1

SCF Energy= -1855.11167315 Predicted Change= -6.695777D-09

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00002	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00098	0.00180	[YES]	0.00098	0.00180	[YES]

Atomic Type	X	Y	Z
N	1.852745	1.102062	0.207702
C	0.525717	0.903264	-0.308416
C	0.414369	0.294427	-1.715597
C	-0.756842	-0.663070	-1.748665
H	-1.590321	-0.154966	-2.245084
C	-0.336365	-1.984704	-2.396750
H	-1.210043	-2.573855	-2.683553
C	0.411502	-2.679712	-1.253157
H	1.403267	-2.224281	-1.123533
H	0.552451	-3.749840	-1.421083
C	-0.456502	-2.392824	-0.019159
H	0.089834	-2.392847	0.927872
C	-1.590640	-3.389667	0.089374
O	-2.131016	-3.935268	-0.843377
O	-1.964410	-3.562119	1.363674
C	-3.189186	-4.275609	1.536976
H	-3.360517	-4.313553	2.611551
H	-3.108660	-5.281256	1.119679
H	-3.999901	-3.738469	1.036763
C	-1.027763	-0.939479	-0.250463
O	-0.203516	-0.023002	0.499981
C	-2.464857	-0.794737	0.219921
H	0.285995	-1.802866	-3.277130
O	1.166714	0.532583	-2.622276
N	0.036666	2.269773	-0.289029
C	-1.372812	2.494669	-0.376329
N	0.779914	3.027608	0.630563
C	1.818916	2.326529	0.874611
C	2.910052	2.694977	1.840516
H	2.452548	2.894882	2.821261
H	3.427399	3.599064	1.511675
O	3.881848	1.679954	1.940761
C	3.319683	0.386493	2.063763
H	2.609270	0.358878	2.903800
C	2.653182	0.000337	0.724166
H	1.976336	-0.847315	0.902969
C	4.486728	-0.594635	2.197388
H	4.151216	-1.516799	2.688501
H	5.288919	-0.159058	2.799292
C	4.874980	-0.842288	0.756424
C	3.843291	-0.454107	-0.101475
C	6.061161	-1.351315	0.247078
H	6.869144	-1.645202	0.911712
C	6.207870	-1.458528	-1.136444
H	7.133055	-1.847833	-1.550618
C	5.184933	-1.049929	-1.989962
H	5.321630	-1.118040	-3.064932
C	3.989661	-0.539970	-1.479026
H	3.207486	-0.188535	-2.144179
C	-2.175018	2.514171	0.780004
C	-1.588159	2.395064	2.162845
H	-2.379492	2.179169	2.886648
H	-1.087452	3.323072	2.453556
H	-0.845451	1.594170	2.208658
C	-3.552534	2.654004	0.624940
H	-4.182460	2.648565	1.510394
C	-4.127778	2.763427	-0.636962
H	-5.205807	2.849591	-0.736972
C	-3.319118	2.778444	-1.764187
H	-3.759490	2.903022	-2.750395
C	-1.929909	2.666556	-1.654044
C	-1.080596	2.774862	-2.897887
H	-1.489602	3.547520	-3.555292
H	-1.062408	1.841902	-3.473714
H	-0.048239	3.027370	-2.651601
C	-3.546085	-0.923456	-0.649377
H	-3.381930	-1.102503	-1.708199
C	-4.853931	-0.839178	-0.169729
H	-5.684505	-0.927956	-0.863231
C	-5.090641	-0.641086	1.185515
H	-6.108261	-0.571246	1.557997
C	-4.012514	-0.541716	2.065654
H	-4.187026	-0.398874	3.128287
C	-2.712076	-0.623352	1.585968
H	-1.871529	-0.552370	2.269060

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -1855.11167315 Predicted Change= -6.695777D-09
Zero-point correction (ZPE)= -1854.4894 0.62223
Internal Energy (U)= -1854.4553 0.65628
Enthalpy (H)= -1854.4544 0.65722
Gibbs Free Energy (G)= -1854.5533 0.55828

Frequencies -- 22.1444 32.4426 38.9729
M06-2X/6-31+G(d,p)/PCM(DCE) SP: -1855.211745

TS-VIIb-*(R,S,S)*

Supporting Information: 0415-post-aldol_spiro-R-R-1.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,modredundant)
Modredundant Input: B 3 21 F
# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest,nofreeze,gdiis) iop(1/8=18)
freq=noraman geom=allcheck guess=read
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C34H33N3O5 C1[X(C34H33N3O5)] #Atoms= 75
Charge = 0 Multiplicity = 1

SCF Energy= -1855.07744994 Predicted Change= -5.140177D-09

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00201	0.00180	[NO]	0.00201	0.00180	[YES]

Atomic Type	X	Y	Z
N	1.477326	-0.801093	-0.746255
C	0.385107	-1.022755	0.011437
C	0.149430	-0.343873	1.335175
C	-1.285439	0.027398	1.735999
H	-1.985524	-0.797885	1.571352
C	-1.321713	0.579072	3.159887
H	-2.361277	0.598256	3.509390
C	-0.775146	2.001787	3.011142
H	0.313211	1.975356	2.911472
H	-1.024670	2.649862	3.856036
C	-1.383638	2.491029	1.698454
H	-2.403520	2.864320	1.844099
C	-0.558824	3.558297	1.025439
O	0.580493	3.851372	1.290131
O	-1.255037	4.155694	0.037416
C	-0.508287	5.084926	-0.737550
H	0.331391	4.581960	-1.224956
H	-0.117695	5.887550	-0.107388
H	-1.201147	5.481350	-1.479294
C	-1.420587	1.223430	0.749643
O	-0.249612	1.128604	0.008330
C	-2.668768	1.240916	-0.118598
H	-0.735723	-0.027788	3.855271
O	1.109155	-0.279439	2.089334
N	-0.323243	-1.941969	-0.639209
C	-1.516049	-2.594195	-0.184655
N	0.223861	-2.237014	-1.865206
C	1.301178	-1.511203	-1.901552
C	2.206876	-1.277773	-3.074401
H	1.629034	-0.746368	-3.846013
H	2.551705	-2.225917	-3.491830
O	3.340616	-0.545785	-2.692618
C	3.055883	0.630032	-1.938941
H	2.369273	1.283375	-2.494079
C	2.500464	0.231781	-0.554493
H	1.988951	1.071264	-0.068091
C	4.414589	1.249200	-1.611845
H	4.291931	2.305526	-1.343755
H	5.086703	1.184334	-2.471455
C	4.857117	0.425344	-0.422507
C	3.758487	-0.192957	0.179157
C	6.136771	0.229230	0.076594
H	6.993003	0.706306	-0.392104
C	6.305582	-0.607132	1.179933
H	7.300950	-0.777687	1.578994
C	5.207626	-1.230450	1.770394
H	5.355384	-1.881217	2.626831
C	3.918385	-1.024277	1.278339
H	3.057325	-1.481875	1.752036
C	-1.436349	-3.397365	0.959379

C	-0.132359	-3.630129	1.680153
H	-0.215808	-4.499508	2.336024
H	0.151420	-2.772177	2.300744
H	0.686620	-3.810678	0.976240
C	-2.623879	-3.963964	1.420671
H	-2.599996	-4.588649	2.308760
C	-3.826508	-3.735889	0.758384
H	-4.742339	-4.178819	1.137625
C	-3.862294	-2.946807	-0.385586
H	-4.803181	-2.764679	-0.896923
C	-2.700460	-2.359274	-0.888063
C	-2.722604	-1.513220	-2.130203
H	-3.718711	-1.091870	-2.284451
H	-2.446639	-2.111249	-3.005119
H	-2.016925	-0.683199	-2.053527
C	-3.892626	0.738017	0.326142
H	-3.966044	0.288776	1.315082
C	-5.027537	0.805265	-0.481236
H	-5.970870	0.404454	-0.120518
C	-4.952293	1.388888	-1.743340
H	-5.836410	1.447592	-2.371556
C	-3.732820	1.893225	-2.195383
H	-3.665226	2.345611	-3.180983
C	-2.600614	1.813435	-1.391514
H	-1.637932	2.180576	-1.732691

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1855.07744994 Predicted Change= -5.140177D-09
Zero-point correction (ZPE)= -1854.4565 0.62094
Internal Energy (U)= -1854.4222 0.65518
Enthalpy (H)= -1854.4213 0.65613
Gibbs Free Energy (G)= -1854.5214 0.55603

Frequencies -- -83.7742 23.1236 26.4872
M06-2X/6-31+G(d,p)/PCM(DCE) SP: -1855.183955

TS-VIIb-*(R,R,R)*

Supporting Information: 0415-post-aldol_spiro-Rent-R-3.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

==========

# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,modredundant)
Modredundant Input: B 3 21 F
# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest,nofreeze,gdiis) iop(1/8=18)
freq=noraman geom=allcheck guess=read
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C34H33N3O5 C1[X(C34H33N3O5)] #Atoms= 75
Charge = 0 Multiplicity = 1

SCF Energy= -1855.07466095 Predicted Change= -1.010715D-09

==========

Optimization completed. {Found 3 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 ||	0.00045	[YES]	0.00000 ||	0.00030	[YES]
Displ	0.00054 ||	0.00180	[YES]	0.00054 ||	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	0.516295	1.092658	-0.698970
C	1.134214	0.070611	-0.060240
C	0.726677	-0.641914	1.206830
C	-0.777858	-0.837499	1.447468
H	-1.288902	0.118311	1.616947
C	-1.005729	-1.805452	2.614901
H	-0.228222	-1.695664	3.374211
C	-1.000259	-3.197143	1.969388
H	-1.496145	-3.950596	2.587865
H	0.032026	-3.514960	1.795665
C	-1.668769	-3.007626	0.599775
H	-1.337019	-3.736281	-0.142518
C	-3.173561	-3.101708	0.614195
O	-3.841825	-3.626915	-0.240770
O	-3.733239	-2.502119	1.693708
C	-5.158577	-2.508937	1.696906
H	-5.537531	-3.533095	1.686709
H	-5.540161	-1.986107	0.815022
H	-5.458272	-1.996456	2.610505
C	-1.102138	-1.617538	0.126865
O	0.169903	-1.832470	-0.374671
C	-2.009330	-0.903846	-0.872391
H	-1.977089	-1.602753	3.069409
O	1.591827	-0.929327	2.011586
N	2.286858	-0.110171	-0.719435
C	3.376639	-0.995869	-0.409849
N	2.362124	0.679986	-1.837221
C	1.284320	1.393352	-1.800047
C	0.809505	2.428361	-2.767919
H	0.158253	1.953091	-3.518142
H	1.659578	2.891240	-3.270238
O	0.110085	3.433183	-2.070345
C	-1.019184	2.918929	-1.384020
H	-1.702284	2.430172	-2.091299
C	-0.586948	1.947355	-0.256807
H	-1.442331	1.313900	-0.018012
C	-1.644496	4.089327	-0.618532
H	-2.709963	3.893553	-0.445943
H	-1.555007	5.012846	-1.196589
C	-0.875335	4.102854	0.683916
C	-0.243774	2.874828	0.888677
C	-0.744517	5.119139	1.620540
H	-1.224236	6.081414	1.465188
C	0.028649	4.890161	2.759303
H	0.147532	5.678645	3.495951
C	0.657995	3.662362	2.957552
H	1.259369	3.500049	3.846367
C	0.524003	2.636805	2.020460
H	1.020315	1.683368	2.185968
C	4.294156	-0.577407	0.558101
C	4.127667	0.726559	1.290638
H	3.780596	1.523190	0.624177
H	5.076294	1.041000	1.732246
H	3.391539	0.607585	2.092020
C	5.368764	-1.422174	0.829017
H	6.095929	-1.126317	1.579858
C	5.514741	-2.624922	0.146806
H	6.357080	-3.272899	0.370106
C	4.597940	-2.994937	-0.830288
H	4.725110	-3.928137	-1.371416
C	3.505807	-2.181601	-1.138182
C	2.518671	-2.561445	-2.207227
H	2.450748	-1.775662	-2.967504
H	1.522765	-2.692079	-1.770835
H	2.830269	-3.486800	-2.697314
C	-3.216112	-0.303191	-0.494666
H	-3.534602	-0.351541	0.545326
C	-4.000321	0.370572	-1.428698
H	-4.932108	0.834424	-1.116813
C	-3.595016	0.443391	-2.760785
H	-4.210307	0.959320	-3.491983
C	-2.396045	-0.154175	-3.145440
H	-2.075892	-0.108018	-4.183236
C	-1.606577	-0.815419	-2.206014
H	-0.659491	-1.271696	-2.479782

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1855.07466095 Predicted Change= -1.010715D-09
Zero-point correction (ZPE)= -1854.4543 0.62028
Internal Energy (U)= -1854.4198 0.65485
Enthalpy (H)= -1854.4188 0.65579
Gibbs Free Energy (G)= -1854.5205 0.55409

Frequencies -- -91.4280 11.4148 27.9296
M06-2X/6-31+G(d,p)/PCM(DCE) SP: -1855.179641

TS-VIIb-*(S,S,S)*

Supporting Information: 0415-post-aldol_spiro-S-R-1.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

==========

# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,modredundant)
Modredundant Input: B 3 21 F
# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest,nofreeze,gdiis) iop(1/8=18)
freq=noraman geom=allcheck guess=read
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C34H33N3O5 C1[X(C34H33N3O5)] #Atoms= 75
Charge = 0 Multiplicity = 1

SCF Energy= -1855.07886613 Predicted Change= -2.023844D-08

==========

Optimization completed. {Found 3 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00003 ||	0.00045	[YES]	0.00000 ||	0.00030	[YES]
Displ	0.00137 ||	0.00180	[YES]	0.00137 ||	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z

N	1.944536	0.491644	0.604424
C	0.827909	0.685883	-0.136880
C	0.448176	-0.152896	-1.323767
C	-1.043772	-0.380455	-1.564783
H	-1.574630	0.570013	-1.679551
C	-1.253868	-1.333986	-2.739458
H	-2.285691	-1.260206	-3.090844
C	-1.010087	-2.718263	-2.128824
H	0.065289	-2.883829	-2.012571
H	-1.424513	-3.525413	-2.738831
C	-1.659561	-2.636659	-0.744033
H	-1.225518	-3.312208	-0.003850
C	-3.145092	-2.882513	-0.814737
O	-3.863881	-2.613940	-1.751396
O	-3.613273	-3.396952	0.335092
C	-5.033326	-3.444685	0.436127
H	-5.445763	-2.435649	0.347791
H	-5.246764	-3.859328	1.420617
H	-5.455306	-4.075799	-0.349584
C	-1.341750	-1.160882	-0.243809
O	-0.124863	-1.151055	0.421964
C	-2.476667	-0.632074	0.621756
H	-0.574535	-1.115154	-3.567716
O	1.340950	-0.564982	-2.040450
N	0.312776	1.843233	0.294469
C	-0.728302	2.626047	-0.303071
N	0.976636	2.310215	1.410179
C	1.936524	1.455783	1.576969
C	2.870572	1.356887	2.747019
H	2.272473	1.110890	3.637426
H	3.374936	2.309581	2.920489
O	3.859345	0.388566	2.516891
C	3.351116	-0.864977	2.072232
H	2.602890	-1.247721	2.779357
C	2.784124	-0.706309	0.644147
H	2.120739	-1.539049	0.384055
C	4.572606	-1.762564	1.875578
H	4.270786	-2.816976	1.876733
H	5.298284	-1.609729	2.678615
C	5.067820	-1.326718	0.513724
C	4.049684	-0.681862	-0.193247
C	6.330746	-1.470224	-0.043206
H	7.125232	-1.967707	0.506154
C	6.568090	-0.945296	-1.313517
H	7.553136	-1.041892	-1.760035
C	5.554089	-0.288929	-2.008850
H	5.754650	0.121152	-2.993879
C	4.279945	-0.155059	-1.455706
H	3.481450	0.333666	-2.001311
C	-0.566188	3.061437	-1.625641
C	0.678748	2.780939	-2.429895
H	0.813673	3.559287	-3.184606
H	0.620805	1.821421	-2.955695
H	1.574874	2.758830	-1.802081
C	-1.616533	3.781191	-2.196138
H	-1.520771	4.124929	-3.222110
C	-2.765411	4.067701	-1.468024
H	-3.574176	4.623721	-1.932099
C	-2.873887	3.657926	-0.144404
H	-3.766317	3.890871	0.429347
C	-1.852148	2.935598	0.472127
C	-1.957513	2.535705	1.917088
H	-1.420629	3.251651	2.548043
H	-1.523395	1.549437	2.092558
H	-3.004971	2.507026	2.224619
C	-3.586464	0.032368	0.097597
H	-3.641780	0.241017	-0.968382
C	-4.641372	0.415054	0.927297
H	-5.494261	0.939205	0.504550
C	-4.605622	0.117441	2.287035
H	-5.431305	0.406411	2.930984
C	-3.502204	-0.552850	2.816269
H	-3.468216	-0.788669	3.876282
C	-2.444511	-0.916399	1.990164
H	-1.569785	-1.426704	2.382378

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1855.07886613 Predicted Change= -2.023844D-08
Zero-point correction (ZPE)= -1854.4574 0.62146
Internal Energy (U)= -1854.4234 0.65542
Enthalpy (H)= -1854.4224 0.65636
Gibbs Free Energy (G)= -1854.5209 0.55788

Frequencies -- -107.6158 30.0089 33.2793
M06-2X/6-31+G(d,p)/PCM(DCE) SP: -1855.183069

TS-VIIb-*(S,R,R)*

Supporting Information: 0415-post-aldol_spiro-Sent-R-2.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

==========

# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,modredundant)
Modredundant Input: B 3 21 F
# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest,nofreeze,gdiis) iop(1/8=18)
freq=noraman geom=allcheck guess=read
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C34H33N3O5 C1[X(C34H33N3O5)] #Atoms= 75
Charge = 0 Multiplicity = 1

SCF Energy= -1855.07799998 Predicted Change= -5.150604D-09

==========

Optimization completed. {Found 3 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00002 ||	0.00045	[YES]	0.00000 ||	0.00030	[YES]
Displ	0.00149 ||	0.00180	[YES]	0.00149 ||	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	1.096772	-0.519687	-0.768894
C	0.008751	-0.965052	-0.098286
C	-0.426889	-0.691970	1.324533
C	-0.097037	0.683825	1.917619
H	0.984274	0.860535	1.968514
C	-0.755173	0.854164	3.292671
H	-0.725369	-0.071512	3.871792
C	-2.178061	1.320358	2.976125
H	-2.681621	1.788718	3.825445
H	-2.788353	0.477831	2.637904
C	-1.975114	2.273844	1.801909
H	-1.573355	3.239871	2.136950
C	-3.234407	2.519407	1.008154
O	-4.323407	2.064835	1.251857
O	-2.994733	3.328904	-0.041473
C	-4.109928	3.538961	-0.899492
H	-4.466644	2.586175	-1.298662
H	-3.750892	4.181537	-1.702931
H	-4.927747	4.021014	-0.358212
C	-0.931307	1.537496	0.903787
O	-1.570428	0.548113	0.177775
C	-0.113065	2.481693	0.033670
H	-0.216073	1.629888	3.849584
O	-0.876363	-1.620800	1.970113
N	-0.595141	-1.819716	-0.932318
C	-1.780801	-2.609853	-0.721815
N	0.022183	-1.860589	-2.153662
C	1.037768	-1.068912	-2.028339
C	2.069259	-0.707201	-3.049238
H	1.731214	0.176180	-3.613440
H	2.217863	-1.537269	-3.741058
O	3.293001	-0.444855	-2.404594
C	3.181361	0.624427	-1.479913
H	2.817645	1.526024	-1.989248
C	2.258801	0.238982	-0.296241
H	1.902932	1.163993	0.163193
C	4.552138	0.792552	-0.817471
H	4.665319	1.822708	-0.457832
H	5.349381	0.590406	-1.537552
C	4.502271	-0.184516	0.335032
C	3.180985	-0.527998	0.626904
C	5.544411	-0.727329	1.073355
H	6.575748	-0.471668	0.846970
C	5.246317	-1.621867	2.101721
H	6.051865	-2.062073	2.681344
C	3.925569	-1.965480	2.385600
H	3.710289	-2.668242	3.184075
C	2.874958	-1.417244	1.648816
H	1.849121	-1.697575	1.877871
C	-2.990386	-2.154833	-1.253753
C	-3.099039	-0.852262	-1.997287
H	-4.079883	-0.772235	-2.472186
H	-2.332444	-0.781022	-2.776309
H	-2.952470	-0.016277	-1.304823
C	-4.107129	-2.970663	-1.063398
H	-5.065402	-2.643277	-1.455829
C	-4.006065	-4.181278	-0.389224
H	-4.888980	-4.798854	-0.253767
C	-2.777480	-4.614157	0.098669
H	-2.696574	-5.569632	0.608904
C	-1.634541	-3.834978	-0.063900
C	-0.295655	-4.292278	0.448471
H	-0.326883	-5.353585	0.705464
H	-0.027610	-3.723464	1.344316
H	0.490578	-4.145619	-0.299765
C	0.771811	3.409057	0.590754
H	0.848983	3.493315	1.674259
C	1.570276	4.210727	-0.222756

H	2.259106	4.921492	0.224806
C	1.478966	4.106581	-1.610137
H	2.094049	4.736179	-2.246311
C	0.584588	3.196169	-2.173109
H	0.497990	3.121217	-3.254462
C	-0.199647	2.384092	-1.356135
H	-0.896348	1.658822	-1.768068

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1855.07799998 Predicted Change= -5.150604D-09
Zero-point correction (ZPE)= -1854.4579 0.62004
Internal Energy (U)= -1854.4232 0.65478
Enthalpy (H)= -1854.4222 0.65572
Gibbs Free Energy (G)= -1854.5245 0.55343

Frequencies -- -71.7826 17.8260 23.4705
M06-2X/6-31+G(d,p)/PCM(DCE) SP: -1855.184412

VIII-*(R,R,R)*

Supporting Information: 0500-lactone-alkoxide-R-ent-R-2-1.log

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Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

==========

# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RM062X/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C34H33N3O5 C1[X(C34H33N3O5)] #Atoms= 75
Charge = 0 Multiplicity = 1

SCF Energy= -1855.08903078 Predicted Change= -7.223927D-09

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00269	0.00180	[NO]	0.00269	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	1.972386	0.201783	0.657598
C	0.846376	0.442612	-0.038045
C	0.210445	-0.671922	-0.918856
C	-0.535929	-1.728387	-0.013335
H	-0.332908	-1.683087	1.061908
C	-0.463637	-3.121543	-0.628484
H	0.558422	-3.346901	-0.950091
C	-1.416872	-3.049832	-1.833618
H	-1.780648	-4.032291	-2.146249
H	-0.891207	-2.577407	-2.667403
C	-2.554712	-2.119487	-1.388385
H	-3.061698	-1.610768	-2.212701
C	-3.581468	-2.826852	-0.539166
O	-3.350023	-3.723910	0.239261
O	-4.802604	-2.290770	-0.693145
C	-5.788463	-2.773283	0.215905
H	-5.491816	-2.541541	1.242518
H	-5.910649	-3.853865	0.112923
H	-6.709946	-2.253210	-0.041813
C	-1.825990	-1.052820	-0.518714
O	-1.108124	-0.160082	-1.380490
C	-2.732398	-0.324043	0.439469
H	-0.803658	-3.874381	0.086513
O	1.066689	-1.033766	-1.796453
N	0.605540	1.741603	0.147582
C	-0.418663	2.573816	-0.429806
N	1.544475	2.336760	0.959076
C	2.358968	1.369591	1.248891
C	3.519086	1.288159	2.186549
H	3.491735	2.112609	2.899639
H	4.472253	1.310159	1.640481
O	3.352167	0.085737	2.915194
C	3.439028	-1.114696	2.155683
H	2.883287	-1.842655	2.748933
C	2.822041	-0.986923	0.715367
H	2.204877	-1.847669	0.447821
C	4.904128	-1.542021	1.925632
H	5.008048	-2.625757	2.056119
H	5.551855	-1.062178	2.666203
C	5.199866	-1.145474	0.500964
C	4.027850	-0.854006	-0.192943
C	6.429730	-1.068572	-0.145063
H	7.350175	-1.291313	0.387511
C	6.458933	-0.695201	-1.486880
H	7.411782	-0.624140	-2.002991
C	5.276593	-0.414252	-2.176010
H	5.320308	-0.135512	-3.224304
C	4.040836	-0.495170	-1.537730
H	3.099005	-0.317926	-2.052345
C	-1.344389	3.158480	0.435503
C	-1.363123	2.834295	1.905149
H	-1.443553	1.750596	2.056655
H	-2.227840	3.299384	2.383477
H	-0.453618	3.181849	2.403637
C	-2.286648	4.017613	-0.130707
H	-3.023549	4.486226	0.515665
C	-2.303661	4.252453	-1.500525
H	-3.048718	4.918326	-1.925545
C	-1.367667	3.642729	-2.330436
H	-1.380962	3.832561	-3.399634
C	-0.389444	2.796050	-1.809480
C	0.651071	2.159780	-2.690903
H	0.615181	2.599594	-3.690260
H	0.502521	1.077176	-2.779117
H	1.657824	2.319212	-2.286439
C	-2.983819	-0.820761	1.721872
H	-2.484730	-1.728227	2.053099
C	-3.885899	-0.173345	2.563812
H	-4.067979	-0.563819	3.560914
C	-4.551284	0.969812	2.126463
H	-5.256380	1.473661	2.781154
C	-4.305836	1.464782	0.847142
H	-4.816584	2.359308	0.500946
C	-3.398410	0.824195	0.008897
H	-3.182310	1.218634	-0.981243

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1855.08903078 Predicted Change= -7.223927D-09
Zero-point correction (ZPE)= -1854.4675 0.62145
Internal Energy (U)= -1854.4328 0.65616
Enthalpy (H)= -1854.4319 0.65710
Gibbs Free Energy (G)= -1854.5344 0.55456

Frequencies -- 12.4783 28.2943 34.0127
M06-2X/6-31+G(d,p)/PCM(DCE) SP: -1855.194782

VIII-*(R,S,S)*

Supporting Information: 0500-lactone-alkoxide-R-S-1-1.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

==========

# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RM062X/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C34H33N3O5 C1[X(C34H33N3O5)] #Atoms= 75
Charge = 0 Multiplicity = 1

SCF Energy= -1855.08730843 Predicted Change= -2.530015D-08

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.03881	0.00180	[NO]	0.03881	0.00180	[NO]

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	1.097864	1.231206	0.565775
C	0.004985	1.067475	-0.212677
C	-0.215854	-0.097829	-1.227183
C	-1.682016	-0.655454	-1.236142
H	-2.484831	0.009746	-0.913102
C	-1.971570	-1.395802	-2.542358
H	-3.050499	-1.564239	-2.641608
C	-1.226662	-2.732501	-2.409240
H	-0.170056	-2.579285	-2.647120
H	-1.619741	-3.522165	-3.053139
C	-1.359244	-3.070376	-0.914192
H	-2.369872	-3.453228	-0.708464
C	-0.372415	-4.084942	-0.385267
O	0.158057	-4.049230	0.697434
O	-0.160978	-5.073892	-1.273000
C	0.761455	-6.072844	-0.845556
H	0.411056	-6.548731	0.073378
H	1.742198	-5.628867	-0.660401
H	0.815284	-6.796298	-1.658021
C	-1.178479	-1.709986	-0.227371
O	0.183070	-1.296738	-0.372176
C	-1.703650	-1.585071	1.180432
H	-1.623091	-0.814551	-3.400478
O	0.424717	0.112036	-2.304782
N	-0.741565	2.147410	0.014911
C	-2.026291	2.466977	-0.544983

N	-0.188001	2.984718	0.944678
C	0.924946	2.396739	1.263751
C	1.878217	2.791258	2.350298
H	1.411253	2.559248	3.320650
H	2.077029	3.863729	2.309046
O	3.100605	2.121637	2.204258
C	2.971517	0.711738	2.073739
H	2.443005	0.298790	2.945485
C	2.276304	0.362653	0.737426
H	1.902657	-0.665561	0.728156
C	4.394501	0.185767	1.881620
H	4.441955	-0.879920	2.136671
H	5.091252	0.727181	2.527013
C	4.619908	0.409780	0.403290
C	3.401012	0.539011	-0.266224
C	5.814979	0.485115	-0.297246
H	6.767249	0.391285	0.217558
C	5.769966	0.696752	-1.675786
H	6.696426	0.766624	-2.238210
C	4.548416	0.816810	-2.336115
H	4.531981	0.972191	-3.410524
C	3.341406	0.731180	-1.639344
H	2.378842	0.774298	-2.145384
C	-2.089765	2.880314	-1.877431
C	-0.846451	3.039502	-2.710087
H	-0.123014	3.686979	-2.201668
H	-1.092333	3.494212	-3.672221
H	-0.361646	2.070124	-2.882899
C	-3.361462	3.140022	-2.392622
H	-3.452783	3.457671	-3.427071
C	-4.495918	3.001883	-1.601299
H	-5.475353	3.204642	-2.023928
C	-4.386053	2.611601	-0.269633
H	-5.275322	2.511900	0.346113
C	-3.139865	2.337047	0.290999
C	-2.993157	1.911128	1.727770
H	-3.959886	1.613540	2.139576
H	-2.593907	2.731469	2.333514
H	-2.309089	1.060952	1.831702
C	-3.078915	-1.661684	1.419818
H	-3.757229	-1.843493	0.587786
C	-3.587072	-1.487170	2.702859
H	-4.658113	-1.548197	2.873271
C	-2.724578	-1.222583	3.765514
H	-3.120072	-1.080551	4.766605
C	-1.353183	-1.149677	3.535169
H	-0.674018	-0.958486	4.361506
C	-0.845673	-1.333151	2.250367
H	0.222770	-1.306914	2.061012

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1855.08730843 Predicted Change= -2.530015D-08
Zero-point correction (ZPE)= -1854.4665 0.62075
Internal Energy (U)= -1854.4316 0.65565
Enthalpy (H)= -1854.4307 0.65659
Gibbs Free Energy (G)= -1854.5350 0.55221

Frequencies -- 5.1131 20.5076 22.6603
M06-2X/6-31+G(d,p)/PCM(DCE) SP: -1855.195955

VIII-*(S,R,R)*

Supporting Information: 0500-lactone-alkoxide-S-ent-R-2-1.log

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Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

==========

# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RM062X/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C34H33N3O5 C1[X(C34H33N3O5)] #Atoms= 75
Charge = 0 Multiplicity = 1

SCF Energy= -1855.08428354 Predicted Change= -5.072045D-08

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00002	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00273	0.00180	[NO]	0.00273	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	2.036695	-0.562717	-0.432467
C	0.787829	-0.418523	0.048173
C	0.083377	0.969500	-0.005905
C	-0.452069	1.259657	-1.463536
H	-0.117266	0.576620	-2.251331
C	-0.348463	2.743132	-1.801066
H	0.648763	3.130610	-1.569588
C	-1.418521	3.400410	-0.920321
H	-1.743518	4.380560	-1.275438
H	-1.020836	3.503888	0.093141
C	-2.561787	2.372541	-0.914584
H	-3.110649	2.432419	-1.866363
C	-3.572335	2.562483	0.192731
O	-4.129170	1.690004	0.810423
O	-3.815316	3.871455	0.402528
C	-4.773525	4.143753	1.421314
H	-4.434296	3.742610	2.378980
H	-5.736549	3.691466	1.172171
H	-4.858966	5.228634	1.468054
C	-1.849819	1.005032	-0.856680
O	-1.311675	0.778177	0.455178
C	-2.668074	-0.151999	-1.370120
H	-0.558873	2.908845	-2.864706
O	0.821344	1.819584	0.605103
N	0.489592	-1.606954	0.575445
C	-0.664921	-2.001940	1.340303
N	1.512460	-2.515925	0.429883
C	2.435472	-1.845046	-0.187088
C	3.751018	-2.254594	-0.765146
H	3.792973	-3.336608	-0.892365
H	4.582638	-1.930184	-0.124472
O	3.813477	-1.666907	-2.051414
C	3.864641	-0.245548	-2.072606
H	3.502056	0.016148	-3.067954
C	2.974662	0.426144	-0.964202
H	2.387770	1.265051	-1.344335
C	5.293024	0.281251	-1.814468
H	5.523172	1.105995	-2.499269
H	6.022139	-0.512561	-2.006078
C	5.272908	0.764003	-0.385318
C	3.968205	0.869836	0.090779
C	6.343787	1.106828	0.434958
H	7.365577	1.024835	0.074726
C	6.081039	1.552222	1.728328
H	6.906825	1.817708	2.381687
C	4.768073	1.665373	2.191964
H	4.584633	2.026496	3.199203
C	3.690652	1.329672	1.374912
H	2.655269	1.441696	1.689424
C	-0.875440	-1.384367	2.576336
C	0.043834	-0.310639	3.092857
H	-0.061854	0.621068	2.525598
H	1.092877	-0.622702	3.020723
H	-0.174831	-0.104387	4.143075
C	-1.975521	-1.817302	3.315139
H	-2.178448	-1.351112	4.274632
C	-2.796909	-2.837755	2.845734
H	-3.644375	-3.163763	3.441065
C	-2.539293	-3.440204	1.619748
H	-3.188055	-4.228993	1.249311
C	-1.467739	-3.022613	0.830139
C	-1.220992	-3.606037	-0.535121
H	-1.167373	-2.809538	-1.287686
H	-2.040658	-4.270964	-0.815765
H	-0.282251	-4.166952	-0.566412
C	-3.394558	-0.949877	-0.485730
H	-3.335998	-0.740926	0.578212
C	-4.180032	-1.991209	-0.973239
H	-4.744357	-2.605335	-0.276522
C	-4.242203	-2.251318	-2.340356
H	-4.854951	-3.066558	-2.714104
C	-3.516919	-1.458900	-3.227158
H	-3.557181	-1.654859	-4.294615
C	-2.736190	-0.413615	-2.741321
H	-2.173171	0.209340	-3.434272

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1855.08428354 Predicted Change= -5.072045D-08
Zero-point correction (ZPE)= -1854.4629 0.62133
Internal Energy (U)= -1854.4284 0.65587
Enthalpy (H)= -1854.4274 0.65682
Gibbs Free Energy (G)= -1854.5288 0.55542

Frequencies -- 19.6109 26.0206 31.5618
M06-2X/6-31+G(d,p)/PCM(DCE) SP: -1855.191036

VIII-*(S,S,S)*

Supporting Information: 0500-lactone-alkoxide-S-S-1-1.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

==========

# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250) freq=noraman

#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RM062X/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C34H33N3O5 C1[X(C34H33N3O5)] #Atoms= 75
Charge = 0 Multiplicity = 1

SCF Energy= -1855.08899583 Predicted Change= -1.391529D-08

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00212	0.00180	[NO]	0.00212	0.00180	[YES]

Atomic Type	X	Y	Z
N	1.744968	0.436245	0.720256
C	0.694316	1.006484	0.092070
C	-0.088607	0.508109	-1.164363
C	-1.639288	0.471911	-0.919448
H	-2.024145	1.065618	-0.088033
C	-2.402198	0.658837	-2.226163
H	-3.454807	0.867929	-2.023541
C	-2.247989	-0.687844	-2.953878
H	-1.277246	-0.709443	-3.456911
H	-3.036543	-0.867658	-3.689705
C	-2.234028	-1.747525	-1.840824
H	-1.708902	-2.668109	-2.109711
C	-3.615604	-2.093980	-1.344843
O	-4.545905	-1.324998	-1.262230
O	-3.682941	-3.367269	-0.920920
C	-4.902795	-3.717897	-0.272877
H	-5.753130	-3.552097	-0.938011
H	-5.031564	-3.114434	0.630101
H	-4.811563	-4.772590	-0.017057
C	-1.454266	-1.040941	-0.695022
O	-0.063209	-0.998786	-1.034711
C	-1.688854	-1.627653	0.675270
H	-1.965226	1.479331	-2.802389
O	0.419100	1.013848	-2.216422
N	0.567760	2.206697	0.660285
C	-0.441425	3.200552	0.403348
N	1.488788	2.423432	1.646372
C	2.190816	1.331627	1.658696
C	3.292546	0.967002	2.605603
H	2.852085	0.696131	3.578122
H	3.958899	1.819123	2.750901
O	4.051495	-0.090894	2.083986
C	3.262771	-1.221438	1.740576
H	2.693345	-1.559255	2.618644
C	2.344767	-0.895892	0.538651
H	1.511048	-1.597503	0.476978
C	4.231973	-2.264109	1.178600
H	3.805252	-3.269404	1.280967
H	5.177303	-2.236240	1.727085
C	4.347044	-1.860975	-0.274315
C	3.271671	-1.052671	-0.647750
C	5.325512	-2.194630	-1.199716
H	6.170489	-2.815797	-0.915640
C	5.209523	-1.702693	-2.500074
H	5.971264	-1.945272	-3.235265
C	4.128317	-0.900550	-2.863697
H	4.053554	-0.529173	-3.881053
C	3.135021	-0.566989	-1.941382
H	2.279306	0.046122	-2.226835
C	-1.525019	3.248496	1.286806
C	-1.611932	2.305787	2.458131
H	-1.488096	1.260182	2.150137
H	-2.581626	2.397683	2.952606
H	-0.828692	2.524602	3.191638
C	-2.509959	4.200586	1.036481
H	-3.371972	4.256796	1.694613
C	-2.393926	5.070282	-0.044520
H	-3.170921	5.805787	-0.228979
C	-1.286717	5.011604	-0.882049
H	-1.194685	5.704348	-1.713256
C	-0.272393	4.073598	-0.672311
C	0.948579	4.010006	-1.546730
H	1.859422	4.077697	-0.941226
H	0.949023	4.837644	-2.259352
H	0.966550	3.056192	-2.087642
C	-0.880382	-2.675918	1.122274
H	-0.092081	-3.042271	0.469666
C	-1.100614	-3.261507	2.365016
H	-0.467839	-4.079246	2.697976
C	-2.140431	-2.810013	3.175622
H	-2.312643	-3.265039	4.146315
C	-2.962689	-1.778219	2.730475
H	-3.780647	-1.427095	3.353023
C	-2.740117	-1.190996	1.485559
H	-3.395869	-0.399008	1.130529

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1855.08899583 Predicted Change= -1.391529D-08

Zero-point correction (ZPE)=	-1854.4676	0.62137
Internal Energy (U)=	-1854.4327	0.65628
Enthalpy (H)=	-1854.4317	0.65722
Gibbs Free Energy (G)=	-1854.5345	0.55442

Frequencies -- 16.3556 25.5806 32.8903
M06-2X/6-31+G(d,p)/PCM(DCE) SP: -1855.196951

IX-*(R,S,S) & -(S,R,R)*

Supporting Information: 0600-Lactone-maj.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

==========

# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RM062X/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C14H14O4 C1[X(C14H14O4)] #Atoms= 32
Charge = 0 Multiplicity = 1

SCF Energy= -842.482413464 Predicted Change= -3.673172D-09

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00046	0.00180	[YES]	0.00046	0.00180	[YES]

Atomic Type	X	Y	Z
C	-0.274526	-0.559747	-0.048173
C	1.223551	-0.474421	-0.058708
C	-1.046074	0.384356	-0.989953
H	-0.469626	0.472257	-1.920323
C	-2.388671	-0.314373	-1.243145
H	-2.875261	0.039973	-2.153894
H	-3.064691	-0.095485	-0.409900
C	-2.033685	-1.806845	-1.281433
H	-1.616910	-2.080954	-2.257338
H	-2.889989	-2.457387	-1.085245
C	-0.944180	-1.950084	-0.215457
H	-0.287420	-2.815859	-0.313314
C	-1.428574	-1.679977	1.203265
O	-2.102438	-2.222692	2.018221
O	-0.831059	-0.450633	1.300163
C	-1.208809	1.772583	-0.404665
O	-2.255873	2.360303	-0.310903
O	-0.032446	2.271039	-0.002795
C	-0.096930	3.563229	0.600861
H	-0.737466	3.534473	1.484774
H	-0.497564	4.292832	-0.106136
H	0.927484	3.811512	0.873452
C	1.917540	-0.839679	-1.213943
H	1.367974	-1.182094	-2.089442
C	3.306032	-0.775851	-1.249623
H	3.837920	-1.063389	-2.151282
C	4.011244	-0.347768	-0.126813
H	5.095405	-0.298723	-0.151891
C	3.321299	0.012873	1.027093
H	3.867484	0.343553	1.905313
C	1.930752	-0.049944	1.063973
H	1.383376	0.229039	1.958065

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -842.482413464 Predicted Change= -3.673172D-09

Zero-point correction (ZPE)=	-842.2214	0.26097
Internal Energy (U)=	-842.2061	0.27621
Enthalpy (H)=	-842.2052	0.27716
Gibbs Free Energy (G)=	-842.2649	0.21746

Frequencies -- 41.2683 46.7945 59.8457
M06-2X/6-31+G(d,p)/PCM(DCE) SP: -842.5352615

IX-*(S,S,S) & -(R,R,R)*

Supporting Information: 0600-Lactone-RSR-min.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

==========

# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250) freq=noraman

#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RM062X/6-31G(d) Freq
---
Pointgroup= C1 Stoichiometry= C14H14O4 C1[X(C14H14O4)] #Atoms= 32
Charge = 0 Multiplicity = 1

SCF Energy= -842.484864325 Predicted Change= -5.071685D-09
==========
Optimization completed. {Found 2 times}
Item Max Val. Criteria Pass? RMS Val. Criteria Pass?
Force 0.00001 || 0.00045 [YES] 0.00000 || 0.00030 [YES]
Displ 0.00110 || 0.00180 [YES] 0.00110 || 0.00180 [YES]

Atomic Coordinates (Angstroms)
Type X Y Z

C -0.767501 -0.358867 -0.184424
C 0.598675 -0.940424 0.039125
C -0.822378 1.056341 -0.809639
H -0.671450 0.972793 -1.889058
C -2.212065 1.584331 -0.412085
H -2.951458 1.201994 -1.123258
H -2.258643 2.675454 -0.429483
C -2.470633 1.010593 0.992077
H -3.534953 0.951643 1.235289
H -1.970076 1.623905 1.744500
C -1.821819 -0.377263 0.951117
H -1.530898 -0.798618 1.914319
C -2.541023 -1.337744 0.014709
O -1.608292 -1.249168 -0.984393
O -3.554632 -1.959495 0.002192
C 0.289407 1.899610 -0.224066
O 0.230964 2.481241 0.834594
O 1.377284 1.881615 -0.999803
C 2.528210 2.516963 -0.441386
H 2.314413 3.563396 -0.215097
H 3.306839 2.433203 -1.197324
H 2.825615 2.001357 0.475370
C 1.337409 -0.583020 1.170022
H 0.905656 0.090165 1.907386
C 2.627718 -1.075122 1.345255
H 3.194842 -0.797345 2.228539
C 3.183639 -1.930762 0.396754
H 4.187496 -2.319670 0.536497
C 2.444549 -2.293991 -0.726100
H 2.870834 -2.966966 -1.463649
C 1.155709 -1.800433 -0.906430
H 0.569810 -2.086125 -1.774321

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
==========
SCF Energy= -842.484864325 Predicted Change= -5.071685D-09
Zero-point correction (ZPE)= -842.2232 0.26159
Internal Energy (U)= -842.2081 0.27673
Enthalpy (H)= -842.2071 0.27767
Gibbs Free Energy (G)= -842.2663 0.21848

Frequencies -- 41.6851 56.4133 60.6445
M06-2X/6-31+G(d,p)/PCM(DCE) SP: -842.5352903

—2F-Ph Substrate—

(R)-**IV**

Supporting Information: 0300-AzF-enolate-2F-R-0002-2.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011
==========
# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RM062X/6-31G(d) Freq
---
Pointgroup= C1 Stoichiometry= C34H32FN3O5 C1[X(C34H32FN3O5)] #Atoms= 75
Charge = 0 Multiplicity = 1

SCF Energy= -1954.29160665 Predicted Change= -9.959896D-09
==========
Optimization completed. {Found 2 times}
Item Max Val. Criteria Pass? RMS Val. Criteria Pass?
Force 0.00001 || 0.00045 [YES] 0.00000 || 0.00030 [YES]
Displ 0.00112 || 0.00180 [YES] 0.00112 || 0.00180 [YES]

Atomic Coordinates (Angstroms)
Type X Y Z

N -1.444138 -1.598403 -0.545335
C -2.068241 -0.438640 -0.263482
C -1.375662 0.897927 -0.297911
C -1.568915 1.692487 0.791333
H -2.248216 1.356393 1.572029
C -0.834927 2.994562 0.955050
H -0.770029 3.505376 -0.011753
C 0.587418 2.819891 1.520229
H 0.555854 2.171941 2.403305
H 0.990208 3.783328 1.848127
C 1.549502 2.204095 0.497869
H 1.049985 1.420201 -0.085884
C 1.951008 3.253365 -0.533433
O 1.512888 4.374416 -0.588511
O 2.873744 2.791325 -1.394003
C 3.260065 3.711473 -2.411621
H 2.397342 3.978464 -3.025674
H 4.011740 3.194767 -3.006995
H 3.675251 4.619691 -1.968979
C 2.794390 1.623466 1.166610
O 3.070094 1.943273 2.305448
C 3.709056 0.652730 0.457598
H -1.396483 3.653216 1.626633
O -0.652787 1.038646 -1.342737
N -3.353628 -0.767594 -0.128380
C -4.451422 0.142572 0.046056
N -3.573522 -2.109379 -0.311741
C -2.388182 -2.584108 -0.563560
C -1.983067 -3.981468 -0.929489
H -2.249640 -4.167447 -1.981400
H -2.507377 -4.706128 -0.304230
O -0.603221 -4.152526 -0.720159
C 0.198035 -3.199961 -1.411623
H -0.026004 -3.238677 -2.486756
C -0.019568 -1.793866 -0.813310
H 0.267079 -0.987648 -1.497541
C 1.656654 -3.513679 -1.066009
H 2.318854 -3.127561 -1.851202
H 1.808541 -4.593738 -0.989374
C 1.864401 -2.769058 0.233202
C 0.872494 -1.805191 0.409147
C 2.870876 -2.919185 1.178623
H 3.658074 -3.654608 1.037308
C 2.850303 -2.113274 2.316283
H 3.631059 -2.218475 3.063257
C 1.839666 -1.169718 2.501892
H 1.844488 -0.539093 3.385528
C 0.843895 -0.996629 1.539248
H 0.072801 -0.239728 1.665344
C -4.772573 0.982849 -1.023659
C -4.016146 0.923707 -2.325742
H -3.993001 -0.101754 -2.712432
H -2.976966 1.258043 -2.220015
H -4.503875 1.554254 -3.072230
C -5.833564 1.866894 -0.831187
H -6.111477 2.537951 -1.638468
C -6.532119 1.893706 0.371576
H -7.353084 2.592037 0.501404
C -6.187261 1.033289 1.408490
H -6.736086 1.058566 2.345384
C -5.129855 0.135636 1.265117
C -4.722068 -0.800659 2.371471
H -3.653642 -0.705161 2.595832
H -4.903937 -1.843053 2.091631
H -5.282373 -0.583532 3.283201
C 4.927064 0.369464 1.088230
C 5.844103 -0.520798 0.548049
H 6.781629 -0.712774 1.059316
C 5.557390 -1.158019 -0.658190
H 6.268674 -1.850868 -1.097389
C 4.353204 -0.906561 -1.303302
H 4.094560 -1.378906 -2.245296
C 3.448289 -0.018153 -0.736465
F 2.287668 0.155586 -1.386027
H 5.124863 0.876341 2.026949

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
==========
SCF Energy= -1954.29160665 Predicted Change= -9.959896D-09
Zero-point correction (ZPE)= -1953.6796 0.61198
Internal Energy (U)= -1953.6429 0.64868
Enthalpy (H)= -1953.6419 0.64963
Gibbs Free Energy (G)= -1953.7473 0.54424

Frequencies -- 25.5307 34.7831 36.9097
M06-2X/6-31+G(d,p)/PCM(DCE) SP: -1954.408151

(S)-**IV**

Supporting Information: 0300-AzF-enolate-S-2F-0004-1.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011
==========
M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)

opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RM062X/6-31G(d) Freq
---
Pointgroup= C1 Stoichiometry= C34H32FN3O5 C1[X(C34H32FN3O5)] #Atoms= 75
Charge = 0 Multiplicity = 1

SCF Energy= -1954.29551405 Predicted Change= -1.432892D-08
==========
Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00003	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00305	0.00180	[NO]	0.00305	0.00180	[YES]

Atomic Type	X	Y	Z
N	-1.297796	1.649689	0.288436
C	-1.848031	0.419143	0.225306
C	-1.090581	-0.845952	0.515336
C	-1.423125	-1.960631	-0.197178
H	-2.211570	-1.923243	-0.943351
C	-0.721946	-3.251756	0.117834
H	-0.537667	-3.293875	1.197607
C	0.625478	-3.441576	-0.599753
H	0.466317	-3.499909	-1.682295
H	1.083248	-4.381827	-0.271900
C	1.616879	-2.295241	-0.349832
H	1.146129	-1.348512	-0.625737
C	2.793590	-2.449772	-1.290916
O	2.730293	-2.300617	-2.486756
O	3.919691	-2.805392	-0.650974
C	5.076947	-2.882041	-1.478262
H	5.896342	-3.165204	-0.819266
H	5.268188	-1.908989	-1.937756
H	4.937236	-3.627284	-2.264065
C	2.042730	-2.195971	1.109914
O	1.907601	-3.125038	1.873765
C	2.617560	-0.897220	1.617717
H	-1.363678	-4.101876	-0.139659
O	-0.204258	-0.688604	1.420812
N	-3.153505	0.640985	0.043307
C	-4.202539	-0.337909	-0.033589
N	-3.454507	1.975355	-0.020162
C	-2.302842	2.560445	0.132962
C	-1.996587	4.024132	0.233656
H	-2.222408	4.366962	1.255580
H	-2.612955	4.589124	-0.467518
O	-0.649248	4.255312	-0.090138
C	0.260866	3.509597	0.712448
H	0.100893	3.747880	1.773122
C	0.119657	2.000237	0.418564
H	0.519362	1.369118	1.221661
C	1.666782	3.842629	0.202103
H	2.399729	3.665103	0.998457
H	1.723239	4.893152	-0.096064
C	1.850211	2.869473	-0.942521
C	0.919081	1.833962	-0.853269
C	2.761894	2.892652	-1.989465
H	3.490561	3.694721	-2.073805
C	2.716243	1.875694	-2.945281
H	3.426592	1.880312	-3.766375
C	1.763125	0.862195	-2.867243
H	1.745463	0.071389	-3.609471
C	0.845875	0.838069	-1.815842
H	0.101176	0.047256	-1.753704
C	-4.570641	-1.005944	1.136298
C	-3.887896	-0.722666	2.447843
H	-3.869700	0.352285	2.657858
H	-2.850877	-1.078012	2.443729
H	-4.415168	-1.219530	3.264886
C	-5.590421	-1.951047	1.027129
H	-5.900968	-2.494386	1.914673
C	-6.204774	-2.201277	-0.195695
H	-6.995911	-2.941904	-0.260079
C	-5.811380	-1.511651	-1.337939
H	-6.290758	-1.713216	-2.291435
C	-4.792667	-0.561669	-1.278639
C	-4.324089	0.183943	-2.500024
H	-4.816505	-0.199364	-3.396027
H	-3.241170	0.076658	-2.633621
H	-4.538605	1.253934	-2.416026
C	3.244458	0.072349	0.842587
C	3.734020	1.257738	1.376488
H	4.224216	1.960017	0.709582
C	3.583302	1.496745	2.737548
H	3.962941	2.419868	3.166210
C	2.957612	0.545824	3.545734
H	2.836119	0.728291	4.608494
C	2.491938	-0.635561	2.985969
H	1.993333	-1.389245	3.586164
F	3.414499	-0.110983	-0.480502

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
==========
SCF Energy= -1954.29551405 Predicted Change= -1.432892D-08
Zero-point correction (ZPE)= -1953.6847 0.61077
Internal Energy (U)= -1953.6477 0.64781
Enthalpy (H)= -1953.6467 0.64875
Gibbs Free Energy (G)= -1953.7542 0.54125

Frequencies -- 12.4830 27.7049 32.3562
M06-2X/6-31+G(d,p)/PCM(DCE) SP: -1954.412102

TS-V-*(S,R,R)*

Supporting Information: 0305-AzF-Re-aldol-R_2-F_ent-1.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011
==========
# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,modredundant)
Modredundant Input: B 4 20 F
# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest,nofreeze,gdiis) iop(1/8=18)
freq=noraman geom=allcheck guess=read
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31G(d) Freq
---
Pointgroup= C1 Stoichiometry= C34H32FN3O5 C1[X(C34H32FN3O5)] #Atoms= 75
Charge = 0 Multiplicity = 1

SCF Energy= -1954.26764788 Predicted Change= -2.285562D-08
==========
Optimization completed. {Found 3 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00002	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00122	0.00180	[YES]	0.00122	0.00180	[YES]

Atomic Type	X	Y	Z
N	1.703823	1.325929	-0.449386
C	0.377551	1.292877	-0.657010
C	-0.280429	0.390128	-1.693345
C	-1.573159	-0.119195	-1.451431
H	-2.260277	0.489622	-0.873230
C	-2.070070	-1.072348	-2.501678
H	-3.126920	-1.296614	-2.344166
C	-1.204944	-2.347484	-2.392447
H	-0.271946	-2.164048	-2.929928
H	-1.704018	-3.204968	-2.850383
C	-0.852223	-2.644501	-0.916918
H	-1.359510	-3.548171	-0.570624
C	0.629201	-2.889833	-0.728100
O	1.528209	-2.299551	-1.282346
O	0.851876	-3.897082	0.130585
C	2.219843	-4.265405	0.293341
H	2.225479	-5.055466	1.043762
H	2.816531	-3.413904	0.624231
H	2.622892	-4.636076	-0.653007
C	-1.274491	-1.501352	0.062679
O	-0.459201	-1.060344	0.913153
C	-2.738431	-1.582574	0.530083
H	-1.965892	-0.659748	-3.512681
O	0.473714	0.152147	-2.645641
N	-0.101305	2.330839	0.032690
C	-1.474669	2.714853	0.210951
N	0.884349	3.050515	0.647585
C	1.972348	2.408606	0.335610
C	3.414793	2.755675	0.526143
H	3.871848	2.140757	1.311108
H	3.509217	3.809928	0.789667
O	4.040843	2.579917	-0.732110
C	4.014572	1.269448	-1.300967
H	3.984689	1.437575	-2.378740
C	2.793940	0.423834	-0.824868
H	2.416199	-0.249681	-1.596883
C	5.234241	0.443562	-0.853044
H	6.087478	1.099863	-0.659624
H	5.522386	-0.258918	-1.644930
C	4.732599	-0.294992	0.365153
C	3.338771	-0.314142	0.383095
C	5.451303	-0.889258	1.396219
H	6.537743	-0.877610	1.393199
C	4.750330	-1.481320	2.446792
H	5.296540	-1.938896	3.266386
C	3.354364	-1.486147	2.458660
H	2.825195	-1.956221	3.282246
C	2.626007	-0.907842	1.417796
H	1.536957	-0.939053	1.397052
C	-2.028759	2.502613	1.476365
C	-1.197395	1.939068	2.598281

H	-0.649830	1.047295	2.268083
H	-1.834799	1.662774	3.441966
H	-0.467045	2.676853	2.945571
C	-3.371191	2.840274	1.640939
H	-3.841050	2.676507	2.606454
C	-4.105160	3.373404	0.586232
H	-5.151132	3.624979	0.731269
C	-3.508064	3.592472	-0.650908
H	-4.083440	4.019849	-1.466919
C	-2.168619	3.268732	-0.866386
C	-1.513992	3.484407	-2.205228
H	-2.103143	4.180844	-2.805880
H	-1.434054	2.543262	-2.761831
H	-0.505127	3.894733	-2.097435
C	-3.077237	-0.831994	1.661345
C	-4.360517	-0.814127	2.190642
H	-4.576420	-0.214340	3.069994
C	-5.363246	-1.581735	1.601894
H	-6.371420	-1.583050	2.004232
C	-5.058107	-2.365627	0.497334
H	-5.795853	-2.998616	0.016129
C	-3.765411	-2.356896	-0.010370
F	-3.545891	-3.166671	-1.069022
H	-2.272356	-0.280193	2.129642

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -1954.26764788 Predicted Change= -2.285562D-08
Zero-point correction (ZPE)= -1953.6559 0.61169
Internal Energy (U)= -1953.6203 0.64733
Enthalpy (H)= -1953.6193 0.64828
Gibbs Free Energy (G)= -1953.7225 0.54510

Frequencies -- -260.3942 20.9477 30.6210
M06-2X/6-31+G(d,p)/PCM(DCE) SP: -1954.377354

TS-V-*(R,S,S)*

Supporting Information: 0305-AzF-Re-aldol-R_2-F-5.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,modredundant)
Modredundant Input: B 4 20 F
# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest,nofreeze,gdiis) iop(1/8=18)
freq=noraman geom=allcheck guess=read
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31G(d) Freq

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Pointgroup= C1 Stoichiometry= C34H32FN3O5 C1[X(C34H32FN3O5)] #Atoms= 75
Charge = 0 Multiplicity = 1

SCF Energy= -1954.27256639 Predicted Change= -6.301316D-09

Optimization completed. {Found 3 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00159	0.00180	[YES]	0.00159	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	1.342784	0.750431	0.667329
C	0.367911	1.075139	-0.193518
C	0.082992	0.318974	-1.483746
C	-1.252707	-0.187223	-1.608116
H	-2.023501	0.475328	-1.218421
C	-1.552923	-0.894553	-2.920460
H	-2.627904	-0.830851	-3.119057
C	-1.143773	-2.359307	-2.732006
H	-0.053654	-2.447992	-2.720839
H	-1.536654	-3.011756	-3.517680
C	-1.678825	-2.710887	-1.351853
H	-2.772041	-2.682364	-1.346670
C	-1.268341	-4.040164	-0.770328
O	-1.784575	-4.542048	0.199603
O	-0.246658	-4.610661	-1.431018
C	0.233231	-5.814604	-0.845646
H	0.598148	-5.622492	0.166271
H	1.044240	-6.157279	-1.487615
H	-0.561583	-6.562973	-0.795494
C	-1.097483	-1.631990	-0.374746
O	0.112305	-1.850169	-0.010910
C	-2.053686	-1.256554	0.761229
H	-1.021931	-0.433466	-3.760267
O	1.064767	0.031307	-2.150838
N	-0.302453	2.076427	0.375206
C	-1.338744	2.875676	-0.219166
N	0.186913	2.375685	1.611436
C	1.170007	1.535089	1.771365
C	1.954609	1.256766	3.017853
H	1.309018	0.674070	3.694341
H	2.229329	2.189297	3.514288
O	3.132732	0.563728	2.714595
C	2.933506	-0.617392	1.938965
H	2.263506	-1.311677	2.462913
C	2.413820	-0.252719	0.533120
H	1.951713	-1.111684	0.035686
C	4.336810	-1.158181	1.660911
H	4.284000	-2.218317	1.386293
H	4.970554	-1.059670	2.546033
C	4.777671	-0.308141	0.489042
C	3.668026	0.242737	-0.155900
C	6.059791	-0.041034	0.031456
H	6.926115	-0.464719	0.531839
C	6.217912	0.795146	-1.074091
H	7.215227	1.022285	-1.438401
C	5.107351	1.343179	-1.713416
H	5.246783	1.989174	-2.574765
C	3.816304	1.063756	-1.263830
H	2.946872	1.455445	-1.781887
C	-2.559667	2.976579	0.457537
C	-2.788779	2.310216	1.785871
H	-2.342319	2.901002	2.592098
H	-2.340208	1.313711	1.823538
H	-3.858514	2.208664	1.978868
C	-3.558059	3.737175	-0.149464
H	-4.521639	3.824616	0.343667
C	-3.335556	4.372587	-1.366109
H	-4.127973	4.955886	-1.824549
C	-2.099123	4.274827	-1.991959
H	-1.920768	4.790281	-2.931018
C	-1.064447	3.527619	-1.428202
C	0.281591	3.469914	-2.106955
H	0.405987	4.343234	-2.751167
H	0.387955	2.578002	-2.733630
H	1.103226	3.467929	-1.383113
C	-1.564835	-1.294947	2.067911
C	-2.390069	-1.063892	3.166756
H	-1.984434	-1.116377	4.172741
C	-3.743609	-0.799171	2.974482
H	-4.400700	-0.635954	3.823178
C	-4.259850	-0.743338	1.681392
H	-5.306236	-0.533896	1.485179
C	-3.407223	-0.959160	0.611283
F	-3.929873	-0.871026	-0.632921
H	-0.516041	-1.556026	2.176698

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -1954.27256639 Predicted Change= -6.301316D-09
Zero-point correction (ZPE)= -1953.6617 0.61081
Internal Energy (U)= -1953.6258 0.64670
Enthalpy (H)= -1953.6249 0.64765
Gibbs Free Energy (G)= -1953.7295 0.54297

Frequencies -- -235.8270 15.2149 24.7379
M06-2X/6-31+G(d,p)/PCM(DCE) SP: -1954.389875

TS-V-*(R,R,R)*

Supporting Information: 0305-AzF-Re-aldol-S_ent-3_2F-dn.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,modredundant)
Modredundant Input: B 4 20 F
# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest,nofreeze,gdiis) iop(1/8=18)
freq=noraman geom=allcheck guess=read
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31G(d) Freq

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Pointgroup= C1 Stoichiometry= C34H32FN3O5 C1[X(C34H32FN3O5)] #Atoms= 75
Charge = 0 Multiplicity = 1

SCF Energy= -1954.27230702 Predicted Change= -2.599199D-10

Optimization completed. {Found 3 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00038	0.00180	[YES]	0.00038	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	2.345361	-1.306017	0.198958

C	1.039841	-1.292753	0.558128
C	0.493904	-0.379372	1.653721
C	-0.902718	-0.229188	1.813244
H	-1.549309	-1.047623	1.532052
C	-1.331485	0.694493	2.936915
H	-2.134946	0.249037	3.527319
C	-1.778006	2.051532	2.343765
H	-1.595764	2.874178	3.041943
H	-2.846827	2.050924	2.116003
C	-0.974696	2.224498	1.065109
H	0.095044	2.290864	1.292390
C	-1.302173	3.419128	0.206102
O	-0.512512	3.995455	-0.503276
O	-2.609113	3.742686	0.257016
C	-3.006432	4.765738	-0.649930
H	-2.818336	4.450926	-1.679747
H	-2.454001	5.687947	-0.455647
H	-4.072942	4.913023	-0.484423
C	-1.125144	0.969643	0.155667
O	-0.235921	0.769868	-0.715369
C	-2.559794	0.696190	-0.347519
H	-0.475250	0.859533	3.597616
O	1.377171	0.285290	2.208824
N	0.464385	-2.237902	-0.190690
C	-0.916167	-2.653216	-0.248111
N	1.353397	-2.855817	-1.012590
C	2.485932	-2.268454	-0.758527
C	3.829284	-2.623171	-1.323150
H	3.746373	-2.781284	-2.399958
H	4.169728	-3.561375	-0.856954
O	4.747691	-1.587842	-1.107288
C	4.815232	-1.184320	0.252826
H	5.067943	-2.048234	0.884889
C	3.493803	-0.505150	0.675955
H	3.408443	-0.456138	1.761894
C	5.829565	-0.039371	0.320452
H	6.664495	-0.233511	-0.358340
H	6.228158	0.049357	1.338577
C	4.993727	1.162607	-0.061169
C	3.634201	0.884247	0.088739
C	5.404844	2.405839	-0.521099
H	6.460958	2.629131	-0.646264
C	4.433863	3.356794	-0.838928
H	4.740857	4.332182	-1.204868
C	3.077447	3.060413	-0.710864
H	2.322191	3.794632	-0.974614
C	2.659688	1.813946	-0.241865
H	1.600688	1.574168	-0.195125
C	-1.431135	-3.386485	0.825154
C	-0.578808	-3.759187	2.010077
H	-1.071631	-4.534033	2.601130
H	-0.408786	-2.894179	2.661867
H	0.397628	-4.141336	1.694743
C	-2.780157	-3.731849	0.766340
H	-3.219743	-4.283746	1.591979
C	-3.557506	-3.374582	-0.331625
H	-4.611331	-3.635342	-0.353462
C	-2.991347	-2.700110	-1.406586
H	-3.598872	-2.429301	-2.264975
C	-1.644297	-2.334207	-1.398542
C	-1.008733	-1.646444	-2.574539
H	-1.777002	-1.359974	-3.296357
H	-0.296981	-2.315850	-3.068670
H	-0.484166	-0.744525	-2.242374
C	-2.745256	0.984522	-1.708951
C	-3.964515	0.809767	-2.352540
H	-4.058824	1.053214	-3.406486
C	-5.058957	0.322328	-1.641095
H	-6.018552	0.175876	-2.127409
C	-4.913402	0.025537	-0.292838
H	-5.731315	-0.361386	0.305853
C	-3.684245	0.222528	0.324695
F	-3.633116	-0.102271	1.633108
H	-1.878569	1.346428	-2.253629

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -1954.27230702 Predicted Change= -2.599199D-10
Zero-point correction (ZPE)= -1953.6598 0.61240
Internal Energy (U)= -1953.6245 0.64773
Enthalpy (H)= -1953.6236 0.64867
Gibbs Free Energy (G)= -1953.7253 0.54693

Frequencies -- -250.0376 22.2972 35.1885
M06-2X/6-31+G(d,p)/PCM(DCE) SP: -1954.382604

TS-V-*(S,S,S)*

Supporting Information: 0305-AzF-Re-aldol-S-2_2F-dn.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250,calcfc,ts,noeigentest,gdiis) iop(1/8=18) freq=noraman #N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31G(d) Freq

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Pointgroup= C1 Stoichiometry= C34H32FN3O5 C1[X(C34H32FN3O5)] #Atoms= 75
Charge = 0 Multiplicity = 1

SCF Energy= -1954.27285391 Predicted Change= -3.511477D-11

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 ||	0.00045	[YES]	0.00000 ||	0.00030	[YES]
Displ	0.00006 ||	0.00180	[YES]	0.00006 ||	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	-1.809513	-0.725489	0.653592
C	-0.782873	-1.176293	-0.087422
C	-0.388088	-0.560612	-1.418442
C	0.999766	-0.349061	-1.627770
H	1.675828	-1.081831	-1.206784
C	1.370559	0.305675	-2.943664
H	2.168445	-0.244304	-3.447803
C	1.793413	1.762474	-2.673296
H	1.596610	2.412542	-3.530942
H	2.863732	1.834081	-2.460095
C	1.014171	2.211896	-1.449722
H	-0.062134	2.263764	-1.654292
C	1.482810	3.547711	-0.927082
O	2.528317	4.082008	-1.210341
O	0.609020	4.077835	-0.049918
C	1.043654	5.293356	0.550668
H	1.980475	5.136176	1.091688
H	0.249254	5.589221	1.235188
H	1.203589	6.062881	-0.208372
C	1.156540	1.161199	-0.303629
O	0.265389	1.137623	0.600422
C	2.595810	1.068174	0.255851
H	0.491054	0.299331	-3.595158
O	-1.333850	-0.098414	-2.061009
N	-0.192073	-2.112716	0.648821
C	0.993858	-2.858888	0.329328
N	-0.782456	-2.254680	1.866107
C	-1.747807	-1.379487	1.848639
C	-2.617463	-0.970029	2.998738
H	-1.977784	-0.472458	3.743572
H	-3.076951	-1.845269	3.462739
O	-3.646684	-0.125713	2.563316
C	-3.191174	0.964250	1.766318
H	-2.424063	1.538787	2.301691
C	-2.675028	0.438787	0.409187
H	-2.032657	1.180902	-0.073799
C	-4.446647	1.749469	1.384319
H	-4.177992	2.771365	1.091213
H	-5.138431	1.802154	2.228993
C	-4.973186	0.958154	0.207753
C	-3.958961	0.176582	-0.349833
C	-6.254683	0.931640	-0.323957
H	-7.046721	1.535859	0.109731
C	-6.511569	0.100519	-1.413981
H	-7.511242	0.059490	-1.835924
C	-5.497189	-0.682177	-1.963511
H	-5.713435	-1.322352	-2.813210
C	-4.204734	-0.645940	-1.440033
H	-3.402857	-1.224458	-1.885034
C	0.943174	-3.784020	-0.715329
C	-0.323535	-4.043079	-1.488896
H	-0.252267	-4.992951	-2.023220
H	-0.497856	-3.255927	-2.232223
H	-1.198882	-4.084838	-0.833654
C	2.133262	-4.433710	-1.040611
H	2.133544	-5.158565	-1.849469
C	3.309394	-4.151141	-0.353680
H	4.228948	-4.656513	-0.632039
C	3.317010	-3.223326	0.682408
H	4.239757	-2.995027	1.208010
C	2.149807	-2.556975	1.056679
C	2.143823	-1.548163	2.173748
H	1.809791	-2.015047	3.106817
H	1.475100	-0.708663	1.955752
H	3.150000	-1.146281	2.322419
C	2.762656	1.704160	1.496713
C	3.975089	1.717375	2.173395
H	4.057336	2.226705	3.128517
C	5.078627	1.062360	1.629090
H	6.031384	1.052391	2.149366
C	4.951619	0.422498	0.403552
H	5.780375	-0.095264	-0.067800
C	3.731978	0.453454	-0.263790

F 3.707162 -0.174652 -1.457906
H 1.879853 2.168436 1.925465

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -1954.27285391 Predicted Change= -3.511477D-11
Zero-point correction (ZPE)= -1953.6609 0.61187
Internal Energy (U)= -1953.6254 0.64744
Enthalpy (H)= -1953.6244 0.64839
Gibbs Free Energy (G)= -1953.7279 0.54487

Frequencies -- -262.7897 21.7884 27.2544
M06-2X/6-31+G(d,p)/PCM(DCE) SP: -1954.384783

—2-OMePh Substrate—

(R)-IV

Supporting Information: 0300-AzF-enolate-2OMe-R-0002-2.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RM062X/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C35H35N3O6 C1[X(C35H35N3O6)] #Atoms= 79
Charge = 0 Multiplicity = 1

SCF Energy= -1969.56513087 Predicted Change= -1.952173D-08

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00002	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00196	0.00180	[NO]	0.00196	0.00180	[YES]

Atomic Type	X	Y	Z
N	-1.512232	-1.594728	-0.500977
C	-2.131657	-0.426604	-0.248231
C	-1.428258	0.906475	-0.283301
C	-1.608468	1.684273	0.819568
H	-2.281833	1.328270	1.597235
C	-0.865456	2.973850	1.031353
H	-0.752048	3.497082	0.075683
C	0.528570	2.760091	1.653539
H	0.450681	2.074230	2.504136
H	0.928925	3.702494	2.039074
C	1.510998	2.168628	0.637661
H	1.004678	1.437633	-0.004192
C	1.984328	3.263293	-0.310657
O	1.586865	4.401311	-0.308847
O	2.922323	2.833084	-1.177722
C	3.396577	3.826358	-2.083255
H	2.584312	4.174046	-2.726159
H	4.175138	3.341882	-2.672457
H	3.804116	4.679833	-1.536965
C	2.710138	1.492763	1.312755
O	2.941236	1.739292	2.480732
C	3.632878	0.547805	0.579476
H	-1.447026	3.631270	1.686996
O	-0.720336	1.053546	-1.340228
N	-3.422435	-0.744483	-0.138586
C	-4.514681	0.174315	0.024925
N	-3.649464	-2.086117	-0.316317
C	-2.462364	-2.572923	-0.536714
C	-2.058839	-3.972571	-0.899756
H	-2.322120	-4.154982	-1.953189
H	-2.589682	-4.696313	-0.278890
O	-0.680891	-4.153804	-0.684781
C	0.134787	-3.194956	-1.351596
H	-0.076284	-3.214299	-2.430312
C	-0.084685	-1.801991	-0.729305
H	0.227677	-0.983380	-1.385192
C	1.588197	-3.516938	-0.991581
H	2.263239	-3.103906	-1.753059
H	1.743508	-4.598267	-0.945329
C	1.772570	-2.807974	0.331266
C	0.779379	-1.846000	0.511715
C	2.759069	-2.985091	1.291898
H	3.546600	-3.719737	1.149038
C	2.719048	-2.204132	2.446955
H	3.485861	-2.327848	3.205387
C	1.710551	-1.259489	2.633595
H	1.706279	-0.642364	3.526474
C	0.733660	-1.060907	1.656086
H	-0.033465	-0.299806	1.780565
C	-4.819237	1.018682	-1.046265
C	-4.053185	0.952679	-2.342308
H	-4.048714	-0.070723	-2.735189
H	-3.008183	1.264350	-2.225224
H	-4.521619	1.598249	-3.088368
C	-5.873166	1.912833	-0.861587
H	-6.137719	2.587620	-1.670259
C	-6.581281	1.945249	0.335431
H	-7.396270	2.651557	0.459524
C	-6.253104	1.080567	1.374147
H	-6.808993	1.110335	2.306726
C	-5.203031	0.173097	1.238600
C	-4.813651	-0.767412	2.347996
H	-3.745529	-0.685517	2.579254
H	-5.006865	-1.807661	2.067838
H	-5.376757	-0.542524	3.256091
C	4.831019	0.239280	1.229904
C	5.788495	-0.583669	0.652214
H	6.714469	-0.797149	1.175899
C	5.554648	-1.114058	-0.613559
H	6.298285	-1.747465	-1.088821
C	4.363502	-0.842362	-1.277317
H	4.175867	-1.266676	-2.258614
C	3.393283	-0.035218	-0.677533
H	4.990808	0.680814	2.208148
O	2.185252	0.170305	-1.255856
C	2.104448	0.293619	-2.662704
H	2.168231	-0.686159	-3.156645
H	1.125105	0.739614	-2.846582
H	2.902166	0.943548	-3.038326

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -1969.56513087 Predicted Change= -1.952173D-08
Zero-point correction (ZPE)= -1968.9121 0.65300
Internal Energy (U)= -1968.8736 0.69149
Enthalpy (H)= -1968.8726 0.69243
Gibbs Free Energy (G)= -1968.9818 0.58330

Frequencies -- 26.2079 32.9433 33.7113
M06-2X/6-31+G(d,p)/PCM(DCE) SP: -1969.682038

(S)-IV

Supporting Information: 0300-AzF-enolate-S-2OMe-0004-1.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RM062X/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C35H35N3O6 C1[X(C35H35N3O6)] #Atoms= 79
Charge = 0 Multiplicity = 1

SCF Energy= -1969.56629281 Predicted Change= -6.492674D-09

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00305	0.00180	[NO]	0.00305	0.00180	[YES]

Atomic Type	X	Y	Z
N	-1.439610	1.628422	0.251870
C	-1.974923	0.393809	0.154844
C	-1.217855	-0.867843	0.455112
C	-1.479912	-1.973247	-0.297143
H	-2.212016	-1.935219	-1.099033
C	-0.781218	-3.254751	0.058513
H	-0.658707	-3.290765	1.146962
C	0.608201	-3.429561	-0.577676
H	0.507427	-3.517965	-1.665996
H	1.064071	-4.353050	-0.203040
C	1.573022	-2.262672	-0.304306
H	1.133501	-1.326660	-0.653043
C	2.804949	-2.483066	-1.157469
O	2.883058	-2.232804	-2.337054
O	3.793290	-3.081539	-0.468752
C	4.958789	-3.387148	-1.225328
H	5.630270	-3.906101	-0.542531
H	5.425847	-2.470957	-1.596907
H	4.706585	-4.022076	-2.077644
C	1.903344	-2.117577	1.181328
O	1.735061	-3.039656	1.948524
C	2.419966	-0.801308	1.709309
H	-1.395208	-4.114595	-0.233039
O	-0.410390	-0.714309	1.432500
N	-3.280939	0.602622	-0.029924

C	-4.315891	-0.391742	-0.097430
N	-3.600032	1.934039	-0.058716
C	-2.456602	2.529277	0.116559
C	-2.172573	3.992448	0.265500
H	-2.415873	4.300353	1.294488
H	-2.787193	4.571328	-0.425832
O	-0.824885	4.249183	-0.033626
C	0.087880	3.492563	0.756000
H	-0.082623	3.697753	1.821705
C	-0.027087	1.987681	0.420007
H	0.361883	1.340247	1.216572
C	1.487740	3.865659	0.261281
H	2.224258	3.656153	1.046464
H	1.532579	4.928598	0.009389
C	1.680153	2.941814	-0.919882
C	0.793213	1.865783	-0.845416
C	2.558757	3.046003	-1.988963
H	3.237349	3.891656	-2.068700
C	2.550955	2.048096	-2.967036
H	3.240375	2.112264	-3.804023
C	1.673426	0.969434	-2.879350
H	1.697884	0.183618	-3.627164
C	0.767554	0.880583	-1.820616
H	0.067676	0.049745	-1.764623
C	-4.662191	-1.057154	1.080921
C	-3.977567	-0.744365	2.385407
H	-4.017380	0.330029	2.597622
H	-2.921700	-1.039290	2.372996
H	-4.469588	-1.269905	3.206475
C	-5.668377	-2.018165	0.987253
H	-5.963182	-2.560236	1.880879
C	-6.290288	-2.284846	-0.228469
H	-7.071074	-3.037412	-0.280716
C	-5.919312	-1.595995	-1.378651
H	-6.406033	-1.809765	-2.325756
C	-4.914463	-0.630473	-1.334789
C	-4.470484	0.119052	-2.562906
H	-4.978898	-0.262445	-3.450754
H	-3.390083	0.014586	-2.716635
H	-4.685478	1.188446	-2.471831
C	3.171267	0.120949	0.965953
C	3.632123	1.299642	1.560906
H	4.228298	1.999511	0.984708
C	3.321952	1.573045	2.889759
H	3.683835	2.493016	3.341331
C	2.565258	0.672059	3.636005
H	2.323418	0.884554	4.672312
C	2.132921	-0.507341	3.042973
O	3.420313	-0.179762	-0.335923
C	4.585533	0.338197	-0.943475
H	4.629460	-0.134837	-1.926945
H	4.526121	1.422718	-1.076313
H	5.474678	0.082431	-0.353444
H	1.542448	-1.233243	3.591746

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1969.56629281 Predicted Change= -6.492674D-09
Zero-point correction (ZPE)= -1968.9138 0.65241
Internal Energy (U)= -1968.8751 0.69117
Enthalpy (H)= -1968.8741 0.69211
Gibbs Free Energy (G)= -1968.9858 0.58043

Frequencies -- 8.9581 25.6388 26.8358
M06-2X/6-31+G(d,p)/PCM(DCE) SP: -1969.685099

TS-V-*(S,R,R)*

Supporting Information: 0305-AzF-Re-aldol-R_ent-6_2OMe-dn.log

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Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

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# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest,gdiis) iop(1/8=18) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C35H35N3O6 C1[X(C35H35N3O6)] #Atoms= 79
Charge = 0 Multiplicity = 1

SCF Energy= -1969.53737937 Predicted Change= -2.642704D-10

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Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00031	0.00180	[YES]	0.00031	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	-1.058229	-0.881811	-0.737129
C	0.006381	-1.248403	0.012783
C	0.484008	-0.751483	1.380790
C	0.144643	0.591195	1.732206
H	-0.875438	0.902899	1.539455
C	0.760498	1.086908	3.025991
H	0.158709	1.917403	3.411475
C	2.172189	1.579227	2.690910
H	2.829772	0.729816	2.480967
H	2.621551	2.163545	3.499354
C	2.017014	2.391504	1.413757
H	1.436352	3.300128	1.600729
C	3.341027	2.789334	0.809114
O	4.432798	2.519954	1.241824
O	3.156713	3.522359	-0.309606
C	4.354315	3.866345	-0.994248
H	4.045526	4.428428	-1.875377
H	4.897474	2.963932	-1.285220
H	5.001700	4.475713	-0.358484
C	1.301174	1.485503	0.368214
O	2.049715	0.635440	-0.205240
C	0.272713	2.174840	-0.536183
H	0.790050	0.301347	3.789393
O	1.294381	-1.478660	1.934606
N	0.674413	-2.130232	-0.733057
C	1.827293	-2.945926	-0.417505
N	0.086808	-2.323695	-1.943383
C	-0.958458	-1.553760	-1.923954
C	-1.974456	-1.352673	-3.002591
H	-2.088138	-2.270937	-3.580388
H	-1.639382	-0.542955	-3.669182
O	-3.214640	-1.040343	-2.417758
C	-3.137046	0.144660	-1.643448
H	-2.773144	0.973896	-2.262026
C	-2.234550	-0.067042	-0.399098
H	-1.880606	0.910634	-0.069599
C	-4.522587	0.382207	-1.038296
H	-5.301226	0.069692	-1.739190
H	-4.656584	1.450920	-0.829433
C	-4.487728	-0.423349	0.240137
C	-3.170203	-0.704319	0.605890
C	-5.541683	-0.869723	1.025508
H	-6.569708	-0.660177	0.743654
C	-5.259210	-1.605766	2.176290
H	-6.073765	-1.968387	2.795609
C	-3.941887	-1.886847	2.535304
H	-3.736621	-2.462926	3.431768
C	-2.880637	-1.432535	1.752265
H	-1.856487	-1.649677	2.043794
C	3.023480	-2.683604	-1.087511
C	3.158237	-1.548709	-2.065163
H	2.925497	-0.597105	-1.576396
H	2.472045	-1.684115	-2.908297
H	4.177081	-1.514374	-2.457843
C	4.094302	-3.535350	-0.809311
H	5.045853	-3.353333	-1.299888
C	3.957342	-4.598634	0.074020
H	4.805243	-5.245901	0.276555
C	2.735816	-4.846414	0.690581
H	2.625384	-5.686595	1.369983
C	1.637860	-4.023978	0.450352
C	0.316602	-4.284228	1.121960
H	0.273478	-5.311135	1.491869
H	-0.526816	-4.137686	0.437886
H	0.193197	-3.604435	1.971274
C	-0.718595	3.085812	-0.115500
C	-1.594352	3.663475	-1.039087
H	-2.352418	4.367301	-0.715265
C	-1.484465	3.353353	-2.395941
H	-2.159578	3.824737	-3.104649
C	-0.520660	2.451175	-2.828391
H	-0.423440	2.214665	-3.884366
C	0.340653	1.873518	-1.894556
H	1.120331	1.176056	-2.189368
O	-0.803004	3.324687	1.224391
C	-1.790700	4.219727	1.684727
H	-2.799128	3.855219	1.450462
H	-1.667395	4.271272	2.766582
H	-1.657983	5.218574	1.253315

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

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SCF Energy= -1969.53737937 Predicted Change= -2.642704D-10
Zero-point correction (ZPE)= -1968.8853 0.65203
Internal Energy (U)= -1968.8475 0.68979
Enthalpy (H)= -1968.8466 0.69073
Gibbs Free Energy (G)= -1968.9554 0.58191

Frequencies -- -286.5602 16.4568 21.3561
M06-2X/6-31+G(d,p)/PCM(DCE) SP: -1969.657747

TS-V-*(R,S,S)*

Supporting Information: 0305-AzF-Re-aldol-R-3_2OMe-dn.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest,gdiis) iop(1/8=18) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31G(d) Freq

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Pointgroup= C1 Stoichiometry= C35H35N3O6 C1[X(C35H35N3O6)] #Atoms= 79
Charge = 0 Multiplicity = 1

SCF Energy= -1969.54226807 Predicted Change= -5.784934D-09

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00186	0.00180	[NO]	0.00186	0.00180	[YES]

Atomic Type	X	Y	Z
N	-1.497691	-0.762816	0.646686
C	-0.505868	-1.086233	-0.194461
C	-0.196528	-0.330743	-1.480284
C	1.142683	0.172059	-1.573040
H	1.902914	-0.493525	-1.170022
C	1.476764	0.882590	-2.874824
H	2.556639	0.814377	-3.045922
C	1.070080	2.348360	-2.689049
H	-0.019876	2.439152	-2.701147
H	1.480835	3.002314	-3.464599
C	1.575804	2.693956	-1.295948
H	2.667989	2.672861	-1.266808
C	1.140570	4.015550	-0.716550
O	1.633186	4.520035	0.264462
O	0.126885	4.581817	-1.395251
C	-0.377805	5.775021	-0.810497
H	-0.768151	5.569220	0.189285
H	-1.174481	6.118583	-1.469948
H	0.408595	6.529726	-0.730567
C	0.977237	1.603669	-0.339713
O	-0.245041	1.827786	-0.010951
C	1.898056	1.221767	0.828141
H	0.964243	0.428185	-3.729929
O	-1.164532	-0.047921	-2.169244
N	0.154750	-2.086087	0.388774
C	1.214719	-2.873039	-0.178447
N	-0.358438	-2.385093	1.615509
C	-1.345256	-1.545342	1.755210
C	-2.151383	-1.262752	2.986918
H	-1.514582	-0.682823	3.674020
H	-2.440070	-2.193380	3.479030
O	-3.320414	-0.563788	2.661954
C	-3.100312	0.615846	1.889159
H	-2.434435	1.305572	2.424096
C	-2.559279	0.246733	0.492926
H	-2.080727	1.101910	0.003963
C	-4.494848	1.166301	1.587103
H	-4.429584	2.226105	1.313778
H	-5.144874	1.072207	2.460831
C	-4.921483	0.320054	0.407191
C	-3.804699	-0.239381	-0.217871
C	-6.197176	0.063482	-0.073843
H	-7.069073	0.493974	0.410828
C	-6.341935	-0.770866	-1.182653
H	-7.334249	-0.989218	-1.565641
C	-5.224350	-1.327791	-1.801791
H	-5.353079	-1.972285	-2.665966
C	-3.939509	-1.059001	-1.328511
H	-3.063550	-1.457271	-1.830143
C	0.987519	-3.513214	-1.403389
C	-0.335459	-3.464838	-2.126799
H	-0.424744	-2.574839	-2.758603
H	-1.181389	-3.465434	-1.431932
H	-0.432377	-4.340518	-2.772573
C	2.049006	-4.240077	-1.943988
H	1.906066	-4.745359	-2.894600
C	3.266628	-4.330635	-1.281783
H	4.079809	-4.899141	-1.722338
C	3.441956	-3.709231	-0.050017
H	4.388974	-3.794705	0.475181
C	2.415116	-2.969430	0.535555
C	2.593854	-2.324341	1.881844
H	3.655662	-2.210130	2.109389
H	2.132648	-2.937969	2.662354
H	2.129909	-1.335344	1.924345
C	1.341286	1.269317	2.103123
C	2.097364	1.038482	3.252642
H	1.636964	1.098916	4.234338
C	3.453307	0.770503	3.128074
H	4.068067	0.609514	4.008974
C	4.041562	0.703070	1.864749
H	5.100513	0.485875	1.784509
C	3.268763	0.909480	0.721544
O	3.781116	0.818566	-0.541525
C	5.126076	0.424916	-0.685284
H	5.298451	-0.563511	-0.239962
H	5.312627	0.376694	-1.758584
H	5.809336	1.151302	-0.229766
H	0.290279	1.539507	2.149151

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -1969.54226807 Predicted Change= -5.784934D-09
Zero-point correction (ZPE)= -1968.8894 0.65280
Internal Energy (U)= -1968.8521 0.69010
Enthalpy (H)= -1968.8512 0.69104
Gibbs Free Energy (G)= -1968.9582 0.58400

Frequencies -- -249.5503 21.5826 22.9568
M06-2X/6-31+G(d,p)/PCM(DCE) SP: -1969.662038

TS-V-*(R,R,R)*

Supporting Information: 0305-AzF-Re-aldol-S_ent-3_2OMe-dn.log

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Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,modredundant)
Modredundant Input: B 4 20 F
# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest,nofreeze,gdiis) iop(1/8=18)
freq=noraman geom=allcheck guess=read
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C35H35N3O6 C1[X(C35H35N3O6)] #Atoms= 79
Charge = 0 Multiplicity = 1

SCF Energy= -1969.53936259 Predicted Change= -7.796367D-10

Optimization completed. {Found 3 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00090	0.00180	[YES]	0.00090	0.00180	[YES]

Atomic Type	X	Y	Z
N	2.449868	-1.330289	0.197894
C	1.136643	-1.301109	0.524722
C	0.581173	-0.406406	1.632179
C	-0.817010	-0.237487	1.750145
H	-1.465578	-1.039321	1.432869
C	-1.271960	0.663532	2.880763
H	-2.098421	0.209986	3.433771
C	-1.692854	2.035212	2.304513
H	-1.523784	2.843448	3.022942
H	-2.754581	2.042957	2.045814
C	-0.856807	2.224748	1.050030
H	0.207952	2.282547	1.302370
C	-1.162181	3.426293	0.193752
O	-0.369739	3.964366	-0.543053
O	-2.454787	3.799219	0.272021
C	-2.843292	4.798400	-0.663983
H	-2.728491	4.420023	-1.683527
H	-2.232363	5.696375	-0.547079
H	-3.890460	5.013153	-0.454151
C	-0.990678	0.980955	0.115845
O	-0.063471	0.784999	-0.719507
C	-2.409228	0.772533	-0.476086
H	-0.436822	0.805958	3.573536
O	1.461521	0.222595	2.230945
N	0.562061	-2.211883	-0.266771
C	-0.823851	-2.598316	-0.376495
N	1.460281	-2.822821	-1.084680
C	2.596773	-2.266049	-0.784582
C	3.947729	-2.630431	-1.324295
H	3.890444	-2.757185	-2.406855
H	4.258502	-3.587540	-0.876065
O	4.880051	-1.619857	-1.055938
C	4.918905	-1.252538	0.315447
H	5.141944	-2.136507	0.930869
C	3.598725	-0.562563	0.723824
H	3.487723	-0.540406	1.808293
C	5.949133	-0.126251	0.439090
H	6.798739	-0.316133	-0.222506
H	6.321899	-0.070795	1.469363

C	5.142220	1.098712	0.067986
C	3.775175	0.838724	0.176431
C	5.584256	2.346181	-0.349847
H	6.646545	2.555989	-0.441865
C	4.636201	3.319313	-0.669873
H	4.966903	4.297986	-1.005080
C	3.272550	3.040805	-0.585155
H	2.536025	3.791992	-0.854085
C	2.823055	1.790705	-0.156714
H	1.759170	1.566071	-0.144081
C	-1.384788	-3.349622	0.660975
C	-0.576205	-3.767963	1.861122
H	-1.100545	-4.548174	2.417184
H	-0.408981	-2.922479	2.538583
H	0.401874	-4.161271	1.565113
C	-2.736440	-3.671550	0.550994
H	-3.209600	-4.239698	1.347102
C	-3.471470	-3.278770	-0.564459
H	-4.526720	-3.528432	-0.630966
C	-2.860310	-2.587991	-1.603613
H	-3.435839	-2.286998	-2.474003
C	-1.509648	-2.240607	-1.541487
C	-0.830688	-1.527164	-2.677347
H	-1.573660	-1.210093	-3.412608
H	-0.111298	-2.190364	-3.168853
H	-0.308149	-0.640852	-2.301248
C	-2.487404	1.183358	-1.812239
C	-3.659189	1.109645	-2.559696
H	-3.669170	1.447002	-3.591565
C	-4.806611	0.601986	-1.966329
H	-5.736406	0.530898	-2.523447
C	-4.770211	0.180956	-0.641218
H	-5.670428	-0.219832	-0.191325
C	-3.589572	0.265718	0.104530
H	-1.574321	1.564030	-2.259759
O	-3.540130	-0.164291	1.396811
C	-4.687400	-0.753117	1.959587
H	-5.002029	-1.636270	1.389551
H	-4.401810	-1.055467	2.968443
H	-5.519751	-0.040932	2.016817

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1969.53936259 Predicted Change= -7.796367D-10
Zero-point correction (ZPE)= -1968.8859 0.65341
Internal Energy (U)= -1968.8488 0.69052
Enthalpy (H)= -1968.8478 0.69147
Gibbs Free Energy (G)= -1968.9538 0.58555

Frequencies -- -278.1862 19.8730 33.1533
M06-2X/6-31+G(d,p)/PCM(DCE) SP: -1969.651892

TS-V-*(S,S,S)*

Supporting Information: 0305-AzF-Re-aldol-S-2_2OMe-dn.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

==========

# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest,gdiis) iop(1/8=18) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C35H35N3O6 C1[X(C35H35N3O6)] #Atoms= 79
Charge = 0 Multiplicity = 1

SCF Energy= -1969.54093721 Predicted Change= -4.659666D-10

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00043	0.00180	[YES]	0.00043	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	-1.977492	-0.743319	0.639006
C	-0.915041	-1.177646	-0.060167
C	-0.505968	-0.588496	-1.401037
C	0.881244	-0.358142	-1.584285
H	1.561763	-1.065965	-1.133330
C	1.278971	0.266857	-2.905387
H	2.076278	-0.305562	-3.388125
C	1.724308	1.718653	-2.653273
H	1.563424	2.357906	-3.526760
H	2.788946	1.767870	-2.408828
C	0.925572	2.205909	-1.457433
H	-0.144083	2.281933	-1.689091
C	1.416747	3.541282	-0.953750
O	2.456821	4.068703	-1.268309
O	0.570563	4.082722	-0.055798
C	1.042710	5.283682	0.544794
H	1.985438	5.100065	1.067642
H	0.267963	5.591628	1.246505
H	1.206044	6.055788	-0.210887
C	1.007831	1.172424	-0.285913
O	0.063953	1.170070	0.566744
C	2.416425	1.110901	0.367766
H	0.409768	0.261836	-3.571201
O	-1.450176	-0.172902	-2.076514
N	-0.320554	-2.081880	0.713715
C	0.919893	-2.764762	0.465356
N	-0.945954	-2.217453	1.914786
C	-1.935007	-1.372072	1.848977
C	-2.847515	-0.962714	2.965762
H	-2.238367	-0.450537	3.726127
H	-3.311812	-1.838794	3.423563
O	-3.871815	-0.135227	2.488988
C	-3.404208	0.947278	1.688606
H	-2.654422	1.534787	2.234531
C	-2.851602	0.405751	0.352630
H	-2.204224	1.146133	-0.127003
C	-4.655230	1.717448	1.265032
H	-4.385996	2.735816	0.960326
H	-5.367207	1.780448	2.092043
C	-5.148721	0.901890	0.090380
C	-4.115615	0.119124	-0.430212
C	-6.417653	0.855183	-0.469246
H	-7.224084	1.460369	-0.064334
C	-6.643281	0.002541	-1.549577
H	-7.633002	-0.054995	-1.992594
C	-5.610416	-0.780872	-2.062188
H	-5.802231	-1.438602	-2.904358
C	-4.330240	-0.724181	-1.510963
H	-3.513588	-1.303155	-1.927253
C	0.979317	-3.700525	-0.569100
C	-0.230539	-4.047971	-1.397075
H	-0.075588	-4.997802	-1.913523
H	-0.417810	-3.280689	-2.157887
H	-1.131112	-4.135802	-0.781871
C	2.224274	-4.269992	-0.834875
H	2.309862	-5.002166	-1.632474
C	3.346652	-3.901423	-0.099752
H	4.310124	-4.347571	-0.328938
C	3.243967	-2.968024	0.926843
H	4.123831	-2.670982	1.491412
C	2.018311	-2.381059	1.242707
C	1.893042	-1.373943	2.353895
H	1.506751	-1.854283	3.259481
H	1.213521	-0.559705	2.080761
H	2.870256	-0.935652	2.574678
C	2.471871	1.825742	1.570056
C	3.621485	1.909582	2.347937
H	3.617530	2.483629	3.269124
C	4.763927	1.236369	1.936551
H	5.673435	1.269507	2.529213
C	4.750323	0.514234	0.747384
H	5.649916	-0.002076	0.434467
C	3.598217	0.466019	-0.047872
H	1.551094	2.300800	1.893745
O	3.583479	-0.214082	-1.229382
C	4.769483	-0.827901	-1.673053
H	5.103771	-1.607416	-0.976927
H	4.525772	-1.285832	-2.632934
H	5.572220	-0.093540	-1.810786

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1969.54093721 Predicted Change= -4.659666D-10
Zero-point correction (ZPE)= -1968.8875 0.65335
Internal Energy (U)= -1968.8504 0.69048
Enthalpy (H)= -1968.8495 0.69143
Gibbs Free Energy (G)= -1968.9555 0.58541

Frequencies -- -280.3552 22.5330 28.8409
M06-2X/6-31+G(d,p)/PCM(DCE) SP: -1969.655002

Energetic Penalty from Loss of Conjugation

(see Table 4)

—Benzaldehyde—

GS-0°

Supporting Information: GS-benzaldehyde.log

```
 Using  Gaussian 09:  AM64L-G09RevC.01 23-Sep-2011
 # M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
 opt=(maxcycle=250) freq=noraman
 #N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RM062X/6-31G(d) Freq
 Pointgroup= C1   Stoichiometry= C7H6O   C1[X(C7H6O)]  #Atoms= 14
 Charge = 0     Multiplicity = 1
 SCF Energy= -345.419894063                  Predicted Change= -1.791021D-07
 Optimization completed.           {Found       2       times}
 Item      Max Val.    Criteria   Pass?      RMS Val.    Criteria    Pass?
 Force      0.00013 ||  0.00045   [ YES ]      0.00004 ||  0.00030   [ YES ]
 Displ      0.00058 ||  0.00180   [ YES ]      0.00058 ||  0.00180   [ YES ]
      Atomic          Coordinates (Angstroms)
       Type          X                   Y                   Z
      C       -0.360987      1.290505      0.000007
      C       -1.732612      1.056242      0.000021
      C       -2.208097     -0.253119      0.000021
      C       -1.318287     -1.329032     -0.000013
      C        0.050244     -1.096007     -0.000041
      C        0.528812      0.216815     -0.000022
      H        0.024685      2.307790      0.000021
      H       -2.428388      1.889205      0.000043
      H       -3.278162     -0.437996      0.000044
      H       -1.697529     -2.346147     -0.000016
      H        0.768276     -1.910737     -0.000061
      C        1.989680      0.470533     -0.000050
      O        2.829951     -0.397579      0.000083
      H        2.278994      1.542893     -0.000229
 Statistical Thermodynamic Analysis
 Temperature= 298.150 Kelvin       Pressure= 1.00000 Atm
 SCF Energy=     -345.419894063              Predicted Change= -1.791021D-07
 Zero-point correction (ZPE)=                  -345.3085   0.11132
 Internal Energy (U)=                          -345.3023   0.11758
 Enthalpy (H)=                                             -345.3013    0.11853
 Gibbs Free Energy (G)=                        -345.3390    0.08082
 Frequencies --   122.6338             223.2633             246.2309
M06-2X/6-31+G(d,p)/PCM(DCE) SP:  -345.445236
```

GS-34°

Supporting Information: GS-benzaldehyde-35.log

```
 Using  Gaussian 09:  AM64L-G09RevC.01 23-Sep-2011
 # M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
 opt=(maxcycle=250,modredundant) freq=noraman
 Modredundant Input:  D      5      6     13     12 F
 #N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RM062X/6-31G(d) Freq
 Pointgroup= C1   Stoichiometry= C7H6O   C1[X(C7H6O)]  #Atoms= 14
 Charge = 0     Multiplicity = 1
 SCF Energy= -345.415883146                  Predicted Change= -2.012823D-08
 Optimization completed.           {Found       2       times}
 Item      Max Val.    Criteria   Pass?      RMS Val.    Criteria    Pass?
 Force      0.00004 ||  0.00045   [ YES ]      0.00001 ||  0.00030   [ YES ]
 Displ      0.00041 ||  0.00180   [ YES ]      0.00041 ||  0.00180   [ YES ]
      Atomic          Coordinates (Angstroms)
       Type          X                   Y                   Z
      C        0.336621      1.286007     -0.000916
      C        1.709244      1.073947     -0.080712
      C        2.211232     -0.225798     -0.056651
      C        1.345615     -1.315490      0.040992
      C       -0.026974     -1.106541      0.095914
      C       -0.530734      0.195424      0.051701
      H       -0.065824      2.296479      0.007444
      H        2.388015      1.918306     -0.147267
      H        3.283448     -0.390668     -0.103506
      H        1.744724     -2.324290      0.078206
      H       -0.725247     -1.935520      0.162201
      C       -1.996448      0.407193      0.181333
      O       -2.827541     -0.351660     -0.256608
      H       -2.296128      1.360522      0.665824
 Statistical Thermodynamic Analysis
 Temperature= 298.150 Kelvin       Pressure= 1.00000 Atm
 SCF Energy=     -345.415883146              Predicted Change= -2.012823D-08
 Zero-point correction (ZPE)=                  -345.3047   0.11113
 Internal Energy (U)=                          -345.2983   0.11751
 Enthalpy (H)=                                             -345.2974    0.11845
 Gibbs Free Energy (G)=                        -345.3354    0.08041
 Frequencies --   108.1004             186.9145             243.2398
M06-2X/6-31+G(d,p)/PCM(DCE) SP:  -345.441798
```

TS-0°

Supporting Information: TS-benzaldehyde.log

```
 Using  Gaussian 09:  AM64L-G09RevC.01 23-Sep-2011
 # M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
 opt=(maxcycle=250,modredundant) freq=noraman
 Modredundant Input:  D      5      6     13     12 F
 Modredundant Input:  B     12     15 F
 #N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RM062X/6-31G(d) Freq
 Pointgroup= C1   Stoichiometry= C7H7O(1-)   C1[X(C7H7O)]  #Atoms= 15
 Charge = -1    Multiplicity = 1
 SCF Energy= -345.946931958                  Predicted Change= -5.220313D-08
 Optimization completed.           {Found       2       times}
 Item      Max Val.    Criteria   Pass?      RMS Val.    Criteria    Pass?
 Force      0.00003 ||  0.00045   [ YES ]      0.00001 ||  0.00030   [ YES ]
 Displ      0.00108 ||  0.00180   [ YES ]      0.00108 ||  0.00180   [ YES ]
      Atomic          Coordinates (Angstroms)
       Type          X                   Y                   Z
      C        0.406585      1.280617     -0.037114
      C        1.770114      1.040985     -0.069863
      C        2.260523     -0.271889     -0.020476
      C        1.355989     -1.326266      0.049036
      C       -0.017770     -1.082607      0.060045
      C       -0.512683      0.224067      0.035838
      H        0.015317      2.296582     -0.020225
      H        2.466349      1.876078     -0.123000
      H        3.331422     -0.460043     -0.033442
      H        1.723418     -2.350854      0.082140
      H       -0.746590     -1.887565      0.084105
      C       -1.994845      0.438685     -0.056635
      O       -2.779586     -0.523667     -0.111872
      H       -2.252093      1.417038     -0.510408
      H       -1.908615      1.476554      1.650817
 Statistical Thermodynamic Analysis
 Temperature= 298.150 Kelvin       Pressure= 1.00000 Atm
 SCF Energy=     -345.946931958              Predicted Change= -5.220313D-08
 Zero-point correction (ZPE)=                  -345.8339   0.11301
 Internal Energy (U)=                          -345.8274   0.11945
 Enthalpy (H)=                                             -345.8265    0.12040
 Gibbs Free Energy (G)=                        -345.8643    0.08258
 Frequencies --   -540.7046             163.1241             223.3664
M06-2X/6-31+G(d,p)/PCM(DCE) SP:  -346.073882
```

TS-34°

Supporting Information: TS-benzaldehyde-35.log

```
 Using  Gaussian 09:  AM64L-G09RevC.01 23-Sep-2011
 # M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
```

opt=(maxcycle=250,modredundant) freq=noraman
Modredundant Input: D 5 6 13 12 F
Modredundant Input: B 12 15 F
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RM062X/6-31G(d) Freq
---
Pointgroup= C1 Stoichiometry= C7H7O(1-) C1[X(C7H7O)] #Atoms= 15
Charge = -1 Multiplicity = 1

SCF Energy= -345.942834096 Predicted Change= -4.870032D-07
==========
Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00024	0.00045	[YES]	0.00005	0.00030	[YES]
Displ	0.00179	0.00180	[YES]	0.00179	0.00180	[YES]

Atomic Type	X	Y	Z
C	0.395907	1.282381	0.013175
C	1.766294	1.052364	0.025561
C	2.267961	-0.252932	0.022974
C	1.375863	-1.321173	-0.007629
C	0.002068	-1.085082	-0.042181
C	-0.509809	0.216794	-0.014334
H	-0.034760	2.279859	0.073903
H	2.455232	1.894450	0.057602
H	3.340648	-0.430498	0.056036
H	1.752471	-2.342580	-0.013926
H	-0.714211	-1.901855	-0.075004
C	-2.003463	0.360136	-0.218915
O	-2.778050	-0.512788	0.212150
H	-2.236950	0.937953	-1.135071
H	-2.106950	2.150054	0.667362

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
==========
SCF Energy= -345.942834096 Predicted Change= -4.870032D-07
Zero-point correction (ZPE)= -345.8294 0.11338
Internal Energy (U)= -345.8230 0.11979
Enthalpy (H)= -345.8220 0.12073
Gibbs Free Energy (G)= -345.8599 0.08290

Frequencies -- -618.6265 146.9034 215.4274
M06-2X/6-31+G(d,p)/PCM(DCE) SP: -346.070968

—2-fluorobenzaldehyde—

GS-0°

Supporting Information: GS-benzaldehyde-2F.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011
==========
# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RM062X/6-31G(d) Freq
---
Pointgroup= C1 Stoichiometry= C7H5FO C1[X(C7H5FO)] #Atoms= 14
Charge = 0 Multiplicity = 1

SCF Energy= -444.624760642 Predicted Change= -5.877905D-08
==========
Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00009	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00056	0.00180	[YES]	0.00056	0.00180	[YES]

Atomic Type	X	Y	Z
C	-0.369974	0.958548	-0.000029
C	-1.743204	0.769216	-0.000068
C	-2.229973	-0.533878	-0.000032
C	-1.355138	-1.623304	0.000025
C	0.014913	-1.405968	0.000077
C	0.527975	-0.104964	0.000064
F	0.109364	2.211472	0.000009
H	-2.398826	1.632519	-0.000114
H	-3.302622	-0.700389	-0.000063
H	-1.747679	-2.634462	0.000047
H	0.725038	-2.227494	0.000152
C	1.994233	0.122789	0.000124
O	2.798164	-0.780694	-0.000187
H	2.321492	1.177494	0.000422

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
==========
SCF Energy= -444.624760642 Predicted Change= -5.877905D-08
Zero-point correction (ZPE)= -444.5213 0.10341
Internal Energy (U)= -444.5142 0.11048
Enthalpy (H)= -444.5133 0.11142
Gibbs Free Energy (G)= -444.5530 0.07167

Frequencies -- 122.1716 197.3278 205.6357
M06-2X/6-31+G(d,p)/PCM(DCE) SP: -444.654146

GS-34°

Supporting Information: GS-benzaldehyde-2F-35.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011
==========
# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,modredundant) freq=noraman
Modredundant Input: D 5 6 13 12 F
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RM062X/6-31G(d) Freq
---
Pointgroup= C1 Stoichiometry= C7H5FO C1[X(C7H5FO)] #Atoms= 14
Charge = 0 Multiplicity = 1

SCF Energy= -444.620981071 Predicted Change= -1.020215D-07
==========
Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00010	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00057	0.00180	[YES]	0.00057	0.00180	[YES]

Atomic Type	X	Y	Z
C	0.336523	0.958232	-0.008146
C	1.713326	0.818759	-0.069935
C	2.249454	-0.465685	-0.044160
C	1.418675	-1.584482	0.037987
C	0.040619	-1.417426	0.082051
C	-0.518832	-0.137499	0.036638
F	-0.196493	2.189464	-0.007841
H	2.336437	1.704136	-0.126480
H	3.326750	-0.592494	-0.083025
H	1.848913	-2.579566	0.073955
H	-0.633701	-2.266307	0.143123
C	-1.988809	0.030490	0.186507
O	-2.786826	-0.767917	-0.243902
H	-2.321094	0.958052	0.688556

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
==========
SCF Energy= -444.620981071 Predicted Change= -1.020215D-07
Zero-point correction (ZPE)= -444.5177 0.10322
Internal Energy (U)= -444.5105 0.11038
Enthalpy (H)= -444.5096 0.11132
Gibbs Free Energy (G)= -444.5497 0.07124

Frequencies -- 103.3907 159.6882 217.3730
M06-2X/6-31+G(d,p)/PCM(DCE) SP: -444.651215

TS-0°

Supporting Information: TS-benzaldehyde-2F.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011
==========
# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,modredundant) freq=noraman
Modredundant Input: D 5 6 13 12 F
Modredundant Input: B 12 15 F
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RM062X/6-31G(d) Freq
---
Pointgroup= C1 Stoichiometry= C7H6FO(1-) C1[X(C7H6FO)] #Atoms= 15
Charge = -1 Multiplicity = 1

SCF Energy= -445.156273357 Predicted Change= -1.745023D-08
==========
Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00003	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00069	0.00180	[YES]	0.00069	0.00180	[YES]

Atomic Type	X	Y	Z
C	0.419406	0.946561	-0.016427

C	1.781473	0.729547	-0.035901
C	2.267375	-0.584541	-0.010316
C	1.359234	-1.637872	0.023560
C	-0.012660	-1.388309	0.033954
C	-0.525278	-0.085400	0.054282
F	-0.020422	2.221981	-0.054442
H	2.445209	1.588531	-0.073161
H	3.338036	-0.768740	-0.027206
H	1.721330	-2.663934	0.026439
H	-0.744851	-2.190283	0.040187
C	-2.001161	0.125787	-0.032097
O	-2.779387	-0.838768	-0.122156
H	-2.287161	1.137438	-0.367110
H	-1.784009	0.974665	1.765749

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -445.156273357 Predicted Change= -1.745023D-08
Zero-point correction (ZPE)= -445.0511 0.10508
Internal Energy (U)= -445.0440 0.11227
Enthalpy (H)= -445.0430 0.11321
Gibbs Free Energy (G)= -445.0827 0.07352

Frequencies -- -499.8950 155.5629 200.2193
M06-2X/6-31+G(d,p)/PCM(DCE) SP: -445.286703

TS-34°

Supporting Information: TS-benzaldehyde-2F-35.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,modredundant) freq=noraman
Modredundant Input: D 5 6 13 12 F
Modredundant Input: B 12 15 F
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RM062X/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C7H6FO(1-) C1[X(C7H6FO)] #Atoms= 15
Charge = -1 Multiplicity = 1

SCF Energy= -445.145357953 Predicted Change= -4.113030D-08

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00002	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00257	0.00180	[NO]	0.00257	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.433771	0.948684	0.014779
C	1.794363	0.692133	0.062277
C	2.255097	-0.626453	0.044882
C	1.328890	-1.662611	-0.031144
C	-0.033594	-1.373961	-0.063056
C	-0.532602	-0.065004	0.047617
F	0.064361	2.235541	-0.072845
H	2.475422	1.537942	0.084522
H	3.322464	-0.829509	0.070369
H	1.669219	-2.694247	-0.089823
H	-0.779936	-2.161255	-0.121670
C	-2.009247	0.090562	-0.186441
O	-2.800146	-0.807046	0.151711
H	-2.254316	0.853185	-0.948496
H	-2.031003	1.610296	1.113535

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -445.145357953 Predicted Change= -4.113030D-08
Zero-point correction (ZPE)= -445.0401 0.10521
Internal Energy (U)= -445.0329 0.11237
Enthalpy (H)= -445.0320 0.11331
Gibbs Free Energy (G)= -445.0717 0.07361

Frequencies -- -581.8833 145.8275 204.6362
M06-2X/6-31+G(d,p)/PCM(DCE) SP: -445.279217

—2-methoxybenzaldehyde—

GS-0°

Supporting Information: GS-benzaldehyde-2OMe.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,modredundant) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RM062X/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H8O2 C1[X(C8H8O2)] #Atoms= 18
Charge = 0 Multiplicity = 1

SCF Energy= -459.897779330 Predicted Change= -2.873977D-08

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00004	0.00045	[YES]	0.00001	0.00030	[YES]
Displ	0.00069	0.00180	[YES]	0.00069	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.652601	-0.084151	0.000120
C	-1.202965	1.199641	0.000006
C	-0.358579	2.307489	-0.000083
C	1.026380	2.160709	-0.000037
C	1.567652	0.882138	0.000057
C	0.744943	-0.243823	0.000199
H	-2.276120	1.346747	0.000186
H	-0.798094	3.300699	-0.000143
H	1.670564	3.033178	-0.000116
H	2.640832	0.715490	0.000094
C	1.366226	-1.590820	0.000197
O	2.565457	-1.762567	-0.000268
H	0.670082	-2.447244	0.000458
O	-1.389496	-1.222601	-0.000025
C	-2.796537	-1.099060	-0.000092
H	-3.147370	-0.572004	-0.894909
H	-3.187399	-2.116100	-0.000296
H	-3.147313	-0.572163	0.894861

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -459.897779330 Predicted Change= -2.873977D-08
Zero-point correction (ZPE)= -459.7525 0.14520
Internal Energy (U)= -459.7438 0.15393
Enthalpy (H)= -459.7429 0.15487
Gibbs Free Energy (G)= -459.7864 0.11128

Frequencies -- 82.2810 122.1542 168.1714
M06-2X/6-31+G(d,p)/PCM(DCE) SP: -459.929073

GS-34°

Supporting Information: GS-benzaldehyde-2OMe-35.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,modredundant) freq=noraman
Modredundant Input: D 5 6 11 12 F
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RM062X/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H8O2 C1[X(C8H8O2)] #Atoms= 18
Charge = 0 Multiplicity = 1

SCF Energy= -459.894522491 Predicted Change= -3.580185D-09

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00044	0.00180	[YES]	0.00044	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.639927	-0.073586	0.000705
C	-1.197696	1.204526	0.052063
C	-0.359233	2.318231	0.036231
C	1.023617	2.179202	-0.028103
C	1.572615	0.902394	-0.068271
C	0.756741	-0.226378	-0.036499
H	-2.270920	1.344120	0.100727
H	-0.803307	3.308676	0.071337
H	1.663162	3.054752	-0.051562
H	2.646780	0.748992	-0.118673
C	1.371148	-1.570777	-0.186888
O	2.471303	-1.843109	0.236663
H	0.750301	-2.332531	-0.692513
O	-1.361998	-1.222376	0.001041
C	-2.770123	-1.114222	0.017828
H	-3.135951	-0.565252	-0.857818
H	-3.150858	-2.134774	-0.006501
H	-3.116501	-0.616450	0.930976

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
==========
SCF Energy= -459.894522491 Predicted Change= -3.580185D-09
Zero-point correction (ZPE)= -459.7495 0.14498
Internal Energy (U)= -459.7407 0.15378
Enthalpy (H)= -459.7397 0.15472
Gibbs Free Energy (G)= -459.7836 0.11090

Frequencies -- 80.0372 106.8365 144.9286
M06-2X/6-31+G(d,p)/PCM(DCE) SP: -459.926539

TS-0°

Supporting Information: TS-benzaldehyde-2OMe-1.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011
==========
# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,modredundant) freq=noraman
Modredundant Input: B 11 14 F
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RM062X/6-31G(d) Freq
---
Pointgroup= C1 Stoichiometry= C8H9O2(1-) C1[X(C8H9O2)] #Atoms= 19
Charge = -1 Multiplicity = 1

SCF Energy= -460.420861330 Predicted Change= -2.252962D-08
==========
Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00002	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00098	0.00180	[YES]	0.00098	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.662216	-0.099900	-0.042036
C	-1.297507	1.134566	-0.053600
C	-0.541124	2.316248	-0.009373
C	0.843669	2.239298	0.034366
C	1.471823	0.993641	0.040680
C	0.745858	-0.198811	0.040809
H	-2.380087	1.198425	-0.102546
H	-1.048514	3.277602	-0.021215
H	1.439564	3.149610	0.053898
H	2.552863	0.892739	0.061210
C	1.491908	-1.494045	-0.005422
O	2.728609	-1.511937	-0.141364
H	0.869838	-2.360618	-0.282479
H	0.740525	-1.766009	1.828010
O	-1.333912	-1.292185	-0.097147
C	-2.724500	-1.253390	0.026307
H	-3.203134	-0.747747	-0.826364
H	-3.061503	-2.291929	0.057454
H	-3.034601	-0.744728	0.949735

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
==========
SCF Energy= -460.420861330 Predicted Change= -2.252962D-08
Zero-point correction (ZPE)= -460.2740 0.14676
Internal Energy (U)= -460.2653 0.15555
Enthalpy (H)= -460.2643 0.15650
Gibbs Free Energy (G)= -460.3077 0.11314

Frequencies -- -511.1198 83.9317 147.6450
M06-2X/6-31+G(d,p)/PCM(DCE) SP: -460.556958

TS-34°

Supporting Information: TS-benzaldehyde-2OMe-35.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011
==========
# M062X/6-31G* gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,modredundant) freq=noraman
Modredundant Input: D 5 6 11 12 F
Modredundant Input: B 11 14 F
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RM062X/6-31G(d) Freq
---
Pointgroup= C1 Stoichiometry= C8H9O2(1-) C1[X(C8H9O2)] #Atoms= 19
Charge = -1 Multiplicity = 1

SCF Energy= -460.413822765 Predicted Change= -2.826828D-08
==========
Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00127	0.00180	[YES]	0.00127	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.707329	0.115605	-0.221212
C	-1.064306	1.459273	-0.134944
C	-0.100979	2.448822	0.059242
C	1.236124	2.073912	0.145361
C	1.579581	0.727325	0.070220
C	0.623880	-0.298160	-0.014285
H	-2.112143	1.717632	-0.271732
H	-0.393444	3.494885	0.109632
H	2.012100	2.829808	0.246524
H	2.616017	0.406552	0.134833
C	1.168356	-1.680707	-0.270146
O	2.267633	-2.017648	0.197949
H	0.696428	-2.186883	-1.130849
H	-0.280664	-2.530065	0.815644
O	-1.689129	-0.782140	-0.574102
C	-2.545135	-1.122030	0.504241
H	-3.107677	-0.240072	0.848695
H	-3.249684	-1.864723	0.119467
H	-1.950122	-1.573077	1.306136

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
==========
SCF Energy= -460.413822765 Predicted Change= -2.826828D-08
Zero-point correction (ZPE)= -460.2673 0.14647
Internal Energy (U)= -460.2585 0.15531
Enthalpy (H)= -460.2575 0.15625
Gibbs Free Energy (G)= -460.3008 0.11293

Frequencies -- -579.5891 128.5224 162.5795
M06-2X/6-31+G(d,p)/PCM(DCE) SP: -460.544673