Electronic Supplementary Information

Intermolecular *exo*-Selective Diels-Alder Reaction Catalysed by Dual-Functional Brønsted Acid: Conformational Restriction of Transition States by Hydrogen Bonds as the Key Interaction

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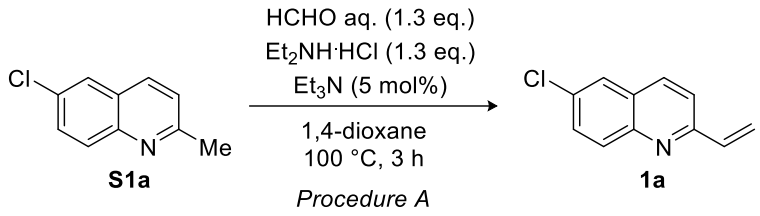
Contents

1. General information

All reactions were carried out under nitrogen atmosphere in flame-dried glassware. Toluene (tol), dichloromethane (DCM) and tetrahydrofuran (THF) were supplied from KANTO Chemical Co., Inc. as "Dehydrated solvent system". Other solvents and reagents were purchased from commercial suppliers (Wako Pure Chemical Industries, Ltd., Tokyo Chemical Industry Co., LTD., Aldrich Inc., and others) and used without further purification. Purification of reaction products was carried out by flash column chromatography using silica gel 60 N (Merck 40-63 μm). Analytical thin layer chromatography (TLC) was performed on Merck precoated TLC plates (silica gel 60 GF 254, 0.25 mm). ^{1}H NMR spectra were recorded on a JEOL ECA-600 (600 MHz) spectrometer. Chemical shifts are reported in ppm from tetramethylsilane or solvent resonance as the internal standard ($CDCl_3$: 7.26 ppm, TMS: 0.00 ppm). ^{13}C NMR spectra were recorded on a JEOL ECA-600 (150 MHz) spectrometer with complete proton decoupling. Chemical shifts are reported in ppm from the solvent resonance as the internal standard ($CDCl_3$: 77.2 ppm). ^{31}P NMR spectra were recorded on a JEOL JNM-ECA600 (243 MHz) spectrometer with complete proton decoupling. Infrared spectra were recorded on a Jasco FT/IR-4100 spectrometer. Chiral stationary phase HPLC analysis was performed on a Jasco LC-2000 Plus Series system with DACIEL chiral analytical column (4.6 mmΦ* 250 mm length). Optical rotations were measured on a Jasco P-1020 digital polarimeter with a sodium lamp and reported as follows; $[\alpha]^{T\,^{\circ}C}D$ (*c* = g/100 mL, solvent, % ee). High resolution mass spectra analysis was performed on a Bruker Daltonics solariX 9.4T FT-ICR-MS spectrometer and a JEOL JMST100GCV Time-of-Flight Mass Spectrometer at the Research and Analytical Center for Giant Molecules, Graduate School of Science, Tohoku University.

2. Preparation of substrates

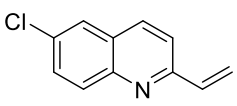
1a was synthesized from corresponding 2-methyl quinoline derivatives **S1a**.



The procedure for the synthesis of 1a was shown below. This procedure was slightly modified from Feng's method[1].

To a frame-dried 50 mL round-bottom flask with a magnetic stirrer bar, 6-chloro-2-methylquinoline (**S1a**) (888 mg, 5.0 mmol), HCHO (30% in H_2O, 6.5 mmol, 1.3 eq.), $Et_2NH{\cdot}HCl$ (713 mg, 6.5 mmol, 1.3 eq.), Et_3N (35 uL, 0.25 mmol, 5 mol %) and 1,4-dioxane (10 mL) were added. This suspension was heated to 100 °C until the starting material **S1a** was fully consumed (checked by TLC). After cooling to room temperature, H_2O (15 mL) was added, and extracted with dichloromethane (10 mL * 3 times). The combined organic layers were dried over $MgSO_4$, and the solvent was removed under reduced pressure. The residue was purified by column chromatography using hexane/ethyl acetate (14/1) as the eluent yielding the 6-chloro-2-vinyl quinoline **1a** (616 mg, 3.8 mmol, 65% yield). **1a** was stored at -20 °C under Ar atmosphere.

6-Chloro-2-vinylquinoline (1a)

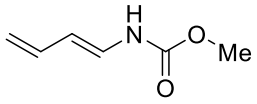


white solid; R_f = 0.40 (Hexane/EtOAc= 6/1); ^1H NMR (600 MHz, $CDCl_3$,) δ 8.02 (d, *J* = 8.4 Hz, 1H), 7.99 (d, *J* = 8.4 Hz, 1H), 7.76 (d, *J* = 2.4 Hz, 1H), 7.65-7.58 (m, 2H), 7.01 (dd, *J* = 17.4, 10.8 Hz, 1H), 6.29 (d, *J* = 17.4 Hz, 1H), 5.69 (d, *J* = 10.6 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 156.4, 146.5, 137.7, 135.6, 132.1, 131.1, 130.7, 128.1, 126.3, 120.5, 119.5; IR (ATR) 3089, 3053, 3020, 2990, 1849, 1592, 1556, 1493, 1421, 1382, 1308, 1192, 1073, 993, 924, 903, 831, 726 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{11}H_8ClN$ 189.03453, found: 189.034498.

Amidodienes (**2**) were prepared following literature from corresponding carboxylic acids[2].

To a solution of corresponding carboxylic acid (1.0 eq.) in DMF (0.5 M) was added NEt_3 (1.1 eq.) and diphenyl phosphoryl azido (1.1 eq.) dropwise at 0 °C and the reaction was allowed to stir for 1 h at the same temperature. Then corresponding benzyl alcohol (3.0 eq.) was added, and the reaction was heated to 85 °C for 4 h. The reaction was quenched with water and extracted with hexane/EA = 3/1. The combined organic layers were washed with water and brine, dried over Na_2SO_4, concentrated in vacuo, and purified by silica-gel chromatography (hexane/AcOEt = 40/1 to 20/1) to afford the amidodienes in moderate yield.

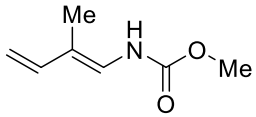
Methyl (*E*)-buta-1,3-dien-1-ylcarbamate (2a)



white solid; R_f = 0.18 (Hexane/EtOAc= 6/1); ^{1}H NMR (600 MHz, $CDCl_3$) δ 6.75 (t, *J* = 13.2 Hz, 1H), 6.54 (brs, 1H), 6.32-6.21 (m, 1H), 5.70 (t, *J* = 13.2 Hz, 1H), 5.04 (dd, *J* = 16.8, 10.2 Hz, 1H), 4.91 (d, *J* = 10.2 Hz, 1H), 3.74 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 154.1, 134.6, 127.2, 113.6, 112.1, 52.8; IR (ATR) 3281, 3080, 3032, 3000, 2950, 1726, 1698, 1670, 1536, 1437, 1316, 1303, 1280, 1239, 1088, 1059, 1003, 938, 866, 769, 676 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_6H_9NO_2$ 127.06333, found: 127.06327.

* **2a showed multiple resonance for the presence of different rotational isomers at 20 °C.**

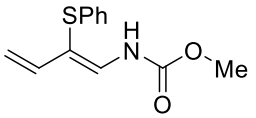
Methyl (*E*)-(2-methylbuta-1,3-dien-1-yl)carbamate (2b)



white solid; R_f = 0.32 (Hexane/EtOAc= 6/1); ^{1}H NMR (600 MHz, $CDCl_3$) δ 6.62 (d, *J* = 10.8 Hz, 1H), 6.34 (dd, *J* = 17.4, 10.8 Hz, 2H), 5.01 (d, *J* = 17.4 Hz, 1H), 4.89 (d, *J* = 10.8 Hz, 1H), 3.74 (s, 3H), 1.67 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 154.1, 138.2, 124.6, 115.5, 109.6, 52.9, 10.2; IR (ATR) 3328, 3088, 2955, 1713, 1660, 1508, 1451, 1359, 1237, 1054, 985, 879, 772 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_7H_{11}NO_2$ 141.07898, found: 141.07897.

* **2b showed multiple resonance for the presence of different rotational isomers at 20 °C.**

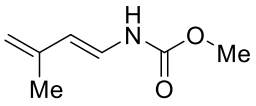
Methyl (*Z*)-(2-(phenylthio)buta-1,3-dien-1-yl)carbamate (2g)



pale yellow oil; R_f = 0.38 (Hexane/EtOAc= 6/1); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.51 (d, *J* = 10.2 Hz, 1H), 7.41 (d, *J* = 10.2 Hz, 1H), 7.24 (t, *J* = 7.8 Hz, 2H), 7.18-7.08 (m, 3H), 6.46 (dd, *J* = 16.2 10.2 Hz, 1H), 5.44 (d, *J* = 16.2 Hz, 1H), 5.00 (d, *J* = 10.2 Hz, 1H), 3.76 (s, 3H) ^{13}C NMR (150 MHz, $CDCl_3$) δ 153.7, 134.7, 134.4, 134.1, 129.2, 126.5, 125.7, 113.7, 110.1, 53.2; IR (ATR) 3346, 3058, 3004, 2955, 1731, 1632, 1476, 1326, 1218, 1069, 1025, 894, 769, 742, 690 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{12}H_{13}NO_2S$ 235.06670, found: 235.06668.

* **2g showed multiple resonance for the presence of different rotational isomers at 20 °C.**

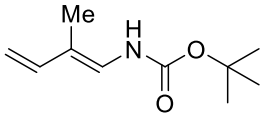
Methyl (*E*)-(3-methylbuta-1,3-dien-1-yl)carbamate (2h)



white solid; R_f = 0.22 (Hexane/EtOAc= 6/1); ^{1}H NMR (600 MHz, $CDCl_3$) δ 6.71 (dd, *J* = 13.8, 11.4 Hz, 1H), 6.46 (brs, 1H), 5.78 (d, *J* = 13.8 Hz, 1H), 4.80 (d, *J* = 4.8 Hz, 2H), 3.74 (s, 3H), 1.86 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 154.3, 140.4, 124.2, 114.2, 113.4, 52.8, 18.9; IR (ATR) 3312, 3075, 3028, 2975, 2952, 2918, 2846, 1723, 1698, 1656, 1530, 1449, 1305, 1246, 1069, 949, 861, 771, 693 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_7H_{11}NO_4$ 141.07898, found: 141.07894.

***2h showed multiple resonance for the presence of different rotational isomers at 20 °C.**

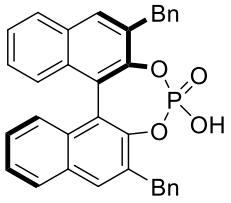
***tert*-Butyl (*E*)-(2-methylbuta-1,3-dien-1-yl)carbamate (2i)**



white solid; R_f = 0.48 (Hexane/EtOAc= 6/1); ^{1}H NMR (600 MHz, $CDCl_3$) δ 6.61 (d, *J* = 10.8 Hz, 1H), 6.35 (dd, *J* = 16.8, 10.8 Hz, 1H), 6.21 (d, *J* = 8.4 Hz, 1H), 4.99 (d, *J* = 16.8 Hz, 1H), 4.87 (d, *J* = 10.8 Hz, 1H), 1.67 (s, 3H), 1.49 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 152.6, 138.6, 124.8, 114.6, 108.9, 81.0, 28.4, 10.2; IR (ATR) 3288, 3092, 3003, 2981, 2930, 1710, 1682, 1655, 1509, 1392, 1366, 1269, 1249, 1158, 1051, 989, 876, 777, 693 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{10}H_{17}NO_2$ 183.12593, found: 183.12588.

* **2i showed multiple resonance for the presence of different rotational isomers at 20 ℃.**

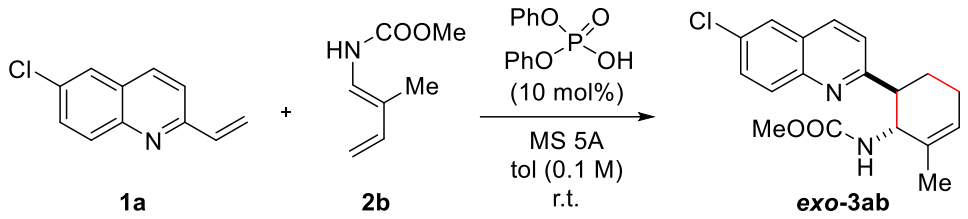
(*R*)-2,6-dibenzyl-4-hydroxydinaphtho[2,1-d:1',2'-f][1,3,2]dioxaphosphepine 4-oxide (5)



white solid; $[\alpha]_D^{23.0}$ = -286.0 (*c* = 1.0, $CHCl_3$, >99% ee); R_f = 0.08 (EtOAc); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.76 (d, *J* = 7.8 Hz, 2H), 7.56 (s, 2H), 7.39 (t, *J* = 7.8 Hz, 2H), 7.29-7.25 (m, 6H), 7.25-7.15 (m, 8H), 6.25 (brs, 1H), 4.42 (d, *J* = 16.2 Hz, 2H), 4.25 (d, *J* = 16.2 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 145.8 (d, *diastereotopic*), 139.1, 133.0, 131.8, 131.3, 130.8, 129.8, 128.7, 128.2, 127.2, 126.5, 126.2, 125.9, 121.9, 36.5; ^{31}P NMR (243 MHz, $CDCl_3$) δ 5.73; IR (ATR) 3060, 3027, 2904, 1714, 1600, 1496, 1453, 1421, 1335, 1267, 1230, 1178, 1147, 1097, 1077, 1014, 971, 927, 908, 887, 750, 701 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{34}H_{25}O_4P_1$ 528.14904, found: 528.14895.

3. Typical procedure for *exo*-selective Diels-Alder reaction of 2-vinylquinoline with amidediene

Representative procedure for the asymmetric Diels-Alder reaction of 6-chloro-2-vinyl quinoline **1a** with amidediene **2b** catalysed by diphenyl phosphate.

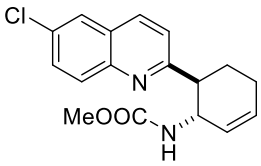


1a **2b** ***exo*-3ab**

To a solution of **1a** (19.0 mg, 0.1 mmol), **2b** (17.0 mg, 0.12 mmol) and pre-activated MS 5A (50 mg) in dry toluene (1.0 ml), diphenyl phosphate (2.5 mg, 10 mol %) was added. The reaction mixture was stirred at room temperature for 48 h. After 48 h, Et_3N (ca. 0.1 mL) was added. This suspension was filtered through celite® (washed by EtOAc) and the solvent was removed under reduced pressure. A corresponding crude residue was purified by column chromatography using hexane/ethyl acetate (4/1 to 2/1) as the eluent to give **3ab** (23.2 mg, 0.07 mmol, 70%) as a mixture of diastereomers. The diastereomeric excess was determined by analysis of crude NMR. The diastereomers were further separated by preparative HPLC using hexane/EtOAc = 7/2 as an eluent.

<u>In all cases, Diels-Alder adducts show multiple resonance for the presence of different rotational isomers at 20 ℃.</u>

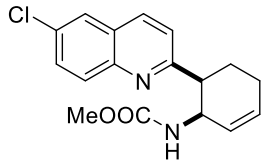
Methyl (6-(6-chloroquinolin-2-yl)cyclohex-2-en-1-yl)carbamate (*exo*-3aa)



white solid; R_f = 0.10 (Hexane/EtOAc= 6/1); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.04 (d, *J* = 9.0 Hz, 1H), 7.97 (d, *J* = 9.0 Hz, 1H), 7.78 (d, *J* = 2.4 Hz, 1H), 7.62 (dd, *J* = 9.0, 2.4 Hz, 1H), 7.44 (d, *J* = 7.8 Hz, 1H), 5.91-5.86 (m, 1H), 5.74 (d, *J* = 9.6 Hz, 1H), 4.81 (d, *J* = 6.6 Hz, 1H), 4.75-4.65 (m, 1H), 3.46 (s, 3H), 3.12-3.02 (m, 1H), 2.33-2.01 (m, 4H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 163.6, 156.6, 146.2, 135.9, 131.8, 130.8, 130.4, 129.2, 129.1, 127.9, 126.4, 120.6, 52.0, 49.8, 28.7, 25.2, one carbon was not found probably due to overlapping; IR (ATR) 3313, 3027, 2938, 2839, 1696, 1599, 1542, 1491, 1451, 1317, 1256, 1190, 1073, 1054, 1026, 878, 831, 758 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{17}H_{17}ClN_2O_2$ 316.09785, found: 316.09781.

* ***<u>exo</u>*<u>-3aa showed multiple resonance for the presence of different rotational isomers at 20 ℃.</u>**

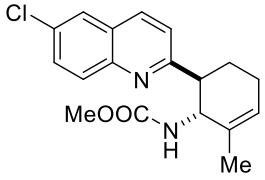
Methyl (6-(6-chloroquinolin-2-yl)cyclohex-2-en-1-yl)carbamate (*endo*-3aa)



colorless oil; R_f = 0.12 (Hexane/EtOAc= 6/1); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.99 (t, *J* = 9.6 Hz, 2H), 7.76 (d, *J* = 2.4 Hz, 1H), 7.61 (d, *J* = 9.0 Hz, 1H), 7.39 (d, *J* = 9.0 Hz, 1H), 5.89 (s, 2H), 5.45 (d, *J* = 8.4 Hz, 1H), 4.64 (s, 1H), 3.46-3.37 (m, 1H), 3.36 (s, 3H), 2.30-1.98 (m, 4H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.6, 156.5, 146.0, 135.2, 131.7, 131.0, 130.2, 129.8, 127.9, 127.6, 126.3, 122.4, 51.9, 48.7, 45.8, 24.7, 23.4; IR (ATR) 3328, 3026, 2946, 2837, 1712, 1599, 1492, 1454, 1337, 1239, 1190, 1073, 834, 756 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{17}H_{17}ClN_2O_2$ 316.09785, found: 316.09777.

*** *endo*-3aa showed multiple resonance for the presence of different rotational isomers at 20 ℃.**

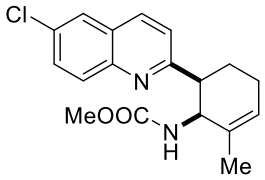
Methyl (6-(6-chloroquinolin-2-yl)-2-methylcyclohex-2-en-1-yl)carbamate (*exo*-3ab)



white solid; $[\alpha]_D^{23.0}$ = -79.8 (*c* = 1.0, $CHCl_3$, 81% ee); R_f = 0.12 (Hexane/EtOAc= 6/1); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.02 (d, *J* = 9.0 Hz, 1H), 7.96 (d, *J* = 9.0 Hz, 1H), 7.77 (d, *J* = 2.4 Hz, 1H), 7.39 (dd, *J* = 9.0, 2.4 Hz, 1H), 7.43 (d, *J* = 9.0 Hz, 1H), 5.63 (s, 1H), 4.69 (dd, *J* = 9.0, 9.0 Hz, 1H), 4.64 (d, *J* = 9.0 Hz, 1H), 3.47 (s, 3H), 3.20 (ddd, *J* = 10.2, 9.0, 3.6 Hz, 1 H), 2.25-1.97 (m, 4H), 1.77 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 163.8, 156.9, 146.2, 135.7, 134.2, 131.6, 130.8, 130.3, 127.8, 126.3, 125.2, 120.8, 54.5, 52.1, 50.1, 28.3, 24.9, 20.3; IR (ATR) 3309, 2969, 2949, 2914, 2844, 1692, 1599, 1543, 1489, 1316, 1265, 1234, 1193, 1074, 1034, 876, 829, 775, 689 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{18}H_{19}ClN_2O_2$ 330.11350, found: 330.11341.; HPLC analysis CHIRALCEL OD-3 (Hexane:*i*PrOH = 97/3, 1.0 mL/min, 40 ℃, 254 nm) 10.3 min (minor), 13.0 min (major).

*** *exo*-3ab showed multiple resonance for the presence of different rotational isomers at 20 ℃.**

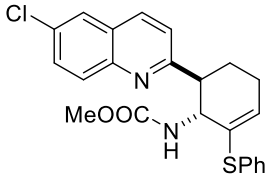
Methyl (6-(6-chloroquinolin-2-yl)-2-methylcyclohex-2-en-1-yl)carbamate (*endo*-3ab)



colorless oil; R_f = 0.15 (Hexane/EtOAc= 6/1); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.98 (t, *J* = 9.0 Hz, 2H), 7.76 (d, *J* = 2.4 Hz, 1H), 7.60 (dd, *J* = 9.0, 2.4 Hz, 1H), 7.40 (d, *J* = 9.0, 2.4 Hz, 1H), 5.61 (s, 1H), 4.97 (d, *J* = 10.2 Hz, 1H), 4.50 (dd, *J* = 10.2, 4.2 Hz, 1H), 3.37 (ddd, *J* = 12.6, 4.2, 3.0 Hz, 1H), 3.28 (s, 3H), 2.23-1.95 (m, 4H), 1.79 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.7, 156.8, 146.1, 135.0, 134.2, 131.5, 131.0, 130.1, 127.6, 126.4, 124.9, 122.3, 52.6, 52.0, 47.1, 25.1, 22.3, 21.2; IR (ATR) 3325, 2942, 2915, 2838, 1721, 1599, 1507, 1453, 1336, 1236, 1192, 1074, 878, 831, 759 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{18}H_{19}ClN_2O_2$ 330.11350, found: 330.11344.

*** *endo*-3ab showed multiple resonance for the presence of different rotational isomers at 20 ℃.**

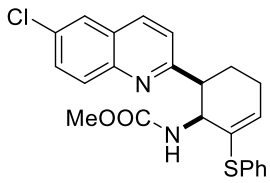
Methyl (-6-(6-chloroquinolin-2-yl)-2-(phenylthio)cyclohex-2-en-1-yl)carbamate (*exo*-3ag)



white solid; R_f = 0.08 (Hexane/EtOAc= 6/1); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.4 Hz, 1H), 7.94 (d, *J* = 9.0 Hz, 1H), 7.76 (d, *J* = 2.4 Hz, 1H), 7.61 (dd, *J* = 9.0, 2.4 Hz, 1H), 7.37 (d, *J* = 8.4 Hz, 3H), 7.26-7.19 (m, 3H), 6.18 (s, 1H), 4.84-4.73 (m, 2H), 3.48 (s, 4H), 2.41-2.26 (m, 2H), 2.24-2.12 (m, 1H), 2.07-2.01 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.8, 156.5, 146.2, 135.8, 135.5, 134.6, 133.1, 131.7, 131.3, 130.9, 130.3, 129.1, 127.8, 127.2, 126.3, 121.4, 53.7, 52.2, 49.2, 26.2, 26.0; IR (ATR) 3423, 3329, 3057, 3018, 2945, 2836, 1720, 1599, 1491, 1307, 1237, 1192, 1075, 1026, 878, 833, 751, 691 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{23}H_{21}ClN_2O_2S$ 424.10123, found: 424.10112.

*** *exo*-3ag showed multiple resonance for the presence of different rotational isomers at 20 °C.**

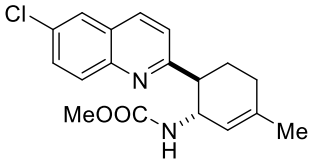
Methyl (-6-(6-chloroquinolin-2-yl)-2-(phenylthio)cyclohex-2-en-1-yl)carbamate (*endo*-3ag)



colorless oil; R_f = 0.10 (Hexane/EtOAc= 6/1); ^{1}H NMR (600 MHz, $CDCl_3$, VT50) δ 7.93 (dd, *J* = 8.4, 4.8 Hz, 2H), 7.72 (s, 1H), 7.58 (dd, *J* = 8.4, 2.4 Hz, 1H), 7.43 (d, *J* = 7.2 Hz, 2H), 7.30 (t, *J* = 8.4 Hz, 3H), 7.24 (t, *J* = 7.2 Hz, 1H), 6.14 (s, 1H), 5.08 (brs, 1H), 4.71 (brs, 1H), 3.44 (d, *J* = 3.0 Hz, 1H), 3.25 (brs, 3H), 2.27 (brs, 2H), 2.20-2.06 (m, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 161.7, 156.3, 146.0, 135.1, 134.5, 134.4, 134.0, 131.7, 131.0, 130.1, 129.2, 127.6, 127.4, 126.3, 122.3, 52.2, 52.0, 47.4, 26.2, 22.5, one carbon was not found probably due to overlapping; IR (ATR) 3424, 3329, 3056, 3018, 2949, 2906, 2833, 1721, 1599, 1492, 1340, 1222, 1191, 1074, 1061, 879, 832, 753, 692 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{23}H_{21}ClN_2O_2S$ 424.10123, found: 424.10118.

*** *endo*-3ag showed multiple resonance for the presence of different rotational isomers even at 50 °C.**

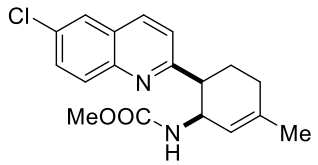
Methyl (6-(6-chloroquinolin-2-yl)-2-methylcyclohex-2-en-1-yl)carbamate (*exo*-3ah)



white solid; R_f = 0.12 (Hexane/EtOAc= 6/1); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.03 (d, *J* = 8.4 Hz, 1H), 7.96 (d, *J* = 9.0 Hz, 1H), 7.77 (d, *J* = 2.4 Hz, 1H), 7.61 (dd, *J* = 9.0, 2.4 Hz, 1H), 7.43 (d, *J* = 8.4 Hz, 1H), 5.45 (s, 1H), 4.81 (d, *J* = 7.2 Hz, 1H), 4.67 (brs, 1H), 3.45 (s, 3H), 3.04-2.83 (m, 1H), 2.25-2.16 (m, 1H), 2.11-1.99 (m, 3H), 1.74 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 163.7, 156.2, 146.2, 137.0, 135.8, 131.7, 131.8, 130.4, 127.9, 126.3, 123.4, 120.5, 52.4, 52.0, 49.8, 30.0, 28.8, 23.3; IR (ATR) 3315, 2935, 2910, 2837, 1695, 1598, 1535, 1490, 1452, 1318, 1254, 1229, 1192, 1128, 1075, 1037, 878, 830, 759 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{18}H_{19}ClN_2O_2$ 330.11350, found: 330.11348.

*** *exo*-3ah showed multiple resonance for the presence of different rotational isomers at 20 °C.**

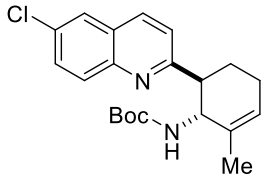
Methyl (6-(6-chloroquinolin-2-yl)-2-methylcyclohex-2-en-1-yl)carbamate (*endo*-3ah)



white solid; R_f = 0.15 (Hexane/EtOAc= 6/1); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.00-7.93 (m, 2H), 7.75 (d, *J* = 2.4 Hz, 1H), 7.60 (d, *J* = 9.0 Hz, 1H), 7.38 (d, *J* = 7.8 Hz, 1H), 5.63 (s, 1H), 5.26 (d, *J* = 7.8 Hz, 1H), 4.59 (s, 1H), 3.21 (s, 4H), 2.17-1.97 (m, 4H), 1.73 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.8, 156.4, 146.1, 137.8, 135.1, 131.6, 131.0, 130.1, 127.6, 126.3, 122.5, 122.1, 51.9, 49.1, 45.8, 29.9, 23.6, 23.3; IR (ATR) 3330, 3013, 2934, 2909, 2833, 1716, 1599, 1492, 1450, 1339, 1308, 1237, 1192, 1074, 972, 878, 834, 759 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{18}H_{19}ClN_2O_2$ 330.11350, found: 330.11342.

*** *endo*-3ah showed multiple resonance for the presence of different rotational isomers at 20 ℃.**

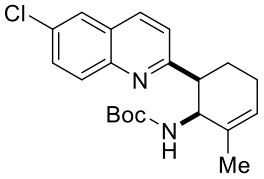
***tert*-Butyl (6-(6-chloroquinolin-2-yl)-2-methylcyclohex-2-en-1-yl)carbamate (*exo*-3ai)**



white solid; R_f = 0.25 (Hexane/EtOAc= 6/1); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.01 (d, *J* = 9.0 Hz, 1H), 7.96 (d, *J* = 9.0 Hz, 1H), 7.76 (d, *J* = 2.4 Hz, 1H), 7.61 (dd, *J* = 9.0, 2.4 Hz, 1H), 7.44 (d, *J* = 9.0 Hz, 1H), 5.62 (s, 1H), 4.60 (dd, *J* = 9.0, 9.0 Hz, 1H), 4.51 (d, *J* = 9.0 Hz, 1H), 3.20 (ddd, *J* = 10.2, 9.0, 3.0 Hz, 1 H), 2.24-1.94 (m, 4H), 1.77 (s, 3H), 1.20 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 164.1, 155.7, 146.2, 135.5, 134.5, 131.5, 130.8, 130.2, 127.8, 126.3, 124.9, 120.9, 79.1, 54.0, 50.3, 28.3, 28.1, 24.9, 20.4; IR (ATR) 3349, 2973, 2937, 2912, 2844, 1678, 1599, 1525, 1490, 1416, 1365, 1319, 1271, 1250, 1233, 1169, 1074, 1017, 999, 828, 764 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{21}H_{25}ClN_2O_2$ 372.16045, found: 372.16039.

*** *exo*-3ai showed multiple resonance for the presence of different rotational isomers at 20 ℃.**

***tert*-Butyl (6-(6-chloroquinolin-2-yl)-2-methylcyclohex-2-en-1-yl)carbamate (*endo*-3ai)**



colorless oil; R_f = 0.30 (Hexane/EtOAc= 6/1); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.99 (t, *J* = 9.0 Hz, 1H), 7.95 (d, *J* = 9.0 Hz, 1H), 7.74 (d, *J* = 2.4 Hz, 1H), 7.59 (dd, *J* = 9.0, 2.4 Hz, 1H), 7.42 (d, *J* = 9.0 Hz, 1H), 5.61 (s, 1H), 4.69 (d, *J* = 10.2 Hz, 1H), 4.43 (dd, *J* = 10.2, 4.2 Hz, 1H), 3.34 (ddd, *J* = 12.6, 4.2, 3.0 Hz, 1H), 2.26-1.92 (m, 4H), 1.78 (s, 3H), 1.01 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.9, 155.3, 146.2, 134.7, 134.4, 131.4, 131.0, 129.9, 127.7, 126.2, 124.9, 122.7, 78.8, 51.9, 47.4, 28.1, 25.4, 21.7, 21.3; IR (ATR) 3438, 2977, 2933, 2837, 1704, 1600, 1492, 1454, 1365, 1238, 1169, 1074, 984, 878, 831, 759 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{21}H_{25}ClN_2O_2$ 372.16045, found: 372.16040.

*** *endo*-3ai showed multiple resonance for the presence of different rotational isomers at 20 ℃.**

4. Computational study by DFT calculations

4-1. Method

All calculations were performed with the Gaussian 16 package[3]. Molecular geometries and transition state structures were optimized and characterized using frequency calculations in the gas-phase at the B3LYP-D3/6-31G(d) level of theory[4,5], unless otherwise noted. A manual conformational search has been performed on possible catalyst substrate orientations. Transition state structures were verified by the presence of a single imaginary vibrational frequency.

4-2. Summary of energies of transition states

Table S1. Summary of model calculations for transition states in the reaction of vinylquinoline **1b** with dienylcarbamates **2a** catalysed by phosphoric acid (*R*)-**4**

VQ	diene	Reactin-face	TS-name	A.u.	kcal/mol	$\Delta\Delta G^{\ddagger}$
s-TRANS	cis-cis	R_endo	TS-Cc(R-en)	-2023.265971	-1269619.629	0.44
		S_endo	TS-Cc(S-en)	-2023.265825	-1269619.538	0.53
		R_exo	TS-Cc(R-ex)	-2023.244898	-1269606.406	13.66
		S_exo	TS-Cc(S-ex)	-2023.242306	-1269604.779	15.29
	cis-trans	R_endo	TS-Ct(R-en)	-2023.260677	-1269616.307	3.76
		S_endo	TS-Ct(S-en)	-2023.260101	-1269615.946	4.12
		R_exo	TS-Ct(R-ex)	-2023.240457	-1269603.619	16.45
		S_exo	TS-Ct(S-ex)	N.D.	-	-
	trans-cis	R_endo	TS-Tc(R-en)	-2023.248883	-1269608.907	11.16
		S_endo	TS-Tc(S-en)	-2023.248044	-1269608.38	11.69
		R_exo	TS-Tc(R-ex)	-2023.266667	-1269620.066	0.00
		S_exo	TS-Tc(S-ex)	-2023.265121	-1269619.096	0.97
	trans-trans	R_endo	TS-Tt(R-en)	-2023.251588	-1269610.604	9.46
		S_endo	TS-Tt(S-en)	-2023.250898	-1269610.171	9.90
		R_exo	TS-Tt(R-ex)	-2023.262974	-1269617.749	2.32
		S_exo	TS-Tt(S-ex)	-2023.26117	-1269616.617	3.45

VQ	diene	Reactin-face	TS-name	A.u.	kcal/mol	$\Delta\Delta G^{\ddagger}$
s-CIS	cis-cis	R_endo	s-cis_TS-Cc(R-en)	-2023.248889	-1269608.91	11.16
		S_endo	s-cis_TS-Cc(S-en)	-2023.24389	-1269605.773	14.29
		R_exo	s-cis_TS-Cc(R-ex)	-2023.25314	-1269611.578	8.49
		S_exo	s-cis_TS-Cc(S-ex)	-2023.254762	-1269612.596	7.47
	trans-cis	R_endo	s-cis_TS-Ct(R-en)	-2023.252217	-1269610.999	9.07
		S_endo	s-cis_TS-Ct(S-en)	-2023.248121	-1269608.428	11.64
		R_exo	s-cis_TS-Ct(R-ex)	-2023.249273	-1269609.151	10.91
		S_exo	s-cis_TS-Ct(S-ex)	-2023.250432	-1269609.879	10.19
	cis-trans	R_endo	s-cis_TS-Tc(R-en)	-2023.257652	-1269614.409	5.66
		S_endo	s-cis_TS-Tc(S-en)	-2023.257691	-1269614.434	5.63
		R_exo	s-cis_TS-Tc(R-ex)	-2023.246881	-1269607.65	12.42
		S_exo	s-cis_TS-Tc(S-ex)	-2023.249192	-1269609.1	10.97
	trans-trans	R_endo	s-cis_TS-Tt(R-en)	-2023.250337	-1269609.819	10.25
		S_endo	s-cis_TS-Tt(S-en)	-2023.249369	-1269609.212	10.85
		R_exo	s-cis_TS-Tt(R-ex)	-2023.25163	-1269610.63	9.44
		S_exo	s-cis_TS-Tt(S-ex)	-2023.255047	-1269612.775	7.29

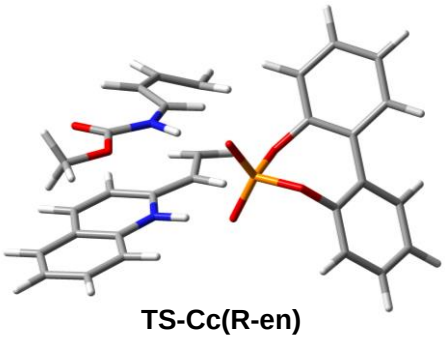
Table S2. DFT calculations for transition states in the reaction of newly designed dienylcarbamates **2** with vinylquinoline **1b** catalysed by phosphoric acid (*R*)-**4**

R	diene	Reactin-face	TS-name	A.u.	kcal/mol	$\Delta\Delta G^{‡}$
Me(**2b**)	cis-cis	R_endo	TS_{Me}-Cc(R-en)	-2062.553752	-1294273.105	5.33
		S_endo	TS_{Me}-Cc(S-en)	-2062.553969	-1294273.241	5.20
	cis-trans	R_endo	TS_{Me}-Ct(R-en)	-2062.547342	-1294269.083	9.36
		S_endo	TS_{Me}-Ct(S-en)	-2062.547486	-1294269.173	9.27
	trans-cis	R_exo	TS_{Me}-Tc(R-ex)	-2062.562251	-1294278.438	0.00
		S_exo	TS_{Me}-Tc(S-ex)	-2062.559024	-1294276.413	2.02
	trans-trans	R_exo	TS_{Me}-Tt(R-ex)	-2062.557978	-1294275.757	2.68
		S_exo	TS_{Me}-Tt(S-ex)	-2062.554628	-1294273.655	4.78
F(**2c**)	cis-cis	R_endo	TS_{F}-Cc(R-en)	-2122.498689	-1331889.152	2.67
		S_endo	TS_{F}-Cc(S-en)	-2122.498794	-1331889.218	2.61
	cis-trans	R_endo	TS_{F}-Ct(R-en)	-2122.494512	-1331886.531	5.29
		S_endo	TS_{F}-Ct(S-en)	-2122.494287	-1331886.39	5.43
	trans-cis	R_exo	TS_{F}-Tc(R-ex)	-2122.502946	-1331891.824	0.00
		S_exo	TS_{F}-Tc(S-ex)	-2122.500877	-1331890.525	1.30
	trans-trans	R_exo	TS_{F}-Tt(R-ex)	-2122.498404	-1331888.973	2.85
		S_exo	TS_{F}-Tt(S-ex)	-2122.497622	-1331888.483	3.34

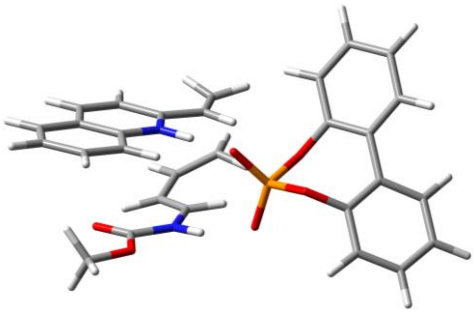
R	diene	Reactin-face	TS-name	A.u.	kcal/mol	$\Delta\Delta G^{‡}$
OMe(**2d**)	cis-cis	R_endo	TS_{OMe}-Cc(R-en)	-2137.751418	-1341460.392	5.74
		S_endo	TS_{OMe}-Cc(S-en)	-2137.751958	-1341460.731	5.40
	cis-trans	R_endo	TS_{OMe}-Ct(R-en)	-2137.74695	-1341457.589	8.54
		S_endo	TS_{OMe}-Ct(S-en)	-2137.746753	-1341457.465	8.67
	trans-cis	R_exo	TS_{OMe}-Tc(R-ex)	-2137.760565	-1341466.132	0.00
		S_exo	TS_{OMe}-Tc(S-ex)	-2137.758529	-1341464.855	1.28
	trans-trans	R_exo	TS_{OMe}-Tt(R-ex)	-2137.756269	-1341463.436	2.70
		S_exo	TS_{OMe}-Tt(S-ex)	-2137.753944	-1341461.977	4.15
I(**2e**)	cis-cis	R_endo	TS_{I}-Cc(R-en)	-2034.012039	-1276362.895	5.70
		S_endo	TS_{I}-Cc(S-en)	-2034.011631	-1276362.639	5.96
	cis-trans	R_endo	TS_{I}-Ct(R-en)	-2034.008199	-1276360.485	8.11
		S_endo	TS_{I}-Ct(S-en)	-2034.008058	-1276360.396	8.20
	trans-cis	R_exo	TS_{I}-Tc(R-ex)	-2034.021128	-1276368.598	0.00
		S_exo	TS_{I}-Tc(S-ex)	-2034.019568	-1276367.619	0.98
	trans-trans	R_exo	TS_{I}-Tt(R-ex)	-2034.016124	-1276365.458	3.14
		S_exo	TS_{I}-Tt(S-ex)	-2034.012585	-1276363.237	5.36

R	diene	Reactin-face	TS-name	A.u.	kcal/mol	$\Delta\Delta G^{\ddagger}$
TMS(**2f**)	cis-cis	R_endo	TS_{TMS}-Cc(R-en)	-2431.854907	-1526013.273	6.35
		S_endo	TS_{TMS}-Cc(S-en)	-2431.855695	-1526013.767	5.86
	cis-trans	R_endo	TS_{TMS}-Ct(R-en)	-2431.848683	-1526009.367	10.26
		S_endo	TS_{TMS}-Ct(S-en)	-2431.84898	-1526009.553	10.07
	trans-cis	R_exo	TS_{TMS}-Tc(R-ex)	-2431.865032	-1526019.626	0.00
		S_exo	TS_{TMS}-Tc(S-ex)	-2431.863214	-1526018.485	1.14
	trans-trans	R_exo	TS_{TMS}-Tt(R-ex)	-2431.861293	-1526017.28	2.35
		S_exo	TS_{TMS}-Tt(S-ex)	-2431.858825	-1526015.731	3.89
SPh(**2g**)	cis-cis	R_endo	TS_{SPh}-Cc(R-en)	-2652.435587	-1664429.855	6.43
		S_endo	TS_{SPh}-Cc(S-en)	-2652.435186	-1664429.604	6.69
	cis-trans	R_endo	TS_{SPh}-Ct(R-en)	-2652.430757	-1664426.824	9.47
		S_endo	TS_{SPh}-Ct(S-en)	-2652.430539	-1664426.688	9.60
	trans-cis	R_exo	TS_{SPh}-Tc(R-ex)	-2652.445841	-1664436.29	0.00
		S_exo	TS_{SPh}-Tc(S-ex)	-2652.445256	-1664435.923	0.37
	trans-trans	R_exo	TS_{SPh}-Tt(R-ex)	-2652.441962	-1664433.856	2.43
		S_exo	TS_{SPh}-Tt(S-ex)	-2652.437919	-1664431.319	4.97

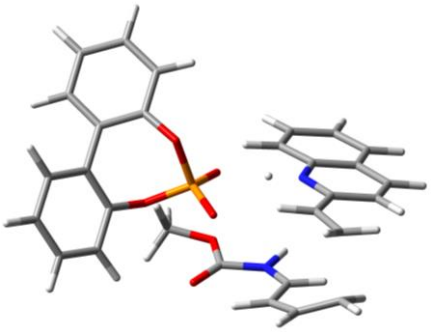
4-3. TS images



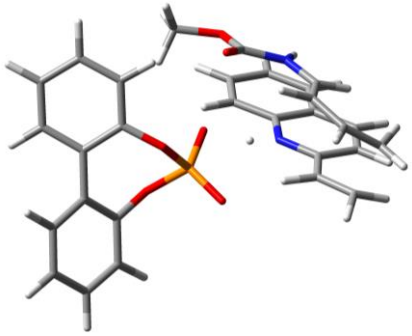
TS-Cc(R-en)
(0.4)



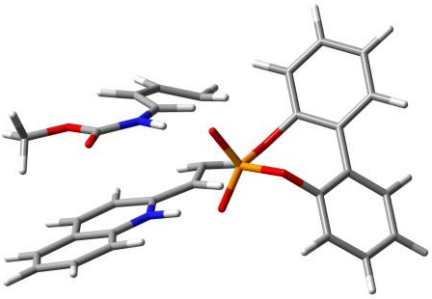
TS-Cc(S-en)
(0.5)



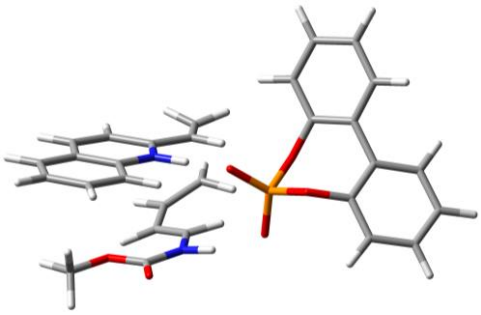
TS-Cc(R-ex)
(13.7)



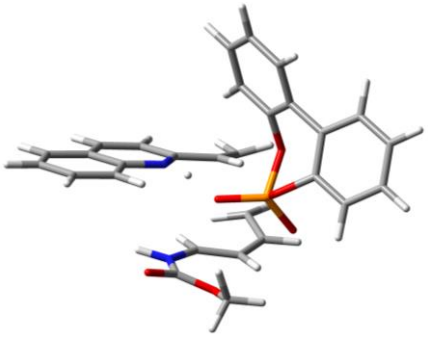
TS-Cc(S-ex)
(15.3)



TS-Ct(R-en)
(3.8)

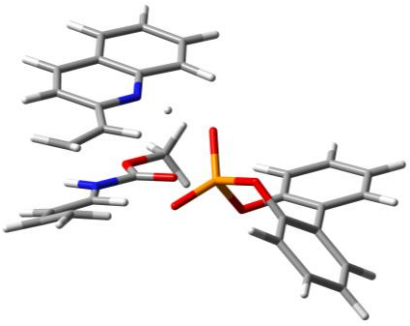


TS-Ct(S-en)
(4.1)

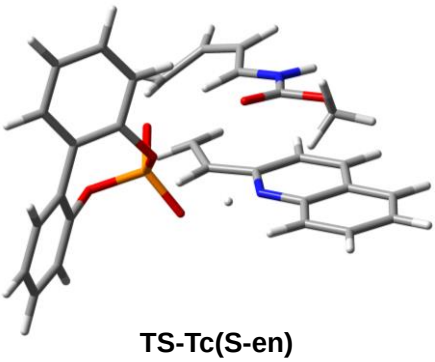


TS-Ct(R-ex)
(16.5)

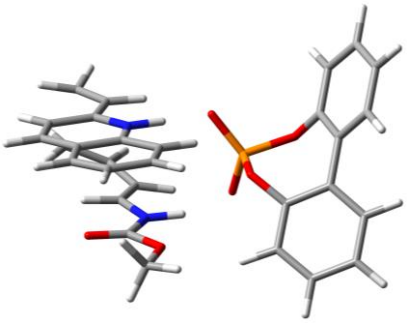
TS-Ct(S-ex)
(N.D.)



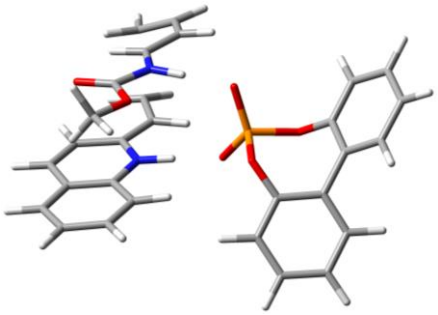
TS-Tc(R-en)
(11.2)



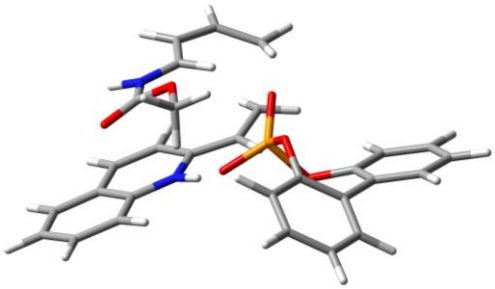
TS-Tc(S-en)
(11.7)



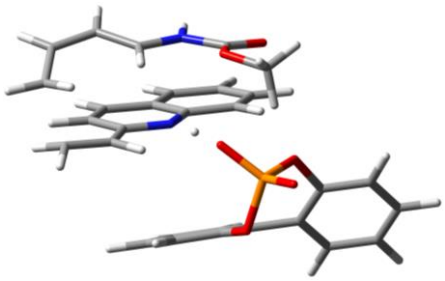
TS-Tc(R-ex)
(0.0 kcal·mol^{-1})



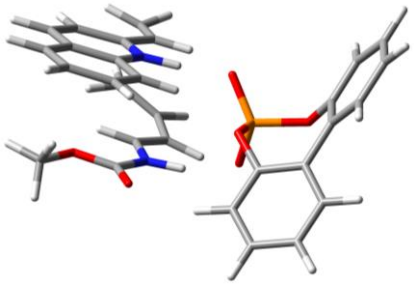
TS-Tc(S-ex)
(1.1)



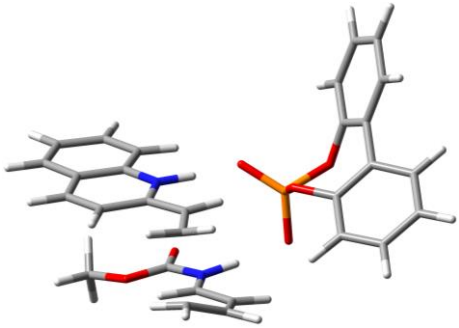
TS-Tt(R-en)
(9.5)



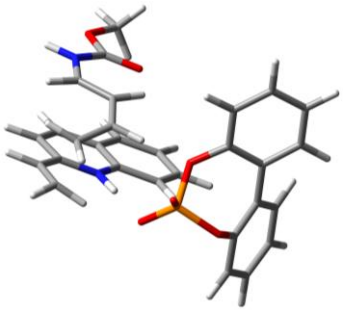
TS-Tt(S-en)
(9.9)



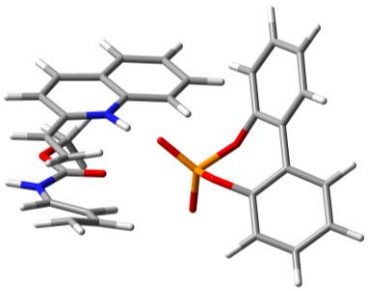
TS-Tt(R-ex)
(2.3)



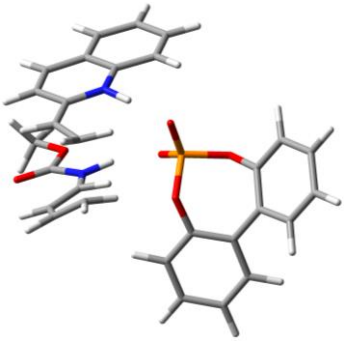
TS-Tt(S-ex)
(3.5)



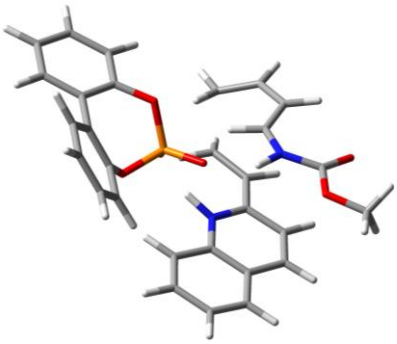
***s-cis*_TS-Cc(R-en)**
(11.2)



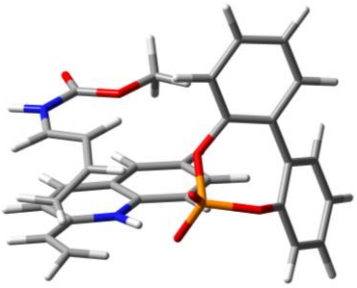
***s-cis*_TS-Cc(S-en)**
(14.3)



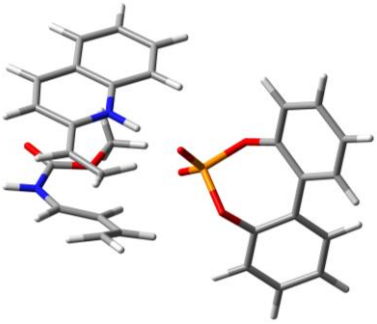
***s-cis*_TS-Cc(R-ex)**
(8.5)



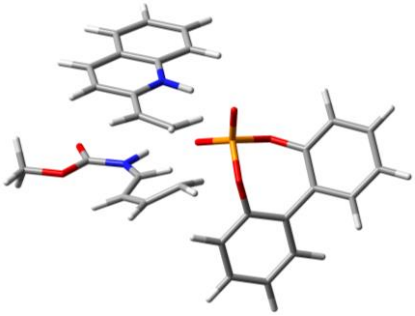
***s-cis*_TS-Cc(S-ex)**
(7.5)



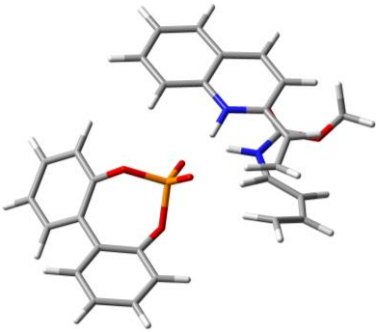
***s-cis*_TS-Ct(R-en)**
(9.1)



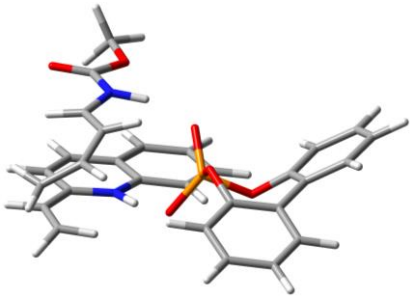
***s-cis*_TS-Ct(S-en)**
(11.6)



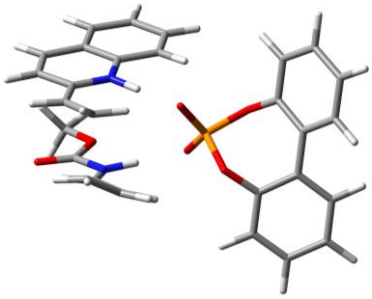
***s-cis*_TS-Ct(R-ex)**
(10.9)



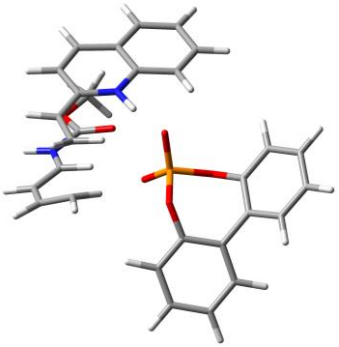
***s-cis*_TS-Ct(S-ex)**
(10.2)



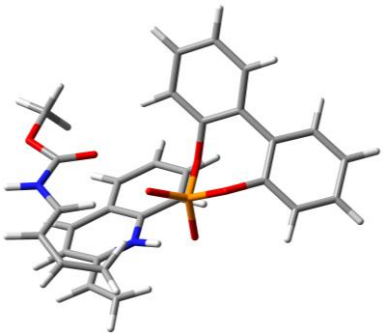
***s-cis*_TS-Tc(R-en)**
(5.7)



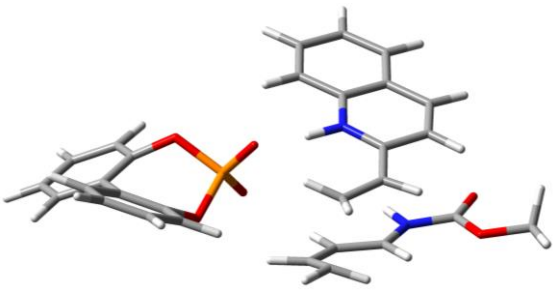
***s-cis*_TS-Tc(S-en)**
(5.6)



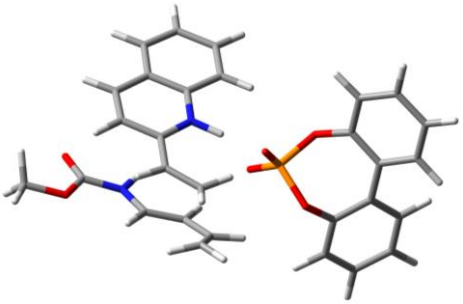
***s-cis*_TS-Tc(R-ex)**
(12.4)



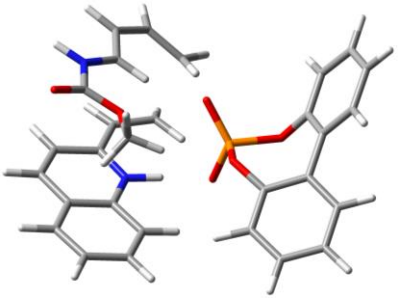
***s-cis*_TS-Tc(S-ex)**
(11.0)



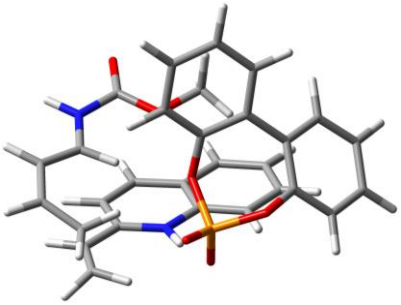
***s-cis*_TS-Tt(R-en)**
(10.3)



***s-cis*_TS-Tt(S-en)**
(10.9)

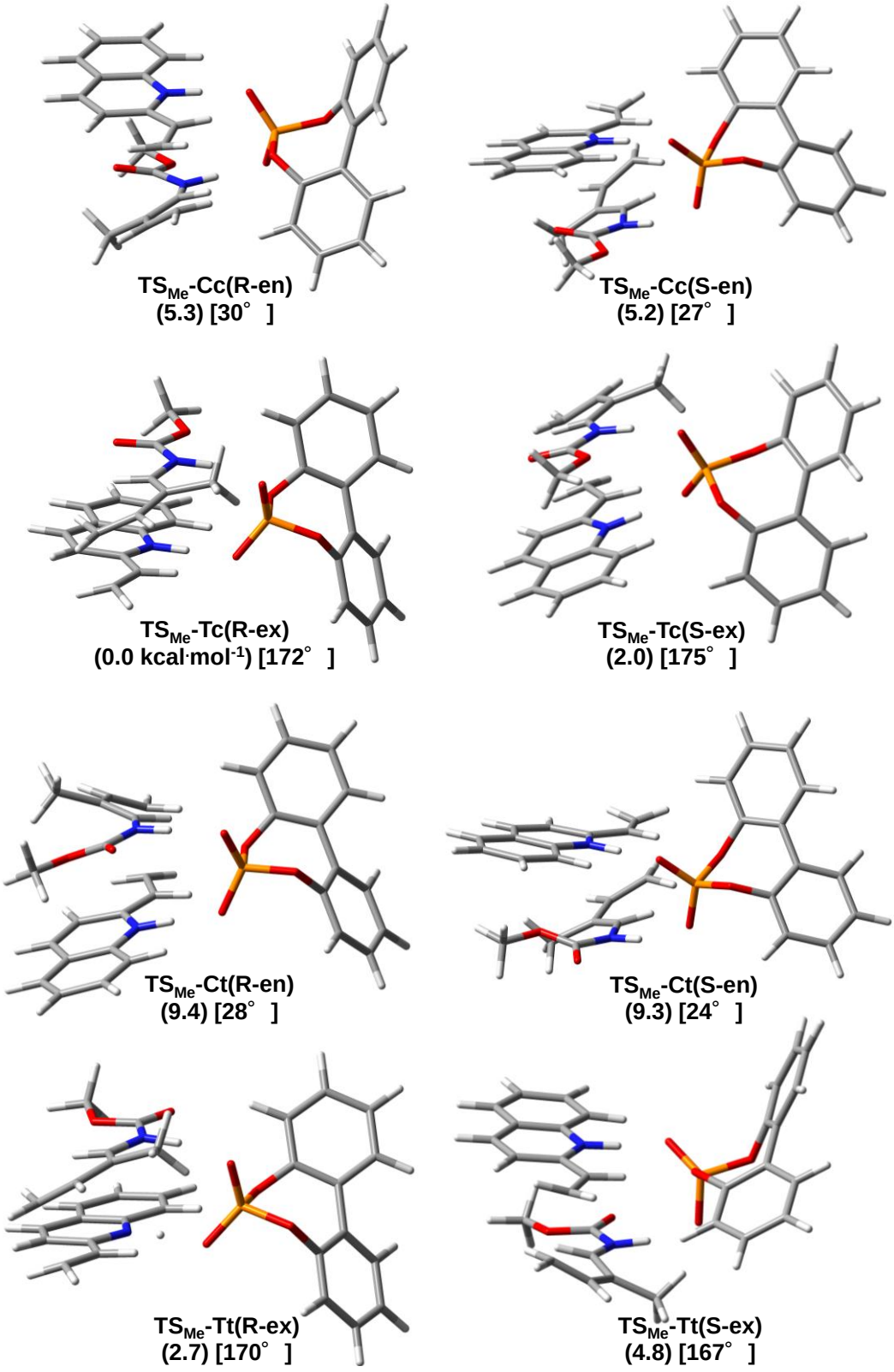


***s-cis*_TS-Tt(R-ex)**
(9.4)

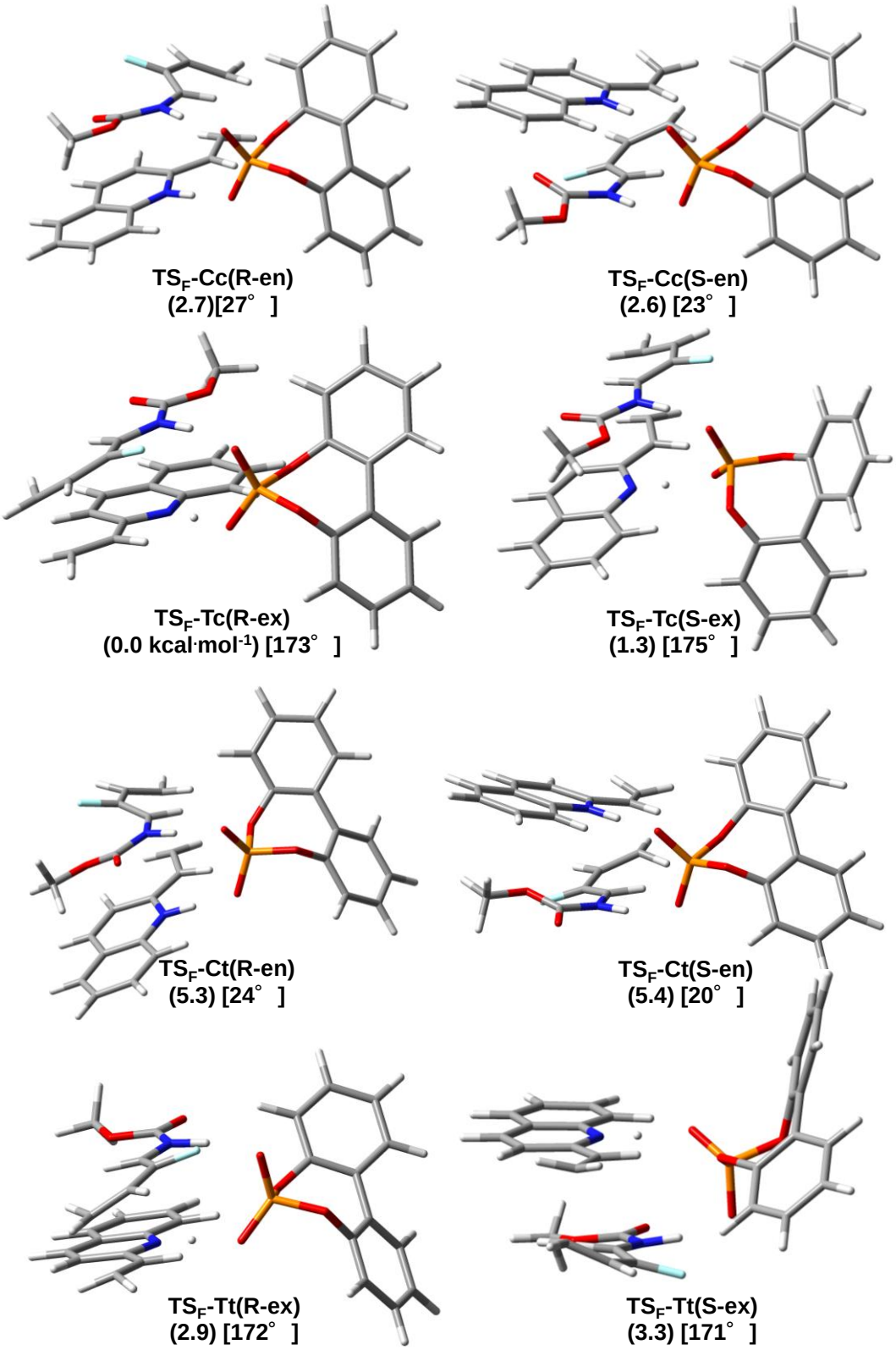


***s-cis*_TS-Tt(S-ex)**
(7.3)

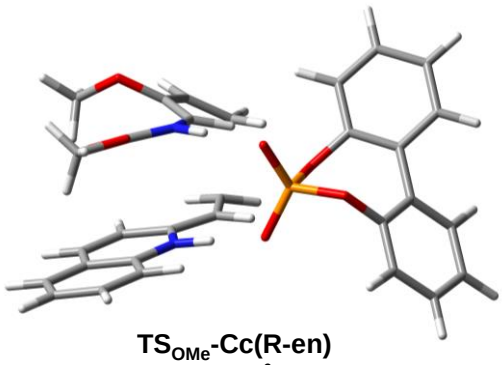
For 2b (R = Me): Dihedral angles (C^1-N^1-C^2-C^3) for dienylcarbamate **2b** were shown in square brackets.



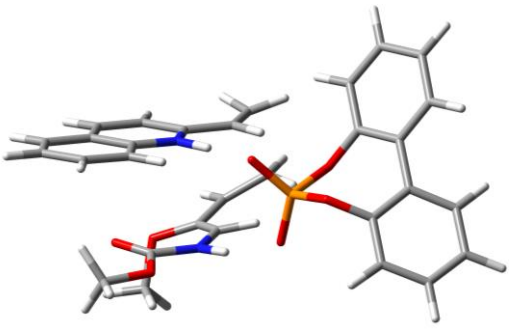
For 2c (R = F) : Dihedral angles (C^1-N^1-C^2-C^3) for dienylcarbamate **2c** were shown in square brackets.



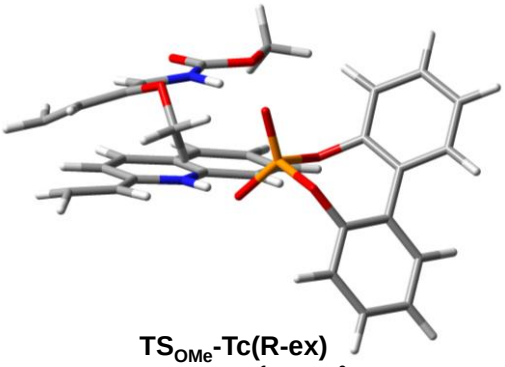
For 2d (R = OMe) : Dihedral angles (C^1-N^1-C^2-C^3) for dienylcarbamate **2d** were shown in square brackets.



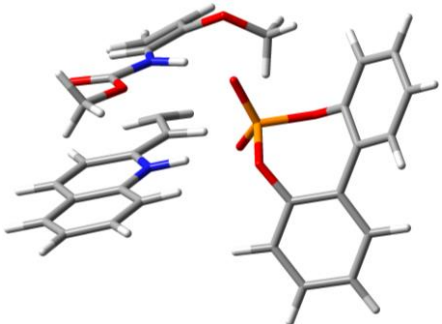
TS_{OMe}-Cc(R-en)
(5.7)[30°]



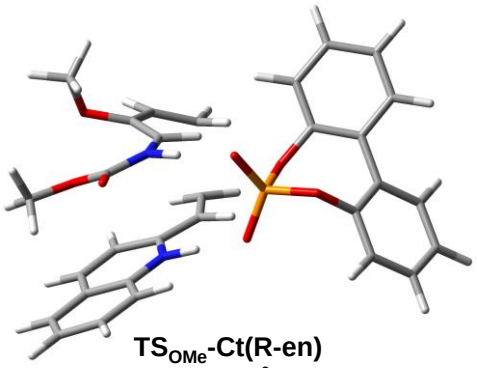
TS_{OMe}-Cc(S-en)
(5.4) [20°]



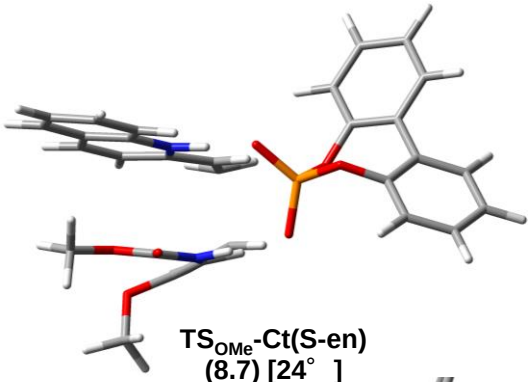
TS_{OMe}-Tc(R-ex)
(0.0 kcal·mol^{-1}) [174°]



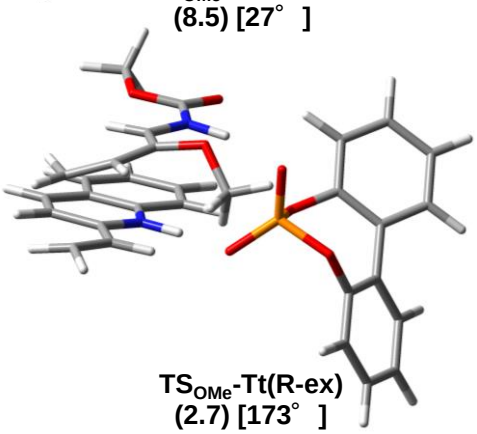
TS_{OMe}-Tc(S-ex)
(1.3) [174°]



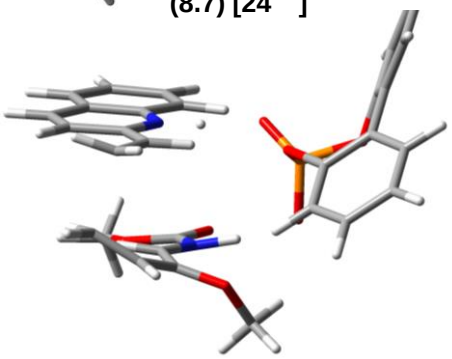
TS_{OMe}-Ct(R-en)
(8.5) [27°]



TS_{OMe}-Ct(S-en)
(8.7) [24°]

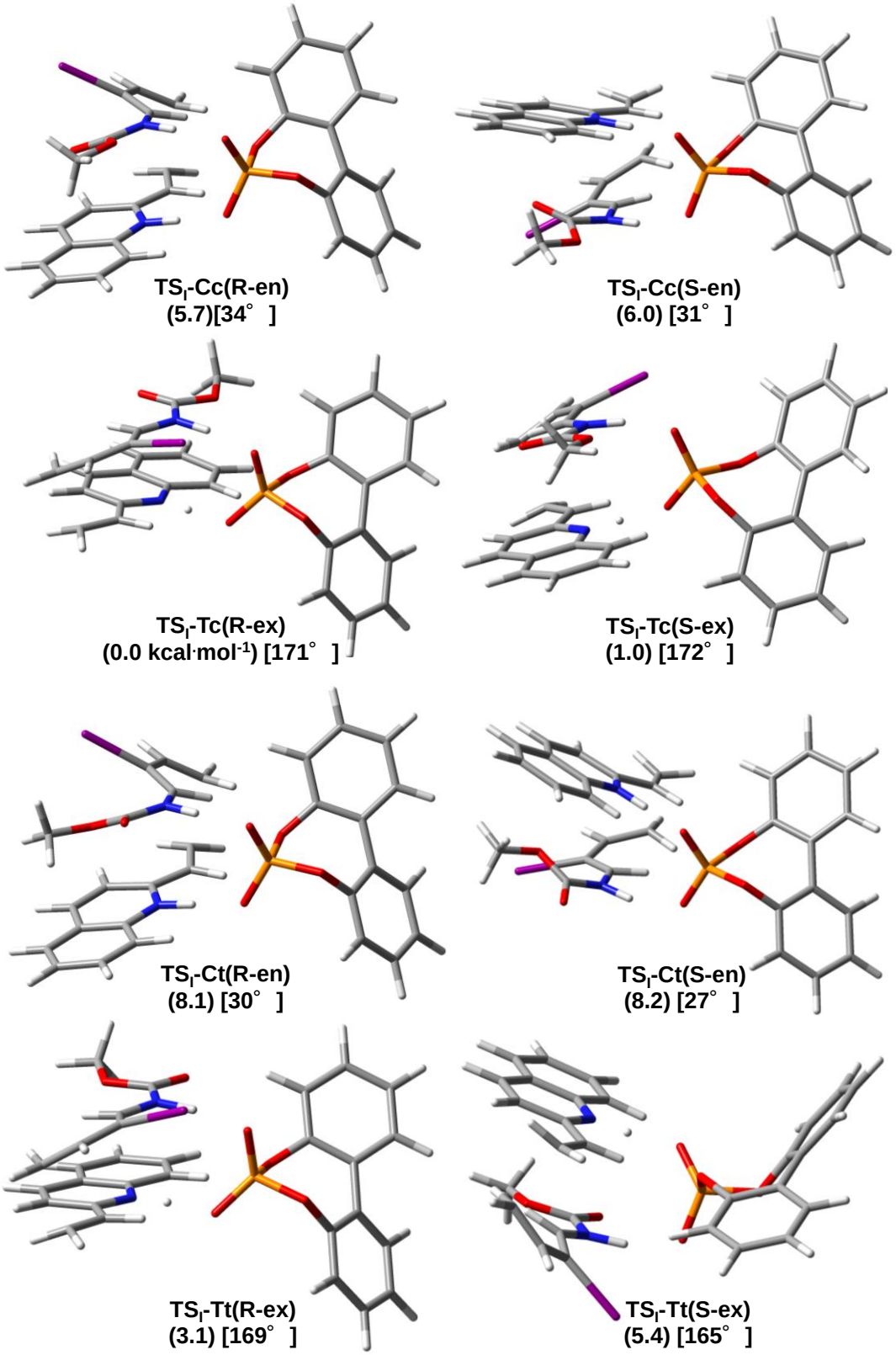


TS_{OMe}-Tt(R-ex)
(2.7) [173°]

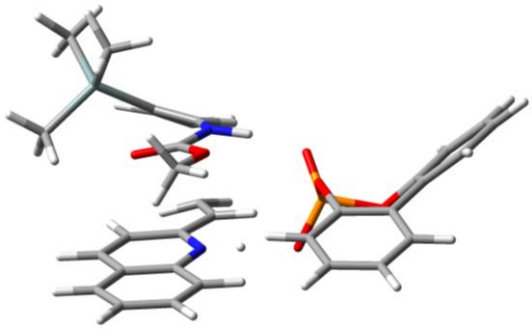


TS_{OMe}-Tt(S-ex)
(4.1) [168°]

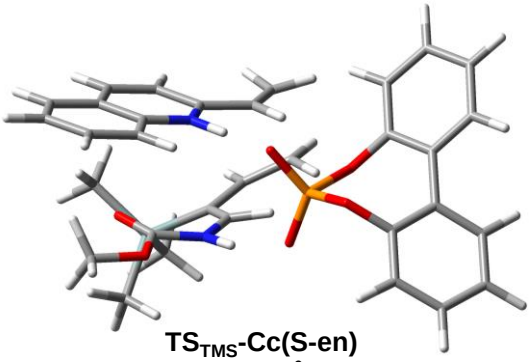
For 2e (R = I) : Dihedral angles (C^1-N^1-C^2-C^3) for dienylcarbamate **2e** were shown in square brackets.



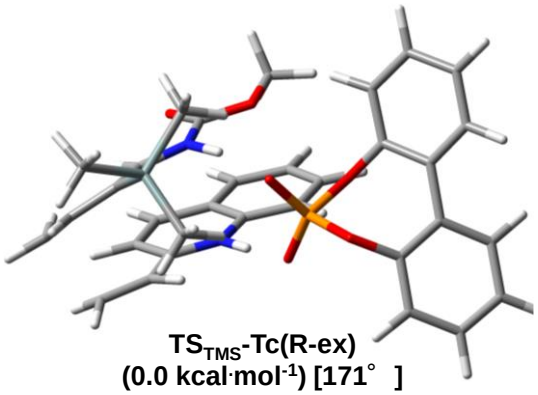
For 2f (R = TMS) : Dihedral angles (C^1-N^1-C^2-C^3) for dienylcarbamate **2f** were shown in square brackets.



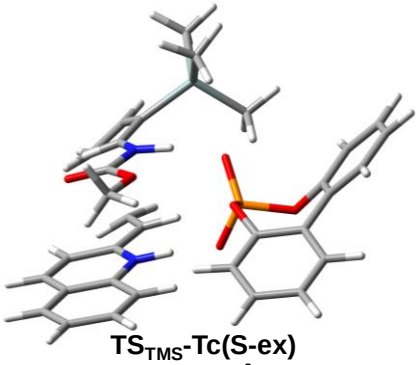
TS_{TMS}-Cc(R-en)
(6.3)[27°]



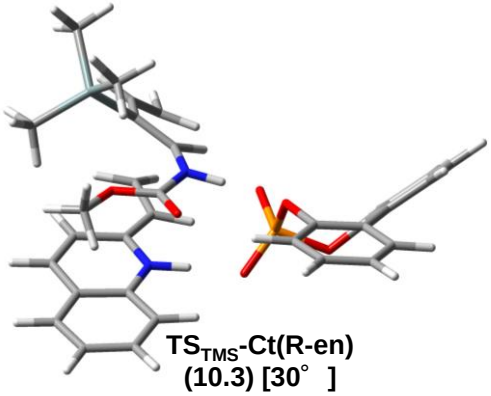
TS_{TMS}-Cc(S-en)
(5.9) [26°]



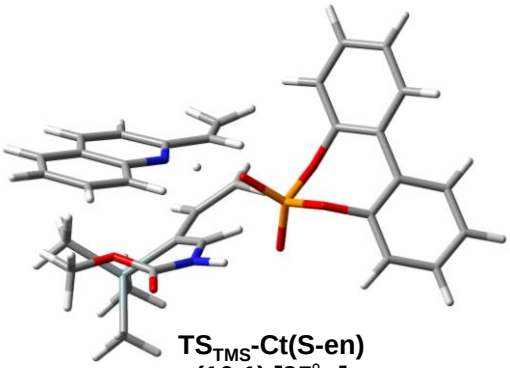
TS_{TMS}-Tc(R-ex)
(0.0 kcal·mol^{-1}) [171°]



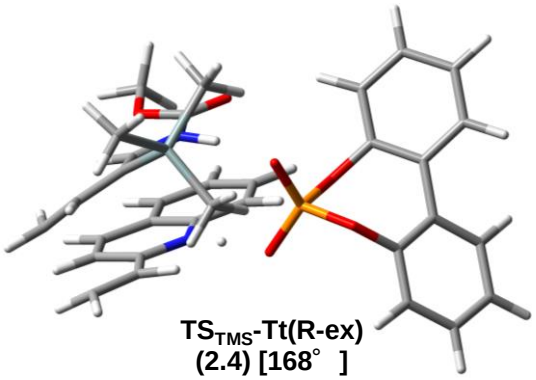
TS_{TMS}-Tc(S-ex)
(1.1) [172°]



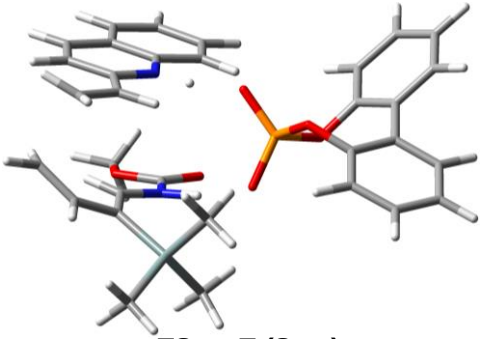
TS_{TMS}-Ct(R-en)
(10.3) [30°]



TS_{TMS}-Ct(S-en)
(10.1) [25°]

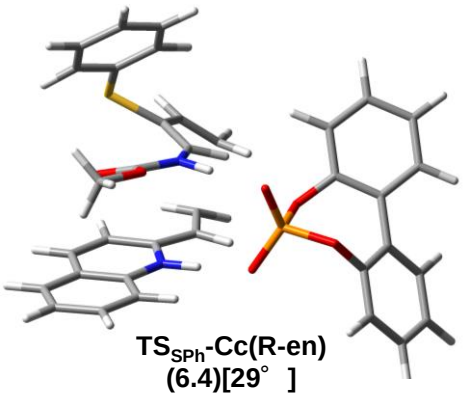


TS_{TMS}-Tt(R-ex)
(2.4) [168°]

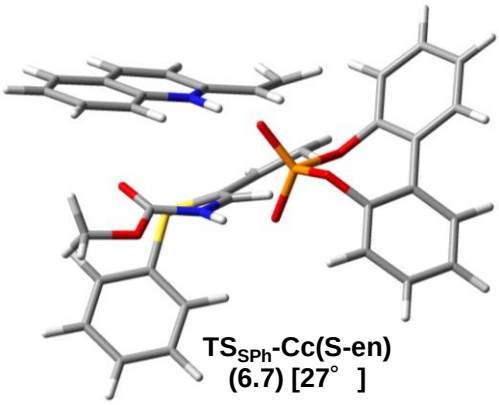


TS_{TMS}-Tt(S-ex)
(3.9) [170°]

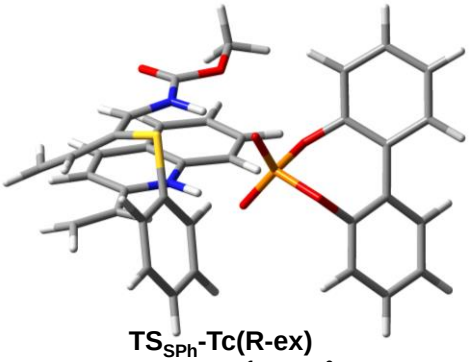
For 2g (R = SPh) : Dihedral angles (C^1-N^1-C^2-C^3) for dienylcarbamate **2g** were shown in square brackets.



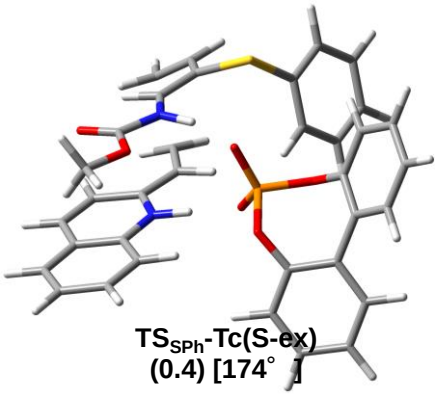
TS_{SPh}-Cc(R-en)
(6.4)[29°]



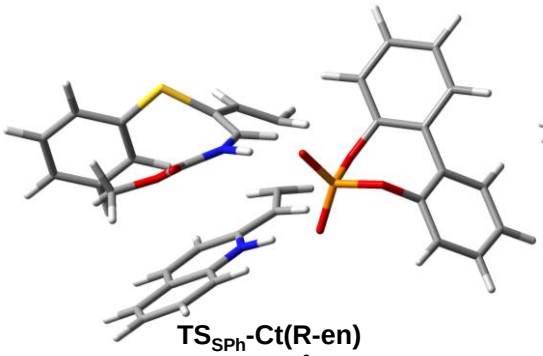
TS_{SPh}-Cc(S-en)
(6.7) [27°]



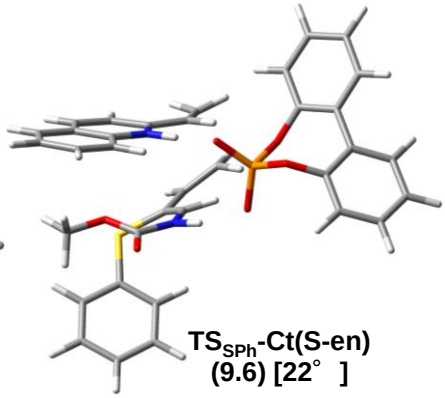
TS_{SPh}-Tc(R-ex)
(0.0 kcal·mol^{-1}) [173°]



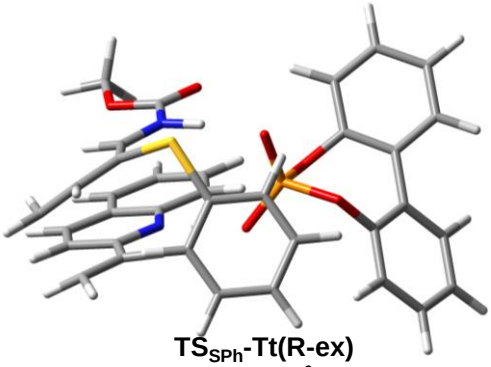
TS_{SPh}-Tc(S-ex)
(0.4) [174°]



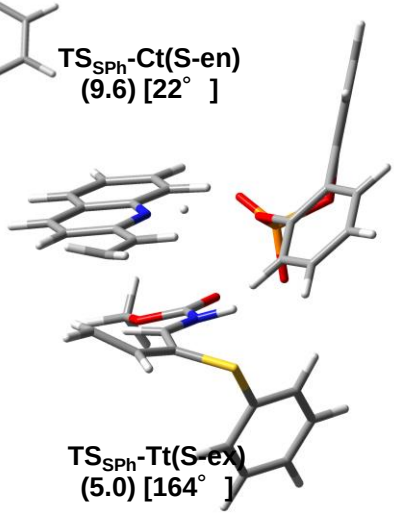
TS_{SPh}-Ct(R-en)
(9.5) [30°]



TS_{SPh}-Ct(S-en)
(9.6) [22°]



TS_{SPh}-Tt(R-ex)
(2.4) [171°]



TS_{SPh}-Tt(S-ex)
(5.0) [164°]

4-3. Coordination

TS-Cc(R-en)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2023.713572 hartree

Sum of electronic and thermal Free Energies = -2023.265971 hartree

The number of imaginary frequency = 1

Imaginary frequency = -334.97

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.047576	3.839671	-1.427458
2	1	0	0.756333	3.285790	-0.952734
3	1	0	0.288027	4.627607	-2.097123
4	6	0	-1.277543	3.990156	-0.793757
5	1	0	-1.939015	4.767880	-1.174014
6	6	0	-1.148672	2.046761	0.692533
7	1	0	-0.083622	1.934528	0.524264
8	1	0	-0.908048	0.391396	1.851001
9	7	0	-1.627825	1.055158	1.490099
10	6	0	-2.960423	0.789949	1.760126
11	8	0	-3.033087	-0.312723	2.530183
12	8	0	-3.919611	1.422408	1.359729
13	1	0	-1.031100	-1.023672	-0.788809
14	6	0	-5.444958	-2.666662	-0.152850
15	6	0	-5.519835	-1.488976	-0.876922
16	6	0	-4.347639	-0.780649	-1.213092
17	6	0	-3.095756	-1.301221	-0.796809
18	6	0	-3.021346	-2.490906	-0.045814
19	6	0	-4.191107	-3.162338	0.263394
20	1	0	-5.283663	0.864496	-2.280035
21	1	0	-6.351075	-3.208822	0.100449
22	1	0	-6.481152	-1.093623	-1.194526
23	6	0	-4.335368	0.441718	-1.958779
24	1	0	-2.047903	-2.849418	0.275186
25	1	0	-4.141377	-4.081939	0.839328
26	6	0	-1.907047	0.533354	-1.832582
27	6	0	-3.167173	1.074574	-2.259149
28	1	0	-3.170663	2.002996	-2.816116
29	7	0	-1.947636	-0.624212	-1.123680
30	6	0	-0.630874	1.084982	-2.118559
31	1	0	0.225558	0.530336	-1.749833
32	6	0	-0.398538	2.270952	-2.809649
33	1	0	-1.193394	2.751126	-3.371662
34	1	0	0.590706	2.415706	-3.233583
35	6	0	4.398447	-1.000404	-0.241767
36	6	0	5.393843	-1.360994	-1.164385
37	6	0	5.492407	-2.661965	-1.653008
38	6	0	4.585075	-3.636028	-1.228355
39	6	0	3.587299	-3.304075	-0.313795
40	6	0	3.503342	-2.002636	0.175257
41	6	0	4.306710	0.378390	0.289657
42	6	0	5.458309	1.085741	0.669726
43	6	0	5.384435	2.385929	1.165579
44	6	0	4.141085	3.006126	1.304041
45	6	0	2.982151	2.324677	0.935748
46	6	0	3.065228	1.029983	0.424171
47	1	0	6.083663	-0.596949	-1.512444
48	1	0	6.268380	-2.912410	-2.370970
49	1	0	4.651168	-4.651062	-1.610273
50	1	0	2.867505	-4.034426	0.039744
51	1	0	6.421977	0.590207	0.590874
52	1	0	6.292167	2.906186	1.457786
53	1	0	4.070291	4.013941	1.703716
54	1	0	2.004858	2.782928	1.046320
55	8	0	2.564382	-1.723704	1.155205
56	8	0	1.911817	0.427173	-0.042431
57	15	0	1.220011	-0.865348	0.770863
58	8	0	0.400320	-1.580185	-0.276943
59	8	0	0.599275	-0.381326	2.047837
60	6	0	-4.364900	-0.713053	2.887884
61	1	0	-4.956710	-0.919273	1.993630
62	1	0	-4.241108	-1.618966	3.481403
63	1	0	-4.853164	0.069371	3.476051
64	6	0	-1.841650	3.114746	0.157199
65	1	0	-2.882873	3.239719	0.424346

TS-Cc-(S-en)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2023.712958 hartree

Sum of electronic and thermal Free Energies = -2023.265825 hartree

The number of imaginary frequency = 1

Imaginary frequency = -330.23

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.918855	3.438811	2.775729
2	1	0	-0.004800	2.869039	2.751766
3	1	0	0.797801	4.479200	3.066167
4	6	0	2.128039	2.806721	3.040493
5	1	0	2.967650	3.437425	3.330906
6	6	0	1.490389	0.557740	2.315518
7	1	0	0.432766	0.798860	2.318320
8	1	0	0.815235	-1.203972	1.597916
9	7	0	1.692068	-0.707993	1.861820
10	6	0	2.912407	-1.301893	1.592185
11	8	0	2.695735	-2.534497	1.091238
12	8	0	4.010592	-0.804013	1.757264
13	1	0	1.016001	0.065224	-1.064178
14	6	0	5.121149	-1.763050	-2.556896
15	6	0	5.385953	-0.536157	-1.974300
16	6	0	4.336851	0.243345	-1.443085
17	6	0	3.013168	-0.260516	-1.514880
18	6	0	2.744113	-1.514424	-2.099476
19	6	0	3.796455	-2.247278	-2.618482
20	1	0	5.524727	1.931732	-0.767895

21	1	0	5.932312	-2.356922	-2.967405
22	1	0	6.402745	-0.156391	-1.918504
23	6	0	4.518608	1.526572	-0.837875
24	1	0	1.719141	-1.871915	-2.124094
25	1	0	3.599026	-3.213005	-3.074909
26	6	0	2.129206	1.702896	-0.418359
27	6	0	3.460317	2.234028	-0.350022
28	1	0	3.610264	3.199460	0.116470
29	7	0	1.983703	0.485649	-0.997079
30	6	0	0.956644	2.357116	0.050727
31	1	0	0.025883	1.812036	-0.062469
32	6	0	0.914911	3.617551	0.636702
33	1	0	1.764224	4.289318	0.567738
34	1	0	-0.046605	4.120440	0.676831
35	6	0	3.886455	-3.279350	0.790541
36	1	0	4.456987	-3.468650	1.704583
37	1	0	3.535888	-4.215863	0.356429
38	1	0	4.510945	-2.736818	0.077979
39	6	0	-4.293241	0.602236	-0.803843
40	6	0	-5.215161	1.225977	-1.659582
41	6	0	-4.874957	2.359127	-2.395441
42	6	0	-3.588021	2.891621	-2.293673
43	6	0	-2.652845	2.290938	-1.452566
44	6	0	-3.004141	1.162475	-0.712499
45	6	0	-4.672906	-0.592714	-0.016168
46	6	0	-5.917056	-0.673125	0.630036
47	6	0	-6.283581	-1.802286	1.359242
48	6	0	-5.401919	-2.881287	1.462361
49	6	0	-4.160640	-2.826618	0.831047
50	6	0	-3.808020	-1.696392	0.097396
51	1	0	-6.207434	0.794334	-1.757255
52	1	0	-5.607270	2.816398	-3.054845
53	1	0	-3.309425	3.769415	-2.870460
54	1	0	-1.646338	2.684946	-1.358177
55	1	0	-6.591453	0.176769	0.570393
56	1	0	-7.249702	-1.835373	1.855087
57	1	0	-5.677382	-3.762081	2.035815
58	1	0	-3.451921	-3.645799	0.887951
59	8	0	-2.089235	0.655718	0.193600
60	8	0	-2.612322	-1.708291	-0.602100
61	15	0	-1.344872	-0.812895	-0.066559
62	8	0	-0.391780	-0.691469	-1.231708
63	8	0	-0.861718	-1.260597	1.284090
64	6	0	2.433923	1.455680	2.775770
65	1	0	3.463512	1.130749	2.848371

TS-Cc-(R-ex)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2023.689597 hartree

Sum of electronic and thermal Free Energies = -2023.244898 hartree

The number of imaginary frequency = 1

Imaginary frequency = -352.86

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.320021	-4.069229	-1.324620
2	1	0	-4.194701	-3.555424	-0.933684
3	1	0	-3.555788	-4.856415	-2.036111
4	6	0	-2.183199	-4.212860	-0.529557
5	1	0	-1.459874	-4.969961	-0.825946
6	6	0	-2.532041	-2.246323	0.854257
7	1	0	-3.558003	-2.167078	0.516420
8	1	0	-2.841521	-0.442816	1.759968
9	7	0	-2.192644	-1.214888	1.685800
10	6	0	-0.949406	-0.988479	2.289977
11	8	0	-0.969814	0.240697	2.828295
12	8	0	-0.047501	-1.791401	2.345765
13	1	0	-1.458059	0.573841	-0.529264
14	6	0	-4.448814	3.825317	1.172322
15	6	0	-5.187760	2.911681	0.442335
16	6	0	-4.550392	1.827516	-0.197487
17	6	0	-3.140421	1.697265	-0.083986
18	6	0	-2.389541	2.626371	0.667136
19	6	0	-3.050202	3.674694	1.283082
20	1	0	-6.320389	0.906827	-1.060496
21	1	0	-4.943431	4.657734	1.663613
22	1	0	-6.266278	3.014578	0.352644
23	6	0	-5.240862	0.828367	-0.955695
24	1	0	-1.316158	2.488778	0.745695
25	1	0	-2.479011	4.393964	1.863082
26	6	0	-3.142716	-0.330186	-1.407566
27	6	0	-4.569497	-0.205820	-1.539073
28	1	0	-5.104580	-0.954240	-2.111513
29	7	0	-2.509737	0.638348	-0.692388
30	6	0	-2.364981	-1.390676	-1.930578
31	1	0	-1.296612	-1.370888	-1.720868
32	6	0	-2.857719	-2.490547	-2.638442
33	1	0	-3.855821	-2.474278	-3.071215
34	1	0	-2.137468	-3.056718	-3.218836
35	6	0	0.308219	0.710840	3.309965
36	1	0	0.992218	0.811081	2.466714
37	1	0	0.098160	1.676897	3.770014
38	1	0	0.716129	0.012028	4.044510
39	6	0	4.104412	1.190888	-0.620423
40	6	0	5.002977	2.252571	-0.426601
41	6	0	4.738826	3.530320	-0.915763
42	6	0	3.551782	3.775494	-1.610368
43	6	0	2.642581	2.739627	-1.816268
44	6	0	2.918079	1.460420	-1.333403
45	6	0	4.398116	-0.160478	-0.090535
46	6	0	5.681237	-0.724185	-0.176084
47	6	0	5.953699	-1.984767	0.352300
48	6	0	4.939281	-2.714203	0.979406
49	6	0	3.656483	-2.178203	1.077258
50	6	0	3.398131	-0.915315	0.549160
51	1	0	5.913097	2.066072	0.137211
52	1	0	5.450989	4.333143	-0.745643
53	1	0	3.333325	4.769958	-1.990562
54	1	0	1.715629	2.892345	-2.359307
55	1	0	6.464375	-0.167081	-0.683329
56	1	0	6.953427	-2.401658	0.265839

57	1	0	5.146148	-3.699560	1.388442
58	1	0	2.840036	-2.704439	1.560668
59	8	0	2.047663	0.441524	-1.656851
60	8	0	2.148156	-0.363357	0.741667
61	15	0	1.078648	-0.275296	-0.517031
62	8	0	0.037045	0.714536	-0.018160
63	8	0	0.663765	-1.603519	-1.053093
64	6	0	-1.761720	-3.324129	0.481383
65	1	0	-0.760571	-3.415146	0.879768

TS-Cc(S-ex)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2023.689596 hartree

Sum of electronic and thermal Free Energies = -2023.242306 hartree

The number of imaginary frequency = 1

Imaginary frequency = -365.26

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.523185	3.718520	1.943594
2	1	0	-4.401384	3.094388	1.797890
3	1	0	-3.752070	4.778068	2.023565
4	6	0	-2.437839	3.221664	2.668542
5	1	0	-1.736759	3.944172	3.081623
6	6	0	-2.775766	0.884177	2.105795
7	1	0	-3.770735	1.102745	1.739235
8	1	0	-3.077254	-0.989357	1.361317
9	7	0	-2.452491	-0.431685	1.928213
10	6	0	-1.233705	-1.053479	2.224085
11	8	0	-1.255606	-2.274553	1.669052
12	8	0	-0.361737	-0.575346	2.912172
13	1	0	-1.382513	0.025793	-0.739932
14	6	0	-4.066720	-3.523322	-2.346602
15	6	0	-4.874549	-2.408610	-2.212152
16	6	0	-4.330858	-1.182942	-1.771948
17	6	0	-2.943028	-1.115843	-1.476846
18	6	0	-2.122537	-2.255849	-1.608735
19	6	0	-2.691438	-3.440508	-2.040983
20	1	0	-6.161826	-0.011985	-1.809223
21	1	0	-4.489010	-4.464244	-2.686083
22	1	0	-5.935659	-2.460410	-2.442668
23	6	0	-5.097109	0.012606	-1.589488
24	1	0	-1.069030	-2.171441	-1.362974
25	1	0	-2.065774	-4.322087	-2.147459
26	6	0	-3.108231	1.219472	-0.857592
27	6	0	-4.513857	1.167001	-1.155074
28	1	0	-5.103450	2.067861	-1.031928
29	7	0	-2.404516	0.068557	-1.034458
30	6	0	-2.414744	2.354805	-0.373778
31	1	0	-1.337351	2.250618	-0.251702
32	6	0	-2.981346	3.597641	-0.070899
33	1	0	-3.979352	3.853856	-0.420910
34	1	0	-2.299267	4.440671	-0.041154
35	6	0	4.160305	-0.555602	0.320150
36	6	0	5.067658	-1.575595	0.652405
37	6	0	4.886300	-2.375571	1.778448
38	6	0	3.780185	-2.166091	2.606023
39	6	0	2.860052	-1.165344	2.298353
40	6	0	3.044056	-0.375992	1.162034
41	6	0	4.398864	0.320760	-0.849503
42	6	0	5.683635	0.811187	-1.135672
43	6	0	5.919551	1.630774	-2.237303
44	6	0	4.862314	1.986055	-3.078974
45	6	0	3.577797	1.514346	-2.816118
46	6	0	3.353034	0.686768	-1.717087
47	1	0	5.920558	-1.744054	0.000468
48	1	0	5.603300	-3.159565	2.006643
49	1	0	3.633536	-2.779341	3.491668
50	1	0	1.988557	-0.972528	2.913172
51	1	0	6.499634	0.558232	-0.464198
52	1	0	6.922354	2.001828	-2.430426
53	1	0	5.035813	2.632506	-3.935105
54	1	0	2.733434	1.769031	-3.447837
55	8	0	2.162508	0.662428	0.949203
56	8	0	2.093824	0.149868	-1.540663
57	15	0	1.111561	0.701431	-0.325113
58	8	0	0.064194	-0.397080	-0.186457
59	8	0	0.681970	2.116289	-0.512439
60	6	0	0.004544	-2.974884	1.674465
61	1	0	0.391746	-3.058975	2.692598
62	1	0	-0.216062	-3.960606	1.263473
63	1	0	0.710887	-2.431485	1.045881
64	6	0	-2.038944	1.870499	2.725049
65	1	0	-1.084530	1.614011	3.166391

TS-Ct(R-en)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2023.707664 hartree

Sum of electronic and thermal Free Energies = -2023.260677 hartree

The number of imaginary frequency = 1

Imaginary frequency = -336.41

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.121292	-3.649361	1.572146
2	1	0	0.691832	-3.140303	1.064482
3	1	0	0.201424	-4.407372	2.281580
4	6	0	-1.355532	-3.814172	0.948791
5	1	0	-2.029290	-4.557127	1.374390
6	6	0	-1.197419	-1.968494	-0.656429
7	1	0	-0.128929	-1.881772	-0.491551
8	1	0	-0.860909	-0.412614	-1.907431
9	7	0	-1.625577	-1.007415	-1.518143
10	6	0	-2.900695	-0.608839	-1.896287
11	8	0	-3.878265	-1.345686	-1.324806
12	8	0	-3.094726	0.324481	-2.645218
13	1	0	-1.004923	1.143325	0.618386
14	6	0	-5.394164	2.829513	-0.108439

15	6	0	-5.480983	1.746241	0.749286
16	6	0	-4.319887	1.040909	1.128697
17	6	0	-3.065242	1.476458	0.628829
18	6	0	-2.980467	2.572672	-0.251019
19	6	0	-4.140193	3.235123	-0.610682
20	1	0	-5.273910	-0.463914	2.373196
21	1	0	-6.291796	3.365817	-0.401047
22	1	0	-6.443426	1.420476	1.136265
23	6	0	-4.323462	-0.109124	1.981930
24	1	0	-2.008890	2.862121	-0.639405
25	1	0	-4.082543	4.074573	-1.296889
26	6	0	-1.903705	-0.293901	1.799941
27	6	0	-3.168058	-0.757158	2.300465
28	1	0	-3.183884	-1.630555	2.940233
29	7	0	-1.928271	0.800437	0.995493
30	6	0	-0.639097	-0.857549	2.109598
31	1	0	0.226941	-0.349284	1.700103
32	6	0	-0.428650	-2.008182	2.865580
33	1	0	-1.229552	-2.437591	3.459530
34	1	0	0.560008	-2.149596	3.292206
35	6	0	-5.210791	-0.959339	-1.707883
36	1	0	-5.386687	0.091913	-1.472603
37	1	0	-5.359619	-1.122001	-2.778779
38	1	0	-5.872796	-1.601995	-1.126207
39	6	0	4.350440	-0.465120	-0.230160
40	6	0	5.493770	-1.218208	-0.540760
41	6	0	5.401299	-2.545722	-0.954433
42	6	0	4.147749	-3.148139	-1.079430
43	6	0	2.996852	-2.421522	-0.778337
44	6	0	3.098386	-1.099488	-0.346612
45	6	0	4.459466	0.944210	0.209896
46	6	0	5.443875	1.347883	1.126344
47	6	0	5.558673	2.676880	1.528395
48	6	0	4.679015	3.636504	1.020740
49	6	0	3.692685	3.262068	0.110133
50	6	0	3.592432	1.932325	-0.292075
51	1	0	6.466091	-0.737914	-0.474805
52	1	0	6.303032	-3.101779	-1.194710
53	1	0	4.063194	-4.177328	-1.417214
54	1	0	2.011614	-2.864495	-0.881059
55	1	0	6.111864	0.596546	1.538773
56	1	0	6.325619	2.961024	2.243521
57	1	0	4.757867	4.673679	1.334713
58	1	0	2.994696	3.980046	-0.306794
59	8	0	1.950301	-0.443949	0.057805
60	8	0	2.668114	1.605761	-1.271016
61	15	0	1.299767	0.797905	-0.862832
62	8	0	0.703414	0.229206	-2.116002
63	8	0	0.465054	1.597249	0.109011
64	6	0	-1.907931	-2.987678	-0.051369
65	1	0	-2.950146	-3.122860	-0.307175

TS-Ct(S-en)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2023.707807 hartree

Sum of electronic and thermal Free Energies = -2023.260101 hartree

The number of imaginary frequency = 1

Imaginary frequency = -330.85

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.184000	3.012520	3.180454
2	1	0	0.237875	2.480788	3.198614
3	1	0	1.139418	4.020276	3.585186
4	6	0	2.382868	2.312676	3.262607
5	1	0	3.273714	2.878702	3.532982
6	6	0	1.576562	0.179539	2.377811
7	1	0	0.542165	0.481000	2.504704
8	1	0	0.686202	-1.432704	1.577379
9	7	0	1.629499	-1.043743	1.788840
10	6	0	2.688794	-1.790303	1.293467
11	8	0	3.885343	-1.185855	1.461735
12	8	0	2.531312	-2.862783	0.749929
13	1	0	0.973073	0.026487	-0.936681
14	6	0	4.988724	-1.554257	-2.898925
15	6	0	5.261966	-0.346519	-2.280970
16	6	0	4.244444	0.349067	-1.594347
17	6	0	2.938960	-0.207640	-1.565080
18	6	0	2.665111	-1.444029	-2.183477
19	6	0	3.688893	-2.101500	-2.842005
20	1	0	5.437491	2.030312	-0.908482
21	1	0	5.775559	-2.087056	-3.424449
22	1	0	6.261905	0.079031	-2.310827
23	6	0	4.444682	1.586912	-0.906330
24	1	0	1.661889	-1.853127	-2.117799
25	1	0	3.487589	-3.057142	-3.316627
26	6	0	2.101825	1.637672	-0.249765
27	6	0	3.420094	2.205920	-0.253723
28	1	0	3.585849	3.137149	0.272905
29	7	0	1.937313	0.464551	-0.909232
30	6	0	0.962787	2.226908	0.364967
31	1	0	0.024919	1.692393	0.263043
32	6	0	0.968379	3.416640	1.086407
33	1	0	1.805184	4.103812	1.017296
34	1	0	0.012150	3.899857	1.262505
35	6	0	5.005370	-1.943229	0.966416
36	1	0	5.112601	-2.873064	1.531569
37	1	0	4.874145	-2.173837	-0.091873
38	1	0	5.873179	-1.299977	1.115142
39	6	0	-4.284650	0.710843	-0.840047
40	6	0	-5.130974	1.375354	-1.741909
41	6	0	-4.706229	2.501541	-2.443941
42	6	0	-3.409404	2.986254	-2.259971
43	6	0	-2.548087	2.344441	-1.371647
44	6	0	-2.984332	1.223143	-0.667215
45	6	0	-4.751729	-0.474874	-0.085907
46	6	0	-6.032929	-0.513096	0.487666
47	6	0	-6.481170	-1.631436	1.187330
48	6	0	-5.646242	-2.742134	1.333649
49	6	0	-4.369709	-2.729960	0.774476
50	6	0	-3.934913	-1.609941	0.069740

51	1	0	-6.130791	0.981645	-1.902690
52	1	0	-5.380854	2.991112	-3.140684
53	1	0	-3.066136	3.858805	-2.809234
54	1	0	-1.535915	2.700415	-1.209189
55	1	0	-6.671684	0.361074	0.395195
56	1	0	-7.474746	-1.631612	1.626860
57	1	0	-5.985646	-3.615038	1.884438
58	1	0	-3.695776	-3.575035	0.865429
59	8	0	-2.143529	0.672083	0.283547
60	8	0	-2.703674	-1.664788	-0.562338
61	15	0	-1.433061	-0.813773	0.032867
62	8	0	-0.433668	-0.708456	-1.094377
63	8	0	-1.008340	-1.285592	1.395415
64	6	0	2.601399	0.986067	2.836914
65	1	0	3.618384	0.620324	2.793848

TS-Ct(R-ex)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2023.687304 hartree

Sum of electronic and thermal Free Energies = -2023.240457 hartree

The number of imaginary frequency = 1

Imaginary frequency = -350.83

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.323006	-2.788704	3.438304
2	1	0	3.349987	-2.546688	3.176423
3	1	0	2.200490	-3.100673	4.472367
4	6	0	1.474267	-3.342179	2.475967
5	1	0	0.576134	-3.844393	2.830262
6	6	0	2.557894	-2.380678	0.528746
7	1	0	3.403719	-2.095812	1.144214
8	1	0	3.510296	-1.341263	-0.935083
9	7	0	2.724529	-1.952793	-0.756827
10	6	0	1.896256	-2.036458	-1.894757
11	8	0	0.944228	-2.945629	-1.746585
12	8	0	2.135358	-1.365430	-2.875580
13	1	0	1.105579	0.411835	-0.106248
14	6	0	4.363730	2.890225	-2.498945
15	6	0	4.859404	2.648338	-1.230427
16	6	0	4.083692	1.941726	-0.286592
17	6	0	2.786635	1.500422	-0.661928
18	6	0	2.290555	1.732507	-1.960336
19	6	0	3.081899	2.422835	-2.860361
20	1	0	5.520892	1.936652	1.343419
21	1	0	4.964086	3.432142	-3.223416
22	1	0	5.850152	2.993267	-0.945307
23	6	0	4.529565	1.614017	1.033856
24	1	0	1.314819	1.340808	-2.227812
25	1	0	2.710794	2.599914	-3.865392
26	6	0	2.423178	0.487967	1.506183
27	6	0	3.738059	0.913672	1.898020
28	1	0	4.083626	0.680686	2.898494
29	7	0	2.024486	0.810952	0.247749
30	6	0	1.515352	-0.235582	2.314335
31	1	0	0.538578	-0.412764	1.881573
32	6	0	1.754516	-0.778798	3.580280
33	1	0	2.631906	-0.479829	4.149867
34	1	0	0.883542	-0.982604	4.193741
35	6	0	-0.095160	-2.929246	-2.748167
36	1	0	-0.393311	-1.898797	-2.944627
37	1	0	0.267169	-3.404785	-3.663911
38	1	0	-0.917667	-3.483661	-2.300685
39	6	0	-3.277359	1.746639	0.493136
40	6	0	-3.579681	3.117388	0.472182
41	6	0	-2.676284	4.070046	0.939750
42	6	0	-1.438658	3.663777	1.443300
43	6	0	-1.113426	2.308693	1.475434
44	6	0	-2.022562	1.361114	1.004843
45	6	0	-4.254164	0.741058	0.015709
46	6	0	-5.614681	0.835555	0.348916
47	6	0	-6.539737	-0.101903	-0.106219
48	6	0	-6.115214	-1.165677	-0.906334
49	6	0	-4.769886	-1.281822	-1.251282
50	6	0	-3.852742	-0.334927	-0.798806
51	1	0	-4.535490	3.432093	0.062176
52	1	0	-2.934655	5.124732	0.903831
53	1	0	-0.726656	4.398495	1.809940
54	1	0	-0.166737	1.964747	1.878429
55	1	0	-5.938442	1.649182	0.992446
56	1	0	-7.585793	-0.009217	0.172373
57	1	0	-6.828693	-1.905621	-1.258843
58	1	0	-4.407140	-2.092911	-1.873780
59	8	0	-1.707514	0.022274	1.131388
60	8	0	-2.547874	-0.409936	-1.242168
61	15	0	-1.336600	-0.888090	-0.217683
62	8	0	-0.081492	-0.310742	-0.849240
63	8	0	-1.434608	-2.322331	0.168140
64	6	0	1.533518	-3.116636	1.085408
65	1	0	0.692123	-3.417166	0.475398

TS-Ct(S-ex)

Not Detected.

TS-Tc(R-en)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2023.694312 hartree

Sum of electronic and thermal Free Energies = -2023.248883 hartree

The number of imaginary frequency = 1

Imaginary frequency = -390.00

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.113075	4.441074	0.548393
2	1	0	-0.283422	3.741966	0.463831
3	1	0	-0.857955	5.481133	0.355151
4	6	0	-2.140173	4.207271	1.468458

5	1	0	-2.779679	5.048223	1.734565
6	6	0	-1.946471	1.746149	1.652386
7	1	0	-0.950993	1.657229	1.211696
8	1	0	-3.512598	0.609643	2.359477
9	7	0	-2.573898	0.574385	1.979446
10	6	0	-2.026694	-0.698085	1.854313
11	8	0	-2.932528	-1.592115	2.304820
12	8	0	-0.932362	-0.953712	1.411314
13	1	0	-1.083445	0.107831	-1.384435
14	6	0	-4.382971	-3.301543	-1.131180
15	6	0	-5.015252	-2.078115	-0.978768
16	6	0	-4.277046	-0.879691	-1.044674
17	6	0	-2.876750	-0.951952	-1.263810
18	6	0	-2.230764	-2.197053	-1.402243
19	6	0	-2.989716	-3.354362	-1.343973
20	1	0	-5.917560	0.513353	-0.724598
21	1	0	-4.958663	-4.221188	-1.086996
22	1	0	-6.088333	-2.026990	-0.811219
23	6	0	-4.846678	0.429664	-0.895389
24	1	0	-1.153749	-2.214593	-1.540613
25	1	0	-2.500762	-4.317772	-1.460207
26	6	0	-2.662244	1.456872	-1.208530
27	6	0	-4.079485	1.553193	-0.983837
28	1	0	-4.521636	2.537400	-0.882144
29	7	0	-2.146076	0.204025	-1.325941
30	6	0	-1.760583	2.532542	-1.370484
31	1	0	-0.740179	2.247240	-1.595325
32	6	0	-2.003224	3.899442	-1.187395
33	1	0	-3.020830	4.261552	-1.062677
34	1	0	-1.372026	4.582230	-1.750684
35	6	0	-2.489070	-2.961944	2.280862
36	1	0	-1.596240	-3.081768	2.900543
37	1	0	-3.320396	-3.539192	2.685923
38	1	0	-2.270711	-3.269289	1.256952
39	6	0	3.879632	-1.453569	0.028387
40	6	0	4.522753	-2.673271	-0.237422
41	6	0	3.845676	-3.886498	-0.127639
42	6	0	2.499698	-3.903312	0.250310
43	6	0	1.836657	-2.707214	0.519341
44	6	0	2.527577	-1.501099	0.412546
45	6	0	4.595282	-0.159682	-0.056822
46	6	0	5.900293	-0.028061	0.445145
47	6	0	6.591579	1.179527	0.376294
48	6	0	5.978934	2.296391	-0.196792
49	6	0	4.684310	2.194091	-0.701515
50	6	0	4.000087	0.979945	-0.637646
51	1	0	5.562232	-2.658544	-0.554003
52	1	0	4.364321	-4.816013	-0.346537
53	1	0	1.967422	-4.847839	0.332010
54	1	0	0.795274	-2.668891	0.819925
55	1	0	6.364390	-0.890946	0.915293
56	1	0	7.598147	1.251307	0.779128
57	1	0	6.505934	3.245405	-0.249815
58	1	0	4.182343	3.039183	-1.161066
59	8	0	1.884091	-0.332645	0.763894
60	8	0	2.773312	0.900046	-1.259891
61	15	0	1.355302	0.669278	-0.432946
62	8	0	0.467735	-0.064550	-1.416711
63	8	0	0.872744	1.925852	0.229159
64	6	0	-2.565326	2.946595	1.927717
65	1	0	-3.506262	2.914457	2.478590

TS-Tc(S-en)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2023.693798 hartree

Sum of electronic and thermal Free Energies = - -2023.248044 hartree

The number of imaginary frequency = 1

Imaginary frequency = -385.27

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.332021	4.286239	-0.267166
2	1	0	0.484478	3.607565	-0.194582
3	1	0	1.089707	5.284321	-0.626337
4	6	0	2.401712	4.178914	0.628355
5	1	0	3.086238	5.023732	0.696698
6	6	0	2.093676	1.823097	1.297907
7	1	0	1.053327	1.728606	0.972012
8	1	0	3.680608	0.641703	1.887350
9	7	0	2.677486	0.671903	1.746969
10	6	0	1.988889	-0.514488	1.987549
11	8	0	2.888893	-1.481190	2.263531
12	8	0	0.788556	-0.644572	1.956699
13	1	0	1.105683	-0.314872	-1.475006
14	6	0	4.295973	-3.695878	-0.473495
15	6	0	4.963085	-2.483893	-0.558722
16	6	0	4.261846	-1.302860	-0.869096
17	6	0	2.861826	-1.377679	-1.087026
18	6	0	2.181940	-2.607511	-0.990863
19	6	0	2.904752	-3.751150	-0.692021
20	1	0	5.942367	0.078724	-0.814298
21	1	0	4.844008	-4.604023	-0.240859
22	1	0	6.035971	-2.430284	-0.390421
23	6	0	4.869487	-0.005862	-0.972243
24	1	0	1.107120	-2.624678	-1.147713
25	1	0	2.387680	-4.704146	-0.622120
26	6	0	2.715945	1.005073	-1.493871
27	6	0	4.135757	1.100793	-1.281095
28	1	0	4.606602	2.073065	-1.366375
29	7	0	2.164689	-0.234204	-1.379284
30	6	0	1.847668	2.058510	-1.852979
31	1	0	0.817758	1.768305	-2.018723
32	6	0	2.135529	3.427664	-1.918170
33	1	0	3.166296	3.771445	-1.885594
34	1	0	1.507066	4.023766	-2.575122
35	6	0	2.313081	-2.757763	2.599701
36	1	0	1.587316	-3.056032	1.842167
37	1	0	3.151924	-3.452727	2.622836
38	1	0	1.823940	-2.703328	3.576684
39	6	0	-4.512370	-0.454517	-0.469695
40	6	0	-5.631737	-1.243976	-0.779637

41	6	0	-5.968098	-1.548199	-2.097036
42	6	0	-5.175894	-1.069324	-3.143234
43	6	0	-4.058902	-0.284509	-2.863758
44	6	0	-3.733847	0.024772	-1.543232
45	6	0	-4.170275	-0.140980	0.936690
46	6	0	-5.156498	0.199393	1.876541
47	6	0	-4.827866	0.469282	3.203686
48	6	0	-3.494434	0.407837	3.619132
49	6	0	-2.495131	0.073161	2.706986
50	6	0	-2.838079	-0.202300	1.384717
51	1	0	-6.230566	-1.638457	0.036924
52	1	0	-6.837091	-2.166470	-2.305094
53	1	0	-5.424689	-1.307234	-4.174081
54	1	0	-3.425506	0.109199	-3.651807
55	1	0	-6.189762	0.271130	1.547522
56	1	0	-5.609214	0.738005	3.909547
57	1	0	-3.233048	0.624581	4.651743
58	1	0	-1.448435	0.010172	2.983494
59	8	0	-2.691915	0.900807	-1.321206
60	8	0	-1.849663	-0.622739	0.517156
61	15	0	-1.271805	0.425308	-0.613952
62	8	0	-0.465152	-0.427172	-1.573441
63	8	0	-0.667094	1.662152	-0.018052
64	6	0	2.806942	3.002553	1.285992
65	1	0	3.791073	3.007742	1.755637

TS-Tc(R-ex)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2023.714856 hartree

Sum of electronic and thermal Free Energies = - -2023.266667 hartree

The number of imaginary frequency = 1

Imaginary frequency = -352.47

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.746135	3.277321	1.086334
2	1	0	5.206095	2.293163	1.100738
3	1	0	5.451779	4.097421	0.981163
4	6	0	3.557832	3.499546	1.778443
5	1	0	3.275613	4.533035	1.972969
6	6	0	2.787556	1.182327	1.799425
7	1	0	3.767970	0.782313	1.566571
8	1	0	0.824858	0.563098	1.970205
9	7	0	1.817897	0.240011	1.899052
10	6	0	2.106235	-1.100549	1.702207
11	8	0	0.971607	-1.822411	1.769259
12	8	0	3.214637	-1.556859	1.493000
13	1	0	1.065782	0.561953	-1.153206
14	6	0	1.725408	-4.057163	-2.090744
15	6	0	2.964987	-3.445830	-2.022218
16	6	0	3.065951	-2.062920	-1.761537
17	6	0	1.874232	-1.317325	-1.567485
18	6	0	0.612135	-1.942519	-1.626692
19	6	0	0.551659	-3.299103	-1.891658
20	1	0	5.231071	-1.907752	-1.824025
21	1	0	1.653493	-5.121366	-2.294435
22	1	0	3.876026	-4.020250	-2.168515
23	6	0	4.305878	-1.354471	-1.685013
24	1	0	-0.283603	-1.357855	-1.445442
25	1	0	-0.417742	-3.786941	-1.938274
26	6	0	3.126921	0.726245	-1.244817
27	6	0	4.339940	-0.013435	-1.442685
28	1	0	5.285276	0.513124	-1.388051
29	7	0	1.963883	0.028136	-1.310059
30	6	0	3.038463	2.121491	-1.004446
31	1	0	2.030723	2.504776	-0.874327
32	6	0	4.107228	3.014100	-0.930611
33	1	0	5.096207	2.718436	-1.271868
34	1	0	3.888337	4.065566	-1.079626
35	6	0	1.139825	-3.241553	1.610733
36	1	0	1.657779	-3.657616	2.480049
37	1	0	0.128507	-3.641689	1.537660
38	1	0	1.705781	-3.464858	0.705559
39	6	0	-4.249073	0.527175	-0.573550
40	6	0	-5.259022	0.282918	-1.518155
41	6	0	-5.488583	1.155412	-2.579904
42	6	0	-4.699174	2.299080	-2.722984
43	6	0	-3.689887	2.565644	-1.799592
44	6	0	-3.473827	1.692453	-0.735555
45	6	0	-4.018297	-0.402425	0.555987
46	6	0	-5.085112	-0.958572	1.279662
47	6	0	-4.861545	-1.834450	2.340566
48	6	0	-3.554697	-2.163850	2.710037
49	6	0	-2.477114	-1.627003	2.007134
50	6	0	-2.714266	-0.768540	0.935939
51	1	0	-5.855692	-0.619941	-1.419581
52	1	0	-6.273495	0.937772	-3.298896
53	1	0	-4.866276	2.981400	-3.551929
54	1	0	-3.061829	3.446783	-1.876526
55	1	0	-6.100008	-0.675400	1.014213
56	1	0	-5.704998	-2.244333	2.889202
57	1	0	-3.374323	-2.831216	3.548574
58	1	0	-1.447851	-1.842057	2.271323
59	8	0	-2.536187	2.046097	0.219847
60	8	0	-1.639063	-0.330372	0.183994
61	15	0	-1.110543	1.238066	0.337386
62	8	0	-0.248764	1.462707	-0.882897
63	8	0	-0.577002	1.479533	1.723072
64	6	0	2.579259	2.523084	2.047579
65	1	0	1.590089	2.832354	2.374113

TS-Tc(S-ex)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2023.710495 hartree

Sum of electronic and thermal Free Energies = - -2023.265121 hartree

The number of imaginary frequency = 1

Imaginary frequency = -348.50

Center Atomic Atomic Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-3.619777	4.276130	-0.904269
2	1	0	-4.369552	3.649757	-0.429461
3	1	0	-4.027674	5.112135	-1.466486
4	6	0	-2.356570	4.405108	-0.331567
5	1	0	-1.735703	5.234443	-0.666888
6	6	0	-2.382826	2.310960	0.925658
7	1	0	-3.459126	2.203300	0.847443
8	1	0	-0.723925	1.239580	1.561678
9	7	0	-1.773227	1.285115	1.562546
10	6	0	-2.509587	0.222867	2.065198
11	8	0	-1.674831	-0.689110	2.592170
12	8	0	-3.722565	0.128760	2.026328
13	1	0	-1.170906	-0.127492	-1.078355
14	6	0	-3.181081	-4.176996	0.366312
15	6	0	-4.187261	-3.317063	-0.038914
16	6	0	-3.875532	-2.026942	-0.517726
17	6	0	-2.513608	-1.635920	-0.576217
18	6	0	-1.491338	-2.503629	-0.142191
19	6	0	-1.832420	-3.762775	0.316758
20	1	0	-5.901211	-1.348106	-0.911156
21	1	0	-3.427617	-5.169524	0.731164
22	1	0	-5.229252	-3.622735	0.007162
23	6	0	-4.850067	-1.075326	-0.956215
24	1	0	-0.463627	-2.156407	-0.164812
25	1	0	-1.050161	-4.437691	0.652465
26	6	0	-3.096849	0.525373	-1.486406
27	6	0	-4.480784	0.151670	-1.422481
28	1	0	-5.227513	0.862524	-1.755741
29	7	0	-2.194930	-0.389123	-1.047505
30	6	0	-2.585343	1.749011	-1.988124
31	1	0	-1.501979	1.827025	-1.988336
32	6	0	-3.327748	2.829920	-2.458804
33	1	0	-4.391817	2.725327	-2.655735
34	1	0	-2.825874	3.534547	-3.112306
35	6	0	-2.319178	-1.817678	3.205271
36	1	0	-2.993108	-2.307951	2.500795
37	1	0	-1.509252	-2.488522	3.491225
38	1	0	-2.882326	-1.496910	4.086764
39	6	0	4.232565	-1.039631	-0.461902
40	6	0	5.143184	-1.856096	-1.151732
41	6	0	4.778359	-3.111636	-1.632611
42	6	0	3.477192	-3.577976	-1.434085
43	6	0	2.553729	-2.786296	-0.754161
44	6	0	2.925987	-1.531810	-0.272119
45	6	0	4.644256	0.283691	0.058930
46	6	0	5.886144	0.464104	0.689104
47	6	0	6.282964	1.711912	1.165113
48	6	0	5.434722	2.813184	1.024047
49	6	0	4.196319	2.660322	0.403467
50	6	0	3.813101	1.410102	-0.076503
51	1	0	6.148016	-1.480955	-1.325136
52	1	0	5.502951	-3.717950	-2.168820
53	1	0	3.179391	-4.553289	-1.809425
54	1	0	1.539297	-3.129484	-0.581228
55	1	0	6.533955	-0.398114	0.821521
56	1	0	7.246279	1.822099	1.655240
57	1	0	5.733773	3.787789	1.399978
58	1	0	3.512766	3.492854	0.275815
59	8	0	2.013441	-0.823759	0.487329
60	8	0	2.622322	1.304955	-0.775021
61	15	0	1.326865	0.580169	-0.067776
62	8	0	0.367737	0.269019	-1.191838
63	8	0	0.872627	1.342240	1.147549
64	6	0	-1.725125	3.436979	0.472866
65	1	0	-0.662111	3.523076	0.681668

TS-Tt(R-en)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2023.698467 hartree

Sum of electronic and thermal Free Energies = - -2023.251588 hartree

The number of imaginary frequency = 1

Imaginary frequency = -348.02

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.174458	4.024303	1.153009
2	1	0	-0.363902	3.312077	1.290851
3	1	0	-0.869089	5.067827	1.113012
4	6	0	-2.451863	3.747713	1.645303
5	1	0	-3.162269	4.572523	1.691551
6	6	0	-2.219082	1.309605	1.897169
7	1	0	-1.128314	1.308397	1.906421
8	1	0	-3.782465	-0.012913	1.660371
9	7	0	-2.801193	0.078039	1.897744
10	6	0	-2.173030	-1.160786	2.093222
11	8	0	-0.977875	-1.013322	2.657502
12	8	0	-2.723349	-2.202754	1.803369
13	1	0	-1.218877	-0.314316	-0.859334
14	6	0	-5.054285	-2.959667	-1.749517
15	6	0	-5.429003	-1.627284	-1.785322
16	6	0	-4.471855	-0.612250	-1.583698
17	6	0	-3.121707	-0.983223	-1.352085
18	6	0	-2.746001	-2.338469	-1.302449
19	6	0	-3.711533	-3.309203	-1.502552
20	1	0	-5.804166	1.098838	-1.748473
21	1	0	-5.795550	-3.737926	-1.903807
22	1	0	-6.463419	-1.346331	-1.967435
23	6	0	-4.775251	0.789435	-1.580058
24	1	0	-1.712459	-2.589617	-1.087734
25	1	0	-3.429158	-4.356875	-1.458585
26	6	0	-2.436748	1.335306	-1.170188
27	6	0	-3.804654	1.725814	-1.382123
28	1	0	-4.044981	2.781948	-1.394174
29	7	0	-2.181034	-0.001422	-1.155267
30	6	0	-1.344348	2.219646	-1.022084
31	1	0	-0.360575	1.770770	-0.992756
32	6	0	-1.406537	3.605659	-0.848361
33	1	0	-2.326248	4.146065	-1.053467
34	1	0	-0.510956	4.169340	-1.096262

35	6	0	-0.182822	-2.214812	2.726684
36	1	0	0.782046	-1.889116	3.111417
37	1	0	-0.658901	-2.938749	3.393305
38	1	0	-0.068649	-2.627955	1.723830
39	6	0	4.340643	0.421737	-0.580505
40	6	0	5.588098	1.065617	-0.567227
41	6	0	5.701090	2.434036	-0.805120
42	6	0	4.555941	3.193249	-1.058381
43	6	0	3.305744	2.577655	-1.075662
44	6	0	3.202898	1.207238	-0.844898
45	6	0	4.225506	-1.036660	-0.349308
46	6	0	5.127611	-1.934540	-0.942295
47	6	0	5.037864	-3.307840	-0.724629
48	6	0	4.027990	-3.816010	0.095494
49	6	0	3.118902	-2.946334	0.695051
50	6	0	3.219531	-1.573153	0.477908
51	1	0	6.475377	0.478585	-0.346266
52	1	0	6.678321	2.908133	-0.781917
53	1	0	4.635141	4.262067	-1.237941
54	1	0	2.396409	3.136435	-1.272345
55	1	0	5.897380	-1.539388	-1.599524
56	1	0	5.746439	-3.978954	-1.201907
57	1	0	3.945830	-4.885829	0.267255
58	1	0	2.328604	-3.309979	1.342950
59	8	0	1.966344	0.603437	-0.961896
60	8	0	2.369573	-0.734544	1.175016
61	15	0	1.165465	0.096318	0.404128
62	8	0	0.796758	1.264456	1.263034
63	8	0	0.121950	-0.871902	-0.114085
64	6	0	-2.976072	2.463132	1.884002
65	1	0	-4.054596	2.371414	2.009893

TS-Tt(S-en)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2023.698491 hartree

Sum of electronic and thermal Free Energies = -2023.250898 hartree

The number of imaginary frequency = 1

Imaginary frequency = -375.61

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.459465	-0.408965	-1.393917
2	1	0	-5.079391	-1.415501	-1.544195
3	1	0	-6.256990	-0.137625	-2.081640
4	6	0	-5.492953	0.122788	-0.101865
5	1	0	-6.160648	0.961354	0.087555
6	6	0	-3.588127	-1.153945	0.782694
7	1	0	-3.609237	-1.908828	0.008144
8	1	0	-2.362504	-0.548906	2.321769
9	7	0	-2.558438	-1.288157	1.657423
10	6	0	-1.612626	-2.334560	1.707645
11	8	0	-2.009903	-3.363450	0.965361
12	8	0	-0.635714	-2.252957	2.417429
13	1	0	-0.644381	-0.184820	-0.091764
14	6	0	0.801542	3.169173	2.997661
15	6	0	-0.293555	3.654851	2.308522
16	6	0	-0.948107	2.849105	1.350653
17	6	0	-0.449372	1.542587	1.101436
18	6	0	0.648683	1.039102	1.828095
19	6	0	1.262233	1.855522	2.759440
20	1	0	-2.504375	4.256847	0.795002
21	1	0	1.304353	3.792965	3.730659
22	1	0	-0.667416	4.658673	2.494119
23	6	0	-2.098678	3.264246	0.614198
24	1	0	0.991742	0.027810	1.640344
25	1	0	2.115801	1.475899	3.313163
26	6	0	-2.146161	1.139250	-0.568075
27	6	0	-2.687135	2.439885	-0.301360
28	1	0	-3.560572	2.766127	-0.851417
29	7	0	-1.060619	0.764214	0.151024
30	6	0	-2.658361	0.227645	-1.536459
31	1	0	-2.089096	-0.686079	-1.676652
32	6	0	-3.811745	0.451738	-2.295824
33	1	0	-4.218205	1.454855	-2.383515
34	1	0	-3.927002	-0.137059	-3.201973
35	6	0	-1.057344	-4.445390	0.814678
36	1	0	-1.645749	-5.288252	0.450997
37	1	0	-0.292446	-4.162902	0.089144
38	1	0	-0.603420	-4.676078	1.780583
39	6	0	3.507460	0.323469	-0.460925
40	6	0	4.810395	0.843164	-0.404529
41	6	0	5.830150	0.172925	0.267971
42	6	0	5.563288	-1.046262	0.896525
43	6	0	4.277521	-1.582317	0.857581
44	6	0	3.260602	-0.902234	0.188308
45	6	0	2.430449	1.043801	-1.176973
46	6	0	2.267903	2.432141	-1.044766
47	6	0	1.263199	3.113789	-1.728875
48	6	0	0.400805	2.413380	-2.576605
49	6	0	0.541183	1.034748	-2.724515
50	6	0	1.539879	0.356252	-2.025344
51	1	0	5.020796	1.777790	-0.917593
52	1	0	6.831921	0.592894	0.289028
53	1	0	6.354579	-1.580054	1.415857
54	1	0	4.032609	-2.521063	1.343118
55	1	0	2.924462	2.970361	-0.366919
56	1	0	1.149181	4.185829	-1.594513
57	1	0	-0.388043	2.935775	-3.111102
58	1	0	-0.120443	0.459116	-3.362561
59	8	0	1.976294	-1.387383	0.287919
60	8	0	1.672426	-1.003567	-2.208129
61	15	0	1.114955	-2.010248	-1.003923
62	8	0	1.484998	-3.409023	-1.324071
63	8	0	-0.317545	-1.618134	-0.668861
64	6	0	-4.567621	-0.184227	0.908818
65	1	0	-4.555167	0.438349	1.801744

TS-Tt(R-ex)

B3LYP-D3/6-31g(d) in ga sphase

SCF Done: E(RB3LYP) = -2023.710855 hartree

Sum of electronic and thermal Free Energies = -2023.262974 hartree
The number of imaginary frequency = 1
Imaginary frequency = -352.13

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.461138	-3.460804	-1.069262
2	1	0	4.963483	-2.497996	-1.032019
3	1	0	5.127732	-4.314670	-0.978229
4	6	0	3.285187	-3.604225	-1.802713
5	1	0	2.960943	-4.617128	-2.035832
6	6	0	2.621864	-1.247839	-1.802918
7	1	0	3.614913	-0.902787	-1.543255
8	1	0	0.679367	-0.581836	-2.004407
9	7	0	1.680227	-0.276902	-1.913748
10	6	0	1.887056	1.081654	-1.759302
11	8	0	3.183401	1.376712	-1.507512
12	8	0	1.000236	1.907293	-1.840733
13	1	0	0.960385	-0.547683	1.082989
14	6	0	2.024853	4.000220	2.070933
15	6	0	3.187692	3.253664	2.140603
16	6	0	3.163953	1.869832	1.866765
17	6	0	1.924403	1.257857	1.539318
18	6	0	0.743541	2.022625	1.456214
19	6	0	0.807183	3.379328	1.720469
20	1	0	5.287877	1.487848	2.114109
21	1	0	2.048026	5.065910	2.277942
22	1	0	4.134585	3.722220	2.397196
23	6	0	4.327430	1.038316	1.873278
24	1	0	-0.186281	1.544300	1.164908
25	1	0	-0.098181	3.974484	1.647973
26	6	0	2.984079	-0.901806	1.281280
27	6	0	4.247825	-0.291241	1.581848
28	1	0	5.136693	-0.910655	1.588236
29	7	0	1.893775	-0.090398	1.279336
30	6	0	2.782321	-2.278068	1.007705
31	1	0	1.752059	-2.569624	0.828907
32	6	0	3.777531	-3.252320	0.932891
33	1	0	4.775564	-3.055024	1.316541
34	1	0	3.469388	-4.287550	1.029116
35	6	0	3.467050	2.784165	-1.415355
36	1	0	2.822139	3.259315	-0.674799
37	1	0	4.512230	2.846417	-1.111002
38	1	0	3.320700	3.262502	-2.388017
39	6	0	-4.069135	0.597468	-0.557996
40	6	0	-5.097007	1.220800	-1.283782
41	6	0	-4.813708	2.133490	-2.298184
42	6	0	-3.486653	2.439161	-2.613208
43	6	0	-2.445160	1.834605	-1.910569
44	6	0	-2.745182	0.930525	-0.894856
45	6	0	-4.362187	-0.351932	0.540960
46	6	0	-5.383409	-0.085918	1.467870
47	6	0	-5.673590	-0.967750	2.506788
48	6	0	-4.934041	-2.144512	2.646221
49	6	0	-3.914410	-2.433332	1.741215
50	6	0	-3.637628	-1.549916	0.699643
51	1	0	-6.128007	0.964299	-1.055720
52	1	0	-5.627450	2.596022	-2.850113
53	1	0	-3.261543	3.144056	-3.409112
54	1	0	-1.401329	2.041348	-2.121942
55	1	0	-5.940336	0.842370	1.373877
56	1	0	-6.466240	-0.731483	3.211323
57	1	0	-5.147923	-2.835274	3.457286
58	1	0	-3.324724	-3.341008	1.814380
59	8	0	-1.704202	0.408475	-0.143684
60	8	0	-2.695616	-1.931193	-0.240084
61	15	0	-1.246541	-1.169886	-0.361915
62	8	0	-0.753096	-1.401343	-1.765380
63	8	0	-0.358902	-1.458732	0.826975
64	6	0	2.361435	-2.576491	-2.072607
65	1	0	1.366861	-2.834007	-2.426862

TS-Tt(S-ex)

B3LYP-D3/6-31g(d) in gas phase
SCF Done: E(RB3LYP) = -2023.709229 hartree
Sum of electronic and thermal Free Energies = -2023.261170 hartree
The number of imaginary frequency = 1
Imaginary frequency = -342.56

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.211113	4.355611	0.926688
2	1	0	2.250346	4.043911	0.868485
3	1	0	1.044281	5.248857	1.523226
4	6	0	0.339260	4.076797	-0.122024
5	1	0	-0.601049	4.625920	-0.146679
6	6	0	1.584810	2.208540	-1.099522
7	1	0	2.508863	2.488961	-0.609354
8	1	0	0.739024	0.672215	-2.175761
9	7	0	1.643722	1.069637	-1.834292
10	6	0	2.771832	0.292896	-2.046140
11	8	0	3.873771	0.834675	-1.471599
12	8	0	2.759838	-0.743509	-2.673502
13	1	0	1.062573	-0.687090	0.526980
14	6	0	5.162381	-3.059657	0.533378
15	6	0	5.341503	-1.896822	1.261306
16	6	0	4.277961	-0.982634	1.416298
17	6	0	3.023134	-1.287663	0.825814
18	6	0	2.846733	-2.465553	0.071701
19	6	0	3.913947	-3.335222	-0.064932
20	1	0	5.340959	0.518262	2.572181
21	1	0	5.984020	-3.759485	0.414110
22	1	0	6.301913	-1.668402	1.716558
23	6	0	4.387457	0.257498	2.119129
24	1	0	1.884449	-2.651296	-0.394087
25	1	0	3.788098	-4.241436	-0.649791
26	6	0	2.054066	0.768152	1.648492
27	6	0	3.324196	1.105039	2.226073
28	1	0	3.419319	2.041059	2.763140

29	7	0	1.978746	-0.409421	0.977794
30	6	0	0.881019	1.560323	1.739460
31	1	0	-0.013333	1.149153	1.283951
32	6	0	0.787573	2.810151	2.347967
33	1	0	1.563955	3.161348	3.022718
34	1	0	-0.204948	3.172244	2.591623
35	6	0	5.092222	0.116472	-1.732578
36	1	0	5.854363	0.616963	-1.134555
37	1	0	4.995830	-0.928700	-1.435338
38	1	0	5.341326	0.170626	-2.796264
39	6	0	-4.365511	0.190770	0.137140
40	6	0	-5.607365	0.841029	0.055226
41	6	0	-5.697203	2.225863	-0.071855
42	6	0	-4.533340	2.996727	-0.122411
43	6	0	-3.288222	2.375471	-0.047138
44	6	0	-3.207745	0.989946	0.079797
45	6	0	-4.277881	-1.277346	0.311912
46	6	0	-5.132702	-1.951337	1.199440
47	6	0	-5.061585	-3.332315	1.369082
48	6	0	-4.119429	-4.073804	0.651757
49	6	0	-3.258704	-3.429686	-0.234916
50	6	0	-3.343975	-2.049386	-0.404151
51	1	0	-6.511825	0.239344	0.075072
52	1	0	-6.671999	2.700452	-0.140461
53	1	0	-4.594174	4.076921	-0.224558
54	1	0	-2.363474	2.941698	-0.075060
55	1	0	-5.846953	-1.370527	1.776676
56	1	0	-5.731574	-3.826472	2.067141
57	1	0	-4.052755	-5.150361	0.782993
58	1	0	-2.519157	-3.973237	-0.813161
59	8	0	-1.963278	0.416273	0.248638
60	8	0	-2.549775	-1.457467	-1.369974
61	15	0	-1.274519	-0.513480	-0.951182
62	8	0	-0.933364	0.326201	-2.149770
63	8	0	-0.210865	-1.308067	-0.231693
64	6	0	0.457624	3.003311	-1.026198
65	1	0	-0.397203	2.725904	-1.636142

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s-cis_Cc(R-en)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2023.696488 hartree

Sum of electronic and thermal Free Energies = -2023.248889 hartree

The number of imaginary frequency = 1

Imaginary frequency = -338.38

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.796413	-4.020231	0.455082
2	1	0	2.860947	-4.235060	0.403591
3	1	0	1.183969	-4.840656	0.819225
4	6	0	1.200093	-3.133278	-0.438083
5	1	0	0.118752	-3.190869	-0.515511
6	6	0	3.170810	-1.790056	-0.984187
7	1	0	3.848012	-2.531954	-0.577304
8	1	0	4.838920	-0.635909	-1.321333
9	7	0	3.834058	-0.660515	-1.424086
10	6	0	3.258723	0.537351	-1.825379
11	8	0	4.245437	1.442894	-2.027993
12	8	0	2.075940	0.749295	-1.972927
13	1	0	0.601931	-0.592301	1.708164
14	6	0	0.797439	3.991989	0.545989
15	6	0	2.091591	3.546344	0.736500
16	6	0	2.339588	2.199432	1.081632
17	6	0	1.239678	1.313651	1.239680
18	6	0	-0.077551	1.779222	1.057052
19	6	0	-0.284587	3.100468	0.708315
20	1	0	4.506063	2.324486	1.179578
21	1	0	0.610212	5.027570	0.277666
22	1	0	2.936337	4.222853	0.628900
23	6	0	3.646976	1.667015	1.287686
24	1	0	-0.904626	1.094541	1.183941
25	1	0	-1.302943	3.445698	0.561755
26	6	0	2.703151	-0.538680	1.736562
27	6	0	3.821877	0.352347	1.603546
28	1	0	4.815581	-0.056449	1.754930
29	7	0	1.467181	-0.000546	1.580218
30	6	0	2.921687	-1.908121	2.036285
31	1	0	3.966838	-2.180772	2.162522
32	6	0	1.952277	-2.907808	2.189940
33	1	0	0.904891	-2.641199	2.303462
34	1	0	2.253224	-3.792397	2.745865
35	6	0	-3.153210	0.115941	-1.385213
36	6	0	-3.903109	0.345217	-2.549241
37	6	0	-3.587613	-0.284887	-3.751349
38	6	0	-2.507416	-1.168793	-3.808964
39	6	0	-1.747961	-1.413603	-2.666485
40	6	0	-2.064393	-0.774342	-1.468244
41	6	0	-3.473846	0.806695	-0.115888
42	6	0	-3.795890	2.173902	-0.093885
43	6	0	-4.083376	2.833968	1.100137
44	6	0	-4.044457	2.132759	2.308834
45	6	0	-3.734217	0.774133	2.313502
46	6	0	-3.464444	0.116287	1.112988
47	1	0	-4.758072	1.013920	-2.495490
48	1	0	-4.189603	-0.096349	-4.635865
49	1	0	-2.258335	-1.670614	-4.740067
50	1	0	-0.903088	-2.094245	-2.683420
51	1	0	-3.796133	2.722842	-1.031871
52	1	0	-4.326831	3.893039	1.088486
53	1	0	-4.255082	2.641874	3.245334
54	1	0	-3.698703	0.197968	3.231825
55	8	0	-1.234289	-0.950234	-0.383340
56	8	0	-3.254555	-1.245130	1.136458
57	15	0	-1.718826	-1.844220	0.956401
58	8	0	-1.806726	-3.294142	0.639450
59	8	0	-0.823255	-1.296402	2.051847
60	6	0	3.783148	2.722852	-2.499523
61	1	0	3.060968	3.148864	-1.799218
62	1	0	4.676835	3.344080	-2.566601
63	1	0	3.312997	2.619321	-3.481394
64	6	0	1.825835	-2.035517	-1.074543

65	1	0	1.186949	-1.303334	-1.550558

s-cis_TS-Cc(S-en)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2023.689022 hartree

Sum of electronic and thermal Free Energies = -2023.243890 hartree

The number of imaginary frequency = 1

Imaginary frequency = -324.72

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.192758	-3.818293	1.120381
2	1	0	-2.106330	-4.291433	1.472218
3	1	0	-0.281670	-4.332383	1.415428
4	6	0	-1.174509	-3.094712	-0.068103
5	1	0	-0.211543	-2.861424	-0.519115
6	6	0	-3.552973	-2.512246	-0.152969
7	1	0	-3.806103	-3.233850	0.615149
8	1	0	-5.537338	-1.971406	-0.116091
9	7	0	-4.648354	-1.768670	-0.551607
10	6	0	-4.638095	-0.642353	-1.361082
11	8	0	-5.887038	-0.117302	-1.385774
12	8	0	-3.680581	-0.191702	-1.949748
13	1	0	-0.790573	-0.122615	1.092231
14	6	0	-2.594417	3.721465	-1.004466
15	6	0	-3.585073	3.157680	-0.223097
16	6	0	-3.335218	1.974934	0.506783
17	6	0	-2.045254	1.383655	0.441308
18	6	0	-1.038509	1.965250	-0.355626
19	6	0	-1.321728	3.115278	-1.068714
20	1	0	-5.311232	1.755336	1.383643
21	1	0	-2.791749	4.628314	-1.568101
22	1	0	-4.569706	3.614806	-0.157084
23	6	0	-4.316363	1.322722	1.312339
24	1	0	-0.060541	1.504347	-0.405729
25	1	0	-0.545963	3.553336	-1.689889
26	6	0	-2.714812	-0.427496	1.884612
27	6	0	-4.020452	0.165294	1.969146
28	1	0	-4.768060	-0.339765	2.571934
29	7	0	-1.783452	0.237160	1.154488
30	6	0	-2.440537	-1.646132	2.556356
31	1	0	-3.282742	-2.064074	3.102417
32	6	0	-1.220833	-2.332181	2.578985
33	1	0	-0.306505	-1.833386	2.267692
34	1	0	-1.094207	-3.070593	3.366828
35	6	0	4.433513	1.177317	0.177679
36	6	0	5.290162	2.065414	0.847507
37	6	0	4.825964	3.269437	1.372897
38	6	0	3.477423	3.607783	1.241662
39	6	0	2.605453	2.743414	0.582158
40	6	0	3.078450	1.543111	0.051215
41	6	0	4.944887	-0.091905	-0.387263
42	6	0	6.168930	-0.143430	-1.073124
43	6	0	6.660287	-1.340045	-1.590864
44	6	0	5.925793	-2.518512	-1.436018
45	6	0	4.707487	-2.493683	-0.759824
46	6	0	4.228186	-1.293900	-0.237172
47	1	0	6.333444	1.787288	0.969878
48	1	0	5.510941	3.934025	1.892155
49	1	0	3.102457	4.540795	1.654072
50	1	0	1.554642	2.986113	0.465745
51	1	0	6.726063	0.778665	-1.215338
52	1	0	7.606905	-1.350535	-2.124127
53	1	0	6.297544	-3.454251	-1.844807
54	1	0	4.111653	-3.389562	-0.621206
55	8	0	2.212941	0.763761	-0.690807
56	8	0	3.069985	-1.312482	0.515447
57	15	0	1.667684	-0.706778	-0.122609
58	8	0	0.785827	-0.455688	1.086327
59	8	0	1.178561	-1.485018	-1.296641
60	6	0	-6.025778	1.034840	-2.237912
61	1	0	-5.834956	0.763147	-3.279860
62	1	0	-7.057502	1.364182	-2.110955
63	1	0	-5.324367	1.817473	-1.939218
64	6	0	-2.282232	-2.433929	-0.656080
65	1	0	-2.074705	-1.755523	-1.473621

s-cis_TS-Cc(R-ex)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2023.700708 hartree

Sum of electronic and thermal Free Energies = -2023.253140 hartree

The number of imaginary frequency = 1

Imaginary frequency = -375.38

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.127231	-2.446875	2.746933
2	1	0	0.719259	-1.815813	2.090299
3	1	0	0.668087	-2.769539	3.633402
4	6	0	-0.793355	-3.353551	2.196234
5	1	0	-1.065630	-4.225198	2.790000
6	6	0	-1.325260	-1.973644	0.302480
7	1	0	-0.440051	-1.398002	0.520925
8	1	0	-1.483359	-0.616625	-1.153220
9	7	0	-1.966066	-1.441119	-0.766445
10	6	0	-3.223643	-1.795264	-1.223422
11	8	0	-3.577070	-0.960529	-2.222609
12	8	0	-3.905920	-2.702057	-0.789313
13	1	0	-0.941641	1.289489	1.557410
14	6	0	-3.405478	3.866403	-1.542490
15	6	0	-4.222940	2.855002	-1.073183
16	6	0	-3.755516	1.955607	-0.092384
17	6	0	-2.434042	2.100227	0.401777
18	6	0	-1.605915	3.132920	-0.078095
19	6	0	-2.095298	3.999434	-1.038754
20	1	0	-5.546054	0.732051	0.055152
21	1	0	-3.767649	4.555860	-2.299094
22	1	0	-5.235716	2.737601	-1.450779

23	6	0	-4.536153	0.878201	0.430810
24	1	0	-0.596017	3.220445	0.305482
25	1	0	-1.453711	4.791205	-1.414362
26	6	0	-2.686803	0.189423	1.867512
27	6	0	-4.030764	0.039063	1.376614
28	1	0	-4.615477	-0.793636	1.750559
29	7	0	-1.965965	1.221781	1.356891
30	6	0	-2.200970	-0.712177	2.839214
31	1	0	-2.943617	-1.443039	3.147776
32	6	0	-0.935456	-0.814386	3.442501
33	1	0	-0.182852	-0.057766	3.228709
34	1	0	-0.920874	-1.189110	4.461639
35	6	0	4.420373	0.438272	-0.289916
36	6	0	5.748330	0.567119	0.148777
37	6	0	6.229630	1.767025	0.668023
38	6	0	5.380991	2.872230	0.767018
39	6	0	4.058382	2.771246	0.339721
40	6	0	3.589212	1.569583	-0.186351
41	6	0	3.923357	-0.843223	-0.842060
42	6	0	4.701884	-1.605855	-1.727354
43	6	0	4.253579	-2.830371	-2.218680
44	6	0	3.004232	-3.320982	-1.831651
45	6	0	2.209380	-2.582432	-0.956693
46	6	0	2.667486	-1.359006	-0.471985
47	1	0	6.399908	-0.300795	0.096636
48	1	0	7.260039	1.835434	1.005395
49	1	0	5.745633	3.809703	1.177748
50	1	0	3.373388	3.610556	0.396451
51	1	0	5.665489	-1.215119	-2.042380
52	1	0	4.874281	-3.396056	-2.907820
53	1	0	2.646856	-4.274343	-2.210980
54	1	0	1.239503	-2.943502	-0.629829
55	8	0	2.304814	1.538031	-0.702189
56	8	0	1.900304	-0.689497	0.465894
57	15	0	1.101673	0.714792	0.055570
58	8	0	0.738466	1.338376	1.384993
59	8	0	0.037436	0.441613	-0.965394
60	6	0	-4.890315	-1.181779	-2.754487
61	1	0	-5.646598	-1.033568	-1.977316
62	1	0	-5.007903	-0.444941	-3.549246
63	1	0	-4.982498	-2.196792	-3.150336
64	6	0	-1.566465	-3.116303	1.041811
65	1	0	-2.382068	-3.777960	0.778511

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s-cis_TS-Cc(S-ex)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2023.700858 hartree

Sum of electronic and thermal Free Energies = -2023.254762 hartree

The number of imaginary frequency = 1

Imaginary frequency = -343.90

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.192758	-3.818293	1.120381
2	1	0	-2.106330	-4.291433	1.472218
3	1	0	-0.281670	-4.332383	1.415428
4	6	0	-1.174509	-3.094712	-0.068103
5	1	0	-0.211543	-2.861424	-0.519115
6	6	0	-3.552973	-2.512246	-0.152969
7	1	0	-3.806103	-3.233850	0.615149
8	1	0	-5.537338	-1.971406	-0.116091
9	7	0	-4.648354	-1.768670	-0.551607
10	6	0	-4.638095	-0.642353	-1.361082
11	8	0	-5.887038	-0.117302	-1.385774
12	8	0	-3.680581	-0.191702	-1.949748
13	1	0	-0.790573	-0.122615	1.092231
14	6	0	-2.594417	3.721465	-1.004466
15	6	0	-3.585073	3.157680	-0.223097
16	6	0	-3.335218	1.974934	0.506783
17	6	0	-2.045254	1.383655	0.441308
18	6	0	-1.038509	1.965250	-0.355626
19	6	0	-1.321728	3.115278	-1.068714
20	1	0	-5.311232	1.755336	1.383643
21	1	0	-2.791749	4.628314	-1.568101
22	1	0	-4.569706	3.614806	-0.157084
23	6	0	-4.316363	1.322722	1.312339
24	1	0	-0.060541	1.504347	-0.405729
25	1	0	-0.545963	3.553336	-1.689889
26	6	0	-2.714812	-0.427496	1.884612
27	6	0	-4.020452	0.165294	1.969146
28	1	0	-4.768060	-0.339765	2.571934
29	7	0	-1.783452	0.237160	1.154488
30	6	0	-2.440537	-1.646132	2.556356
31	1	0	-3.282742	-2.064074	3.102417
32	6	0	-1.220833	-2.332181	2.578985
33	1	0	-0.306505	-1.833386	2.267692
34	1	0	-1.094207	-3.070593	3.366828
35	6	0	4.433513	1.177317	0.177679
36	6	0	5.290162	2.065414	0.847507
37	6	0	4.825964	3.269437	1.372897
38	6	0	3.477423	3.607783	1.241662
39	6	0	2.605453	2.743414	0.582158
40	6	0	3.078450	1.543111	0.051215
41	6	0	4.944887	-0.091905	-0.387263
42	6	0	6.168930	-0.143430	-1.073124
43	6	0	6.660287	-1.340045	-1.590864
44	6	0	5.925793	-2.518512	-1.436018
45	6	0	4.707487	-2.493683	-0.759824
46	6	0	4.228186	-1.293900	-0.237172
47	1	0	6.333444	1.787288	0.969878
48	1	0	5.510941	3.934025	1.892155
49	1	0	3.102457	4.540795	1.654072
50	1	0	1.554642	2.986113	0.465745
51	1	0	6.726063	0.778665	-1.215338
52	1	0	7.606905	-1.350535	-2.124127
53	1	0	6.297544	-3.454251	-1.844807
54	1	0	4.111653	-3.389562	-0.621206
55	8	0	2.212941	0.763761	-0.690807
56	8	0	3.069985	-1.312482	0.515447
57	15	0	1.667684	-0.706778	-0.122609
58	8	0	0.785827	-0.455688	1.086327

59	8	0	1.178561	-1.485018	-1.296641
60	6	0	-6.025778	1.034840	-2.237912
61	1	0	-5.834956	0.763147	-3.279860
62	1	0	-7.057502	1.364182	-2.110955
63	1	0	-5.324367	1.817473	-1.939218
64	6	0	-2.282232	-2.433929	-0.656080
65	1	0	-2.074705	-1.755523	-1.473621

s-cis_TS-Ct(R-en)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2023.701474 hartree

Sum of electronic and thermal Free Energies = -2023.252217 hartree

The number of imaginary frequency = 1

Imaginary frequency = -332.07

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.922332	-3.619353	-0.791428
2	1	0	-3.988854	-3.493904	-0.623181
3	1	0	-2.656545	-4.521717	-1.335795
4	6	0	-1.984753	-3.102987	0.096810
5	1	0	-0.965248	-3.472364	0.002969
6	6	0	-3.359402	-1.343779	1.119402
7	1	0	-4.277925	-1.792094	0.756453
8	1	0	-4.557835	0.145510	1.854787
9	7	0	-3.595765	-0.154299	1.779829
10	6	0	-2.733124	0.854037	2.220346
11	8	0	-1.448609	0.515983	2.094534
12	8	0	-3.160342	1.904743	2.656098
13	1	0	-0.992048	-0.278143	-1.706557
14	6	0	-0.161061	4.131741	-0.199190
15	6	0	-1.528598	3.927869	-0.189302
16	6	0	-2.068826	2.695596	-0.616175
17	6	0	-1.189427	1.663994	-1.041673
18	6	0	0.202732	1.881003	-1.053149
19	6	0	0.699722	3.102725	-0.636427
20	1	0	-4.162481	3.191335	-0.321619
21	1	0	0.251716	5.081457	0.127849
22	1	0	-2.207257	4.707153	0.146924
23	6	0	-3.469613	2.422349	-0.652249
24	1	0	0.860210	1.089982	-1.387086
25	1	0	1.773343	3.258328	-0.648173
26	6	0	-3.032763	0.171608	-1.493180
27	6	0	-3.931833	1.217629	-1.089246
28	1	0	-4.996417	1.010994	-1.126517
29	7	0	-1.705634	0.455166	-1.455440
30	6	0	-3.556155	-1.071316	-1.930828
31	1	0	-4.642592	-1.113740	-1.957567
32	6	0	-2.847201	-2.210182	-2.328186
33	1	0	-1.771622	-2.163384	-2.479487
34	1	0	-3.365910	-2.907474	-2.980997
35	6	0	3.080624	-0.335451	1.138399
36	6	0	3.941279	-0.264326	2.245833
37	6	0	3.615728	-0.866674	3.459309
38	6	0	2.414582	-1.568899	3.585675
39	6	0	1.544037	-1.656580	2.500947
40	6	0	1.867814	-1.037693	1.292658
41	6	0	3.422804	0.322512	-0.142663
42	6	0	3.996782	1.604400	-0.169686
43	6	0	4.315330	2.234192	-1.371969
44	6	0	4.052702	1.589896	-2.584404
45	6	0	3.491042	0.314498	-2.585193
46	6	0	3.191869	-0.318015	-1.377630
47	1	0	4.889532	0.254862	2.136649
48	1	0	4.303649	-0.801757	4.297537
49	1	0	2.157872	-2.053065	4.523903
50	1	0	0.607374	-2.199045	2.570279
51	1	0	4.171884	2.116536	0.772827
52	1	0	4.756338	3.227286	-1.363015
53	1	0	4.286285	2.077808	-3.526637
54	1	0	3.281035	-0.217976	-3.506587
55	8	0	0.933714	-1.028478	0.281348
56	8	0	2.737559	-1.616315	-1.408834
57	15	0	1.142928	-1.959509	-1.105269
58	8	0	1.032151	-3.411778	-0.807404
59	8	0	0.260880	-1.252213	-2.115169
60	6	0	-0.491216	1.510164	2.520854
61	1	0	-0.592347	1.683439	3.595270
62	1	0	0.479951	1.081236	2.283344
63	1	0	-0.651092	2.441994	1.977712
64	6	0	-2.160620	-1.983455	0.946012
65	1	0	-1.268717	-1.555227	1.378431

s-cis_TS-Ct(S-en)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2023.695583 hartree

Sum of electronic and thermal Free Energies = -2023.248121 hartree

The number of imaginary frequency = 1

Imaginary frequency = -333.31

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.848509	-3.007083	2.702596
2	1	0	-1.796707	-3.448314	2.997139
3	1	0	-0.020446	-3.240636	3.366671
4	6	0	-0.563121	-2.746845	1.367689
5	1	0	0.475785	-2.550357	1.117701
6	6	0	-2.853973	-2.621234	0.507575
7	1	0	-3.249753	-3.123236	1.384475
8	1	0	-4.806779	-2.468301	-0.099126
9	7	0	-3.858513	-2.230521	-0.354218
10	6	0	-3.836294	-1.368847	-1.461109
11	8	0	-2.597401	-1.003964	-1.763526
12	8	0	-4.860688	-1.029386	-2.020174
13	1	0	-1.084519	0.636300	1.289195
14	6	0	-3.166607	3.489227	-1.862849
15	6	0	-4.155818	2.780859	-1.207104
16	6	0	-3.822188	1.881747	-0.170786

17	6	0	-2.457093	1.705166	0.180410
18	6	0	-1.454699	2.441488	-0.484841
19	6	0	-1.815919	3.316896	-1.491612
20	1	0	-5.840008	1.230514	0.295982
21	1	0	-3.425378	4.178231	-2.661098
22	1	0	-5.201179	2.900594	-1.478630
23	6	0	-4.790446	1.126977	0.557197
24	1	0	-0.418803	2.314715	-0.198759
25	1	0	-1.040823	3.876519	-2.006790
26	6	0	-3.022968	0.098589	1.889194
27	6	0	-4.408229	0.286586	1.560025
28	1	0	-5.144263	-0.278007	2.122797
29	7	0	-2.120369	0.821267	1.180257
30	6	0	-2.660606	-0.783466	2.941000
31	1	0	-3.505002	-1.240139	3.452140
32	6	0	-1.375586	-1.093955	3.392730
33	1	0	-0.513909	-0.549089	3.017746
34	1	0	-1.284648	-1.450549	4.415297
35	6	0	4.418005	0.764538	0.205839
36	6	0	5.554559	1.178970	0.918381
37	6	0	5.561307	2.364900	1.649949
38	6	0	4.416134	3.164142	1.688477
39	6	0	3.274639	2.774826	0.990106
40	6	0	3.279632	1.592483	0.252134
41	6	0	4.421985	-0.491675	-0.578314
42	6	0	5.521444	-0.849342	-1.374865
43	6	0	5.534451	-2.036678	-2.104212
44	6	0	4.433174	-2.894960	-2.056181
45	6	0	3.328734	-2.562946	-1.273544
46	6	0	3.329415	-1.378689	-0.539260
47	1	0	6.435643	0.543030	0.908271
48	1	0	6.452927	2.658047	2.197219
49	1	0	4.409637	4.086536	2.262962
50	1	0	2.370043	3.373997	0.996400
51	1	0	6.366191	-0.168273	-1.432224
52	1	0	6.395943	-2.284970	-2.717872
53	1	0	4.431288	-3.818198	-2.629227
54	1	0	2.457241	-3.206643	-1.213058
55	8	0	2.170737	1.287405	-0.512956
56	8	0	2.266948	-1.125264	0.308457
57	15	0	1.156639	0.051700	-0.071900
58	8	0	0.510233	0.393433	1.257276
59	8	0	0.338113	-0.301894	-1.267701
60	6	0	-2.411413	-0.115167	-2.885153
61	1	0	-3.039827	0.769338	-2.770550
62	1	0	-1.353655	0.135864	-2.841322
63	1	0	-2.670912	-0.635913	-3.811215
64	6	0	-1.498526	-2.492135	0.336049
65	1	0	-1.107933	-2.060652	-0.576027

s-cis_TS-Ct(R-ex)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2023.696603 hartree

Sum of electronic and thermal Free Energies = -2023.249273 hartree

The number of imaginary frequency = 1

Imaginary frequency = -380.04

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.075389	-2.319305	2.727594
2	1	0	0.553847	-1.719218	2.076954
3	1	0	0.434151	-2.649226	3.629910
4	6	0	-1.011384	-3.202609	2.166057
5	1	0	-1.323531	-4.059207	2.762239
6	6	0	-1.464879	-1.832883	0.239127
7	1	0	-0.564744	-1.286822	0.473068
8	1	0	-1.492492	-0.502679	-1.243187
9	7	0	-2.042486	-1.285316	-0.861547
10	6	0	-3.288782	-1.490509	-1.433562
11	8	0	-3.979068	-2.467059	-0.803008
12	8	0	-3.699211	-0.849703	-2.377055
13	1	0	-0.891702	1.424594	1.485788
14	6	0	-3.040856	4.105662	-1.753113
15	6	0	-3.939652	3.150820	-1.316945
16	6	0	-3.577707	2.241667	-0.300646
17	6	0	-2.277002	2.316411	0.259910
18	6	0	-1.365651	3.292323	-0.186635
19	6	0	-1.753266	4.171216	-1.181414
20	1	0	-5.443011	1.132835	-0.232179
21	1	0	-3.320536	4.801062	-2.538591
22	1	0	-4.933496	3.081666	-1.751159
23	6	0	-4.448501	1.224201	0.196739
24	1	0	-0.372815	3.325465	0.246992
25	1	0	-1.047773	4.918573	-1.532682
26	6	0	-2.715109	0.442829	1.727494
27	6	0	-4.042503	0.372298	1.179396
28	1	0	-4.697670	-0.410710	1.544698
29	7	0	-1.909844	1.423380	1.244923
30	6	0	-2.323493	-0.482908	2.720575
31	1	0	-3.119028	-1.168352	3.000306
32	6	0	-1.093081	-0.648404	3.379799
33	1	0	-0.295827	0.070920	3.202873
34	1	0	-1.143955	-1.022186	4.398174
35	6	0	4.454506	0.239177	-0.232624
36	6	0	5.781002	0.298032	0.225058
37	6	0	6.320382	1.473383	0.743369
38	6	0	5.532741	2.624401	0.822191
39	6	0	4.212962	2.593221	0.375847
40	6	0	3.685431	1.415401	-0.149082
41	6	0	3.896044	-1.017387	-0.783404
42	6	0	4.643807	-1.828903	-1.651565
43	6	0	4.134820	-3.030066	-2.141493
44	6	0	2.854186	-3.447081	-1.770581
45	6	0	2.089079	-2.658871	-0.912643
46	6	0	2.608232	-1.459797	-0.428771
47	1	0	6.384357	-0.604848	0.188332
48	1	0	7.348036	1.487402	1.095495
49	1	0	5.942635	3.543516	1.231771
50	1	0	3.574809	3.469591	0.416258
51	1	0	5.632165	-1.494846	-1.954892
52	1	0	4.732818	-3.634502	-2.817696

53	1	0	2.449524	-4.381347	-2.149997
54	1	0	1.095201	-2.961208	-0.598313
55	8	0	2.409431	1.452175	-0.684220
56	8	0	1.866130	-0.740790	0.491939
57	15	0	1.149626	0.698416	0.054108
58	8	0	0.791789	1.351475	1.371217
59	8	0	0.093693	0.470507	-0.985686
60	6	0	-5.296734	-2.693253	-1.329713
61	1	0	-5.247525	-2.967088	-2.386624
62	1	0	-5.709264	-3.510390	-0.737207
63	1	0	-5.909093	-1.792959	-1.224162
64	6	0	-1.749990	-2.958113	0.990755
65	1	0	-2.570568	-3.611285	0.722739

s-cis_TS-Ct(S-ex)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2023.696984 hartree

Sum of electronic and thermal Free Energies = -2023.250432 hartree

The number of imaginary frequency = 1

Imaginary frequency = -348.88

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.094836	-3.774730	-0.791969
2	1	0	-0.336765	-3.001056	-0.703295
3	1	0	-0.760296	-4.665003	-1.319337
4	6	0	-2.067134	-3.938181	0.200600
5	1	0	-2.581618	-4.897126	0.252326
6	6	0	-2.016126	-1.649933	0.953172
7	1	0	-1.096032	-1.537623	0.398144
8	1	0	-1.585273	0.231821	1.459191
9	7	0	-2.336114	-0.469786	1.546755
10	6	0	-3.519380	-0.032928	2.119692
11	8	0	-4.470318	-0.994937	2.114806
12	8	0	-3.675350	1.090717	2.547758
13	1	0	-0.910224	-0.190020	-1.823493
14	6	0	-1.635349	4.425369	-1.097918
15	6	0	-2.823239	3.751925	-0.881861
16	6	0	-2.910152	2.363181	-1.114842
17	6	0	-1.759677	1.667814	-1.566723
18	6	0	-0.554491	2.358775	-1.790747
19	6	0	-0.502665	3.720784	-1.553938
20	1	0	-4.983422	2.102518	-0.522534
21	1	0	-1.571550	5.493428	-0.913835
22	1	0	-3.704600	4.278779	-0.525928
23	6	0	-4.098426	1.597818	-0.900962
24	1	0	0.323791	1.817794	-2.123332
25	1	0	0.430635	4.250820	-1.721997
26	6	0	-2.954504	-0.436625	-1.608956
27	6	0	-4.127567	0.259996	-1.158950
28	1	0	-5.028123	-0.321235	-0.994317
29	7	0	-1.829529	0.306165	-1.779575
30	6	0	-3.010095	-1.826824	-1.855806
31	1	0	-3.977259	-2.269283	-1.635094
32	6	0	-2.008614	-2.685478	-2.327385
33	1	0	-1.076374	-2.268466	-2.698430
34	1	0	-2.341634	-3.580345	-2.843285
35	6	0	4.254173	0.740489	0.562087
36	6	0	5.240519	1.393786	1.318182
37	6	0	5.120259	2.739953	1.657997
38	6	0	3.996039	3.464191	1.252944
39	6	0	3.002388	2.839795	0.501055
40	6	0	3.140897	1.497954	0.154473
41	6	0	4.383390	-0.688884	0.195785
42	6	0	5.608570	-1.218479	-0.240129
43	6	0	5.741467	-2.564721	-0.574120
44	6	0	4.637800	-3.416343	-0.483351
45	6	0	3.409731	-2.916325	-0.054183
46	6	0	3.288535	-1.570272	0.284845
47	1	0	6.099867	0.822843	1.658986
48	1	0	5.894906	3.218639	2.250511
49	1	0	3.889747	4.510368	1.526539
50	1	0	2.111696	3.366730	0.174657
51	1	0	6.460115	-0.550111	-0.333954
52	1	0	6.700488	-2.945251	-0.914350
53	1	0	4.731307	-4.466212	-0.747433
54	1	0	2.533631	-3.550476	0.035492
55	8	0	2.193433	0.928001	-0.678891
56	8	0	2.083402	-1.133287	0.805583
57	15	0	1.094514	-0.140612	-0.062245
58	8	0	0.156313	0.519596	0.902232
59	8	0	0.536579	-0.877205	-1.266365
60	6	0	-5.732088	-0.580539	2.662875
61	1	0	-6.149447	0.245296	2.079399
62	1	0	-6.376387	-1.458249	2.602522
63	1	0	-5.614271	-0.257325	3.700325
64	6	0	-2.589087	-2.904515	1.007504
65	1	0	-3.455625	-3.092145	1.628730

s-cis_TS-Tc(R-en)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2023.704067 hartree

Sum of electronic and thermal Free Energies = -2023.257652 hartree

The number of imaginary frequency = 1

Imaginary frequency = -362.62

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.179273	-4.489308	0.452986
2	1	0	-2.231522	-4.510919	0.715198
3	1	0	-0.781997	-5.441643	0.111220
4	6	0	-0.312132	-3.611901	1.096107
5	1	0	0.754074	-3.812867	1.005901
6	6	0	-1.906628	-1.844085	1.729251
7	1	0	-2.809216	-2.437733	1.625776
8	1	0	-1.298933	0.114604	1.700697
9	7	0	-2.108722	-0.507815	1.890961
10	6	0	-3.382038	0.018661	2.013723

11	8	0	-3.319198	1.362879	1.930491
12	8	0	-4.398620	-0.632711	2.162183
13	1	0	-1.098753	-0.673871	-1.333273
14	6	0	-3.036621	3.643931	-1.588875
15	6	0	-4.054077	2.721730	-1.429474
16	6	0	-3.764888	1.342501	-1.359764
17	6	0	-2.414576	0.913871	-1.449851
18	6	0	-1.384382	1.857175	-1.637400
19	6	0	-1.702470	3.201788	-1.698942
20	1	0	-5.804789	0.633966	-1.111221
21	1	0	-3.262535	4.704818	-1.639589
22	1	0	-5.090355	3.042907	-1.358552
23	6	0	-4.763272	0.334160	-1.195371
24	1	0	-0.359919	1.524208	-1.742276
25	1	0	-0.905123	3.925912	-1.839313
26	6	0	-3.055610	-1.409095	-1.230474
27	6	0	-4.424838	-0.983533	-1.136557
28	1	0	-5.184431	-1.744678	-0.999714
29	7	0	-2.122989	-0.431863	-1.363537
30	6	0	-2.764031	-2.797933	-1.246032
31	1	0	-3.653368	-3.422765	-1.198786
32	6	0	-1.538575	-3.456044	-1.375404
33	1	0	-0.621164	-2.884023	-1.488581
34	1	0	-1.542335	-4.422932	-1.870132
35	6	0	4.219960	1.206714	0.231684
36	6	0	5.205977	1.980280	0.864671
37	6	0	4.982296	3.317304	1.187337
38	6	0	3.753442	3.910705	0.887237
39	6	0	2.757673	3.164581	0.259444
40	6	0	2.996292	1.832522	-0.069839
41	6	0	4.462959	-0.210520	-0.123188
42	6	0	5.684027	-0.618069	-0.683837
43	6	0	5.924576	-1.950084	-1.014671
44	6	0	4.934077	-2.910479	-0.796410
45	6	0	3.712943	-2.531922	-0.241789
46	6	0	3.485160	-1.199788	0.096958
47	1	0	6.151283	1.510719	1.122625
48	1	0	5.760216	3.890828	1.683486
49	1	0	3.568325	4.949685	1.145805
50	1	0	1.790312	3.590283	0.013901
51	1	0	6.443357	0.134276	-0.878609
52	1	0	6.876929	-2.235093	-1.452814
53	1	0	5.109404	-3.950022	-1.059615
54	1	0	2.922800	-3.252782	-0.058619
55	8	0	2.029923	1.142301	-0.781040
56	8	0	2.304871	-0.879416	0.744047
57	15	0	1.123618	-0.013304	-0.024076
58	8	0	0.263496	0.592667	1.045806
59	8	0	0.514991	-0.833123	-1.139636
60	6	0	-4.577653	2.035641	2.064353
61	1	0	-4.995193	1.874757	3.062667
62	1	0	-4.358474	3.090752	1.901366
63	1	0	-5.288336	1.672397	1.317517
64	6	0	-0.637112	-2.368312	1.670903
65	1	0	0.186520	-1.717202	1.938650

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s-cis_TS-Tc(S-en)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2023.703942 hartree

Sum of electronic and thermal Free Energies = -2023.257691 hartree

The number of imaginary frequency = 1

Imaginary frequency = -359.42

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.075747	-3.516160	2.695128
2	1	0	-2.122951	-3.747048	2.530906
3	1	0	-0.653841	-3.955049	3.595495
4	6	0	-0.226454	-3.296209	1.615602
5	1	0	0.844524	-3.327058	1.808149
6	6	0	-1.863587	-2.494842	-0.047724
7	1	0	-2.756883	-2.861345	0.447760
8	1	0	-1.286389	-1.045909	-1.381621
9	7	0	-2.085296	-1.637985	-1.082706
10	6	0	-3.366924	-1.351436	-1.518754
11	8	0	-3.323696	-0.320578	-2.385736
12	8	0	-4.373672	-1.934277	-1.163367
13	1	0	-1.132617	0.443919	1.327644
14	6	0	-3.220793	3.682554	-1.436675
15	6	0	-4.207804	2.908427	-0.855304
16	6	0	-3.869863	1.873974	0.042475
17	6	0	-2.502445	1.638340	0.342661
18	6	0	-1.502910	2.444171	-0.237704
19	6	0	-1.868008	3.445735	-1.119029
20	1	0	-5.888333	1.175282	0.446234
21	1	0	-3.484294	4.475012	-2.130699
22	1	0	-5.257112	3.083571	-1.079831
23	6	0	-4.834831	1.027428	0.669912
24	1	0	-0.463625	2.276909	0.011658
25	1	0	-1.093112	4.057028	-1.571910
26	6	0	-3.063685	-0.183022	1.834517
27	6	0	-4.449605	0.042982	1.527702
28	1	0	-5.183810	-0.604882	1.992920
29	7	0	-2.163821	0.618453	1.208272
30	6	0	-2.722904	-1.163334	2.801578
31	1	0	-3.589443	-1.662712	3.229659
32	6	0	-1.472702	-1.521219	3.313818
33	1	0	-0.576636	-1.006746	2.976118
34	1	0	-1.440263	-1.875709	4.339965
35	6	0	4.354525	0.894120	0.194137
36	6	0	5.491617	1.306434	0.907412
37	6	0	5.465704	2.432102	1.728163
38	6	0	4.287544	3.171485	1.858128
39	6	0	3.144530	2.782761	1.161899
40	6	0	3.183130	1.661245	0.336198
41	6	0	4.393354	-0.295924	-0.686446
42	6	0	5.487629	-0.536494	-1.532787
43	6	0	5.540585	-1.663400	-2.350514
44	6	0	4.486077	-2.579455	-2.341684
45	6	0	3.387330	-2.363422	-1.511956
46	6	0	3.346160	-1.236652	-0.693295

47	1	0	6.399977	0.715852	0.825582
48	1	0	6.358774	2.724440	2.273350
49	1	0	4.256428	4.046134	2.502050
50	1	0	2.214423	3.336333	1.237647
51	1	0	6.296119	0.188979	-1.556515
52	1	0	6.396851	-1.820130	-3.000458
53	1	0	4.515752	-3.457594	-2.980808
54	1	0	2.555164	-3.059263	-1.477757
55	8	0	2.064144	1.360450	-0.420659
56	8	0	2.290017	-1.106129	0.192204
57	15	0	1.129636	0.052395	-0.041128
58	8	0	0.490110	0.243784	1.316111
59	8	0	0.290659	-0.229824	-1.252771
60	6	0	-4.591766	0.060084	-2.935898
61	1	0	-5.300325	0.296441	-2.138192
62	1	0	-4.388930	0.943980	-3.540205
63	1	0	-5.000565	-0.746967	-3.551130
64	6	0	-0.585155	-2.811778	0.342516
65	1	0	0.221894	-2.501044	-0.308762

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s-cis_TS-Tc(R-ex)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2023.692914 hartree

Sum of electronic and thermal Free Energies = -2023.246881 hartree

The number of imaginary frequency = 1

Imaginary frequency = -357.15

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.029486	3.181944	1.378104
2	1	0	-0.232737	2.362433	0.716378
3	1	0	-0.790095	3.556618	1.986660
4	6	0	1.002265	4.090319	0.953055
5	1	0	1.023345	5.083832	1.399504
6	6	0	2.265902	2.496482	-0.418282
7	1	0	1.485605	1.735211	-0.427405
8	1	0	4.169027	2.810433	-1.173750
9	7	0	3.398435	2.156106	-1.107777
10	6	0	3.581929	0.911834	-1.705398
11	8	0	4.821917	0.868175	-2.247541
12	8	0	2.767434	0.020738	-1.732101
13	1	0	0.895301	-0.589005	1.532492
14	6	0	3.322059	-4.077671	-0.532626
15	6	0	4.223614	-3.105795	-0.143171
16	6	0	3.776346	-1.935456	0.507404
17	6	0	2.388639	-1.777508	0.765149
18	6	0	1.473724	-2.776681	0.372830
19	6	0	1.945629	-3.904394	-0.271919
20	1	0	5.711752	-0.974507	0.735327
21	1	0	3.668503	-4.974316	-1.037766
22	1	0	5.288066	-3.226850	-0.330832
23	6	0	4.643578	-0.878543	0.915371
24	1	0	0.418418	-2.631435	0.575449
25	1	0	1.241281	-4.669513	-0.585574
26	6	0	2.735606	0.395210	1.749169
27	6	0	4.143784	0.245491	1.502657
28	1	0	4.798245	1.059007	1.796290
29	7	0	1.940748	-0.645866	1.402624
30	6	0	2.254076	1.581581	2.356527
31	1	0	3.036256	2.299257	2.586661
32	6	0	0.943236	1.920480	2.728466
33	1	0	0.164056	1.162555	2.690748
34	1	0	0.849052	2.621551	3.551979
35	6	0	-4.444190	-0.974650	-0.220742
36	6	0	-5.636114	-1.636914	0.114443
37	6	0	-5.649201	-2.991202	0.441642
38	6	0	-4.455302	-3.716463	0.445348
39	6	0	-3.258394	-3.082573	0.117528
40	6	0	-3.254704	-1.728969	-0.215208
41	6	0	-4.443797	0.461510	-0.581548
42	6	0	-5.433193	1.002568	-1.417945
43	6	0	-5.443832	2.356256	-1.748366
44	6	0	-4.450361	3.202080	-1.248828
45	6	0	-3.456528	2.689958	-0.416766
46	6	0	-3.460023	1.336547	-0.083289
47	1	0	-6.560137	-1.065504	0.135028
48	1	0	-6.585753	-3.475651	0.703547
49	1	0	-4.454506	-4.771565	0.705398
50	1	0	-2.314949	-3.618561	0.102948
51	1	0	-6.189516	0.338429	-1.827398
52	1	0	-6.217276	2.746905	-2.403845
53	1	0	-4.445947	4.257044	-1.509616
54	1	0	-2.669947	3.318862	-0.012547
55	8	0	-2.067836	-1.161700	-0.637296
56	8	0	-2.524330	0.875800	0.822643
57	15	0	-1.263139	-0.067905	0.303644
58	8	0	-0.734853	-0.729409	1.561945
59	8	0	-0.328432	0.695799	-0.580710
60	6	0	5.121790	-0.367813	-2.921425
61	1	0	4.452133	-0.509171	-3.774204
62	1	0	6.155111	-0.271514	-3.256088
63	1	0	5.007827	-1.213604	-2.238542
64	6	0	2.088912	3.754081	0.123480
65	1	0	2.868887	4.500478	-0.028919

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s-cis_TS-Tc(S-ex)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2023.696747 hartree

Sum of electronic and thermal Free Energies = -2023.249192 hartree

The number of imaginary frequency = 1

Imaginary frequency = -348.00

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.498287	4.003001	0.918675
2	1	0	0.745018	3.218024	0.974888
3	1	0	1.107911	5.003807	0.747420
4	6	0	2.652747	3.889163	1.694820

5	1	0	3.208192	4.793247	1.942593
6	6	0	2.753639	1.443093	1.669302
7	1	0	1.739032	1.323192	1.291764
8	1	0	4.349987	0.270556	2.288859
9	7	0	3.418460	0.264852	1.890820
10	6	0	2.892912	-0.973729	1.546279
11	8	0	3.789771	-1.937169	1.852226
12	8	0	1.804895	-1.157184	1.048000
13	1	0	0.813315	1.021657	-1.627049
14	6	0	1.368597	-3.579263	-2.573923
15	6	0	2.612741	-3.049982	-2.287524
16	6	0	2.752780	-1.676483	-1.991321
17	6	0	1.599527	-0.847697	-1.999287
18	6	0	0.335806	-1.390387	-2.307026
19	6	0	0.233092	-2.741081	-2.581359
20	1	0	4.898511	-1.675367	-1.649619
21	1	0	1.262348	-4.636867	-2.796424
22	1	0	3.499798	-3.679257	-2.287643
23	6	0	3.999515	-1.063685	-1.665188
24	1	0	-0.534297	-0.746266	-2.292294
25	1	0	-0.743211	-3.162234	-2.802507
26	6	0	2.890404	1.090571	-1.366762
27	6	0	4.066287	0.264294	-1.365238
28	1	0	5.011103	0.730513	-1.107592
29	7	0	1.722632	0.492002	-1.709845
30	6	0	3.007582	2.468055	-1.057620
31	1	0	4.029156	2.779985	-0.859315
32	6	0	2.019096	3.461407	-1.020361
33	1	0	1.005312	3.219266	-1.331707
34	1	0	2.344010	4.469951	-1.255815
35	6	0	-3.557237	-0.927311	1.015317
36	6	0	-4.243503	-1.662971	1.994933
37	6	0	-3.563314	-2.495030	2.882178
38	6	0	-2.171522	-2.604532	2.809310
39	6	0	-1.464053	-1.884463	1.848102
40	6	0	-2.157857	-1.061849	0.962928
41	6	0	-4.273809	-0.065814	0.046484
42	6	0	-5.465093	-0.500296	-0.557671
43	6	0	-6.151187	0.294488	-1.473500
44	6	0	-5.648416	1.552611	-1.813885
45	6	0	-4.468137	2.008423	-1.230020
46	6	0	-3.792957	1.211768	-0.306112
47	1	0	-5.322818	-1.558921	2.066781
48	1	0	-4.117094	-3.047509	3.636469
49	1	0	-1.637293	-3.246477	3.505205
50	1	0	-0.384650	-1.937368	1.755213
51	1	0	-5.840088	-1.490337	-0.312391
52	1	0	-7.067585	-0.071620	-1.928253
53	1	0	-6.171538	2.177210	-2.533022
54	1	0	-4.052446	2.982398	-1.465848
55	8	0	-1.455523	-0.430504	-0.043993
56	8	0	-2.692843	1.750306	0.331568
57	15	0	-1.162910	1.197137	0.050837
58	8	0	-0.332881	1.545546	1.246525
59	8	0	-0.700321	1.577111	-1.343765
60	6	0	3.341604	-3.274116	1.557817
61	1	0	3.059155	-3.360665	0.505802
62	1	0	4.188880	-3.919614	1.790844
63	1	0	2.480617	-3.531887	2.180906
64	6	0	3.271938	2.667413	2.031205
65	1	0	4.243106	2.701111	2.525536

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s-cis_TS-Tt(R-en)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2023.693730 hartree

Sum of electronic and thermal Free Energies = -2023.250337 hartree

The number of imaginary frequency = 1

Imaginary frequency = -357.08

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.861820	-3.397298	-0.572150
2	1	0	1.829621	-3.887833	-0.634760
3	1	0	0.032924	-4.077302	-0.389893
4	6	0	0.600775	-2.249759	-1.320699
5	1	0	-0.437446	-1.969607	-1.465807
6	6	0	2.902269	-1.431117	-1.538974
7	1	0	3.367367	-2.357745	-1.234299
8	1	0	3.411849	0.512002	-2.013477
9	7	0	3.783130	-0.400465	-1.774300
10	6	0	5.150607	-0.400350	-1.562450
11	8	0	5.588724	-1.618309	-1.172484
12	8	0	5.849528	0.580598	-1.711473
13	1	0	0.730644	0.038748	1.301268
14	6	0	2.556464	4.400718	1.131676
15	6	0	3.605613	3.502171	1.164473
16	6	0	3.355034	2.115397	1.252276
17	6	0	2.010426	1.657014	1.292030
18	6	0	0.944547	2.580645	1.276689
19	6	0	1.227046	3.931659	1.194731
20	1	0	5.423902	1.452887	1.278088
21	1	0	2.751828	5.466532	1.062272
22	1	0	4.635965	3.846090	1.125778
23	6	0	4.386843	1.130295	1.312372
24	1	0	-0.074207	2.218164	1.335082
25	1	0	0.405879	4.642279	1.177117
26	6	0	2.718910	-0.648705	1.370627
27	6	0	4.081492	-0.195825	1.395235
28	1	0	4.862945	-0.946686	1.426510
29	7	0	1.754686	0.304547	1.348546
30	6	0	2.435764	-2.039308	1.383671
31	1	0	3.315208	-2.674625	1.455405
32	6	0	1.178844	-2.657850	1.321974
33	1	0	0.275774	-2.062650	1.432901
34	1	0	1.112498	-3.661082	1.736399
35	6	0	-4.852317	0.514916	-0.497248
36	6	0	-6.003996	0.823475	-1.238779
37	6	0	-6.139126	2.044064	-1.897088
38	6	0	-5.110256	2.986867	-1.831270
39	6	0	-3.956415	2.705291	-1.102199
40	6	0	-3.833673	1.485959	-0.438344

41	6	0	-4.721306	-0.781265	0.207017
42	6	0	-5.795775	-1.335156	0.921069
43	6	0	-5.681387	-2.562696	1.570846
44	6	0	-4.474642	-3.265076	1.523877
45	6	0	-3.392789	-2.736018	0.822636
46	6	0	-3.518581	-1.512121	0.167887
47	1	0	-6.791737	0.078426	-1.311061
48	1	0	-7.038598	2.253395	-2.469410
49	1	0	-5.203362	3.937751	-2.348949
50	1	0	-3.139281	3.415049	-1.027637
51	1	0	-6.725958	-0.776417	0.978120
52	1	0	-6.527482	-2.964038	2.121664
53	1	0	-4.374706	-4.219269	2.034264
54	1	0	-2.441538	-3.255771	0.763407
55	8	0	-2.727952	1.281015	0.363644
56	8	0	-2.463592	-1.062114	-0.599930
57	15	0	-1.537276	0.222028	-0.084901
58	8	0	-0.745317	0.693205	-1.256633
59	8	0	-0.860852	-0.154385	1.221376
60	6	0	7.005574	-1.692552	-0.936257
61	1	0	7.293455	-1.017200	-0.125505
62	1	0	7.198069	-2.729430	-0.660036
63	1	0	7.559749	-1.422686	-1.838513
64	6	0	1.552645	-1.292104	-1.728482
65	1	0	1.150295	-0.345660	-2.082000

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s-cis_TS-Tt(S-en)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2023.693585 hartree

Sum of electronic and thermal Free Energies = -2023.249369 hartree

The number of imaginary frequency = 1

Imaginary frequency = -352.18

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.072835	-2.939095	2.211981
2	1	0	-2.086891	-3.284588	2.393792
3	1	0	-0.336853	-3.331020	2.909244
4	6	0	-0.648672	-2.640468	0.919427
5	1	0	0.422723	-2.572569	0.751823
6	6	0	-2.831915	-2.097391	-0.063066
7	1	0	-3.420106	-2.529079	0.734336
8	1	0	-3.072165	-0.976857	-1.778989
9	7	0	-3.567005	-1.460723	-1.037581
10	6	0	-4.934064	-1.250287	-1.053039
11	8	0	-5.537526	-1.857867	-0.005963
12	8	0	-5.501746	-0.599772	-1.905935
13	1	0	-0.759576	0.794490	1.092839
14	6	0	-2.285125	3.999687	-2.043290
15	6	0	-3.391091	3.401058	-1.471217
16	6	0	-3.233139	2.429932	-0.458542
17	6	0	-1.922688	2.067683	-0.045098
18	6	0	-0.799730	2.695790	-0.621563
19	6	0	-0.990639	3.644568	-1.608706
20	1	0	-5.340232	2.030818	-0.119289
21	1	0	-2.408887	4.743144	-2.824834
22	1	0	-4.396040	3.665956	-1.789316
23	6	0	-4.328072	1.780815	0.186979
24	1	0	0.194749	2.428390	-0.289048
25	1	0	-0.123126	4.117856	-2.058918
26	6	0	-2.784180	0.461072	1.537594
27	6	0	-4.113605	0.853523	1.163300
28	1	0	-4.943904	0.352753	1.648241
29	7	0	-1.758280	1.101511	0.924062
30	6	0	-2.598657	-0.540262	2.526969
31	1	0	-3.523763	-0.921103	2.953119
32	6	0	-1.391615	-1.057106	3.013343
33	1	0	-0.448314	-0.594400	2.735972
34	1	0	-1.413724	-1.485756	4.012279
35	6	0	4.745138	0.444331	0.246425
36	6	0	5.883353	0.767030	1.002491
37	6	0	5.955345	1.947089	1.739958
38	6	0	4.875378	2.833302	1.740325
39	6	0	3.733653	2.535840	0.998565
40	6	0	3.673858	1.358216	0.255499
41	6	0	4.680729	-0.805376	-0.545290
42	6	0	5.778990	-1.243487	-1.302334
43	6	0	5.729131	-2.425295	-2.038910
44	6	0	4.564279	-3.196413	-2.038309
45	6	0	3.459594	-2.783237	-1.295773
46	6	0	3.521965	-1.605230	-0.553788
47	1	0	6.712022	0.064352	1.021385
48	1	0	6.846168	2.168481	2.321207
49	1	0	4.919514	3.752158	2.318805
50	1	0	2.879231	3.204267	0.974888
51	1	0	6.674979	-0.629073	-1.323008
52	1	0	6.591851	-2.736463	-2.621373
53	1	0	4.513300	-4.114564	-2.617241
54	1	0	2.540144	-3.359161	-1.273041
55	8	0	2.573566	1.141474	-0.551369
56	8	0	2.450290	-1.276315	0.255099
57	15	0	1.450516	-0.009209	-0.146869
58	8	0	0.798098	0.377011	1.168110
59	8	0	0.632316	-0.287335	-1.362581
60	6	0	-6.962456	-1.675041	0.045185
61	1	0	-7.431147	-2.048169	-0.868656
62	1	0	-7.296216	-2.246262	0.911777
63	1	0	-7.207659	-0.615600	0.164147
64	6	0	-1.468356	-2.199113	-0.142206
65	1	0	-0.954258	-1.775768	-1.002812

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s-cis_TS-Tt(R-ex)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2023.700029 hartree

Sum of electronic and thermal Free Energies = -2023.251630 hartree

The number of imaginary frequency = 1

Imaginary frequency = -332.94

Center Atomic Atomic Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-1.131836	3.811641	-1.160957
2	1	0	-0.484575	3.047182	-0.736112
3	1	0	-0.655852	4.477145	-1.877526
4	6	0	-2.177649	4.327670	-0.396147
5	1	0	-2.588441	5.299704	-0.667904
6	6	0	-2.538599	2.329260	0.969297
7	1	0	-1.606971	1.867229	0.647913
8	1	0	-4.134292	1.944430	2.235876
9	7	0	-3.269653	1.583615	1.850814
10	6	0	-2.935797	0.311615	2.335591
11	8	0	-1.799305	-0.116960	1.789037
12	8	0	-3.624480	-0.271203	3.147311
13	1	0	-1.221430	-0.175500	-1.727285
14	6	0	-2.473416	-4.341234	0.108726
15	6	0	-3.553115	-3.483606	0.216024
16	6	0	-3.477718	-2.171667	-0.298021
17	6	0	-2.274198	-1.739837	-0.914767
18	6	0	-1.177354	-2.619099	-1.025993
19	6	0	-1.289842	-3.902243	-0.520243
20	1	0	-5.481703	-1.534348	0.251700
21	1	0	-2.535627	-5.350709	0.503499
22	1	0	-4.473244	-3.804990	0.696905
23	6	0	-4.554436	-1.234443	-0.229149
24	1	0	-0.267825	-2.264654	-1.498104
25	1	0	-0.449149	-4.584435	-0.611222
26	6	0	-3.190354	0.449541	-1.354815
27	6	0	-4.421012	0.016409	-0.750665
28	1	0	-5.235552	0.730515	-0.699416
29	7	0	-2.184348	-0.459294	-1.411497
30	6	0	-3.094266	1.757698	-1.884154
31	1	0	-4.021154	2.320294	-1.820871
32	6	0	-1.997029	2.398631	-2.468828
33	1	0	-1.078300	1.843385	-2.644755
34	1	0	-2.214014	3.168558	-3.201738
35	6	0	4.011808	-0.981904	0.026323
36	6	0	5.075846	-1.868523	-0.207955
37	6	0	4.861280	-3.224646	-0.443351
38	6	0	3.558989	-3.728285	-0.445697
39	6	0	2.485175	-2.869028	-0.223153
40	6	0	2.704833	-1.509678	-0.000143
41	6	0	4.271223	0.444697	0.326218
42	6	0	5.312063	0.828246	1.187804
43	6	0	5.565690	2.169763	1.465367
44	6	0	4.771671	3.163281	0.886530
45	6	0	3.731869	2.808559	0.029349
46	6	0	3.493486	1.464482	-0.249136
47	1	0	6.087335	-1.471981	-0.217089
48	1	0	5.705579	-3.882935	-0.627491
49	1	0	3.378250	-4.785512	-0.620770
50	1	0	1.464756	-3.232835	-0.194059
51	1	0	5.911569	0.054437	1.659392
52	1	0	6.372872	2.438594	2.141048
53	1	0	4.958121	4.211203	1.105062
54	1	0	3.095742	3.552346	-0.438569
55	8	0	1.613350	-0.723975	0.310982
56	8	0	2.520025	1.140051	-1.175938
57	15	0	1.082027	0.524814	-0.657405
58	8	0	0.411002	-0.014300	-1.903708
59	8	0	0.351623	1.462065	0.252303
60	6	0	-1.232431	-1.329039	2.324582
61	1	0	-1.880297	-2.179086	2.100480
62	1	0	-0.269786	-1.421774	1.824226
63	1	0	-1.107460	-1.234388	3.406249
64	6	0	-2.880416	3.612993	0.597305
65	1	0	-3.765459	4.072694	1.036887

s-cis_TS-Tt(S-ex)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2023.706196 hartree

Sum of electronic and thermal Free Energies = -2023.255047 hartree

The number of imaginary frequency = 1

Imaginary frequency = -366.00

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.873915	2.512515	-1.489427
2	1	0	1.868627	2.311816	-1.143644
3	1	0	2.898128	3.260459	-2.276450
4	6	0	3.940134	2.454705	-0.588673
5	1	0	4.846868	3.012089	-0.818804
6	6	0	2.976046	0.722162	0.845976
7	1	0	2.003143	0.776339	0.375852
8	1	0	3.929667	-0.304028	2.369233
9	7	0	3.059633	-0.189373	1.863506
10	6	0	2.013526	-0.950943	2.394172
11	8	0	0.880218	-0.743201	1.719060
12	8	0	2.171428	-1.684770	3.347131
13	1	0	0.594028	-0.549770	-2.021621
14	6	0	-1.476240	-4.245271	0.069952
15	6	0	-0.115849	-4.336634	0.296801
16	6	0	0.763149	-3.368183	-0.234545
17	6	0	0.228983	-2.299528	-1.003332
18	6	0	-1.158315	-2.215940	-1.237665
19	6	0	-1.990800	-3.181848	-0.701425
20	1	0	2.609880	-4.194038	0.559144
21	1	0	-2.149972	-4.990072	0.482918
22	1	0	0.297493	-5.149955	0.887904
23	6	0	2.176077	-3.391856	-0.032255
24	1	0	-1.546686	-1.391300	-1.823675
25	1	0	-3.058834	-3.104174	-0.872163
26	6	0	2.415333	-1.335633	-1.325464
27	6	0	2.969686	-2.418423	-0.560331
28	1	0	4.042447	-2.428127	-0.402639
29	7	0	1.073686	-1.343788	-1.519944
30	6	0	3.275724	-0.335889	-1.843302
31	1	0	4.324329	-0.505567	-1.618070
32	6	0	2.956951	0.795077	-2.612306
33	1	0	1.954089	0.904172	-3.019946
34	1	0	3.744495	1.167695	-3.259756

35	6	0	-2.002085	1.546226	1.282597
36	6	0	-2.405120	2.047643	2.531558
37	6	0	-1.551855	2.822132	3.314415
38	6	0	-0.271532	3.130204	2.847558
39	6	0	0.151037	2.649036	1.610347
40	6	0	-0.698508	1.850539	0.843335
41	6	0	-2.917819	0.716554	0.466696
42	6	0	-3.736224	-0.258170	1.062330
43	6	0	-4.635477	-1.014022	0.312936
44	6	0	-4.727553	-0.814891	-1.067431
45	6	0	-3.919731	0.138390	-1.685900
46	6	0	-3.029073	0.900035	-0.927396
47	1	0	-3.414938	1.841276	2.875353
48	1	0	-1.892162	3.201386	4.273757
49	1	0	0.394815	3.749941	3.441300
50	1	0	1.137095	2.883117	1.223665
51	1	0	-3.653306	-0.424439	2.133134
52	1	0	-5.257003	-1.758295	0.803117
53	1	0	-5.426729	-1.397371	-1.661514
54	1	0	-3.969809	0.324531	-2.753544
55	8	0	-0.206899	1.268319	-0.303495
56	8	0	-2.333156	1.906545	-1.553709
57	15	0	-0.703950	1.781050	-1.838841
58	8	0	-0.170952	3.130919	-2.144055
59	8	0	-0.408100	0.558979	-2.687327
60	6	0	-0.310484	-1.341292	2.270366
61	1	0	-0.612333	-0.788635	3.163775
62	1	0	-1.062016	-1.244816	1.490114
63	1	0	-0.130118	-2.389086	2.512527
64	6	0	4.001350	1.584195	0.517142
65	1	0	4.923035	1.543581	1.096475

(R=Me)

TS_{Me}-Cc(R-en)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2063.028159 hartree

Sum of electronic and thermal Free Energies = -2062.553752 hartree

The number of imaginary frequency = 1

Imaginary frequency = -340.27

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.160605	3.517073	1.634478
2	1	0	-0.909988	2.894865	1.156744
3	1	0	-0.566232	4.245745	2.332053
4	6	0	1.028980	3.834169	0.989989
5	1	0	1.583641	4.683736	1.388718
6	6	0	1.087865	1.969543	-0.545021
7	1	0	0.046610	1.781775	-0.311157
8	1	0	0.806811	0.450792	-1.860240
9	7	0	1.551875	1.048650	-1.440917
10	6	0	2.857683	0.640031	-1.656873
11	8	0	2.871807	-0.223330	-2.693181
12	8	0	3.838857	0.954529	-1.010699
13	1	0	0.948797	-1.209328	0.745824
14	6	0	5.328812	-2.926975	0.074174
15	6	0	5.421556	-1.797135	0.868587
16	6	0	4.263120	-1.080690	1.231536
17	6	0	3.005585	-1.543206	0.766854
18	6	0	2.911547	-2.686311	-0.050900
19	6	0	4.068971	-3.367767	-0.384615
20	1	0	5.225305	0.476839	2.400226
21	1	0	6.225171	-3.474842	-0.200604
22	1	0	6.388091	-1.444470	1.218882
23	6	0	4.271664	0.099535	2.040403
24	1	0	1.933886	-3.002897	-0.402245
25	1	0	4.005122	-4.251670	-1.012792
26	6	0	1.850515	0.259792	1.886364
27	6	0	3.115554	0.748769	2.354695
28	1	0	3.132336	1.642379	2.966255
29	7	0	1.871032	-0.856581	1.114058
30	6	0	0.578751	0.798410	2.216299
31	1	0	-0.280814	0.256031	1.835707
32	6	0	0.347426	1.945971	2.965321
33	1	0	1.155449	2.436059	3.499657
34	1	0	-0.624138	2.049106	3.439008
35	6	0	-4.484122	-0.965615	0.209533
36	6	0	-5.487344	-1.327188	1.122944
37	6	0	-5.624166	-2.640784	1.566738
38	6	0	-4.748291	-3.626624	1.104847
39	6	0	-3.743763	-3.293949	0.197840
40	6	0	-3.621330	-1.979563	-0.246532
41	6	0	-4.350418	0.426422	-0.276070
42	6	0	-5.478080	1.181786	-0.634167
43	6	0	-5.359941	2.491359	-1.095910
44	6	0	-4.096072	3.071267	-1.223096
45	6	0	-2.959931	2.342186	-0.874829
46	6	0	-3.088183	1.039903	-0.392981
47	1	0	-6.152649	-0.554869	1.499430
48	1	0	-6.405329	-2.892375	2.278667
49	1	0	-4.844247	-4.651813	1.451747
50	1	0	-3.048050	-4.033430	-0.183832
51	1	0	-6.457845	0.716933	-0.567388
52	1	0	-6.249647	3.050084	-1.372211
53	1	0	-3.991491	4.085270	-1.599029
54	1	0	-1.967653	2.768279	-0.978688
55	8	0	-2.678584	-1.695337	-1.220971
56	8	0	-1.957729	0.383001	0.059675
57	15	0	-1.305430	-0.892352	-0.814785
58	8	0	-0.501592	-1.677126	0.194571
59	8	0	-0.684486	-0.367601	-2.074604
60	6	0	4.162226	-0.769402	-3.004634
61	1	0	4.577848	-1.297008	-2.143394
62	1	0	3.988392	-1.459537	-3.830745
63	1	0	4.850028	0.025799	-3.307196
64	6	0	1.697160	3.101062	-0.027964
65	6	0	3.037155	3.619456	-0.499052
66	1	0	3.869367	3.115919	0.000949
67	1	0	3.173965	3.455077	-1.571320
68	1	0	3.108244	4.696104	-0.309311

TS_{Me}-Cc(S-en)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2063.027155 hartree

Sum of electronic and thermal Free Energies = -2062.553969 hartree

The number of imaginary frequency = 1

Imaginary frequency = -329.00

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.499912	3.502914	-2.248226
2	1	0	0.358016	2.849206	-2.127002
3	1	0	-0.248870	4.540128	-2.454700
4	6	0	-1.711839	3.017507	-2.716041
5	1	0	-2.423081	3.758749	-3.081073
6	6	0	-1.385961	0.707532	-2.108946
7	1	0	-0.331072	0.921092	-1.976803
8	1	0	-0.746596	-1.130097	-1.621972
9	7	0	-1.624012	-0.603232	-1.812825
10	6	0	-2.814278	-1.227016	-1.481455
11	8	0	-2.577882	-2.548419	-1.334739
12	8	0	-3.896652	-0.700972	-1.307304
13	1	0	-0.950824	-0.085675	1.249930
14	6	0	-5.087246	-1.984793	2.575912
15	6	0	-5.334020	-0.713575	2.088115
16	6	0	-4.273642	0.092930	1.626159
17	6	0	-2.956117	-0.429782	1.669460
18	6	0	-2.704053	-1.726122	2.159866
19	6	0	-3.768137	-2.486547	2.611934
20	1	0	-5.441608	1.833164	1.057222
21	1	0	-5.908126	-2.600041	2.931919
22	1	0	-6.346932	-0.321299	2.051517
23	6	0	-4.439556	1.415127	1.107262
24	1	0	-1.682597	-2.095188	2.167530
25	1	0	-3.584328	-3.486028	2.995742
26	6	0	-2.045944	1.599715	0.730981
27	6	0	-3.370521	2.144802	0.677487
28	1	0	-3.504879	3.143460	0.280570
29	7	0	-1.916121	0.340838	1.217760
30	6	0	-0.851144	2.280762	0.370358
31	1	0	0.065646	1.715597	0.492688
32	6	0	-0.759015	3.578489	-0.109925
33	1	0	-1.614488	4.245892	-0.087614
34	1	0	0.201499	4.078824	-0.032979
35	6	0	-3.728917	-3.329858	-0.980429
36	1	0	-4.475521	-3.291240	-1.779348
37	1	0	-3.356313	-4.346961	-0.854960
38	1	0	-4.174871	-2.965702	-0.052573
39	6	0	4.405161	0.540273	0.778144
40	6	0	5.373921	1.130344	1.605759
41	6	0	5.079008	2.235203	2.401495
42	6	0	3.790343	2.772562	2.389898
43	6	0	2.809165	2.204807	1.579037
44	6	0	3.113565	1.103594	0.778633
45	6	0	4.742350	-0.623437	-0.072984
46	6	0	5.951754	-0.679205	-0.784621
47	6	0	6.278936	-1.781036	-1.571942
48	6	0	5.392009	-2.856435	-1.668438
49	6	0	4.184717	-2.825476	-0.973013
50	6	0	3.871896	-1.722679	-0.181903
51	1	0	6.368556	0.693980	1.632526
52	1	0	5.847844	2.666055	3.036641
53	1	0	3.545956	3.628473	3.013225
54	1	0	1.800931	2.604500	1.557433
55	1	0	6.629313	0.168452	-0.729236
56	1	0	7.218221	-1.795473	-2.117743
57	1	0	5.636747	-3.715603	-2.286879
58	1	0	3.472376	-3.641856	-1.024003
59	8	0	2.147783	0.637567	-0.095008
60	8	0	2.712149	-1.756740	0.574987
61	15	0	1.421966	-0.851974	0.113146
62	8	0	0.496933	-0.797418	1.305198
63	8	0	0.918641	-1.240813	-1.247548
64	6	0	-2.210465	1.688244	-2.635607
65	6	0	-3.614571	1.436297	-3.137235
66	1	0	-3.698395	0.460500	-3.621715
67	1	0	-4.346907	1.443040	-2.324657
68	1	0	-3.890974	2.203939	-3.868507

TS_{Me}-Ct(R-en)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2063.021822 hartree

Sum of electronic and thermal Free Energies = -2062.547342 hartree

The number of imaginary frequency = 1

Imaginary frequency = -335.28

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.085618	3.408101	1.697747
2	1	0	-0.855071	2.833282	1.193918
3	1	0	-0.464855	4.108991	2.437208
4	6	0	1.109721	3.722323	1.064081
5	1	0	1.690721	4.533504	1.503608
6	6	0	1.104491	1.946099	-0.573610
7	1	0	0.059030	1.787638	-0.333624
8	1	0	0.711911	0.536808	-1.969658
9	7	0	1.503233	1.055585	-1.528600
10	6	0	2.744771	0.563840	-1.907294
11	8	0	3.732805	0.909588	-1.053627
12	8	0	2.897963	-0.146928	-2.877723
13	1	0	0.945270	-1.245058	0.495161
14	6	0	5.292302	-3.090769	-0.100704
15	6	0	5.378056	-2.062727	0.822184
16	6	0	4.233372	-1.314942	1.167296
17	6	0	2.991548	-1.655683	0.570158
18	6	0	2.908855	-2.692116	-0.379797
19	6	0	4.055007	-3.395461	-0.706457
20	1	0	5.188926	0.088614	2.523712
21	1	0	6.178021	-3.659548	-0.366971

22	1	0	6.329625	-1.809624	1.283202
23	6	0	4.245743	-0.202321	2.067422
24	1	0	1.949609	-2.910824	-0.839114
25	1	0	3.999031	-4.191545	-1.442801
26	6	0	1.847216	0.089099	1.788588
27	6	0	3.105197	0.486578	2.354334
28	1	0	3.124393	1.325851	3.038469
29	7	0	1.866432	-0.953470	0.918837
30	6	0	0.582929	0.638757	2.126570
31	1	0	-0.281881	0.145717	1.695842
32	6	0	0.365921	1.741248	2.943351
33	1	0	1.174659	2.181422	3.518546
34	1	0	-0.612469	1.842430	3.402829
35	6	0	5.045714	0.508439	-1.479728
36	1	0	5.088747	-0.572063	-1.624311
37	1	0	5.312074	1.012802	-2.413174
38	1	0	5.714019	0.813594	-0.674264
39	6	0	-4.412267	0.450050	-0.158811
40	6	0	-5.560474	1.219538	-0.403416
41	6	0	-5.472253	2.561017	-0.770774
42	6	0	-4.219402	3.160270	-0.916830
43	6	0	-3.063512	2.417762	-0.679648
44	6	0	-3.161128	1.082848	-0.289235
45	6	0	-4.512227	-0.976947	0.222066
46	6	0	-5.466715	-1.419910	1.151667
47	6	0	-5.572392	-2.765702	1.496534
48	6	0	-4.713563	-3.702718	0.916188
49	6	0	-3.757280	-3.289165	-0.009535
50	6	0	-3.665860	-1.942691	-0.354127
51	1	0	-6.533157	0.741833	-0.324834
52	1	0	-6.377548	3.130583	-0.960860
53	1	0	-4.139359	4.199883	-1.222232
54	1	0	-2.079095	2.857212	-0.801983
55	1	0	-6.118261	-0.686749	1.619493
56	1	0	-6.315923	-3.080884	2.223302
57	1	0	-4.785442	-4.753014	1.185031
58	1	0	-3.076589	-3.988932	-0.482305
59	8	0	-2.006755	0.403672	0.057488
60	8	0	-2.774477	-1.573463	-1.348226
61	15	0	-1.389277	-0.787826	-0.950961
62	8	0	-0.839187	-0.150517	-2.191147
63	8	0	-0.524879	-1.639610	-0.051946
64	6	0	1.751588	3.028268	0.002072
65	6	0	3.099364	3.548266	-0.446664
66	1	0	3.925175	3.064329	0.085359
67	1	0	3.261942	3.379674	-1.514234
68	1	0	3.159629	4.626604	-0.262873

TS_{Me}-Ct(S-en)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2063.021633 hartree

Sum of electronic and thermal Free Energies = -2062.547486 hartree

The number of imaginary frequency = 1

Imaginary frequency = -323.58

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.883000	3.585553	-2.237758
2	1	0	0.031387	3.001749	-2.261710
3	1	0	-0.740450	4.651085	-2.397236
4	6	0	-2.099469	3.026249	-2.596799
5	1	0	-2.902814	3.725051	-2.831834
6	6	0	-1.531410	0.725312	-2.169358
7	1	0	-0.495217	1.041932	-2.124143
8	1	0	-0.631193	-1.028307	-1.852560
9	7	0	-1.584013	-0.616076	-1.928101
10	6	0	-2.589045	-1.498286	-1.557506
11	8	0	-3.757075	-0.886986	-1.271875
12	8	0	-2.401306	-2.693190	-1.464395
13	1	0	-0.863172	-0.258273	1.035905
14	6	0	-4.806752	-2.268537	2.735943
15	6	0	-5.106357	-0.961813	2.393151
16	6	0	-4.116527	-0.125853	1.834744
17	6	0	-2.809729	-0.648085	1.649848
18	6	0	-2.510269	-1.984645	1.980912
19	6	0	-3.507903	-2.777681	2.520289
20	1	0	-5.346473	1.639461	1.530527
21	1	0	-5.572377	-2.908280	3.164409
22	1	0	-6.107125	-0.564338	2.542965
23	6	0	-4.348436	1.222729	1.418405
24	1	0	-1.506615	-2.357852	1.801302
25	1	0	-3.286089	-3.808984	2.778074
26	6	0	-2.018278	1.451958	0.761062
27	6	0	-3.344577	1.982162	0.892824
28	1	0	-3.530111	3.001909	0.579208
29	7	0	-1.830840	0.162229	1.133237
30	6	0	-0.879034	2.187970	0.332187
31	1	0	0.063918	1.652703	0.330801
32	6	0	-0.875236	3.514456	-0.071678
33	1	0	-1.739573	4.151687	0.083532
34	1	0	0.074514	4.039872	-0.074358
35	6	0	-4.842771	-1.786272	-0.988648
36	1	0	-5.057561	-2.408271	-1.862237
37	1	0	-4.599049	-2.424364	-0.138183
38	1	0	-5.692084	-1.144506	-0.754370
39	6	0	4.400381	0.483419	0.960614
40	6	0	5.277966	0.905321	1.972098
41	6	0	4.879516	1.814952	2.949488
42	6	0	3.577889	2.320878	2.937357
43	6	0	2.685817	1.917312	1.945286
44	6	0	3.095150	1.012665	0.966305
45	6	0	4.841122	-0.470076	-0.083094
46	6	0	6.102373	-0.352833	-0.689287
47	6	0	6.525852	-1.255809	-1.662119
48	6	0	5.685579	-2.300415	-2.055815
49	6	0	4.428504	-2.439081	-1.470261
50	6	0	4.018749	-1.535656	-0.492511
51	1	0	6.282194	0.491190	1.994499
52	1	0	5.578467	2.117912	3.724033
53	1	0	3.254804	3.024392	3.699955
54	1	0	1.669400	2.296040	1.912905

55	1	0	6.744595	0.474868	-0.400841
56	1	0	7.504077	-1.137815	-2.119876
57	1	0	6.005574	-3.003964	-2.819452
58	1	0	3.750941	-3.238862	-1.749268
59	8	0	2.221108	0.715085	-0.063870
60	8	0	2.808962	-1.755317	0.145115
61	15	0	1.521062	-0.793228	-0.185480
62	8	0	0.550817	-0.988029	0.955612
63	8	0	1.068895	-0.905105	-1.613835
64	6	0	-2.484576	1.657124	-2.551545
65	6	0	-3.912118	1.331179	-2.930681
66	1	0	-3.987109	0.364177	-3.432870
67	1	0	-4.569267	1.291060	-2.055149
68	1	0	-4.297216	2.097241	-3.612541

TS_{Me}-Tc(R-ex)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2063.036231 hartree

Sum of electronic and thermal Free Energies = -2062.562251 hartree

The number of imaginary frequency = 1

Imaginary frequency = -340.04

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.213823	-2.778370	0.214728
2	1	0	-5.454525	-1.724934	0.323641
3	1	0	-6.050594	-3.400883	-0.091273
4	6	0	-4.196073	-3.353406	0.964057
5	1	0	-4.178619	-4.441723	1.016028
6	6	0	-2.993051	-1.314640	1.428079
7	1	0	-3.868716	-0.719634	1.199961
8	1	0	-0.945416	-0.986290	1.749079
9	7	0	-1.901262	-0.563563	1.743738
10	6	0	-2.012143	0.818221	1.796103
11	8	0	-0.801966	1.369917	2.007096
12	8	0	-3.049414	1.442447	1.665789
13	1	0	-1.025894	-0.167230	-1.299061
14	6	0	-1.342272	4.571272	-1.286725
15	6	0	-2.623089	4.054473	-1.363276
16	6	0	-2.828460	2.658567	-1.398823
17	6	0	-1.698292	1.802156	-1.343430
18	6	0	-0.393265	2.329479	-1.262510
19	6	0	-0.230322	3.702730	-1.239771
20	1	0	-4.994895	2.681074	-1.536011
21	1	0	-1.189511	5.646098	-1.262204
22	1	0	-3.486684	4.713395	-1.399274
23	6	0	-4.114714	2.044518	-1.496866
24	1	0	0.453823	1.655358	-1.199850
25	1	0	0.772176	4.115931	-1.175669
26	6	0	-3.096880	-0.162986	-1.466423
27	6	0	-4.248124	0.687665	-1.540180
28	1	0	-5.228691	0.232641	-1.611418
29	7	0	-1.889104	0.442847	-1.364267
30	6	0	-3.123390	-1.584795	-1.491913
31	1	0	-2.161013	-2.072569	-1.368329
32	6	0	-4.259116	-2.363578	-1.684690
33	1	0	-5.171620	-1.924905	-2.078986
34	1	0	-4.118866	-3.405459	-1.948477
35	6	0	-0.799553	2.801631	2.141787
36	1	0	-1.233969	3.086478	3.105065
37	1	0	0.249646	3.092212	2.092686
38	1	0	-1.363381	3.268882	1.333936
39	6	0	4.323105	-0.490859	-0.703062
40	6	0	5.354048	-0.105375	-1.574713
41	6	0	5.532153	-0.725932	-2.809471
42	6	0	4.668941	-1.751489	-3.202968
43	6	0	3.637450	-2.154062	-2.356495
44	6	0	3.472644	-1.534664	-1.119322
45	6	0	4.145878	0.163501	0.613184
46	6	0	5.239055	0.458788	1.442869
47	6	0	5.060350	1.058391	2.688477
48	6	0	3.772567	1.359896	3.139783
49	6	0	2.670099	1.080122	2.333604
50	6	0	2.864171	0.508726	1.078225
51	1	0	6.009478	0.708737	-1.277032
52	1	0	6.335086	-0.403203	-3.466401
53	1	0	4.796015	-2.236168	-4.167131
54	1	0	2.952283	-2.950230	-2.627498
55	1	0	6.236706	0.186453	1.109355
56	1	0	5.922682	1.269286	3.314834
57	1	0	3.625875	1.803660	4.120863
58	1	0	1.653233	1.272185	2.656020
59	8	0	2.506049	-2.032438	-0.262243
60	8	0	1.773125	0.341138	0.243934
61	15	0	1.133938	-1.177979	0.042436
62	8	0	0.277010	-1.076918	-1.198287
63	8	0	0.567567	-1.691270	1.335838
64	6	0	-3.058528	-2.693955	1.493233
65	6	0	-1.906845	-3.501400	2.049099
66	1	0	-1.022583	-3.444186	1.406486
67	1	0	-1.592043	-3.119382	3.027454
68	1	0	-2.190583	-4.551649	2.167816

TS_{Me}-Tc(S-ex)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2063.033023 hartree

Sum of electronic and thermal Free Energies = -2062.559024 hartree

The number of imaginary frequency = 1

Imaginary frequency = -342.03

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.968945	-3.776307	-1.431598
2	1	0	4.626305	-3.111976	-0.878845
3	1	0	4.487040	-4.474817	-2.083716
4	6	0	2.733851	-4.146760	-0.909908
5	1	0	2.244691	-5.005277	-1.370180
6	6	0	2.491741	-2.287143	0.601531

7	1	0	3.555750	-2.095021	0.537076
8	1	0	0.799643	-1.345733	1.456843
9	7	0	1.844869	-1.391941	1.388759
10	6	0	2.565058	-0.375458	2.006437
11	8	0	1.726716	0.416789	2.692932
12	8	0	3.770643	-0.222120	1.927943
13	1	0	1.083740	0.280390	-0.962041
14	6	0	2.735029	4.324322	0.944934
15	6	0	3.799528	3.634177	0.391673
16	6	0	3.594174	2.391140	-0.243714
17	6	0	2.276870	1.867565	-0.307473
18	6	0	1.197626	2.560662	0.277758
19	6	0	1.434992	3.778950	0.889198
20	1	0	5.659015	1.991328	-0.786469
21	1	0	2.899428	5.281479	1.430551
22	1	0	4.807431	4.038202	0.439847
23	6	0	4.640471	1.615110	-0.835366
24	1	0	0.204196	2.125060	0.259062
25	1	0	0.605413	4.315504	1.340456
26	6	0	3.038044	-0.079818	-1.523150
27	6	0	4.377920	0.427302	-1.449799
28	1	0	5.177685	-0.149965	-1.897818
29	7	0	2.066393	0.665767	-0.935182
30	6	0	2.638302	-1.271863	-2.179499
31	1	0	1.570479	-1.467006	-2.171611
32	6	0	3.477353	-2.190794	-2.804232
33	1	0	4.518688	-1.949002	-3.001269
34	1	0	3.035237	-2.862799	-3.530892
35	6	0	2.358147	1.485637	3.415182
36	1	0	2.949790	2.110049	2.743308
37	1	0	1.539214	2.059397	3.848548
38	1	0	3.003989	1.081851	4.200580
39	6	0	-4.187128	0.995593	-0.686500
40	6	0	-5.070236	1.664434	-1.549153
41	6	0	-4.672223	2.786852	-2.272321
42	6	0	-3.365124	3.263083	-2.150311
43	6	0	-2.467799	2.617031	-1.301756
44	6	0	-2.876796	1.499882	-0.574866
45	6	0	-4.627571	-0.189644	0.084118
46	6	0	-5.881806	-0.224635	0.714357
47	6	0	-6.304801	-1.345998	1.424976
48	6	0	-5.471216	-2.462850	1.524880
49	6	0	-4.220956	-2.453283	0.909147
50	6	0	-3.811674	-1.330398	0.193856
51	1	0	-6.078795	1.276517	-1.662378
52	1	0	-5.375796	3.279851	-2.937259
53	1	0	-3.041928	4.132733	-2.715975
54	1	0	-1.447986	2.969148	-1.187135
55	1	0	-6.518720	0.653866	0.657480
56	1	0	-7.277325	-1.343807	1.909232
57	1	0	-5.790892	-3.337750	2.084271
58	1	0	-3.548374	-3.302643	0.964380
59	8	0	-1.993790	0.949638	0.338472
60	8	0	-2.608604	-1.382455	-0.489728
61	15	0	-1.312179	-0.541238	0.075869
62	8	0	-0.344854	-0.465179	-1.082499
63	8	0	-0.854788	-1.045122	1.414821
64	6	0	1.938606	-3.400368	-0.005637
65	6	0	0.482942	-3.770731	0.173465
66	1	0	0.093089	-3.478830	1.151514
67	1	0	-0.137993	-3.264909	-0.575607
68	1	0	0.344662	-4.850591	0.052076

TS_{Me}-Tt(R-ex)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2063.032556 hartree

Sum of electronic and thermal Free Energies = -2062.557978 hartree

The number of imaginary frequency = 1

Imaginary frequency = -339.75

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.917981	-3.005968	0.223965
2	1	0	-5.203249	-1.957901	0.237022
3	1	0	-5.716474	-3.684273	-0.065632
4	6	0	-3.916870	-3.479418	1.062431
5	1	0	-3.859140	-4.559417	1.194560
6	6	0	-2.821471	-1.360294	1.457722
7	1	0	-3.710676	-0.824172	1.154658
8	1	0	-0.794434	-0.971190	1.829178
9	7	0	-1.760025	-0.566559	1.776580
10	6	0	-1.790338	0.816334	1.835377
11	8	0	-3.033040	1.311912	1.622215
12	8	0	-0.813180	1.502116	2.057940
13	1	0	-0.907341	-0.217428	-1.190968
14	6	0	-1.681387	4.486908	-1.424280
15	6	0	-2.877474	3.836593	-1.668063
16	6	0	-2.941254	2.427065	-1.637208
17	6	0	-1.755065	1.693007	-1.366649
18	6	0	-0.540008	2.358605	-1.106579
19	6	0	-0.517450	3.741584	-1.137878
20	1	0	-5.064918	2.223639	-2.042183
21	1	0	-1.636561	5.571647	-1.445578
22	1	0	-3.783543	4.399028	-1.879100
23	6	0	-4.143433	1.682368	-1.841336
24	1	0	0.347756	1.782979	-0.865637
25	1	0	0.414383	4.258904	-0.929845
26	6	0	-2.937866	-0.407610	-1.531081
27	6	0	-4.148397	0.319478	-1.783066
28	1	0	-5.067575	-0.233693	-1.933134
29	7	0	-1.809450	0.320934	-1.339934
30	6	0	-2.836566	-1.823624	-1.467980
31	1	0	-1.847388	-2.214679	-1.251659
32	6	0	-3.894491	-2.707463	-1.653680
33	1	0	-4.814981	-2.383849	-2.131863
34	1	0	-3.657639	-3.752797	-1.815717
35	6	0	-3.135968	2.739672	1.762773
36	1	0	-2.417193	3.244971	1.116279
37	1	0	-4.156637	2.984223	1.467306
38	1	0	-2.957057	3.029544	2.802191
39	6	0	4.176091	0.407251	0.614338

40	6	0	5.231129	0.841663	1.432849
41	6	0	4.989568	1.579942	2.589974
42	6	0	3.678248	1.894095	2.958561
43	6	0	2.610565	1.475265	2.165778
44	6	0	2.869931	0.748439	1.006848
45	6	0	4.422361	-0.359198	-0.629216
46	6	0	5.462998	-0.000424	-1.501564
47	6	0	5.709650	-0.710975	-2.674368
48	6	0	4.905496	-1.803765	-3.006495
49	6	0	3.865374	-2.181503	-2.159422
50	6	0	3.631927	-1.470941	-0.983463
51	1	0	6.248616	0.573754	1.161325
52	1	0	5.823015	1.897466	3.210711
53	1	0	3.485884	2.459666	3.866406
54	1	0	1.577022	1.689116	2.415605
55	1	0	6.070986	0.865788	-1.255013
56	1	0	6.519031	-0.405705	-3.331795
57	1	0	5.085173	-2.360154	-3.922414
58	1	0	3.225796	-3.029145	-2.381747
59	8	0	1.809524	0.420002	0.177189
60	8	0	2.664251	-1.951249	-0.118865
61	15	0	1.258811	-1.141207	0.141534
62	8	0	0.751284	-1.578602	1.487406
63	8	0	0.357554	-1.189458	-1.072188
64	6	0	-2.834809	-2.737097	1.596833
65	6	0	-1.675991	-3.458263	2.248887
66	1	0	-0.766487	-3.396446	1.642633
67	1	0	-1.423909	-3.008234	3.216457
68	1	0	-1.918565	-4.512289	2.414781

TS_{Me}-Tt(S-ex)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2063.029231 hartree

Sum of electronic and thermal Free Energies = -2062.554628 hartree

The number of imaginary frequency = 1

Imaginary frequency = -332.13

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.554586	-4.181233	1.340954
2	1	0	-2.522375	-3.688950	1.314590
3	1	0	-1.488268	-5.007691	2.043565
4	6	0	-0.737809	-4.197337	0.219387
5	1	0	0.071656	-4.927136	0.213578
6	6	0	-1.685566	-2.264514	-0.884958
7	1	0	-2.582601	-2.337750	-0.284582
8	1	0	-0.733394	-0.852339	-2.087891
9	7	0	-1.651891	-1.193656	-1.729897
10	6	0	-2.715077	-0.336637	-1.972165
11	8	0	-3.853426	-0.762637	-1.367695
12	8	0	-2.632276	0.661805	-2.653723
13	1	0	-1.010954	0.859108	0.499175
14	6	0	-5.070802	3.283104	0.421394
15	6	0	-5.254988	2.174343	1.227057
16	6	0	-4.203313	1.253124	1.421329
17	6	0	-2.956656	1.493819	0.784885
18	6	0	-2.775203	2.617622	-0.047534
19	6	0	-3.829918	3.496272	-0.217712
20	1	0	-5.264901	-0.142474	2.702205
21	1	0	-5.882464	3.988914	0.272545
22	1	0	-6.209047	1.994036	1.715879
23	6	0	-4.318044	0.068602	2.211038
24	1	0	-1.819923	2.755173	-0.542789
25	1	0	-3.700580	4.360975	-0.861712
26	6	0	-2.008849	-0.522841	1.717292
27	6	0	-3.267368	-0.790932	2.350618
28	1	0	-3.368508	-1.689029	2.947660
29	7	0	-1.924706	0.606710	0.972397
30	6	0	-0.861208	-1.357022	1.812878
31	1	0	0.019449	-1.035238	1.268824
32	6	0	-0.789010	-2.533758	2.546707
33	1	0	-1.513233	-2.759214	3.324346
34	1	0	0.191734	-2.964608	2.712876
35	6	0	-5.018612	0.020139	-1.678003
36	1	0	-5.814135	-0.388341	-1.053995
37	1	0	-4.852241	1.073157	-1.447546
38	1	0	-5.270549	-0.083423	-2.737472
39	6	0	4.298314	-0.157830	0.222748
40	6	0	5.504747	-0.876853	0.213461
41	6	0	5.523413	-2.270213	0.214037
42	6	0	4.321343	-2.981556	0.228057
43	6	0	3.109836	-2.293014	0.230195
44	6	0	3.100589	-0.898580	0.216722
45	6	0	4.289772	1.322135	0.292038
46	6	0	5.175072	2.005298	1.142555
47	6	0	5.179422	3.396016	1.222863
48	6	0	4.283306	4.140168	0.451426
49	6	0	3.393414	3.487756	-0.399405
50	6	0	3.403459	2.096747	-0.479208
51	1	0	6.439440	-0.323421	0.191813
52	1	0	6.472662	-2.798265	0.199167
53	1	0	4.325826	-4.068246	0.233146
54	1	0	2.158501	-2.814341	0.250369
55	1	0	5.852332	1.425278	1.763414
56	1	0	5.871739	3.896500	1.894099
57	1	0	4.275035	5.224959	0.512758
58	1	0	2.687949	4.032136	-1.018047
59	8	0	1.885671	-0.252169	0.308301
60	8	0	2.584173	1.490575	-1.414304
61	15	0	1.259400	0.638813	-0.957926
62	8	0	0.894833	-0.251495	-2.109899
63	8	0	0.229082	1.516687	-0.288831
64	6	0	-0.721584	-3.257193	-0.842581
65	6	0	0.360093	-3.331397	-1.898696
66	1	0	-0.081851	-3.325688	-2.902742
67	1	0	1.039033	-2.475302	-1.856492
68	1	0	0.945257	-4.249914	-1.790408

(R=F)

TS_{F}-Cc(R-en)

B3LYP-D3/6-31g(d) in gas phase
SCF Done: E(RB3LYP) = -2122.936896 hartree
Sum of electronic and thermal Free Energies = -2122.498689 hartree
The number of imaginary frequency = 1
Imaginary frequency = -364.42

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.082591	3.580321	1.648950
2	1	0	-0.883375	3.027240	1.167863
3	1	0	-0.425351	4.331669	2.355674
4	6	0	1.103096	3.835732	0.966051
5	1	0	1.755231	4.632489	1.317105
6	6	0	1.057675	1.913497	-0.579444
7	1	0	0.014130	1.745914	-0.346339
8	1	0	0.831439	0.383381	-1.884568
9	7	0	1.553911	1.001847	-1.456290
10	6	0	2.887951	0.663562	-1.652674
11	8	0	2.957292	-0.196012	-2.690207
12	8	0	3.832824	1.027332	-0.985522
13	1	0	0.938867	-1.196819	0.749119
14	6	0	5.323042	-2.901990	0.083783
15	6	0	5.412475	-1.774196	0.880658
16	6	0	4.251558	-1.059385	1.241101
17	6	0	2.995874	-1.523653	0.772712
18	6	0	2.905482	-2.665486	-0.047709
19	6	0	4.064783	-3.343404	-0.380310
20	1	0	5.208883	0.500073	2.409859
21	1	0	6.220755	-3.448045	-0.190136
22	1	0	6.377409	-1.420321	1.233838
23	6	0	4.256857	0.120349	2.048844
24	1	0	1.929249	-2.982846	-0.402281
25	1	0	4.004423	-4.225318	-1.011526
26	6	0	1.837701	0.283208	1.880475
27	6	0	3.099325	0.770833	2.356436
28	1	0	3.115339	1.668086	2.962402
29	7	0	1.859623	-0.837758	1.115975
30	6	0	0.565449	0.838761	2.186822
31	1	0	-0.294857	0.304231	1.797204
32	6	0	0.337858	1.988285	2.939975
33	1	0	1.143254	2.446429	3.506164
34	1	0	-0.639814	2.093221	3.401727
35	6	0	-4.477753	-0.965052	0.211161
36	6	0	-5.478891	-1.314216	1.131885
37	6	0	-5.619934	-2.623225	1.587540
38	6	0	-4.750594	-3.617185	1.130729
39	6	0	-3.748157	-3.296978	0.217020
40	6	0	-3.621674	-1.987031	-0.238865
41	6	0	-4.340556	0.422850	-0.285534
42	6	0	-5.467781	1.180622	-0.640320
43	6	0	-5.348977	2.488642	-1.106189
44	6	0	-4.084558	3.065564	-1.240476
45	6	0	-2.948808	2.333836	-0.896612
46	6	0	-3.077257	1.032152	-0.412813
47	1	0	-6.139051	-0.535744	1.504645
48	1	0	-6.399361	-2.864940	2.304731
49	1	0	-4.849973	-4.638875	1.486751
50	1	0	-3.057405	-4.042895	-0.161081
51	1	0	-6.448503	0.718960	-0.566481
52	1	0	-6.238730	3.048657	-1.379514
53	1	0	-3.979256	4.078569	-1.618763
54	1	0	-1.956118	2.757738	-1.007617
55	8	0	-2.680512	-1.715595	-1.219203
56	8	0	-1.944722	0.375439	0.034022
57	15	0	-1.302742	-0.918307	-0.823658
58	8	0	-0.502886	-1.690182	0.198723
59	8	0	-0.675577	-0.414754	-2.089092
60	6	0	4.275399	-0.690954	-2.970704
61	1	0	4.680222	-1.221724	-2.105793
62	1	0	4.152344	-1.370224	-3.814751
63	1	0	4.944510	0.133148	-3.234343
64	6	0	1.655756	3.039356	-0.050850
65	9	0	2.872696	3.427247	-0.490715

TS_F-Cc(S-en)

B3LYP-D3/6-31g(d) in gas phase
SCF Done: E(RB3LYP) = -2122.935806 hartree
Sum of electronic and thermal Free Energies = -2122.498794 hartree
The number of imaginary frequency = 1
Imaginary frequency = -353.90

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.624781	3.556470	2.280448
2	1	0	-0.276574	2.953728	2.226872
3	1	0	0.448223	4.607773	2.491277
4	6	0	1.815753	2.994686	2.723922
5	1	0	2.618519	3.647886	3.059122
6	6	0	1.354904	0.658474	2.094637
7	1	0	0.301259	0.886388	1.989129
8	1	0	0.754683	-1.182052	1.587230
9	7	0	1.618605	-0.637790	1.789507
10	6	0	2.845071	-1.218963	1.493130
11	8	0	2.653846	-2.547211	1.339378
12	8	0	3.905508	-0.649405	1.349243
13	1	0	0.940205	-0.070618	-1.236471
14	6	0	5.065234	-1.983416	-2.571065
15	6	0	5.319044	-0.714395	-2.082534
16	6	0	4.262805	0.095827	-1.615790
17	6	0	2.942856	-0.421375	-1.657004
18	6	0	2.683883	-1.716543	-2.148032
19	6	0	3.743600	-2.480348	-2.603232
20	1	0	5.440317	1.826802	-1.041700
21	1	0	5.882369	-2.601945	-2.929975
22	1	0	6.333560	-0.326447	-2.047354
23	6	0	4.436218	1.414476	-1.093547
24	1	0	1.660939	-2.081356	-2.153443
25	1	0	3.555156	-3.479081	-2.986590
26	6	0	2.046194	1.606010	-0.703816

27	6	0	3.371827	2.146771	-0.656225
28	1	0	3.513991	3.141038	-0.251440
29	7	0	1.907552	0.352216	-1.199345
30	6	0	0.858780	2.286311	-0.312313
31	1	0	-0.063052	1.726168	-0.420240
32	6	0	0.783240	3.590049	0.166072
33	1	0	1.637080	4.256361	0.092774
34	1	0	-0.178051	4.091384	0.098206
35	6	0	3.837402	-3.286208	1.000671
36	1	0	4.576077	-3.210889	1.804008
37	1	0	3.506093	-4.318160	0.880757
38	1	0	4.274888	-2.912039	0.072415
39	6	0	-4.402082	0.549539	-0.771453
40	6	0	-5.367524	1.153585	-1.592809
41	6	0	-5.067109	2.266942	-2.374562
42	6	0	-3.776270	2.798828	-2.355298
43	6	0	-2.798282	2.217309	-1.550282
44	6	0	-3.108650	1.108187	-0.763466
45	6	0	-4.744078	-0.624022	0.064138
46	6	0	-5.954187	-0.684771	0.774153
47	6	0	-6.285872	-1.795711	1.546650
48	6	0	-5.403007	-2.875560	1.629527
49	6	0	-4.195110	-2.839935	0.935328
50	6	0	-3.877896	-1.727863	0.159272
51	1	0	-6.363806	0.721511	-1.626246
52	1	0	-5.833441	2.708622	-3.005245
53	1	0	-3.527701	3.660951	-2.968287
54	1	0	-1.788171	2.612022	-1.523152
55	1	0	-6.628697	0.165926	0.729376
56	1	0	-7.225602	-1.813958	2.091526
57	1	0	-5.651354	-3.741931	2.236319
58	1	0	-3.485982	-3.659685	0.975824
59	8	0	-2.145730	0.626832	0.105921
60	8	0	-2.717244	-1.756382	-0.597412
61	15	0	-1.425349	-0.861668	-0.124808
62	8	0	-0.499775	-0.790877	-1.315683
63	8	0	-0.919047	-1.269507	1.229687
64	6	0	2.176686	1.641756	2.608153
65	9	0	3.436276	1.345710	2.995465

TS_F-Ct(R-en)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2122.932397 hartree

Sum of electronic and thermal Free Energies = -2122.494512 hartree

The number of imaginary frequency = 1

Imaginary frequency = -359.31

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.027596	3.421634	1.749630
2	1	0	-0.839951	2.903804	1.249656
3	1	0	-0.352543	4.136838	2.500745
4	6	0	1.153769	3.699394	1.068740
5	1	0	1.817581	4.469910	1.454972
6	6	0	1.072230	1.867072	-0.580828
7	1	0	0.029112	1.709426	-0.336232
8	1	0	0.756773	0.437112	-1.970382
9	7	0	1.517574	0.988696	-1.517001
10	6	0	2.802036	0.596056	-1.882597
11	8	0	3.737242	1.004087	-1.006274
12	8	0	3.016144	-0.092016	-2.857606
13	1	0	0.925910	-1.269740	0.523214
14	6	0	5.273470	-3.072656	-0.168384
15	6	0	5.370406	-2.047608	0.756036
16	6	0	4.225596	-1.313932	1.131763
17	6	0	2.974700	-1.665063	0.560538
18	6	0	2.879383	-2.702599	-0.387249
19	6	0	4.024745	-3.391637	-0.743334
20	1	0	5.194892	0.086238	2.480595
21	1	0	6.158944	-3.629543	-0.459338
22	1	0	6.329804	-1.785490	1.195074
23	6	0	4.246050	-0.208364	2.038868
24	1	0	1.911509	-2.931128	-0.823170
25	1	0	3.960361	-4.186698	-1.480018
26	6	0	1.844011	0.078000	1.793312
27	6	0	3.106884	0.474494	2.346691
28	1	0	3.134456	1.312820	3.031542
29	7	0	1.852263	-0.969010	0.929898
30	6	0	0.583834	0.643329	2.128207
31	1	0	-0.286150	0.155282	1.701965
32	6	0	0.377663	1.748266	2.950177
33	1	0	1.191041	2.161911	3.538907
34	1	0	-0.598168	1.845293	3.417191
35	6	0	5.088027	0.717119	-1.401526
36	1	0	5.225176	-0.355640	-1.549883
37	1	0	5.333053	1.248602	-2.325426
38	1	0	5.707938	1.074366	-0.578914
39	6	0	-4.382535	0.478144	-0.194913
40	6	0	-5.513226	1.266914	-0.459406
41	6	0	-5.396119	2.600748	-0.845936
42	6	0	-4.130870	3.173434	-0.990837
43	6	0	-2.991807	2.411302	-0.735179
44	6	0	-3.118195	1.083569	-0.328293
45	6	0	-4.515546	-0.938531	0.213855
46	6	0	-5.486242	-1.340785	1.145399
47	6	0	-5.623708	-2.676166	1.518136
48	6	0	-4.781313	-3.643943	0.964836
49	6	0	-3.809376	-3.271184	0.038155
50	6	0	-3.686341	-1.934745	-0.334114
51	1	0	-6.495823	0.810235	-0.379736
52	1	0	-6.288670	3.184990	-1.050876
53	1	0	-4.028002	4.206902	-1.309778
54	1	0	-1.998395	2.830602	-0.857390
55	1	0	-6.125017	-0.583985	1.592659
56	1	0	-6.379266	-2.959344	2.245629
57	1	0	-4.878097	-4.686368	1.255452
58	1	0	-3.140608	-3.995510	-0.414167
59	8	0	-1.978579	0.388491	0.035001
60	8	0	-2.778908	-1.606399	-1.328822
61	15	0	-1.380612	-0.845061	-0.936679
62	8	0	-0.799759	-0.253730	-2.185579

63	8	0	-0.544101	-1.688413	-0.003767
64	6	0	1.687767	2.956707	0.002412
65	9	0	2.905774	3.364139	-0.426773

TS_F-Ct(S-en)

F_s-trans_s-cis-B_S-endo

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2122.931994 hartree

Sum of electronic and thermal Free Energies = -2122.494287 hartree

The number of imaginary frequency = 1

Imaginary frequency = -349.74

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.968224	3.460272	-2.465906
2	1	0	-0.029362	2.917692	-2.513902
3	1	0	-0.885143	4.519485	-2.693395
4	6	0	-2.161462	2.819200	-2.774497
5	1	0	-3.035312	3.417697	-3.023312
6	6	0	-1.488787	0.528071	-2.183747
7	1	0	-0.454563	0.850883	-2.181299
8	1	0	-0.638750	-1.213491	-1.720989
9	7	0	-1.578335	-0.781798	-1.840018
10	6	0	-2.636496	-1.598177	-1.453141
11	8	0	-3.783440	-0.923062	-1.272352
12	8	0	-2.490784	-2.787390	-1.261564
13	1	0	-0.864491	-0.184233	1.052534
14	6	0	-4.826279	-2.080556	2.836819
15	6	0	-5.119673	-0.795629	2.416774
16	6	0	-4.123163	0.003315	1.816645
17	6	0	-2.816594	-0.532542	1.672395
18	6	0	-2.523003	-1.847686	2.085029
19	6	0	-3.527096	-2.604964	2.661271
20	1	0	-5.346152	1.749009	1.399518
21	1	0	-5.596941	-2.692695	3.295480
22	1	0	-6.120353	-0.387637	2.534756
23	6	0	-4.348819	1.323762	1.318821
24	1	0	-1.519178	-2.233474	1.935992
25	1	0	-3.310922	-3.620347	2.979647
26	6	0	-2.018064	1.502656	0.650687
27	6	0	-3.341473	2.045389	0.748165
28	1	0	-3.525001	3.042360	0.367724
29	7	0	-1.833037	0.241784	1.111040
30	6	0	-0.881380	2.201156	0.153479
31	1	0	0.061431	1.666361	0.181691
32	6	0	-0.882204	3.502232	-0.338152
33	1	0	-1.736765	4.153300	-0.184005
34	1	0	0.070557	4.021920	-0.377173
35	6	0	-4.916920	-1.750104	-0.960126
36	1	0	-5.123505	-2.436357	-1.786122
37	1	0	-4.734963	-2.321575	-0.048290
38	1	0	-5.745648	-1.056108	-0.820418
39	6	0	4.401384	0.563016	0.908097
40	6	0	5.282183	1.078396	1.872407
41	6	0	4.885043	2.072136	2.764725
42	6	0	3.581397	2.570312	2.713581
43	6	0	2.686108	2.074938	1.767029
44	6	0	3.094489	1.086696	0.872248
45	6	0	4.840505	-0.481163	-0.045657
46	6	0	6.098736	-0.416897	-0.665919
47	6	0	6.520774	-1.404675	-1.553193
48	6	0	5.682208	-2.483545	-1.844907
49	6	0	4.428132	-2.571103	-1.243249
50	6	0	4.020057	-1.582314	-0.351334
51	1	0	6.287977	0.671239	1.927546
52	1	0	5.586626	2.446798	3.504720
53	1	0	3.259235	3.338991	3.410836
54	1	0	1.667750	2.444855	1.706227
55	1	0	6.739663	0.435557	-0.457981
56	1	0	7.496635	-1.326804	-2.024329
57	1	0	6.001160	-3.253733	-2.541710
58	1	0	3.751974	-3.395161	-1.444024
59	8	0	2.216298	0.693866	-0.122578
60	8	0	2.813063	-1.745422	0.309349
61	15	0	1.522235	-0.821609	-0.103454
62	8	0	0.552556	-0.914121	1.050914
63	8	0	1.065270	-1.063731	-1.514647
64	6	0	-2.424220	1.447254	-2.618228
65	9	0	-3.699618	1.076877	-2.877635

TS_F-Tc(R-ex)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2122.940557 hartree

Sum of electronic and thermal Free Energies = -2122.502946 hartree

The number of imaginary frequency = 1

Imaginary frequency = -371.52

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.019979	-3.000385	0.423886
2	1	0	-5.392283	-1.983127	0.506698
3	1	0	-5.781770	-3.733130	0.171739
4	6	0	-3.948354	-3.409956	1.213138
5	1	0	-3.755989	-4.471993	1.345660
6	6	0	-2.925492	-1.188723	1.517881
7	1	0	-3.836551	-0.670913	1.250109
8	1	0	-0.898068	-0.810739	1.860759
9	7	0	-1.864083	-0.394065	1.793766
10	6	0	-2.018040	0.984031	1.746394
11	8	0	-0.832472	1.588352	1.939892
12	8	0	-3.073499	1.559758	1.551654
13	1	0	-1.014360	-0.272300	-1.237414
14	6	0	-1.464484	4.448302	-1.613220
15	6	0	-2.728560	3.889408	-1.665885
16	6	0	-2.893385	2.489618	-1.591225
17	6	0	-1.739828	1.674205	-1.452707
18	6	0	-0.451874	2.244982	-1.394097
19	6	0	-0.328880	3.619834	-1.479606

20	1	0	-5.056909	2.437110	-1.759092
21	1	0	-1.342722	5.525657	-1.673530
22	1	0	-3.609802	4.517477	-1.766694
23	6	0	-4.159881	1.832110	-1.655224
24	1	0	0.413245	1.603766	-1.263325
25	1	0	0.660015	4.066829	-1.433680
26	6	0	-3.079966	-0.333775	-1.432422
27	6	0	-4.254231	0.472599	-1.588940
28	1	0	-5.219990	-0.016017	-1.639367
29	7	0	-1.890864	0.313143	-1.366830
30	6	0	-3.059768	-1.753472	-1.343875
31	1	0	-2.078073	-2.194381	-1.196026
32	6	0	-4.165513	-2.594263	-1.471878
33	1	0	-5.097820	-2.214217	-1.882563
34	1	0	-3.973324	-3.634420	-1.710966
35	6	0	-0.881750	3.025588	1.975391
36	1	0	-1.360703	3.359738	2.900747
37	1	0	0.158513	3.348885	1.943290
38	1	0	-1.429722	3.416217	1.117366
39	6	0	4.303689	-0.559492	-0.685819
40	6	0	5.320188	-0.289727	-1.615994
41	6	0	5.480207	-1.063915	-2.763348
42	6	0	4.612751	-2.131320	-3.008006
43	6	0	3.595406	-2.421356	-2.100591
44	6	0	3.448451	-1.647930	-0.950884
45	6	0	4.145631	0.260667	0.536666
46	6	0	5.250514	0.662495	1.303694
47	6	0	5.089239	1.421540	2.461649
48	6	0	3.807842	1.781109	2.888037
49	6	0	2.694206	1.397642	2.142260
50	6	0	2.870384	0.664387	0.971253
51	1	0	5.978662	0.555839	-1.435901
52	1	0	6.272267	-0.828517	-3.468808
53	1	0	4.725739	-2.736240	-3.903558
54	1	0	2.907948	-3.246075	-2.255575
55	1	0	6.243577	0.348129	0.994330
56	1	0	5.960340	1.712597	3.042072
57	1	0	3.675101	2.350641	3.804006
58	1	0	1.681738	1.630822	2.451409
59	8	0	2.497171	-2.032966	-0.022058
60	8	0	1.767786	0.386636	0.183611
61	15	0	1.129049	-1.148783	0.197819
62	8	0	0.249981	-1.200906	-1.032264
63	8	0	0.587824	-1.487123	1.555703
64	6	0	-2.928975	-2.559554	1.660246
65	9	0	-1.830201	-3.140150	2.189947

TS_F-Tc(S-ex)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2122.938184 hartree

Sum of electronic and thermal Free Energies = -2122.500877 hartree

The number of imaginary frequency = 1

Imaginary frequency = -370.81

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.743182	-3.901187	-1.489953
2	1	0	4.486523	-3.332148	-0.939193
3	1	0	4.163847	-4.637601	-2.169182
4	6	0	2.511167	-4.180050	-0.899700
5	1	0	1.887070	-4.970480	-1.309762
6	6	0	2.462042	-2.244583	0.623617
7	1	0	3.524050	-2.070756	0.513891
8	1	0	0.759676	-1.355924	1.489572
9	7	0	1.814422	-1.369092	1.420633
10	6	0	2.530843	-0.342851	2.026966
11	8	0	1.695612	0.440638	2.723151
12	8	0	3.734271	-0.181868	1.929146
13	1	0	1.070929	0.275572	-0.967778
14	6	0	2.833218	4.295164	0.898325
15	6	0	3.877815	3.577425	0.342882
16	6	0	3.639237	2.334961	-0.282361
17	6	0	2.309274	1.842069	-0.332300
18	6	0	1.249621	2.563021	0.256126
19	6	0	1.519813	3.779820	0.856064
20	1	0	5.688584	1.885326	-0.842708
21	1	0	3.022831	5.251806	1.375685
22	1	0	4.894882	3.958772	0.381430
23	6	0	4.661607	1.531063	-0.877358
24	1	0	0.246926	2.147681	0.248790
25	1	0	0.706820	4.339157	1.309786
26	6	0	3.015340	-0.132896	-1.532676
27	6	0	4.366707	0.343460	-1.479134
28	1	0	5.148189	-0.254670	-1.932454
29	7	0	2.065917	0.641358	-0.947311
30	6	0	2.576454	-1.324256	-2.168870
31	1	0	1.502094	-1.481227	-2.154820
32	6	0	3.375128	-2.277478	-2.801349
33	1	0	4.425017	-2.073587	-2.999537
34	1	0	2.901015	-2.903931	-3.548997
35	6	0	2.327201	1.511534	3.443468
36	1	0	2.911660	2.139558	2.768723
37	1	0	1.508268	2.080092	3.883548
38	1	0	2.979526	1.108393	4.223753
39	6	0	-4.168962	1.016442	-0.680763
40	6	0	-5.051439	1.695850	-1.535679
41	6	0	-4.649549	2.819689	-2.254533
42	6	0	-3.338736	3.286404	-2.135861
43	6	0	-2.442086	2.629526	-1.294964
44	6	0	-2.854380	1.511015	-0.571540
45	6	0	-4.613573	-0.169895	0.085517
46	6	0	-5.865301	-0.200813	0.720985
47	6	0	-6.290656	-1.322896	1.428984
48	6	0	-5.461940	-2.444137	1.521101
49	6	0	-4.214442	-2.438997	0.899731
50	6	0	-3.803327	-1.315332	0.186772
51	1	0	-6.063028	1.315109	-1.646388
52	1	0	-5.352888	3.321000	-2.913518
53	1	0	-3.012200	4.156947	-2.698329
54	1	0	-1.419290	2.974142	-1.183803
55	1	0	-6.497863	0.681265	0.670625

56	1	0	-7.261035	-1.317818	1.917606
57	1	0	-5.783363	-3.319405	2.078951
58	1	0	-3.544880	-3.290960	0.949274
59	8	0	-1.971534	0.950791	0.334113
60	8	0	-2.604648	-1.370889	-0.504371
61	15	0	-1.301390	-0.547171	0.061775
62	8	0	-0.336443	-0.454915	-1.098165
63	8	0	-0.845827	-1.050733	1.400362
64	6	0	1.885624	-3.352874	0.040158
65	9	0	0.590487	-3.613778	0.335462

TS_F-Tt(R-ex)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2122.936705 hartree

Sum of electronic and thermal Free Energies = -2122.498404 hartree

The number of imaginary frequency = 1

Imaginary frequency = -369.34

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.772423	-3.181172	0.361508
2	1	0	-5.174518	-2.172105	0.388720
3	1	0	-5.504048	-3.943998	0.108974
4	6	0	-3.723923	-3.531296	1.208548
5	1	0	-3.506077	-4.582420	1.381992
6	6	0	-2.777770	-1.269028	1.513124
7	1	0	-3.692604	-0.788266	1.198953
8	1	0	-0.762216	-0.875923	1.906097
9	7	0	-1.731670	-0.462322	1.815033
10	6	0	-1.779636	0.921727	1.818310
11	8	0	-3.028130	1.388463	1.572868
12	8	0	-0.814580	1.628692	2.020734
13	1	0	-0.906226	-0.277652	-1.146918
14	6	0	-1.726971	4.405740	-1.614429
15	6	0	-2.916450	3.732861	-1.826894
16	6	0	-2.966298	2.325801	-1.728064
17	6	0	-1.772527	1.617409	-1.422771
18	6	0	-0.564160	2.306816	-1.194293
19	6	0	-0.555675	3.686779	-1.291976
20	1	0	-5.087132	2.082036	-2.124530
21	1	0	-1.692788	5.488555	-1.688067
22	1	0	-3.827749	4.275615	-2.065092
23	6	0	-4.160608	1.560309	-1.896950
24	1	0	0.329402	1.751951	-0.926513
25	1	0	0.370720	4.222910	-1.108901
26	6	0	-2.933770	-0.499583	-1.489214
27	6	0	-4.151782	0.201309	-1.775363
28	1	0	-5.064311	-0.368448	-1.903537
29	7	0	-1.812802	0.248128	-1.330647
30	6	0	-2.812268	-1.910559	-1.365780
31	1	0	-1.812205	-2.275031	-1.151454
32	6	0	-3.852944	-2.828311	-1.510512
33	1	0	-4.787642	-2.532730	-1.980951
34	1	0	-3.582151	-3.863116	-1.689407
35	6	0	-3.153798	2.819552	1.652118
36	1	0	-2.440380	3.306963	0.986256
37	1	0	-4.176942	3.035412	1.343372
38	1	0	-2.982743	3.155869	2.678660
39	6	0	4.170061	0.460512	0.553485
40	6	0	5.236921	0.957465	1.319277
41	6	0	5.012173	1.784736	2.418157
42	6	0	3.706263	2.126969	2.780895
43	6	0	2.627264	1.647586	2.039409
44	6	0	2.869604	0.832685	0.936699
45	6	0	4.397309	-0.403204	-0.628332
46	6	0	5.424698	-0.117016	-1.542197
47	6	0	5.653509	-0.919632	-2.657835
48	6	0	4.844282	-2.034492	-2.888967
49	6	0	3.817026	-2.341627	-1.998761
50	6	0	3.601208	-1.538701	-0.880208
51	1	0	6.250394	0.668118	1.054807
52	1	0	5.854549	2.149489	2.999641
53	1	0	3.527015	2.761058	3.645103
54	1	0	1.597417	1.878816	2.289199
55	1	0	6.036631	0.765243	-1.374959
56	1	0	6.453010	-0.669257	-3.349674
57	1	0	5.010234	-2.663029	-3.759713
58	1	0	3.174431	-3.203880	-2.142182
59	8	0	1.798125	0.441194	0.150452
60	8	0	2.646841	-1.947460	0.034251
61	15	0	1.245301	-1.119334	0.248648
62	8	0	0.750720	-1.445641	1.628090
63	8	0	0.332531	-1.253833	-0.951902
64	6	0	-2.750072	-2.639001	1.674182
65	9	0	-1.654646	-3.175103	2.254975

TS_F-Tt(S-ex)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2122.936091 hartree

Sum of electronic and thermal Free Energies = -2122.497622 hartree

The number of imaginary frequency = 1

Imaginary frequency = -366.18

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.289735	4.140794	1.562709
2	1	0	2.318386	3.802271	1.472971
3	1	0	1.146887	4.945101	2.279375
4	6	0	0.446449	4.091790	0.456078
5	1	0	-0.471391	4.674923	0.461672
6	6	0	1.594224	2.273763	-0.767595
7	1	0	2.514223	2.420261	-0.220575
8	1	0	0.649837	0.915058	-2.039206
9	7	0	1.572917	1.257778	-1.664098
10	6	0	2.671867	0.472664	-1.987438
11	8	0	3.803140	0.922177	-1.387354
12	8	0	2.617751	-0.487729	-2.722096
13	1	0	1.057246	-0.820946	0.498132

14	6	0	5.192249	-3.119954	0.192498
15	6	0	5.368728	-2.043546	1.042818
16	6	0	4.296571	-1.165488	1.311113
17	6	0	3.038319	-1.417527	0.701888
18	6	0	2.864477	-2.507371	-0.176220
19	6	0	3.938880	-3.343724	-0.418900
20	1	0	5.351642	0.204188	2.625039
21	1	0	6.019594	-3.792521	-0.012922
22	1	0	6.332023	-1.856542	1.510560
23	6	0	4.397373	-0.015149	2.152127
24	1	0	1.897540	-2.652025	-0.647000
25	1	0	3.816051	-4.182148	-1.097892
26	6	0	2.055807	0.516686	1.757726
27	6	0	3.323710	0.800427	2.365898
28	1	0	3.413051	1.669631	3.006413
29	7	0	1.986932	-0.575629	0.959743
30	6	0	0.876509	1.292347	1.927081
31	1	0	-0.009091	0.943898	1.405375
32	6	0	0.772830	2.442044	2.709734
33	1	0	1.522018	2.665724	3.465238
34	1	0	-0.225793	2.775826	2.969541
35	6	0	4.996567	0.213176	-1.763971
36	1	0	5.788316	0.632947	-1.142838
37	1	0	4.887092	-0.855686	-1.576371
38	1	0	5.212088	0.375909	-2.823827
39	6	0	-4.353985	0.035628	0.158268
40	6	0	-5.631222	0.616591	0.104528
41	6	0	-5.799210	1.986855	-0.083456
42	6	0	-4.680267	2.808638	-0.237925
43	6	0	-3.400842	2.258145	-0.189126
44	6	0	-3.242674	0.889184	0.018647
45	6	0	-4.186358	-1.421780	0.357774
46	6	0	-4.970507	-2.125489	1.286279
47	6	0	-4.828705	-3.500303	1.462020
48	6	0	-3.886364	-4.205017	0.708521
49	6	0	-3.094648	-3.530419	-0.218930
50	6	0	-3.250733	-2.157169	-0.393417
51	1	0	-6.500654	-0.029476	0.189924
52	1	0	-6.799675	2.408099	-0.128491
53	1	0	-4.802363	3.875531	-0.405119
54	1	0	-2.512945	2.862044	-0.329937
55	1	0	-5.686201	-1.572583	1.888665
56	1	0	-5.444669	-4.018445	2.191838
57	1	0	-3.765339	-5.276324	0.844146
58	1	0	-2.354902	-4.044369	-0.823320
59	8	0	-1.963235	0.389704	0.182173
60	8	0	-2.518068	-1.532033	-1.388643
61	15	0	-1.251791	-0.572171	-0.978240
62	8	0	-0.874072	0.233608	-2.184600
63	8	0	-0.215376	-1.364295	-0.211303
64	6	0	0.556839	3.164699	-0.587284
65	9	0	-0.492210	3.082528	-1.441266

(R=OMe)

TS$_{OMe}$-Cc(R-en)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2138.229020 hartree

Sum of electronic and thermal Free Energies = -2137.751418 hartree

The number of imaginary frequency = 1

Imaginary frequency = -351.89

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.081855	3.444690	1.618397
2	1	0	-0.869393	2.847957	1.170454
3	1	0	-0.438076	4.205347	2.308708
4	6	0	1.093316	3.706119	0.924060
5	1	0	1.695676	4.549727	1.254271
6	6	0	1.034715	1.780779	-0.580580
7	1	0	-0.013279	1.642591	-0.348682
8	1	0	0.741550	0.267149	-1.892824
9	7	0	1.490909	0.845138	-1.458706
10	6	0	2.799059	0.433983	-1.656440
11	8	0	2.825833	-0.409746	-2.709693
12	8	0	3.766978	0.719284	-0.980103
13	1	0	0.767746	-1.326266	0.723073
14	6	0	5.028196	-3.310213	0.032816
15	6	0	5.190009	-2.214014	0.862129
16	6	0	4.079584	-1.428739	1.233624
17	6	0	2.798462	-1.788445	0.742879
18	6	0	2.634416	-2.899686	-0.107362
19	6	0	3.745929	-3.648860	-0.450796
20	1	0	5.130034	0.013222	2.471844
21	1	0	5.887423	-3.910908	-0.249993
22	1	0	6.174281	-1.940816	1.233415
23	6	0	4.158963	-0.278968	2.080365
24	1	0	1.640825	-3.138323	-0.475113
25	1	0	3.628570	-4.507372	-1.105803
26	6	0	1.759673	0.068539	1.886579
27	6	0	3.048201	0.447133	2.391776
28	1	0	3.118636	1.316332	3.033959
29	7	0	1.710535	-1.032922	1.095882
30	6	0	0.526546	0.697437	2.207278
31	1	0	-0.366442	0.212269	1.825323
32	6	0	0.369344	1.858710	2.955297
33	1	0	1.211253	2.305056	3.476002
34	1	0	-0.588401	2.019285	3.440963
35	6	0	-4.633020	-0.825210	0.220038
36	6	0	-5.649082	-1.121824	1.142734
37	6	0	-5.854705	-2.421100	1.601799
38	6	0	-5.036573	-3.458182	1.146304
39	6	0	-4.020720	-3.190518	0.230474
40	6	0	-3.829408	-1.889602	-0.228938
41	6	0	-4.426967	0.552778	-0.280315
42	6	0	-5.514504	1.365072	-0.638077
43	6	0	-5.328997	2.663163	-1.109917
44	6	0	-4.036711	3.174022	-1.247135
45	6	0	-2.939223	2.387535	-0.899792
46	6	0	-3.134461	1.096699	-0.409583
47	1	0	-6.269107	-0.310383	1.514157
48	1	0	-6.644286	-2.621971	2.320522

49	1	0	-5.186269	-4.472841	1.504917
50	1	0	-3.368699	-3.970970	-0.146731
51	1	0	-6.517414	0.954078	-0.562401
52	1	0	-6.189051	3.266699	-1.385824
53	1	0	-3.880003	4.178510	-1.630328
54	1	0	-1.926448	2.760215	-1.011602
55	8	0	-2.877981	-1.668208	-1.211450
56	8	0	-2.037764	0.382949	0.040734
57	15	0	-1.461207	-0.936677	-0.822918
58	8	0	-0.695577	-1.749336	0.195002
59	8	0	-0.815916	-0.464462	-2.090500
60	6	0	4.113028	-0.977083	-2.992380
61	1	0	4.484055	-1.541719	-2.133709
62	1	0	3.953810	-1.637287	-3.845569
63	1	0	4.830228	-0.190440	-3.244237
64	6	0	1.674985	2.906976	-0.089487
65	8	0	2.860805	3.305594	-0.657190
66	6	0	3.996216	3.399210	0.203901
67	1	0	4.194051	2.438574	0.685337
68	1	0	4.838534	3.659943	-0.439878
69	1	0	3.870675	4.185974	0.960978

TS$_{OMe}$-Cc(S-en)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2138.227023 hartree

Sum of electronic and thermal Free Energies = -2137.751958 hartree

The number of imaginary frequency = 1

Imaginary frequency = -344.86

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.659315	3.730282	1.769798
2	1	0	-0.229337	3.109143	1.825244
3	1	0	0.468744	4.794725	1.880134
4	6	0	1.892174	3.243308	2.181996
5	1	0	2.691728	3.955606	2.376859
6	6	0	1.439684	0.865734	1.874484
7	1	0	0.382194	1.101290	1.858884
8	1	0	0.713249	-0.973023	1.580627
9	7	0	1.620334	-0.469005	1.669740
10	6	0	2.768279	-1.175344	1.344437
11	8	0	2.437648	-2.483580	1.246105
12	8	0	3.881983	-0.731503	1.157702
13	1	0	0.764483	-0.241003	-1.350917
14	6	0	4.797800	-2.334248	-2.697000
15	6	0	5.090761	-1.033657	-2.326667
16	6	0	4.067305	-0.166768	-1.890680
17	6	0	2.739234	-0.660846	-1.835693
18	6	0	2.440951	-1.988171	-2.202238
19	6	0	3.468877	-2.807029	-2.634913
20	1	0	5.294120	1.583239	-1.506111
21	1	0	5.590078	-2.995503	-3.034983
22	1	0	6.111769	-0.663255	-2.364244
23	6	0	4.281395	1.189669	-1.492719
24	1	0	1.413796	-2.333909	-2.132384
25	1	0	3.249190	-3.830573	-2.925051
26	6	0	1.909472	1.464607	-1.046355
27	6	0	3.245400	1.980869	-1.093403
28	1	0	3.419478	3.002221	-0.779122
29	7	0	1.734943	0.169425	-1.408405
30	6	0	0.747570	2.201454	-0.686959
31	1	0	-0.184256	1.647649	-0.689161
32	6	0	0.707172	3.548982	-0.349396
33	1	0	1.561812	4.192602	-0.532138
34	1	0	-0.252518	4.053061	-0.417534
35	6	0	3.536564	-3.358445	0.952091
36	1	0	4.257188	-3.353214	1.775803
37	1	0	3.092800	-4.348212	0.840224
38	1	0	4.039321	-3.055646	0.031594
39	6	0	-4.546511	0.472879	-0.772571
40	6	0	-5.533568	0.945242	-1.652329
41	6	0	-5.252422	1.919269	-2.608054
42	6	0	-3.960603	2.440058	-2.707885
43	6	0	-2.961536	1.987430	-1.847807
44	6	0	-3.252846	1.018373	-0.888043
45	6	0	-4.864499	-0.551240	0.248464
46	6	0	-6.053140	-0.491273	0.993858
47	6	0	-6.362755	-1.462127	1.943931
48	6	0	-5.478264	-2.519144	2.173436
49	6	0	-4.291338	-2.601470	1.447711
50	6	0	-3.995826	-1.630085	0.494178
51	1	0	-6.531234	0.519503	-1.590106
52	1	0	-6.035002	2.260480	-3.279859
53	1	0	-3.728012	3.193223	-3.455857
54	1	0	-1.950127	2.375436	-1.908376
55	1	0	-6.728217	0.344778	0.832628
56	1	0	-7.286170	-1.387860	2.511520
57	1	0	-5.709113	-3.275893	2.918151
58	1	0	-3.582201	-3.408365	1.598094
59	8	0	-2.268287	0.672150	0.019945
60	8	0	-2.859686	-1.788391	-0.282079
61	15	0	-1.550847	-0.833766	-0.012494
62	8	0	-0.682980	-0.951524	-1.241796
63	8	0	-0.981650	-1.029263	1.364645
64	6	0	2.318369	1.892970	2.190503
65	8	0	3.660461	1.718704	2.430065
66	6	0	3.977099	0.990038	3.615211
67	1	0	5.062251	0.872721	3.618192
68	1	0	3.659160	1.546233	4.508377
69	1	0	3.515992	-0.002536	3.626554

TS$_{OMe}$-Ct(R-en)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2138.223584 hartree

Sum of electronic and thermal Free Energies = -2137.746950 hartree

The number of imaginary frequency = 1

Imaginary frequency = -349.18

Center Atomic Atomic Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-0.042781	3.164601	1.998132
2	1	0	-0.842888	2.676838	1.451105
3	1	0	-0.384048	3.827278	2.789460
4	6	0	1.158206	3.477421	1.373437
5	1	0	1.808373	4.214552	1.840773
6	6	0	1.090069	1.794708	-0.398995
7	1	0	0.033085	1.677579	-0.192873
8	1	0	0.702768	0.456999	-1.864600
9	7	0	1.493025	0.937481	-1.381631
10	6	0	2.741689	0.440476	-1.731962
11	8	0	3.707076	0.806998	-0.868225
12	8	0	2.910941	-0.274057	-2.698430
13	1	0	0.798383	-1.441206	0.465294
14	6	0	5.072238	-3.412745	-0.238579
15	6	0	5.193840	-2.449632	0.747939
16	6	0	4.076651	-1.682861	1.139451
17	6	0	2.825872	-1.937149	0.518797
18	6	0	2.706984	-2.908135	-0.494338
19	6	0	3.826323	-3.632599	-0.863062
20	1	0	5.079207	-0.406600	2.584193
21	1	0	5.937055	-3.995925	-0.540174
22	1	0	6.152630	-2.262177	1.224975
23	6	0	4.127413	-0.632396	2.109598
24	1	0	1.742425	-3.059089	-0.969311
25	1	0	3.743321	-4.377389	-1.648798
26	6	0	1.745545	-0.226589	1.840517
27	6	0	3.013782	0.081956	2.436294
28	1	0	3.064331	0.878613	3.167798
29	7	0	1.727895	-1.212190	0.906842
30	6	0	0.502041	0.355035	2.203757
31	1	0	-0.378531	-0.070449	1.734798
32	6	0	0.323053	1.402252	3.101175
33	1	0	1.144376	1.757175	3.716292
34	1	0	-0.653455	1.501219	3.565808
35	6	0	5.035911	0.435048	-1.264910
36	1	0	5.105392	-0.642417	-1.422884
37	1	0	5.315435	0.956379	-2.185496
38	1	0	5.676701	0.747175	-0.440037
39	6	0	-4.464407	0.559023	-0.158512
40	6	0	-5.565821	1.401791	-0.375402
41	6	0	-5.401017	2.756776	-0.656652
42	6	0	-4.116209	3.297118	-0.741681
43	6	0	-3.005534	2.481247	-0.531113
44	6	0	-3.179595	1.131306	-0.228147
45	6	0	-4.647059	-0.880355	0.135321
46	6	0	-5.642829	-1.324131	1.020254
47	6	0	-5.826279	-2.679863	1.283883
48	6	0	-5.005943	-3.626769	0.665175
49	6	0	-4.010006	-3.212678	-0.217461
50	6	0	-3.840709	-1.855459	-0.480838
51	1	0	-6.563319	0.972334	-0.343498
52	1	0	-6.271575	3.383862	-0.826817
53	1	0	-3.976285	4.348172	-0.978747
54	1	0	-1.997599	2.875797	-0.606899
55	1	0	-6.264482	-0.585218	1.518683
56	1	0	-6.600329	-2.995869	1.977666
57	1	0	-5.138524	-4.685383	0.870833
58	1	0	-3.357345	-3.919742	-0.718065
59	8	0	-2.068882	0.373147	0.095283
60	8	0	-2.910224	-1.477933	-1.435315
61	15	0	-1.494147	-0.792914	-0.968107
62	8	0	-0.884165	-0.117876	-2.159631
63	8	0	-0.693888	-1.737068	-0.103186
64	6	0	1.745477	2.825343	0.261929
65	8	0	3.012676	3.268842	-0.044953
66	6	0	3.177396	3.774160	-1.368650
67	1	0	2.488329	4.608340	-1.557018
68	1	0	4.207877	4.131297	-1.429443
69	1	0	3.020358	3.006711	-2.134385

TS$_{OMe}$-Ct(S-en)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2138.223407 hartree

Sum of electronic and thermal Free Energies = --2137.746753 hartree

The number of imaginary frequency = 1

Imaginary frequency = -340.64

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.892923	-3.281730	-2.515544
2	1	0	0.031442	-3.144545	-1.963396
3	1	0	-0.783039	-3.835651	-3.444085
4	6	0	-2.107567	-3.358113	-1.850071
5	1	0	-2.961697	-3.783155	-2.374086
6	6	0	-1.482393	-2.092596	0.140032
7	1	0	-0.446106	-2.234837	-0.143388
8	1	0	-0.596414	-1.120339	1.641515
9	7	0	-1.545492	-1.334300	1.270857
10	6	0	-2.559597	-0.614837	1.889782
11	8	0	-3.716390	-0.635774	1.203196
12	8	0	-2.382629	-0.015780	2.930979
13	1	0	-0.719352	1.210697	-0.195020
14	6	0	-4.601563	3.684579	0.947846
15	6	0	-4.912240	2.873298	-0.129073
16	6	0	-3.942793	2.001488	-0.668513
17	6	0	-2.644189	1.990626	-0.095607
18	6	0	-2.334209	2.802933	1.013258
19	6	0	-3.312196	3.639583	1.520965
20	1	0	-5.185180	1.069193	-2.187281
21	1	0	-5.351806	4.352280	1.360664
22	1	0	-5.906675	2.889813	-0.567998
23	6	0	-4.190259	1.099796	-1.750124
24	1	0	-1.338874	2.747495	1.443204
25	1	0	-3.082850	4.267876	2.376417
26	6	0	-1.886902	0.328364	-1.672736
27	6	0	-3.207126	0.285503	-2.229684
28	1	0	-3.407473	-0.402211	-3.041513
29	7	0	-1.684765	1.166753	-0.627335
30	6	0	-0.765000	-0.394936	-2.165699

31	1	0	0.176283	-0.225239	-1.655473
32	6	0	-0.776077	-1.268713	-3.244996
33	1	0	-1.628723	-1.317933	-3.914433
34	1	0	0.175147	-1.497738	-3.715728
35	6	0	-4.818484	-0.002584	1.873242
36	1	0	-5.052777	-0.533485	2.800773
37	1	0	-4.585230	1.038660	2.100641
38	1	0	-5.650962	-0.066962	1.172727
39	6	0	4.551855	0.586761	-0.797160
40	6	0	5.475510	1.291719	-1.585332
41	6	0	5.119566	1.826669	-2.821685
42	6	0	3.815200	1.670793	-3.295670
43	6	0	2.877888	0.976754	-2.532400
44	6	0	3.244710	0.437314	-1.299986
45	6	0	4.947283	0.007964	0.507219
46	6	0	6.176604	-0.651689	0.667418
47	6	0	6.558356	-1.185197	1.896535
48	6	0	5.707157	-1.073511	2.998916
49	6	0	4.481107	-0.424176	2.866790
50	6	0	4.113235	0.112885	1.635387
51	1	0	6.482556	1.434024	-1.203125
52	1	0	5.853951	2.373367	-3.406512
53	1	0	3.525167	2.091700	-4.254616
54	1	0	1.858034	0.842045	-2.877767
55	1	0	6.826526	-0.760319	-0.196602
56	1	0	7.512312	-1.696508	1.990963
57	1	0	5.994486	-1.493605	3.958861
58	1	0	3.796346	-0.316464	3.701109
59	8	0	2.322917	-0.336658	-0.618038
60	8	0	2.937289	0.840438	1.556540
61	15	0	1.628415	0.203711	0.798280
62	8	0	0.712453	1.365614	0.496902
63	8	0	1.111858	-1.031902	1.480203
64	6	0	-2.436856	-2.777641	-0.600794
65	8	0	-3.764422	-2.891311	-0.252003
66	6	0	-4.006313	-3.612545	0.954808
67	1	0	-5.088962	-3.608090	1.100012
68	1	0	-3.651254	-4.648456	0.868097
69	1	0	-3.528603	-3.144038	1.822212

TS_{OMe}-Tc(R-ex)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2138.237409 hartree

Sum of electronic and thermal Free Energies = -2137.760565 hartree

The number of imaginary frequency = 1

Imaginary frequency = -352.95

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.118561	-2.705984	0.181359
2	1	0	-5.414668	-1.665403	0.277159
3	1	0	-5.925282	-3.374971	-0.107016
4	6	0	-4.087934	-3.210787	0.966451
5	1	0	-3.995258	-4.290525	1.064107
6	6	0	-2.975198	-1.077486	1.413871
7	1	0	-3.862730	-0.507134	1.174271
8	1	0	-0.954408	-0.777374	1.853846
9	7	0	-1.894178	-0.329107	1.745239
10	6	0	-1.999116	1.053317	1.764306
11	8	0	-0.799867	1.608959	2.018797
12	8	0	-3.028169	1.675798	1.570412
13	1	0	-0.985962	-0.089710	-1.244729
14	6	0	-1.278309	4.659047	-1.394636
15	6	0	-2.555890	4.140997	-1.508315
16	6	0	-2.762758	2.745175	-1.513339
17	6	0	-1.637939	1.888348	-1.390491
18	6	0	-0.337125	2.417209	-1.269980
19	6	0	-0.171779	3.790604	-1.278171
20	1	0	-4.922313	2.770084	-1.733819
21	1	0	-1.124372	5.733969	-1.393875
22	1	0	-3.416198	4.799260	-1.596759
23	6	0	-4.046789	2.132303	-1.643513
24	1	0	0.506802	1.746224	-1.153143
25	1	0	0.828533	4.203450	-1.184110
26	6	0	-3.038259	-0.076351	-1.520391
27	6	0	-4.182999	0.775481	-1.657506
28	1	0	-5.161056	0.320826	-1.759662
29	7	0	-1.831521	0.528923	-1.383706
30	6	0	-3.067663	-1.496689	-1.525608
31	1	0	-2.105906	-1.979962	-1.387062
32	6	0	-4.200520	-2.286820	-1.706077
33	1	0	-5.114948	-1.857476	-2.107055
34	1	0	-4.048375	-3.326372	-1.974454
35	6	0	-0.813269	3.042639	2.132947
36	1	0	-1.312786	3.339092	3.060309
37	1	0	0.234939	3.340475	2.150786
38	1	0	-1.323225	3.495372	1.281996
39	6	0	4.307051	-0.543000	-0.752513
40	6	0	5.305843	-0.291568	-1.706601
41	6	0	5.424972	-1.068621	-2.857027
42	6	0	4.533009	-2.120276	-3.080588
43	6	0	3.532463	-2.391866	-2.149082
44	6	0	3.426368	-1.616307	-0.996239
45	6	0	4.192510	0.279718	0.473079
46	6	0	5.321212	0.661572	1.215286
47	6	0	5.198608	1.420071	2.378371
48	6	0	3.933355	1.798573	2.835787
49	6	0	2.796884	1.435645	2.114685
50	6	0	2.935209	0.704500	0.937739
51	1	0	5.983337	0.542145	-1.542583
52	1	0	6.204136	-0.847437	-3.581155
53	1	0	4.613754	-2.727048	-3.978368
54	1	0	2.826783	-3.204016	-2.288077
55	1	0	6.301671	0.331647	0.882803
56	1	0	6.087403	1.695533	2.939227
57	1	0	3.831060	2.366726	3.756439
58	1	0	1.795153	1.681854	2.447748
59	8	0	2.490662	-1.984272	-0.045314
60	8	0	1.810041	0.447118	0.174170
61	15	0	1.142684	-1.073266	0.212830
62	8	0	0.225296	-1.125181	-0.989592

63	8	0	0.632653	-1.405437	1.582903
64	6	0	-3.008246	-2.459211	1.477090
65	8	0	-1.931181	-3.088844	2.048958
66	6	0	-1.134338	-3.893755	1.168314
67	1	0	-0.862061	-3.334008	0.268565
68	1	0	-0.225111	-4.129911	1.720645
69	1	0	-1.659523	-4.819060	0.892887

TS_{OMe}-Tc(S-ex)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2138.234980 hartree

Sum of electronic and thermal Free Energies = -2137.758529 hartree

The number of imaginary frequency = 1

Imaginary frequency = -350.80

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.989578	3.679087	-1.390977
2	1	0	-4.662569	2.992184	-0.886924
3	1	0	-4.486424	4.393643	-2.041898
4	6	0	-2.795475	4.055657	-0.785153
5	1	0	-2.287714	4.940339	-1.162887
6	6	0	-2.588436	2.113267	0.686090
7	1	0	-3.639022	1.873817	0.590047
8	1	0	-0.840806	1.306102	1.524632
9	7	0	-1.884446	1.254904	1.458944
10	6	0	-2.530453	0.181318	2.058644
11	8	0	-1.643733	-0.561924	2.737345
12	8	0	-3.723616	-0.050385	1.972250
13	1	0	-1.067922	-0.362689	-0.966758
14	6	0	-2.723427	-4.435327	0.876944
15	6	0	-3.786683	-3.738027	0.330894
16	6	0	-3.580082	-2.486274	-0.286615
17	6	0	-2.263036	-1.960338	-0.337189
18	6	0	-1.184889	-2.660704	0.241504
19	6	0	-1.423226	-3.888594	0.832690
20	1	0	-5.641895	-2.084252	-0.837232
21	1	0	-2.888473	-5.399629	1.347976
22	1	0	-4.794430	-4.143231	0.370572
23	6	0	-4.623945	-1.705103	-0.874316
24	1	0	-0.192048	-2.223534	0.233655
25	1	0	-0.594747	-4.431433	1.278419
26	6	0	-3.021336	0.002468	-1.526991
27	6	0	-4.360018	-0.508410	-1.471859
28	1	0	-5.157710	0.072961	-1.918521
29	7	0	-2.051289	-0.749596	-0.946036
30	6	0	-2.619816	1.207974	-2.160403
31	1	0	-1.552845	1.403795	-2.137478
32	6	0	-3.451454	2.130872	-2.787310
33	1	0	-4.485759	1.884332	-3.013306
34	1	0	-2.997139	2.820175	-3.490209
35	6	0	-2.207604	-1.667961	3.459241
36	1	0	-2.778266	-2.316323	2.791971
37	1	0	-1.353187	-2.201933	3.874842
38	1	0	-2.859802	-1.304016	4.258903
39	6	0	4.179810	-1.073763	-0.700130
40	6	0	5.060753	-1.728119	-1.575899
41	6	0	4.659695	-2.836383	-2.318950
42	6	0	3.351828	-3.312212	-2.203767
43	6	0	2.456793	-2.680232	-1.342252
44	6	0	2.868707	-1.577462	-0.595211
45	6	0	4.622326	0.096068	0.092178
46	6	0	5.876117	0.116339	0.723742
47	6	0	6.300265	1.222092	1.457730
48	6	0	5.467480	2.337096	1.580887
49	6	0	4.217879	2.341712	0.963818
50	6	0	3.807274	1.235372	0.223580
51	1	0	6.069929	-1.340052	-1.683154
52	1	0	5.361421	-3.318562	-2.993715
53	1	0	3.026197	-4.170734	-2.784856
54	1	0	1.436559	-3.032751	-1.233423
55	1	0	6.511668	-0.761843	0.649298
56	1	0	7.272368	1.208644	1.942623
57	1	0	5.786786	3.199300	2.159827
58	1	0	3.546886	3.190799	1.040791
59	8	0	1.988978	-1.040947	0.329181
60	8	0	2.606634	1.303618	-0.462173
61	15	0	1.303633	0.452537	0.083853
62	8	0	0.356139	0.381768	-1.094525
63	8	0	0.832340	0.943854	1.418138
64	6	0	-2.067990	3.273102	0.136955
65	8	0	-0.804800	3.628513	0.537896
66	6	0	0.183132	3.791865	-0.487721
67	1	0	1.139511	3.860796	0.031824
68	1	0	0.205871	2.921725	-1.150736
69	1	0	0.016009	4.708901	-1.068270

TS_{OMe}-Tt(R-ex)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2138.234087 hartree

Sum of electronic and thermal Free Energies = -2137.756269 hartree

The number of imaginary frequency = 1

Imaginary frequency = -350.73

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.903647	-2.866889	0.066822
2	1	0	-5.214529	-1.827724	0.126900
3	1	0	-5.691746	-3.551921	-0.235321
4	6	0	-3.896898	-3.342679	0.899702
5	1	0	-3.791186	-4.419415	1.015122
6	6	0	-2.835610	-1.185624	1.390541
7	1	0	-3.725782	-0.634695	1.123129
8	1	0	-0.825633	-0.904411	1.873670
9	7	0	-1.760821	-0.443645	1.758062
10	6	0	-1.743817	0.937035	1.855353
11	8	0	-2.963286	1.479041	1.616521
12	8	0	-0.752053	1.583048	2.123733

13	1	0	-0.885463	-0.088292	-1.165689
14	6	0	-1.513730	4.647035	-1.333797
15	6	0	-2.722111	4.034928	-1.613702
16	6	0	-2.825162	2.627578	-1.615277
17	6	0	-1.665349	1.854089	-1.339088
18	6	0	-0.438756	2.480813	-1.041404
19	6	0	-0.377150	3.863224	-1.042100
20	1	0	-4.945606	2.495762	-2.065095
21	1	0	-1.438857	5.730300	-1.330807
22	1	0	-3.608366	4.626377	-1.829505
23	6	0	-4.044007	1.923303	-1.860586
24	1	0	0.428616	1.876248	-0.797748
25	1	0	0.564982	4.348783	-0.805699
26	6	0	-2.903080	-0.207730	-1.586106
27	6	0	-4.087615	0.560433	-1.840478
28	1	0	-5.017494	0.037205	-2.027752
29	7	0	-1.758169	0.482993	-1.346958
30	6	0	-2.841429	-1.626005	-1.577743
31	1	0	-1.862470	-2.047921	-1.377540
32	6	0	-3.919370	-2.482249	-1.791361
33	1	0	-4.836074	-2.119123	-2.248649
34	1	0	-3.698786	-3.519959	-2.016098
35	6	0	-3.023843	2.905348	1.791049
36	1	0	-2.273858	3.402073	1.174039
37	1	0	-4.028562	3.190436	1.477858
38	1	0	-2.860748	3.163796	2.841258
39	6	0	4.191873	0.467258	0.527274
40	6	0	5.274850	0.929766	1.292091
41	6	0	5.073858	1.720261	2.422236
42	6	0	3.776638	2.058925	2.818245
43	6	0	2.681900	1.613480	2.078598
44	6	0	2.901317	0.836222	0.944558
45	6	0	4.391963	-0.357612	-0.686799
46	6	0	5.407004	-0.048800	-1.607046
47	6	0	5.610730	-0.814040	-2.753399
48	6	0	4.787658	-1.913071	-3.009763
49	6	0	3.772127	-2.241907	-2.113882
50	6	0	3.581361	-1.477087	-0.964350
51	1	0	6.281723	0.642386	1.001566
52	1	0	5.928216	2.058650	3.002167
53	1	0	3.616398	2.663351	3.707048
54	1	0	1.657763	1.841204	2.353808
55	1	0	6.029507	0.821890	-1.419504
56	1	0	6.401251	-0.546576	-3.449111
57	1	0	4.933625	-2.512257	-3.904449
58	1	0	3.119406	-3.093007	-2.277212
59	8	0	1.814472	0.479554	0.161644
60	8	0	2.638396	-1.909754	-0.049615
61	15	0	1.246811	-1.075420	0.225516
62	8	0	0.778361	-1.448163	1.600711
63	8	0	0.303631	-1.174586	-0.955713
64	6	0	-2.849307	-2.569747	1.443672
65	8	0	-1.778983	-3.179922	2.046660
66	6	0	-0.943831	-3.975367	1.191294
67	1	0	-0.665527	-3.417597	0.292507
68	1	0	-0.041812	-4.183476	1.766061
69	1	0	-1.441917	-4.915307	0.915714

TS$_{OMe}$-Tt(S-ex)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2138.231474 hartree

Sum of electronic and thermal Free Energies = -2137.753944 hartree

The number of imaginary frequency = 1

Imaginary frequency = -357.67

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.641931	3.878263	-1.952548
2	1	0	-2.611533	3.410991	-1.802456
3	1	0	-1.623937	4.625450	-2.742014
4	6	0	-0.766569	4.034807	-0.885135
5	1	0	0.068640	4.723285	-0.995330
6	6	0	-1.670784	2.263563	0.530740
7	1	0	-2.624977	2.355041	0.031637
8	1	0	-0.654267	0.912052	1.772975
9	7	0	-1.589123	1.261822	1.450702
10	6	0	-2.659272	0.482858	1.863143
11	8	0	-3.828706	0.896334	1.311515
12	8	0	-2.554706	-0.451102	2.628421
13	1	0	-1.068571	-0.968320	-0.524006
14	6	0	-5.136736	-3.326428	0.057027
15	6	0	-5.359702	-2.315253	-0.860148
16	6	0	-4.315666	-1.435239	-1.217067
17	6	0	-3.037160	-1.616028	-0.625591
18	6	0	-2.815331	-2.639786	0.318308
19	6	0	-3.863113	-3.480848	0.646638
20	1	0	-5.435731	-0.186276	-2.596360
21	1	0	-5.942791	-4.000689	0.330508
22	1	0	-6.338583	-2.181716	-1.313701
23	6	0	-4.465012	-0.350073	-2.134562
24	1	0	-1.833686	-2.731222	0.771174
25	1	0	-3.702636	-4.268066	1.377161
26	6	0	-2.128072	0.264268	-1.837175
27	6	0	-3.417528	0.472128	-2.432231
28	1	0	-3.544842	1.292698	-3.127825
29	7	0	-2.013300	-0.768273	-0.966871
30	6	0	-0.980745	1.062495	-2.088789
31	1	0	-0.076670	0.800642	-1.548283
32	6	0	-0.942402	2.145603	-2.965040
33	1	0	-1.694674	2.257665	-3.741545
34	1	0	0.033035	2.532398	-3.238621
35	6	0	-4.987511	0.180767	1.772132
36	1	0	-5.817932	0.566471	1.179734
37	1	0	-4.868993	-0.892087	1.614537
38	1	0	-5.152484	0.374545	2.835974
39	6	0	4.388045	-0.019487	-0.235788
40	6	0	5.643800	0.607131	-0.187929
41	6	0	5.760488	1.993541	-0.113013
42	6	0	4.610841	2.786254	-0.071753
43	6	0	3.350795	2.191433	-0.117410
44	6	0	3.247125	0.804896	-0.208601

45	6	0	4.271752	-1.493259	-0.319144
46	6	0	5.108184	-2.243148	-1.161836
47	6	0	5.013418	-3.631503	-1.230872
48	6	0	4.066379	-4.304177	-0.454507
49	6	0	3.223247	-3.583815	0.389573
50	6	0	3.332435	-2.196774	0.457698
51	1	0	6.535770	-0.013413	-0.187740
52	1	0	6.744813	2.451664	-0.070081
53	1	0	4.693312	3.867477	0.002775
54	1	0	2.438422	2.774465	-0.066106
55	1	0	5.827551	-1.716898	-1.783373
56	1	0	5.669504	-4.185738	-1.896364
57	1	0	3.981578	-5.386173	-0.507499
58	1	0	2.478616	-4.071845	1.009314
59	8	0	1.990390	0.244580	-0.365689
60	8	0	2.549201	-1.520331	1.378483
61	15	0	1.280579	-0.615842	0.864700
62	8	0	0.889538	0.289958	1.998279
63	8	0	0.248563	-1.476730	0.174456
64	6	0	-0.693130	3.211057	0.262331
65	8	0	0.461355	3.358704	0.980220
66	6	0	0.405452	3.355390	2.417480
67	1	0	1.204814	4.024856	2.744644
68	1	0	-0.559071	3.740154	2.768707
69	1	0	0.590753	2.352265	2.803773

(R=I)

TSI-Cc(R-en)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2034.445573 hartree

Sum of electronic and thermal Free Energies = -2034.012039 hartree

The number of imaginary frequency = 1

Imaginary frequency = -375.39

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.029874	-2.775568	2.053027
2	1	0	0.872717	-2.383033	1.493833
3	1	0	0.303378	-3.506693	2.810210
4	6	0	-1.218098	-2.934857	1.452029
5	1	0	-1.912396	-3.617729	1.933698
6	6	0	-0.948764	-1.237654	-0.288656
7	1	0	0.116315	-1.269623	-0.078617
8	1	0	-0.378142	0.033917	-1.750224
9	7	0	-1.226554	-0.329879	-1.259365
10	6	0	-2.409430	0.373867	-1.467566
11	8	0	-2.300066	1.058497	-2.621870
12	8	0	-3.363246	0.414729	-0.719894
13	1	0	-0.009185	1.939579	0.684840
14	6	0	-3.848273	4.631642	-0.104506
15	6	0	-4.187417	3.645699	0.806162
16	6	0	-3.229749	2.699742	1.226253
17	6	0	-1.916008	2.783901	0.697939
18	6	0	-1.572405	3.782091	-0.235071
19	6	0	-2.536910	4.695532	-0.623993
20	1	0	-4.505882	1.549043	2.554465
21	1	0	-4.590827	5.356544	-0.424184
22	1	0	-5.196910	3.582451	1.203592
23	6	0	-3.502315	1.640551	2.148033
24	1	0	-0.561306	3.808213	-0.630706
25	1	0	-2.280646	5.469029	-1.342255
26	6	0	-1.208830	0.858353	1.972748
27	6	0	-2.534957	0.749663	2.506246
28	1	0	-2.753269	-0.054398	3.197823
29	7	0	-0.976575	1.868072	1.095664
30	6	0	-0.098340	0.048446	2.331888
31	1	0	0.855112	0.330059	1.896531
32	6	0	-0.122347	-1.048470	3.191411
33	1	0	-1.012413	-1.276830	3.770484
34	1	0	0.805908	-1.304004	3.694767
35	6	0	5.154064	0.215814	0.086682
36	6	0	6.251738	0.372984	0.948485
37	6	0	6.740895	1.636242	1.275599
38	6	0	6.132644	2.777498	0.745646
39	6	0	5.041365	2.648656	-0.112220
40	6	0	4.566100	1.380895	-0.440234
41	6	0	4.646044	-1.126355	-0.276494
42	6	0	5.525535	-2.174635	-0.590727
43	6	0	5.054992	-3.439897	-0.938208
44	6	0	3.680038	-3.678795	-0.992146
45	6	0	2.785231	-2.654134	-0.685327
46	6	0	3.264443	-1.397063	-0.317022
47	1	0	6.708785	-0.514349	1.378042
48	1	0	7.587777	1.730229	1.949563
49	1	0	6.504129	3.765929	1.001468
50	1	0	4.547122	3.512121	-0.544203
51	1	0	6.593822	-1.977039	-0.582010
52	1	0	5.758555	-4.230460	-1.183117
53	1	0	3.302122	-4.655948	-1.279576
54	1	0	1.713585	-2.815990	-0.734773
55	8	0	3.543708	1.276077	-1.369735
56	8	0	2.360448	-0.434726	0.099695
57	15	0	2.028587	0.898006	-0.867743
58	8	0	1.498465	1.941703	0.086670
59	8	0	1.237989	0.456763	-2.064126
60	6	0	-3.429176	1.888340	-2.935887
61	1	0	-3.586956	2.637116	-2.156027
62	1	0	-3.177512	2.366886	-3.882728
63	1	0	-4.331790	1.279447	-3.039619
64	6	0	-1.721920	-2.180749	0.365114
65	53	0	-3.708029	-2.731824	-0.261516

TSI-Cc(S-en)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2034.444487 hartree

Sum of electronic and thermal Free Energies = -2034.011631 hartree

The number of imaginary frequency = 1

Imaginary frequency = -358.11

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.306854	-3.363426	1.339394
2	1	0	-0.577404	-2.921204	0.890921
3	1	0	0.107258	-4.241852	1.948204
4	6	0	1.543552	-3.298551	0.704896
5	1	0	2.301972	-4.005637	1.029527
6	6	0	1.081940	-1.316975	-0.641913
7	1	0	0.027087	-1.498570	-0.452203
8	1	0	0.308681	0.170277	-1.722120
9	7	0	1.228088	-0.200766	-1.398244
10	6	0	2.330498	0.637203	-1.526463
11	8	0	2.060626	1.548952	-2.482159
12	8	0	3.348243	0.600104	-0.868646
13	1	0	0.092940	1.608118	1.016274
14	6	0	3.805177	4.548182	0.713628
15	6	0	4.220816	3.391981	1.350735
16	6	0	3.312865	2.337919	1.583183
17	6	0	1.971640	2.491116	1.148016
18	6	0	1.548071	3.665961	0.495679
19	6	0	2.464961	4.681856	0.288747
20	1	0	4.686752	0.963810	2.552557
21	1	0	4.509294	5.355874	0.537798
22	1	0	5.251836	3.277983	1.674726
23	6	0	3.661134	1.108186	2.223987
24	1	0	0.515067	3.743059	0.168956
25	1	0	2.148524	5.592809	-0.211209
26	6	0	1.385875	0.299380	1.971238
27	6	0	2.736716	0.123538	2.413273
28	1	0	3.011481	-0.810005	2.888235
29	7	0	1.081023	1.470362	1.358774
30	6	0	0.316547	-0.616905	2.166921
31	1	0	-0.648831	-0.290113	1.798740
32	6	0	0.387051	-1.853155	2.800823
33	1	0	1.287053	-2.154406	3.328355
34	1	0	-0.529646	-2.248474	3.229324
35	6	0	3.101232	2.515144	-2.697660
36	1	0	4.016331	2.019214	-3.033887
37	1	0	2.718312	3.179959	-3.472487
38	1	0	3.308648	3.071286	-1.780612
39	6	0	-5.016140	-0.303558	0.741920
40	6	0	-6.082955	-0.355386	1.653925
41	6	0	-5.867982	-0.515309	3.021345
42	6	0	-4.563686	-0.619089	3.509314
43	6	0	-3.486685	-0.568645	2.625617
44	6	0	-3.708916	-0.418285	1.256279
45	6	0	-5.268005	-0.146290	-0.708550
46	6	0	-6.297930	-0.853254	-1.350795
47	6	0	-6.548261	-0.690426	-2.711884
48	6	0	-5.763069	0.186819	-3.465116
49	6	0	-4.734010	0.899349	-2.851612
50	6	0	-4.498677	0.735423	-1.488505
51	1	0	-7.095034	-0.246909	1.274164
52	1	0	-6.713323	-0.545292	3.702898
53	1	0	-4.382445	-0.733470	4.574581
54	1	0	-2.466186	-0.641837	2.985408
55	1	0	-6.891573	-1.553631	-0.769707
56	1	0	-7.346563	-1.254678	-3.185802
57	1	0	-5.947337	0.312721	-4.528406
58	1	0	-4.104724	1.588154	-3.404728
59	8	0	-2.623046	-0.486177	0.401722
60	8	0	-3.532660	1.522045	-0.880979
61	15	0	-2.097986	0.842611	-0.466574
62	8	0	-1.416761	1.815551	0.465469
63	8	0	-1.381601	0.273485	-1.659210
64	6	0	1.955889	-2.297764	-0.208106
65	53	0	3.968159	-2.526140	-0.938190

TS$_I$-Ct(R-en)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2034.441589 hartree

Sum of electronic and thermal Free Energies = -2034.008199 hartree

The number of imaginary frequency = 1

Imaginary frequency = -364.98

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.030788	-2.654715	2.091799
2	1	0	0.879853	-2.296162	1.519853
3	1	0	0.292084	-3.349655	2.886224
4	6	0	-1.216486	-2.826294	1.494884
5	1	0	-1.919094	-3.480325	2.003747
6	6	0	-0.927348	-1.211736	-0.322375
7	1	0	0.133506	-1.240459	-0.089198
8	1	0	-0.302954	-0.049221	-1.848032
9	7	0	-1.168340	-0.353119	-1.344759
10	6	0	-2.315339	0.334658	-1.742110
11	8	0	-3.252413	0.358365	-0.778169
12	8	0	-2.400662	0.894479	-2.812304
13	1	0	-0.011947	1.956131	0.453179
14	6	0	-3.823973	4.699281	-0.328334
15	6	0	-4.125400	3.815079	0.692973
16	6	0	-3.176916	2.859283	1.113849
17	6	0	-1.903970	2.841411	0.485978
18	6	0	-1.601838	3.736139	-0.559265
19	6	0	-2.561305	4.650433	-0.957416
20	1	0	-4.401911	1.855787	2.601873
21	1	0	-4.560329	5.427967	-0.653292
22	1	0	-5.099974	3.835366	1.174259
23	6	0	-3.428185	1.872092	2.118444
24	1	0	-0.626904	3.682624	-1.034463
25	1	0	-2.338382	5.337568	-1.768078
26	6	0	-1.176747	0.993352	1.860494
27	6	0	-2.476471	0.959866	2.466460
28	1	0	-2.677850	0.213553	3.224733
29	7	0	-0.967659	1.928641	0.899369
30	6	0	-0.068713	0.189195	2.238632
31	1	0	0.878275	0.434286	1.769387
32	6	0	-0.089278	-0.860747	3.153407

33	1	0	-0.972161	-1.056206	3.755040
34	1	0	0.845056	-1.107749	3.649192
35	6	0	-4.512423	0.914258	-1.187865
36	1	0	-4.383210	1.945136	-1.522021
37	1	0	-4.943012	0.314318	-1.994259
38	1	0	-5.144895	0.872043	-0.301607
39	6	0	4.698830	-1.118978	-0.178948
40	6	0	5.597164	-2.174659	-0.401499
41	6	0	5.148595	-3.464181	-0.682882
42	6	0	3.778111	-3.721351	-0.762469
43	6	0	2.864986	-2.689837	-0.545657
44	6	0	3.321959	-1.407923	-0.241049
45	6	0	5.181285	0.250204	0.110865
46	6	0	6.251378	0.476892	0.991587
47	6	0	6.716494	1.764892	1.250192
48	6	0	6.111303	2.861621	0.630352
49	6	0	5.047258	2.663657	-0.248341
50	6	0	4.596005	1.371331	-0.506982
51	1	0	6.662847	-1.964934	-0.375014
52	1	0	5.866388	-4.260475	-0.857959
53	1	0	3.418355	-4.718307	-1.001001
54	1	0	1.796553	-2.864474	-0.618092
55	1	0	6.705728	-0.374997	1.490229
56	1	0	7.542273	1.913101	1.940407
57	1	0	6.464166	3.869224	0.831976
58	1	0	4.556672	3.490922	-0.749754
59	8	0	2.398126	-0.430760	0.088995
60	8	0	3.602706	1.194339	-1.457126
61	15	0	2.078169	0.826518	-0.979176
62	8	0	1.330143	0.288403	-2.162591
63	8	0	1.500231	1.922967	-0.115523
64	6	0	-1.708025	-2.121250	0.369667
65	53	0	-3.692362	-2.710295	-0.249331

TS_I-Ct(S-en)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2034.441067 hartree

Sum of electronic and thermal Free Energies = -2034.008058 hartree

The number of imaginary frequency = 1

Imaginary frequency = -352.54

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.728246	-2.835546	2.428389
2	1	0	-0.194907	-2.772990	1.861249
3	1	0	0.656063	-3.427879	3.336945
4	6	0	1.962451	-2.796757	1.788899
5	1	0	2.815547	-3.182559	2.340284
6	6	0	1.233889	-1.561068	-0.184623
7	1	0	0.219908	-1.807328	0.120070
8	1	0	0.211692	-0.746505	-1.681719
9	7	0	1.184103	-0.809528	-1.311122
10	6	0	2.088390	0.045151	-1.940122
11	8	0	3.143812	0.337279	-1.163839
12	8	0	1.884660	0.501148	-3.044049
13	1	0	-0.028643	1.610940	0.198967
14	6	0	3.396290	4.692625	-0.925681
15	6	0	3.836495	3.936109	0.146002
16	6	0	3.022241	2.914594	0.680432
17	6	0	1.741206	2.696918	0.108959
18	6	0	1.299177	3.458181	-0.991679
19	6	0	2.128581	4.444230	-1.496521
20	1	0	4.404404	2.183720	2.188857
21	1	0	4.027966	5.474616	-1.336067
22	1	0	4.816501	4.110219	0.583013
23	6	0	3.417881	2.053615	1.751006
24	1	0	0.322373	3.248792	-1.417251
25	1	0	1.798174	5.033766	-2.346487
26	6	0	1.274973	0.911186	1.662444
27	6	0	2.585109	1.079344	2.218768
28	1	0	2.897528	0.426074	3.023725
29	7	0	0.931370	1.721510	0.632597
30	6	0	0.285889	0.007831	2.143106
31	1	0	-0.677951	0.047532	1.648261
32	6	0	0.436623	-0.883351	3.199870
33	1	0	1.306819	-0.836273	3.847020
34	1	0	-0.466197	-1.229241	3.694426
35	6	0	4.180489	1.084975	-1.821414
36	1	0	4.555984	0.529368	-2.684867
37	1	0	3.801310	2.055998	-2.144423
38	1	0	4.962625	1.205793	-1.072822
39	6	0	-5.119124	0.167753	0.802258
40	6	0	-6.140748	0.722373	1.590069
41	6	0	-5.870290	1.315111	2.822106
42	6	0	-4.556100	1.370857	3.292127
43	6	0	-3.522761	0.829135	2.528822
44	6	0	-3.803210	0.229975	1.301055
45	6	0	-5.421262	-0.474716	-0.497214
46	6	0	-6.529157	-1.324627	-0.648585
47	6	0	-6.823244	-1.920526	-1.873494
48	6	0	-6.004011	-1.680156	-2.979960
49	6	0	-4.897941	-0.840739	-2.856318
50	6	0	-4.618616	-0.243196	-1.629347
51	1	0	-7.158669	0.700666	1.210944
52	1	0	-6.680265	1.742186	3.406637
53	1	0	-4.333602	1.838632	4.247340
54	1	0	-2.493655	0.859542	2.871780
55	1	0	-7.150470	-1.530973	0.218617
56	1	0	-7.682568	-2.579393	-1.961501
57	1	0	-6.222282	-2.147523	-3.936151
58	1	0	-4.241921	-0.629848	-3.693979
59	8	0	-2.771974	-0.391596	0.618875
60	8	0	-3.574011	0.664487	-1.557675
61	15	0	-2.179732	0.244226	-0.803847
62	8	0	-1.451807	1.535485	-0.512716
63	8	0	-1.479310	-0.900288	-1.483070
64	6	0	2.238901	-2.165715	0.550753
65	53	0	4.285071	-2.369776	-0.105592

TS_I-Tc(R-ex)

B3LYP-D3/6-31g(d) in gas phase
SCF Done: E(RB3LYP) = -2034.453793 hartree
Sum of electronic and thermal Free Energies = -2034.021128 hartree
The number of imaginary frequency = 1
Imaginary frequency = -366.73

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.381996	-0.636051	0.999375
2	1	0	5.319774	0.347805	0.543516
3	1	0	6.322015	-0.832144	1.509488
4	6	0	4.711349	-1.719325	0.436406
5	1	0	5.030232	-2.714385	0.734242
6	6	0	3.016495	-0.408158	-0.728486
7	1	0	3.683542	0.447694	-0.708897
8	1	0	0.975676	-0.757706	-1.182965
9	7	0	1.814738	-0.126180	-1.283676
10	6	0	1.606506	1.155676	-1.790755
11	8	0	0.332786	1.293208	-2.189773
12	8	0	2.459094	2.023051	-1.855609
13	1	0	0.519826	1.041771	1.356462
14	6	0	-0.223648	5.466683	-0.202672
15	6	0	1.122892	5.335327	0.085064
16	6	0	1.628556	4.117980	0.591582
17	6	0	0.731364	3.034684	0.785130
18	6	0	-0.641871	3.170609	0.492840
19	6	0	-1.102456	4.381188	0.008010
20	1	0	3.703873	4.721174	0.794150
21	1	0	-0.608332	6.405398	-0.589920
22	1	0	1.807996	6.164448	-0.070998
23	6	0	2.998301	3.906494	0.935281
24	1	0	-1.306196	2.325292	0.632769
25	1	0	-2.158276	4.492079	-0.221582
26	6	0	2.508401	1.619017	1.596860
27	6	0	3.424581	2.708761	1.432408
28	1	0	4.466520	2.558928	1.688416
29	7	0	1.216339	1.840558	1.257451
30	6	0	2.855365	0.323979	2.075071
31	1	0	2.056435	-0.411545	2.068607
32	6	0	4.109127	-0.031112	2.573788
33	1	0	4.808496	0.738146	2.891403
34	1	0	4.176216	-0.947360	3.149836
35	6	0	0.018757	2.554545	-2.806129
36	1	0	0.437509	2.587020	-3.816739
37	1	0	-1.069378	2.595103	-2.839534
38	1	0	0.413266	3.384166	-2.218781
39	6	0	-4.536920	-0.776110	0.888726
40	6	0	-5.682298	-0.446299	1.631072
41	6	0	-5.767865	-0.719780	2.995007
42	6	0	-4.695110	-1.330124	3.650362
43	6	0	-3.546512	-1.668596	2.936467
44	6	0	-3.473168	-1.401025	1.570577
45	6	0	-4.453865	-0.495764	-0.562486
46	6	0	-5.532794	-0.745468	-1.425383
47	6	0	-5.436044	-0.499196	-2.794321
48	6	0	-4.241834	-0.012342	-3.333411
49	6	0	-3.157085	0.247330	-2.496662
50	6	0	-3.276212	0.028796	-1.125879
51	1	0	-6.505651	0.049843	1.124195
52	1	0	-6.664047	-0.448533	3.546107
53	1	0	-4.750482	-1.540678	4.714923
54	1	0	-2.697646	-2.148493	3.411724
55	1	0	-6.446280	-1.164198	-1.012006
56	1	0	-6.282929	-0.708553	-3.441874
57	1	0	-4.151776	0.155361	-4.403273
58	1	0	-2.204661	0.596990	-2.878459
59	8	0	-2.363167	-1.846576	0.874925
60	8	0	-2.233818	0.397642	-0.295542
61	15	0	-1.237715	-0.782609	0.321445
62	8	0	-0.523349	-0.116066	1.477201
63	8	0	-0.475608	-1.463408	-0.776093
64	6	0	3.519099	-1.625740	-0.313890
65	53	0	2.447440	-3.447506	-0.677802

TS_I-Tc(S-ex)
B3LYP-D3/6-31g(d) in gas phase
SCF Done: E(RB3LYP) = -2034.452220 hartree
Sum of electronic and thermal Free Energies = -2034.019568 hartree
The number of imaginary frequency = 1
Imaginary frequency = -363.22

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.390861	-2.674721	-1.592275
2	1	0	4.907535	-1.915519	-1.012741
3	1	0	5.037258	-3.243258	-2.256445
4	6	0	3.268919	-3.318103	-1.071953
5	1	0	2.967036	-4.252626	-1.536685
6	6	0	2.655019	-1.552815	0.495558
7	1	0	3.676217	-1.187621	0.453368
8	1	0	0.809426	-0.862088	1.303930
9	7	0	1.862448	-0.792759	1.280853
10	6	0	2.436426	0.293018	1.947123
11	8	0	1.496517	0.953795	2.631391
12	8	0	3.617533	0.588036	1.904965
13	1	0	0.968438	1.014878	-1.011890
14	6	0	2.311037	5.067605	1.104079
15	6	0	3.433644	4.474541	0.553825
16	6	0	3.327662	3.248886	-0.139189
17	6	0	2.050226	2.641298	-0.258093
18	6	0	0.909860	3.239063	0.318674
19	6	0	1.050133	4.442915	0.985302
20	1	0	5.424366	3.015638	-0.653731
21	1	0	2.398167	6.011258	1.634082
22	1	0	4.410331	4.942090	0.647234
23	6	0	4.435330	2.573096	-0.739207
24	1	0	-0.051612	2.741884	0.248550
25	1	0	0.175223	4.906616	1.431622
26	6	0	2.968204	0.798221	-1.518816

27	6	0	4.267078	1.394909	-1.406404
28	1	0	5.114205	0.891125	-1.856211
29	7	0	1.935834	1.452053	-0.931245
30	6	0	2.669334	-0.414355	-2.197955
31	1	0	1.625953	-0.714617	-2.178498
32	6	0	3.587444	-1.209871	-2.884281
33	1	0	4.567897	-0.818025	-3.143929
34	1	0	3.192751	-1.914834	-3.607562
35	6	0	1.978134	2.054648	3.419223
36	1	0	2.533958	2.760787	2.799944
37	1	0	1.083679	2.523961	3.827808
38	1	0	2.623158	1.687909	4.223320
39	6	0	-4.380671	1.299598	-0.632319
40	6	0	-5.354719	1.938538	-1.416564
41	6	0	-5.098555	3.152583	-2.051124
42	6	0	-3.845029	3.754230	-1.917420
43	6	0	-2.859936	3.140142	-1.145511
44	6	0	-3.126915	1.930149	-0.505287
45	6	0	-4.670691	0.014892	0.044337
46	6	0	-5.894890	-0.208246	0.695381
47	6	0	-6.173148	-1.423637	1.318065
48	6	0	-5.221242	-2.446994	1.306474
49	6	0	-3.998170	-2.250290	0.667436
50	6	0	-3.734171	-1.035080	0.039303
51	1	0	-6.319982	1.455441	-1.540581
52	1	0	-5.869659	3.620163	-2.656917
53	1	0	-3.631714	4.696421	-2.414963
54	1	0	-1.879149	3.588092	-1.023553
55	1	0	-6.623893	0.596918	0.726146
56	1	0	-7.125300	-1.567674	1.821072
57	1	0	-5.427910	-3.393888	1.797645
58	1	0	-3.235791	-3.021410	0.637282
59	8	0	-2.164674	1.407839	0.339376
60	8	0	-2.554611	-0.898020	-0.671214
61	15	0	-1.339626	0.018193	-0.050788
62	8	0	-0.407357	0.295471	-1.209725
63	8	0	-0.812365	-0.529398	1.242966
64	6	0	2.375035	-2.745987	-0.141808
65	53	0	0.494684	-3.736995	0.152731

TS_I-Tt(R-ex)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2034.449718 hartree

Sum of electronic and thermal Free Energies = -2034.016124 hartree

The number of imaginary frequency = 1

Imaginary frequency = -366.11

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.160657	-0.911283	1.176649
2	1	0	5.134885	0.100297	0.781475
3	1	0	6.076963	-1.158037	1.707732
4	6	0	4.495336	-1.945058	0.520793
5	1	0	4.782863	-2.961587	0.774533
6	6	0	2.881909	-0.542424	-0.666363
7	1	0	3.568475	0.291139	-0.577982
8	1	0	0.850470	-0.863266	-1.171807
9	7	0	1.700173	-0.236918	-1.253584
10	6	0	1.412530	1.002963	-1.814156
11	8	0	2.482258	1.833921	-1.797344
12	8	0	0.328465	1.297191	-2.270121
13	1	0	0.447346	0.978636	1.303289
14	6	0	0.177218	5.510536	-0.187239
15	6	0	1.448517	5.294763	0.312629
16	6	0	1.812510	4.023626	0.808326
17	6	0	0.847724	2.979313	0.794458
18	6	0	-0.445030	3.200424	0.275709
19	6	0	-0.763375	4.457214	-0.207234
20	1	0	3.868218	4.492941	1.325632
21	1	0	-0.098886	6.488225	-0.570604
22	1	0	2.184592	6.094573	0.325790
23	6	0	3.112538	3.711228	1.309717
24	1	0	-1.159000	2.384144	0.242234
25	1	0	-1.754750	4.629744	-0.615388
26	6	0	2.423338	1.420012	1.749625
27	6	0	3.413527	2.457584	1.758613
28	1	0	4.405242	2.231501	2.131113
29	7	0	1.195102	1.739866	1.272671
30	6	0	2.642961	0.084955	2.187917
31	1	0	1.802313	-0.593610	2.082490
32	6	0	3.840792	-0.379958	2.732493
33	1	0	4.563551	0.317216	3.148892
34	1	0	3.821224	-1.339735	3.237045
35	6	0	2.268016	3.095251	-2.455387
36	1	0	1.393453	3.602155	-2.045553
37	1	0	3.172021	3.674653	-2.266337
38	1	0	2.128742	2.939288	-3.528959
39	6	0	-4.469588	-0.237282	-0.663751
40	6	0	-5.514301	-0.363542	-1.593796
41	6	0	-5.338552	-0.002817	-2.928887
42	6	0	-4.103303	0.485833	-3.365643
43	6	0	-3.047918	0.621081	-2.464267
44	6	0	-3.244717	0.271026	-1.130723
45	6	0	-4.646638	-0.599735	0.761601
46	6	0	-5.818252	-0.249498	1.452977
47	6	0	-6.002276	-0.583089	2.793462
48	6	0	-5.002085	-1.276043	3.480139
49	6	0	-3.828972	-1.635548	2.818751
50	6	0	-3.656903	-1.306865	1.474814
51	1	0	-6.465020	-0.771357	-1.261274
52	1	0	-6.159940	-0.117715	-3.630929
53	1	0	-3.959149	0.753662	-4.408955
54	1	0	-2.068961	0.983058	-2.759194
55	1	0	-6.583811	0.312162	0.924542
56	1	0	-6.917538	-0.293662	3.302412
57	1	0	-5.132733	-1.535051	4.527334
58	1	0	-3.035280	-2.181217	3.318038
59	8	0	-2.223011	0.498688	-0.224018
60	8	0	-2.529419	-1.785624	0.833014
61	15	0	-1.329614	-0.787052	0.321167
62	8	0	-0.625436	-1.490008	-0.802228

63	8	0	-0.547692	-0.219189	1.487901
64	6	0	3.341916	-1.787076	-0.277051
65	53	0	2.251796	-3.566536	-0.773384

TS_I-Tt(S-ex)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2034.445986 hartree

Sum of electronic and thermal Free Energies = -2034.012585 hartree

The number of imaginary frequency = 1

Imaginary frequency = -364.93

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.768803	-3.255357	2.513505
2	1	0	-2.708264	-2.751980	2.304268
3	1	0	-1.782736	-3.874813	3.406935
4	6	0	-0.929164	-3.642029	1.472861
5	1	0	-0.179031	-4.397028	1.691974
6	6	0	-1.722766	-2.005018	-0.165845
7	1	0	-2.655359	-1.922589	0.380210
8	1	0	-0.658791	-0.900049	-1.593904
9	7	0	-1.607933	-1.164491	-1.223648
10	6	0	-2.653676	-0.389461	-1.717344
11	8	0	-3.828892	-0.685534	-1.106787
12	8	0	-2.523243	0.431923	-2.596221
13	1	0	-1.153413	1.413810	0.448085
14	6	0	-5.281870	3.601888	-0.297156
15	6	0	-5.466344	2.698025	0.732807
16	6	0	-4.395535	1.885593	1.166552
17	6	0	-3.131781	2.020794	0.531023
18	6	0	-2.949153	2.936418	-0.527545
19	6	0	-4.021514	3.713826	-0.926073
20	1	0	-5.461079	0.788637	2.707679
21	1	0	-6.107106	4.224576	-0.629289
22	1	0	-6.433365	2.597872	1.218999
23	6	0	-4.504366	0.913865	2.206395
24	1	0	-1.978504	2.995142	-1.008111
25	1	0	-3.891696	4.417070	-1.743239
26	6	0	-2.164574	0.303742	1.922099
27	6	0	-3.433911	0.148180	2.571657
28	1	0	-3.531175	-0.587979	3.360170
29	7	0	-2.083550	1.235589	0.943044
30	6	0	-1.006816	-0.469669	2.220392
31	1	0	-0.119964	-0.276353	1.626883
32	6	0	-0.939802	-1.431852	3.226207
33	1	0	-1.645243	-1.420918	4.052864
34	1	0	0.041926	-1.808754	3.491359
35	6	0	-4.973576	-0.012989	-1.659195
36	1	0	-5.808684	-0.291040	-1.015666
37	1	0	-4.828560	1.067932	-1.655145
38	1	0	-5.149159	-0.351595	-2.684345
39	6	0	4.220841	0.825728	0.503499
40	6	0	5.500279	0.271449	0.674384
41	6	0	5.674751	-1.074827	0.989573
42	6	0	4.559767	-1.903506	1.139424
43	6	0	3.279530	-1.379361	0.971443
44	6	0	3.113930	-0.032008	0.655478
45	6	0	4.046485	2.266786	0.209110
46	6	0	4.814899	3.238134	0.872423
47	6	0	4.664163	4.596048	0.598292
48	6	0	3.727227	5.014934	-0.350252
49	6	0	2.950931	4.071795	-1.021473
50	6	0	3.116419	2.715583	-0.746976
51	1	0	6.366860	0.912488	0.538010
52	1	0	6.676993	-1.477157	1.107710
53	1	0	4.684800	-2.956166	1.378421
54	1	0	2.394527	-1.996997	1.072676
55	1	0	5.524251	2.913474	1.628729
56	1	0	5.268168	5.325369	1.130940
57	1	0	3.598669	6.072234	-0.565338
58	1	0	2.217403	4.358889	-1.767285
59	8	0	1.830220	0.473570	0.594759
60	8	0	2.404778	1.801472	-1.503581
61	15	0	1.151154	0.976874	-0.842850
62	8	0	0.857057	-0.187541	-1.739408
63	8	0	0.054536	1.920419	-0.397184
64	6	0	-0.847687	-3.006380	0.214526
65	53	0	0.729597	-3.641157	-1.097509

(R=TMS) (TMS=$SiMe_3$)

TS_{TMS}-Cc(R-en)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2432.396072 hartree

Sum of electronic and thermal Free Energies = -2431.854907 hartree

The number of imaginary frequency = 1

Imaginary frequency = -342.87

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.316257	-3.593948	-1.532616
2	1	0	2.277426	-3.887453	-1.420210
3	1	0	3.914485	-4.279450	-2.127498
4	6	0	3.954859	-2.846512	-0.553574
5	1	0	5.043086	-2.874596	-0.582529
6	6	0	3.373091	-1.938504	0.387216
7	6	0	1.993450	-1.803711	0.335329
8	1	0	1.396284	-2.520940	-0.219110
9	1	0	0.153876	-1.155860	0.790628
10	7	0	1.150265	-0.927419	0.959714
11	6	0	1.441580	0.349690	1.393788
12	8	0	0.321891	0.927363	1.863727
13	8	0	2.532097	0.890756	1.348526
14	1	0	0.132874	0.505723	-1.834985
15	6	0	1.565215	4.811851	-0.505330
16	6	0	2.689663	4.061640	-0.801394
17	6	0	2.562990	2.728761	-1.246307
18	6	0	1.263442	2.174960	-1.367371
19	6	0	0.116901	2.942613	-1.079130

20	6	0	0.278842	4.249401	-0.654697
21	1	0	4.674754	2.290336	-1.503594
22	1	0	1.669839	5.837491	-0.164317
23	1	0	3.683940	4.487792	-0.696387
24	6	0	3.668165	1.891560	-1.593888
25	1	0	-0.861635	2.489294	-1.200084
26	1	0	-0.599779	4.848680	-0.432333
27	6	0	2.157127	0.057540	-2.103205
28	6	0	3.477081	0.608896	-2.014148
29	1	0	4.322302	-0.024304	-2.251541
30	7	0	1.126290	0.870430	-1.772536
31	6	0	1.841085	-1.259055	-2.543087
32	1	0	0.790901	-1.535742	-2.496100
33	6	0	2.757331	-2.169029	-3.051269
34	1	0	3.763416	-1.855479	-3.308847
35	1	0	2.378914	-2.988225	-3.654157
36	6	0	-4.793972	0.519099	0.409756
37	6	0	-5.806935	1.491397	0.438573
38	6	0	-5.512716	2.846004	0.583028
39	6	0	-4.184142	3.260100	0.705950
40	6	0	-3.159433	2.315931	0.675551
41	6	0	-3.462787	0.963364	0.522044
42	6	0	-5.114776	-0.924319	0.315912
43	6	0	-6.174595	-1.472074	1.057622
44	6	0	-6.490291	-2.826956	0.985745
45	6	0	-5.738473	-3.673172	0.167144
46	6	0	-4.680735	-3.156403	-0.578248
47	6	0	-4.378014	-1.798011	-0.506614
48	1	0	-6.839356	1.170815	0.329843
49	1	0	-6.317446	3.575675	0.594930
50	1	0	-3.946511	4.314162	0.823747
51	1	0	-2.117231	2.598072	0.779000
52	1	0	-6.740512	-0.818966	1.716212
53	1	0	-7.311873	-3.222785	1.576155
54	1	0	-5.972314	-4.732724	0.110148
55	1	0	-4.079882	-3.782239	-1.229525
56	8	0	-2.432951	0.049091	0.579602
57	8	0	-3.397370	-1.306099	-1.348448
58	15	0	-1.952369	-0.773334	-0.775646
59	8	0	-1.432275	0.182942	-1.824845
60	8	0	-1.074916	-1.884107	-0.267143
61	14	0	4.581462	-1.203644	1.673841
62	6	0	5.547082	0.295913	1.044933
63	1	0	4.893843	1.160540	0.918765
64	1	0	6.342466	0.552537	1.756181
65	1	0	6.027507	0.074463	0.083431
66	6	0	3.736237	-0.909111	3.344339
67	1	0	4.360281	-1.294664	4.158883
68	1	0	3.554709	0.154649	3.516870
69	1	0	2.770036	-1.424399	3.395772
70	6	0	5.872368	-2.571562	1.972565
71	1	0	5.401676	-3.526420	2.234958
72	1	0	6.531272	-2.748293	1.114354
73	1	0	6.513095	-2.276364	2.813332
74	6	0	0.498994	2.238326	2.423147
75	1	0	0.951329	2.914556	1.695578
76	1	0	-0.505180	2.570820	2.686664
77	1	0	1.131429	2.185606	3.314507

TS_{TMS}-Cc(S-en)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2432.396885 hartree

Sum of electronic and thermal Free Energies = -2431.855695 hartree

The number of imaginary frequency = 1

Imaginary frequency = -321.11

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.499520	-3.567180	1.172435
2	1	0	-0.399374	-3.129715	0.749529
3	1	0	0.327543	-4.448914	1.784617
4	6	0	1.734218	-3.427252	0.558446
5	1	0	2.500850	-4.121074	0.898814
6	6	0	2.167125	-2.402614	-0.342896
7	6	0	1.205843	-1.486203	-0.743776
8	1	0	0.153825	-1.694061	-0.566419
9	1	0	0.385790	0.062970	-1.738210
10	7	0	1.310468	-0.324043	-1.453477
11	6	0	2.409619	0.500704	-1.550657
12	8	0	2.100557	1.572513	-2.304741
13	8	0	3.493377	0.318207	-1.024956
14	1	0	0.228774	1.451984	0.953458
15	6	0	3.932824	4.407118	0.751790
16	6	0	4.350457	3.234049	1.356277
17	6	0	3.445543	2.170138	1.553068
18	6	0	2.107316	2.329150	1.111504
19	6	0	1.683210	3.519873	0.489124
20	6	0	2.595512	4.546550	0.321751
21	1	0	4.811778	0.779794	2.512504
22	1	0	4.633785	5.223644	0.606605
23	1	0	5.378947	3.116851	1.687521
24	6	0	3.788891	0.930171	2.177952
25	1	0	0.652326	3.599896	0.156968
26	1	0	2.277776	5.470545	-0.152725
27	6	0	1.514618	0.124216	1.897217
28	6	0	2.863267	-0.056112	2.346291
29	1	0	3.135591	-0.995987	2.809574
30	7	0	1.217477	1.301628	1.294192
31	6	0	0.444526	-0.793126	2.080631
32	1	0	-0.519246	-0.468014	1.706521
33	6	0	0.520041	-2.029657	2.700908
34	1	0	1.417347	-2.341579	3.225477
35	1	0	-0.398158	-2.463822	3.083655
36	14	0	3.958222	-2.587900	-0.986450
37	6	0	3.190265	2.478116	-2.544046
38	1	0	3.954480	1.991911	-3.158165
39	1	0	2.750291	3.319969	-3.078863
40	1	0	3.635135	2.810345	-1.604937
41	6	0	5.256104	-1.897805	0.203784
42	1	0	5.129002	-2.327297	1.205758
43	1	0	6.262730	-2.166388	-0.141145

44	1	0	5.186550	-0.811508	0.277571
45	6	0	4.145538	-1.955691	-2.763850
46	1	0	4.683112	-1.004651	-2.794157
47	1	0	4.692512	-2.686641	-3.370516
48	1	0	3.167968	-1.801083	-3.235278
49	6	0	4.267779	-4.465435	-1.069657
50	1	0	4.338624	-4.944364	-0.086102
51	1	0	3.487178	-4.983510	-1.639238
52	1	0	5.222555	-4.642085	-1.581317
53	6	0	-4.919957	-0.264548	0.791227
54	6	0	-5.962774	-0.270952	1.731550
55	6	0	-5.716898	-0.432356	3.093270
56	6	0	-4.405049	-0.584138	3.546542
57	6	0	-3.351114	-0.579462	2.634575
58	6	0	-3.605130	-0.425879	1.271537
59	6	0	-5.203681	-0.107010	-0.653387
60	6	0	-6.276581	-0.777979	-1.262432
61	6	0	-6.556697	-0.616243	-2.617521
62	6	0	-5.758423	0.223324	-3.398745
63	6	0	-4.686820	0.899771	-2.818891
64	6	0	-4.421364	0.737162	-1.461398
65	1	0	-6.980053	-0.125948	1.378687
66	1	0	-6.543975	-0.426525	3.797559
67	1	0	-4.199868	-0.701188	4.607212
68	1	0	-2.324441	-0.691500	2.966120
69	1	0	-6.881277	-1.450223	-0.659875
70	1	0	-7.388670	-1.152697	-3.065151
71	1	0	-5.966014	0.348206	-4.457901
72	1	0	-4.046129	1.559398	-3.394121
73	8	0	-2.546770	-0.538871	0.387912
74	8	0	-3.411055	1.492366	-0.887668
75	15	0	-1.992344	0.767615	-0.492287
76	8	0	-1.270573	1.723196	0.427462
77	8	0	-1.307937	0.176631	-1.691782

TS_{TMS}-Ct(R-en)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2432.391406 hartree

Sum of electronic and thermal Free Energies = -2431.848683 hartree

The number of imaginary frequency = 1

Imaginary frequency = -336.93

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.412359	-3.886093	1.218612
2	1	0	-0.375030	-3.563657	1.234168
3	1	0	-1.595240	-4.850467	1.686835
4	6	0	-2.278748	-3.490300	0.206721
5	1	0	-3.188745	-4.080312	0.113385
6	6	0	-2.188368	-2.325662	-0.621413
7	6	0	-1.039606	-1.564261	-0.479973
8	1	0	-0.188307	-1.961974	0.067537
9	1	0	0.316755	-0.148332	-1.004810
10	7	0	-0.688340	-0.347230	-1.016358
11	6	0	-1.419444	0.758941	-1.409575
12	8	0	-2.737304	0.646531	-1.156054
13	8	0	-0.902678	1.744272	-1.900828
14	1	0	-0.309988	0.867432	1.815335
15	6	0	-3.090302	4.616324	0.975681
16	6	0	-3.900434	3.552345	1.333524
17	6	0	-3.338072	2.289674	1.612941
18	6	0	-1.928084	2.141753	1.543798
19	6	0	-1.104926	3.222244	1.168298
20	6	0	-1.692602	4.443196	0.887403
21	1	0	-5.188524	1.207849	1.977038
22	1	0	-3.528959	5.585122	0.756458
23	1	0	-4.979527	3.671739	1.391721
24	6	0	-4.105226	1.124167	1.933592
25	1	0	-0.031905	3.067565	1.104198
26	1	0	-1.065826	5.279582	0.592607
27	6	0	-2.070261	-0.192076	2.157258
28	6	0	-3.501414	-0.073200	2.177028
29	1	0	-4.091065	-0.949352	2.416488
30	7	0	-1.366752	0.923506	1.832637
31	6	0	-1.336338	-1.344331	2.533824
32	1	0	-0.256466	-1.243746	2.561447
33	6	0	-1.867824	-2.593346	2.834041
34	1	0	-2.940724	-2.745023	2.910082
35	1	0	-1.281260	-3.248743	3.470232
36	14	0	-3.574900	-2.131410	-1.912743
37	6	0	-3.525377	1.753681	-1.637913
38	1	0	-3.127003	2.696281	-1.263233
39	1	0	-3.528393	1.762450	-2.731434
40	1	0	-4.529285	1.578454	-1.255990
41	6	0	-5.110019	-1.278207	-1.191550
42	1	0	-5.676897	-0.747281	-1.965981
43	1	0	-5.780418	-2.024232	-0.748184
44	1	0	-4.836198	-0.563266	-0.411930
45	6	0	-2.939118	-1.366848	-3.523834
46	1	0	-2.037446	-1.898332	-3.851465
47	1	0	-3.696394	-1.503473	-4.306131
48	1	0	-2.697676	-0.303341	-3.480514
49	6	0	-4.105809	-3.887993	-2.405975
50	1	0	-3.253848	-4.493740	-2.735574
51	1	0	-4.612362	-4.431061	-1.599941
52	1	0	-4.811718	-3.825607	-3.244039
53	6	0	5.050701	-0.315178	-0.317137
54	6	0	6.127560	-0.992791	-0.910952
55	6	0	6.736564	-2.076942	-0.282117
56	6	0	6.272634	-2.511790	0.962047
57	6	0	5.205027	-1.856241	1.572975
58	6	0	4.609893	-0.768530	0.938817
59	6	0	4.415641	0.848373	-0.976928
60	6	0	5.195901	1.840180	-1.592632
61	6	0	4.612206	2.933407	-2.229258
62	6	0	3.221628	3.057686	-2.258193
63	6	0	2.420582	2.090145	-1.652614
64	6	0	3.016521	0.999031	-1.023618
65	1	0	6.471332	-0.668892	-1.889503
66	1	0	7.563860	-2.587925	-0.766799
67	1	0	6.737917	-3.361076	1.454855

68	1	0	4.819812	-2.164073	2.539142
69	1	0	6.277912	1.751663	-1.547935
70	1	0	5.241107	3.688660	-2.692538
71	1	0	2.755966	3.906718	-2.751394
72	1	0	1.338277	2.155252	-1.678715
73	8	0	3.616618	-0.070858	1.606961
74	8	0	2.195898	-0.000828	-0.515357
75	15	0	2.051936	-0.245513	1.143924
76	8	0	1.546948	-1.648026	1.286441
77	8	0	1.300307	0.922597	1.739202

TS_{TMS}-Ct(S-en)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2432.390310 hartree

Sum of electronic and thermal Free Energies = -2431.848980 hartree

The number of imaginary frequency = 1

Imaginary frequency = -316.79

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.849192	-2.942084	2.448410
2	1	0	-0.082160	-2.851566	1.898860
3	1	0	0.775286	-3.509444	3.372545
4	6	0	2.074919	-2.894745	1.804240
5	1	0	2.914009	-3.285529	2.377400
6	6	0	2.400817	-2.281776	0.551223
7	6	0	1.346913	-1.707076	-0.147694
8	1	0	0.327839	-1.938023	0.151418
9	1	0	0.315974	-0.847150	-1.631318
10	7	0	1.288937	-0.935748	-1.270475
11	6	0	2.184729	-0.081875	-1.890359
12	8	0	3.338213	0.075254	-1.201198
13	8	0	1.927723	0.491849	-2.927532
14	1	0	0.142099	1.503509	0.165577
15	6	0	3.605116	4.524875	-1.000171
16	6	0	4.025738	3.796208	0.098368
17	6	0	3.197105	2.796430	0.650056
18	6	0	1.924340	2.567931	0.064891
19	6	0	1.502379	3.300683	-1.062253
20	6	0	2.344040	4.268903	-1.580769
21	1	0	4.542788	2.116091	2.214524
22	1	0	4.247338	5.291591	-1.422948
23	1	0	4.999787	3.977968	0.545546
24	6	0	3.565946	1.972744	1.759257
25	1	0	0.532087	3.082596	-1.497556
26	1	0	2.028764	4.836583	-2.451093
27	6	0	1.421497	0.831383	1.664015
28	6	0	2.720435	1.017225	2.241592
29	1	0	3.013308	0.392896	3.076276
30	7	0	1.101741	1.610648	0.603149
31	6	0	0.419899	-0.050144	2.158142
32	1	0	-0.539261	-0.013392	1.653872
33	6	0	0.560008	-0.922111	3.225051
34	1	0	1.435236	-0.894401	3.865614
35	1	0	-0.341107	-1.284700	3.708561
36	14	0	4.189897	-2.550255	-0.045530
37	6	0	4.313953	0.891951	-1.877531
38	1	0	4.639524	0.402893	-2.799840
39	1	0	3.894563	1.870301	-2.112196
40	1	0	5.145266	0.984930	-1.181056
41	6	0	5.395617	-1.252213	0.634549
42	1	0	5.747438	-1.552325	1.629076
43	1	0	6.278448	-1.152052	-0.008715
44	1	0	4.918966	-0.274264	0.725198
45	6	0	4.275576	-2.793607	-1.920209
46	1	0	5.279783	-3.143910	-2.190738
47	1	0	3.568729	-3.576904	-2.219679
48	1	0	4.060048	-1.907115	-2.518760
49	6	0	4.748895	-4.221811	0.667490
50	1	0	4.878521	-4.209198	1.755847
51	1	0	4.046171	-5.026346	0.421964
52	1	0	5.720880	-4.486999	0.232108
53	6	0	-4.986266	0.228280	0.818357
54	6	0	-5.986268	0.820983	1.605720
55	6	0	-5.691712	1.417064	2.830205
56	6	0	-4.374180	1.437814	3.292739
57	6	0	-3.361823	0.858000	2.529973
58	6	0	-3.666471	0.256453	1.309440
59	6	0	-5.315030	-0.417471	-0.472996
60	6	0	-6.449714	-1.233334	-0.610200
61	6	0	-6.769326	-1.831691	-1.827126
62	6	0	-5.949134	-1.628596	-2.939921
63	6	0	-4.816695	-0.823638	-2.830591
64	6	0	-4.511498	-0.223496	-1.611334
65	1	0	-7.006485	0.826198	1.232096
66	1	0	-6.485404	1.873985	3.414578
67	1	0	-4.132635	1.907615	4.242374
68	1	0	-2.330405	0.860532	2.867132
69	1	0	-7.072539	-1.411353	0.262221
70	1	0	-7.649500	-2.463972	-1.903843
71	1	0	-6.187457	-2.098257	-3.890249
72	1	0	-4.158525	-0.642040	-3.673442
73	8	0	-2.658220	-0.402930	0.629090
74	8	0	-3.438934	0.651510	-1.555112
75	15	0	-2.052644	0.198625	-0.803057
76	8	0	-1.289676	1.472948	-0.527862
77	8	0	-1.387233	-0.969431	-1.473912

TS_{TMS}-Tc(R-ex)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2432.406690 hartree

Sum of electronic and thermal Free Energies = -2431.865032 hartree

The number of imaginary frequency = 1

Imaginary frequency = -333.25

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.395555	1.065561	-1.002188

2	1	0	5.387257	0.085530	-0.533971
3	1	0	6.318834	1.308789	-1.522307
4	6	0	4.623871	2.103197	-0.497920
5	1	0	4.895475	3.100174	-0.841582
6	6	0	3.415794	1.997028	0.254145
7	6	0	3.063288	0.735451	0.703542
8	1	0	3.790412	-0.071389	0.725071
9	1	0	1.000364	0.896677	1.049207
10	7	0	1.872201	0.360192	1.246515
11	6	0	1.745783	-0.894928	1.824869
12	8	0	0.467329	-1.099907	2.195762
13	8	0	2.651498	-1.694447	1.973243
14	1	0	0.664451	-1.039979	-1.410157
15	6	0	0.269891	-5.385240	0.445055
16	6	0	1.606126	-5.155669	0.171107
17	6	0	2.016795	-3.933765	-0.403835
18	6	0	1.035045	-2.947199	-0.680233
19	6	0	-0.326867	-3.181191	-0.399419
20	6	0	-0.693033	-4.394870	0.153368
21	1	0	4.140290	-4.365327	-0.534058
22	1	0	-0.041313	-6.328054	0.884853
23	1	0	2.356041	-5.910987	0.390982
24	6	0	3.370730	-3.625873	-0.739985
25	1	0	-1.055799	-2.404873	-0.604022
26	1	0	-1.740007	-4.582017	0.373946
27	6	0	2.702730	-1.435557	-1.557047
28	6	0	3.703977	-2.430130	-1.306129
29	1	0	4.734963	-2.205709	-1.551377
30	7	0	1.427722	-1.749373	-1.224412
31	6	0	2.946422	-0.149674	-2.113137
32	1	0	2.092597	0.520316	-2.148322
33	6	0	4.170074	0.281738	-2.610682
34	1	0	4.948693	-0.432255	-2.863632
35	1	0	4.184225	1.184810	-3.209809
36	14	0	2.450671	3.616317	0.581235
37	6	0	1.389136	4.072885	-0.908381
38	1	0	1.976922	4.072905	-1.834780
39	1	0	0.565784	3.360550	-1.007043
40	1	0	0.960555	5.075378	-0.784525
41	6	0	1.438868	3.499660	2.169701
42	1	0	0.510293	2.945408	2.014140
43	1	0	2.008680	3.022420	2.975886
44	1	0	1.175479	4.511111	2.503823
45	6	0	3.767690	4.962943	0.832183
46	1	0	4.332848	5.189201	-0.079574
47	1	0	3.274309	5.892247	1.143364
48	1	0	4.485564	4.690392	1.614782
49	6	0	0.217957	-2.340779	2.878238
50	1	0	0.623841	-2.294758	3.893648
51	1	0	-0.866889	-2.440693	2.902005
52	1	0	0.667705	-3.176843	2.342180
53	6	0	-4.543900	0.521406	-0.776391
54	6	0	-5.738702	0.045994	-1.339843
55	6	0	-5.974727	0.118554	-2.711166
56	6	0	-5.007083	0.669015	-3.555197
57	6	0	-3.812098	1.148915	-3.021859
58	6	0	-3.588725	1.080509	-1.648434
59	6	0	-4.303032	0.455289	0.683015
60	6	0	-5.303582	0.786915	1.610105
61	6	0	-5.061727	0.742205	2.982124
62	6	0	-3.798487	0.379299	3.456669
63	6	0	-2.788254	0.041473	2.557145
64	6	0	-3.051700	0.060680	1.189555
65	1	0	-6.480032	-0.403379	-0.684542
66	1	0	-6.906106	-0.262534	-3.120652
67	1	0	-5.179982	0.723183	-4.626536
68	1	0	-3.041314	1.587197	-3.646823
69	1	0	-6.272948	1.109017	1.239640
70	1	0	-5.850957	1.011486	3.678526
71	1	0	-3.596944	0.367607	4.524441
72	1	0	-1.788014	-0.219723	2.882672
73	8	0	-2.437532	1.661667	-1.142772
74	8	0	-2.075277	-0.383235	0.313567
75	15	0	-1.214409	0.730365	-0.560867
76	8	0	-0.558473	-0.055695	-1.670773
77	8	0	-0.396907	1.604295	0.349933

TS_{TMS}-Tc(S-ex)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2432.404134 hartree

Sum of electronic and thermal Free Energies = -2431.863214 hartree

The number of imaginary frequency = 1

Imaginary frequency = -323.82

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.278792	-1.806349	-0.724416
2	1	0	5.379625	-0.825137	-0.270058
3	1	0	6.185019	-2.186041	-1.189732
4	6	0	4.331639	-2.711142	-0.269818
5	1	0	4.472210	-3.740543	-0.595980
6	6	0	3.106907	-2.417724	0.400516
7	6	0	2.922109	-1.117936	0.845278
8	1	0	3.760740	-0.432221	0.935547
9	1	0	0.837055	-0.975860	1.027456
10	7	0	1.762396	-0.572108	1.293499
11	6	0	1.748186	0.698009	1.855832
12	8	0	0.474158	1.055703	2.089154
13	8	0	2.730126	1.377459	2.093024
14	1	0	0.957576	1.081817	-1.358512
15	6	0	1.310294	5.451600	0.401211
16	6	0	2.589895	4.953838	0.235950
17	6	0	2.791303	3.668507	-0.311527
18	6	0	1.657652	2.892657	-0.664445
19	6	0	0.354089	3.406513	-0.508811
20	6	0	0.195448	4.676198	0.015611
21	1	0	4.962231	3.674918	-0.294101
22	1	0	1.161125	6.442669	0.818979
23	1	0	3.456510	5.545625	0.518485
24	6	0	4.078020	3.100021	-0.556737
25	1	0	-0.489027	2.792652	-0.805191

26	1	0	-0.806165	5.080970	0.132068
27	6	0	3.050182	1.074474	-1.428108
28	6	0	4.206440	1.861590	-1.114168
29	1	0	5.187506	1.441026	-1.297350
30	7	0	1.841242	1.628799	-1.172518
31	6	0	3.089199	-0.240616	-1.968157
32	1	0	2.137547	-0.759334	-2.033958
33	6	0	4.240720	-0.875736	-2.413463
34	1	0	5.136780	-0.306824	-2.642873
35	1	0	4.130202	-1.785715	-2.991438
36	14	0	1.864273	-3.856713	0.609872
37	6	0	0.827402	-4.074773	-0.952289
38	1	0	0.161430	-3.215849	-1.073701
39	1	0	1.457899	-4.170901	-1.844969
40	1	0	0.211009	-4.980134	-0.880176
41	6	0	2.908298	-5.421827	0.873663
42	1	0	3.619657	-5.303349	1.699469
43	1	0	2.243002	-6.256905	1.126292
44	1	0	3.472721	-5.719357	-0.017858
45	6	0	0.785510	-3.614284	2.138589
46	1	0	1.372613	-3.260735	2.994419
47	1	0	-0.025820	-2.907145	1.949456
48	1	0	0.336096	-4.575260	2.419157
49	6	0	0.284757	2.301373	2.774816
50	1	0	0.858403	3.099626	2.301174
51	1	0	-0.784795	2.499516	2.705923
52	1	0	0.590084	2.202840	3.821360
53	6	0	-4.503947	0.610808	-0.189820
54	6	0	-5.624264	1.414203	-0.457641
55	6	0	-5.568901	2.803096	-0.359443
56	6	0	-4.376702	3.424343	0.018612
57	6	0	-3.248332	2.650928	0.284091
58	6	0	-3.306704	1.261496	0.170655
59	6	0	-4.596624	-0.866733	-0.240655
60	6	0	-5.706351	-1.542213	0.293160
61	6	0	-5.797381	-2.931908	0.252268
62	6	0	-4.767079	-3.681545	-0.321436
63	6	0	-3.655011	-3.035865	-0.858427
64	6	0	-3.580569	-1.645321	-0.822515
65	1	0	-6.548538	0.930274	-0.760952
66	1	0	-6.451493	3.396937	-0.579491
67	1	0	-4.324645	4.506339	0.106630
68	1	0	-2.313020	3.100059	0.601367
69	1	0	-6.493105	-0.961252	0.766545
70	1	0	-6.663738	-3.429254	0.679316
71	1	0	-4.826828	-4.766130	-0.347633
72	1	0	-2.836276	-3.584092	-1.312520
73	8	0	-2.191802	0.536971	0.535623
74	8	0	-2.516426	-1.023824	-1.451321
75	15	0	-1.315488	-0.354946	-0.551605
76	8	0	-0.555254	0.538769	-1.500876
77	8	0	-0.599106	-1.400826	0.258342

TS$_{TMS}$-Tt(R-ex)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2432.403020 hartree

Sum of electronic and thermal Free Energies = -2431.861293 hartree

The number of imaginary frequency = 1

Imaginary frequency = -333.58

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.122851	1.446180	1.158901
2	1	0	-5.181124	0.431747	0.774536
3	1	0	-6.006861	1.773286	1.701005
4	6	0	-4.337931	2.404597	0.531629
5	1	0	-4.547655	3.436007	0.810519
6	6	0	-3.181823	2.187922	-0.274952
7	6	0	-2.909725	0.885499	-0.663217
8	1	0	-3.673509	0.118597	-0.588341
9	1	0	-0.860243	0.966787	-1.100855
10	7	0	-1.754973	0.442654	-1.235773
11	6	0	-1.583150	-0.797793	-1.826278
12	8	0	-2.728332	-1.519921	-1.852104
13	8	0	-0.522868	-1.187130	-2.273052
14	1	0	-0.603305	-0.925384	1.335758
15	6	0	-0.765145	-5.401599	-0.297421
16	6	0	-2.014155	-5.075574	0.199143
17	6	0	-2.257152	-3.789298	0.726874
18	6	0	-1.194824	-2.846027	0.748787
19	6	0	0.074410	-3.177258	0.232202
20	6	0	0.273486	-4.445687	-0.282831
21	1	0	-4.354395	-4.066141	1.216707
22	1	0	-0.582368	-6.391143	-0.705487
23	1	0	-2.824934	-5.799602	0.184727
24	6	0	-3.525071	-3.362960	1.228999
25	1	0	0.863799	-2.432829	0.225282
26	1	0	1.246681	-4.703597	-0.689710
27	6	0	-2.618543	-1.164086	1.740132
28	6	0	-3.705761	-2.099359	1.710985
29	1	0	-4.674477	-1.785654	2.080376
30	7	0	-1.424368	-1.593370	1.262001
31	6	0	-2.704990	0.170966	2.218720
32	1	0	-1.802025	0.766423	2.128973
33	6	0	-3.850195	0.741938	2.761381
34	1	0	-4.659928	0.122346	3.136320
35	1	0	-3.750810	1.694439	3.269191
36	14	0	-2.161872	3.736395	-0.756280
37	6	0	-1.243037	3.474780	-2.382920
38	1	0	-0.331061	2.890319	-2.239917
39	1	0	-1.873211	2.974322	-3.127721
40	1	0	-0.956280	4.450922	-2.794006
41	6	0	-1.001627	4.230207	0.644575
42	1	0	-1.532687	4.298172	1.602115
43	1	0	-0.197291	3.495366	0.733695
44	1	0	-0.549081	5.209254	0.442837
45	6	0	-3.430116	5.126171	-1.024083
46	1	0	-3.927900	5.441098	-0.099471
47	1	0	-2.913975	6.006627	-1.426834
48	1	0	-4.205680	4.838658	-1.743773
49	6	0	-2.623385	-2.779271	-2.539278

50	1	0	-1.813281	-3.380810	-2.124953
51	1	0	-3.584529	-3.270678	-2.385584
52	1	0	-2.443756	-2.612223	-3.605221
53	6	0	4.363026	0.110015	-0.746756
54	6	0	5.365967	0.264803	-1.717316
55	6	0	5.103453	0.042293	-3.067828
56	6	0	3.821568	-0.334558	-3.478678
57	6	0	2.805661	-0.495492	-2.537450
58	6	0	3.087988	-0.281173	-1.191110
59	6	0	4.635943	0.326580	0.693153
60	6	0	5.816549	-0.154349	1.282564
61	6	0	6.090166	0.043745	2.634274
62	6	0	5.173765	0.728847	3.435525
63	6	0	3.993663	1.216392	2.877089
64	6	0	3.732788	1.021440	1.522205
65	1	0	6.354966	0.585261	-1.401203
66	1	0	5.894894	0.176772	-3.800130
67	1	0	3.610633	-0.497233	-4.532272
68	1	0	1.795092	-0.779616	-2.809652
69	1	0	6.516320	-0.709496	0.663794
70	1	0	7.009829	-0.345086	3.062627
71	1	0	5.374769	0.882395	4.492268
72	1	0	3.262971	1.759231	3.467347
73	8	0	2.096035	-0.534050	-0.255606
74	8	0	2.604932	1.620583	0.987917
75	15	0	1.323735	0.737718	0.463413
76	8	0	0.608477	1.593231	-0.547100
77	8	0	0.563289	0.121515	1.614702

TS$_{TMS}$-Tt(S-ex)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2432.398798 hartree

Sum of electronic and thermal Free Energies = -2431.858825 hartree

The number of imaginary frequency = 1

Imaginary frequency = -323.82

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.255857	-2.923765	1.426530
2	1	0	-4.715317	-2.022258	1.031498
3	1	0	-4.906515	-3.523149	2.058647
4	6	0	-3.215969	-3.552505	0.757003
5	1	0	-2.999679	-4.569214	1.081293
6	6	0	-2.288251	-2.966556	-0.154550
7	6	0	-2.562963	-1.685147	-0.609039
8	1	0	-3.559737	-1.269497	-0.501102
9	1	0	-0.670020	-0.993432	-1.190706
10	7	0	-1.705566	-0.863540	-1.272770
11	6	0	-2.057996	0.327314	-1.889886
12	8	0	-3.399280	0.526358	-1.892478
13	8	0	-1.250318	1.094065	-2.370642
14	1	0	-1.000791	1.014818	1.039886
15	6	0	-3.020705	4.982810	-0.580106
16	6	0	-4.000778	4.230817	0.041970
17	6	0	-3.683471	2.978090	0.610024
18	6	0	-2.343509	2.514351	0.534977
19	6	0	-1.347776	3.279761	-0.105569
20	6	0	-1.695462	4.500577	-0.653395
21	1	0	-5.669880	2.455683	1.315190
22	1	0	-3.268897	5.944983	-1.017904
23	1	0	-5.025142	4.590103	0.098520
24	6	0	-4.635546	2.126719	1.250391
25	1	0	-0.339176	2.885245	-0.162034
26	1	0	-0.936579	5.093606	-1.155136
27	6	0	-2.905422	0.475069	1.697442
28	6	0	-4.266688	0.920864	1.772844
29	1	0	-4.999361	0.283199	2.252169
30	7	0	-2.023881	1.296157	1.078945
31	6	0	-2.422363	-0.759483	2.209873
32	1	0	-1.372835	-0.970282	2.030350
33	6	0	-3.197667	-1.691062	2.886807
34	1	0	-4.147731	-1.411411	3.332408
35	1	0	-2.692501	-2.506184	3.391689
36	14	0	-0.786460	-4.039545	-0.660773
37	6	0	0.555129	-3.966197	0.664749
38	1	0	0.973085	-2.957817	0.713008
39	1	0	0.162288	-4.239929	1.651761
40	1	0	1.368338	-4.662766	0.423277
41	6	0	-0.135875	-3.561547	-2.364391
42	1	0	-0.954200	-3.392469	-3.074343
43	1	0	0.485971	-2.664583	-2.320733
44	1	0	0.479149	-4.380971	-2.757415
45	6	0	-1.432251	-5.823596	-0.767562
46	1	0	-0.640275	-6.465293	-1.173614
47	1	0	-1.716429	-6.240948	0.205498
48	1	0	-2.298205	-5.904147	-1.435164
49	6	0	-3.826003	1.697495	-2.609640
50	1	0	-4.899843	1.767424	-2.432779
51	1	0	-3.316479	2.588276	-2.239928
52	1	0	-3.620364	1.580195	-3.677553
53	6	0	4.814782	0.022145	0.184482
54	6	0	6.072504	-0.433497	-0.242816
55	6	0	6.386415	-1.790799	-0.258660
56	6	0	5.436478	-2.729121	0.152224
57	6	0	4.180095	-2.304084	0.580029
58	6	0	3.877949	-0.943799	0.597101
59	6	0	4.495380	1.468054	0.210638
60	6	0	5.429144	2.409252	0.673304
61	6	0	5.146692	3.773688	0.676384
62	6	0	3.909870	4.228812	0.213223
63	6	0	2.964823	3.315120	-0.249330
64	6	0	3.255816	1.952109	-0.248805
65	1	0	6.801365	0.295616	-0.585966
66	1	0	7.364944	-2.115476	-0.601321
67	1	0	5.670810	-3.790083	0.137137
68	1	0	3.421182	-3.005363	0.909640
69	1	0	6.383046	2.052547	1.051959
70	1	0	5.886137	4.478250	1.046661
71	1	0	3.680487	5.290983	0.213287
72	1	0	2.000459	3.635620	-0.630182
73	8	0	2.660950	-0.547444	1.123044

74	8	0	2.333730	1.084397	-0.802772
75	15	0	1.474934	0.048031	0.147273
76	8	0	0.940031	-1.025463	-0.760123
77	8	0	0.550152	0.805868	1.069600

(R=SPh)

TS$_{SPh}$-Cc(R-en)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2652.956697 hartree

Sum of electronic and thermal Free Energies = -2652.435587 hartree

The number of imaginary frequency = 1

Imaginary frequency = -362.51

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.402358	-1.911053	3.114362
2	1	0	1.153596	-1.717993	2.356099
3	1	0	0.789827	-2.397846	4.006310
4	6	0	-0.914503	-2.193444	2.762455
5	1	0	-1.528468	-2.695829	3.508008
6	6	0	-0.898586	-1.104826	0.585998
7	1	0	0.182116	-1.184936	0.612137
8	1	0	-0.545995	-0.378206	-1.265034
9	7	0	-1.305978	-0.503923	-0.560401
10	6	0	-2.521576	0.110111	-0.831214
11	8	0	-2.594128	0.355735	-2.153072
12	8	0	-3.364314	0.423351	-0.015816
13	1	0	0.142149	2.128277	0.365372
14	6	0	-3.798548	4.557592	-0.712457
15	6	0	-3.983613	3.949169	0.516913
16	6	0	-2.963494	3.160063	1.085690
17	6	0	-1.745503	3.010607	0.374861
18	6	0	-1.558584	3.624641	-0.878831
19	6	0	-2.582171	4.390660	-1.408618
20	1	0	-4.014736	2.565490	2.890552
21	1	0	-4.589583	5.162297	-1.145792
22	1	0	-4.920715	4.062897	1.055549
23	6	0	-3.085689	2.473733	2.334408
24	1	0	-0.619418	3.475956	-1.403678
25	1	0	-2.446733	4.866557	-2.375651
26	6	0	-0.841651	1.573628	2.093377
27	6	0	-2.071048	1.704566	2.819252
28	1	0	-2.176667	1.181424	3.761426
29	7	0	-0.749566	2.237165	0.912401
30	6	0	0.311714	0.871720	2.532503
31	1	0	1.189672	0.958943	1.900187
32	6	0	0.415103	0.098239	3.686147
33	1	0	-0.382653	0.092328	4.423031
34	1	0	1.406237	-0.036981	4.109386
35	6	0	5.212043	0.144971	-0.361130
36	6	0	6.418153	0.541890	0.238243
37	6	0	6.925942	1.827351	0.062325
38	6	0	6.227784	2.750929	-0.719961
39	6	0	5.028094	2.382128	-1.325937
40	6	0	4.533799	1.091814	-1.150841
41	6	0	4.681859	-1.226551	-0.190065
42	6	0	5.526442	-2.345350	-0.263429
43	6	0	5.034682	-3.639921	-0.107367
44	6	0	3.670914	-3.842436	0.113616
45	6	0	2.810575	-2.748100	0.189975
46	6	0	3.313697	-1.454615	0.053718
47	1	0	6.947851	-0.169972	0.865536
48	1	0	7.858371	2.110733	0.542520
49	1	0	6.613993	3.757325	-0.856086
50	1	0	4.461215	3.071826	-1.941950
51	1	0	6.581482	-2.187545	-0.469416
52	1	0	5.710692	-4.487521	-0.175395
53	1	0	3.274426	-4.848392	0.220076
54	1	0	1.746177	-2.883946	0.350215
55	8	0	3.391984	0.720381	-1.842149
56	8	0	2.460737	-0.383444	0.254643
57	15	0	1.968470	0.567421	-1.039662
58	8	0	1.553695	1.878653	-0.417673
59	8	0	1.030825	-0.220792	-1.905405
60	6	0	-3.797064	1.017868	-2.571406
61	1	0	-3.918928	1.967981	-2.045149
62	1	0	-3.675011	1.183057	-3.642298
63	1	0	-4.661887	0.376993	-2.377822
64	6	0	-1.600321	-1.758485	1.596354
65	16	0	-3.352445	-2.121663	1.603535
66	6	0	-3.685018	-2.639523	-0.078903
67	6	0	-2.796583	-3.438076	-0.808711
68	6	0	-4.897906	-2.242108	-0.656927
69	6	0	-3.113613	-3.820186	-2.111775
70	1	0	-1.853983	-3.742148	-0.364307
71	6	0	-5.220631	-2.652827	-1.950672
72	1	0	-5.566422	-1.589789	-0.104113
73	6	0	-4.327091	-3.434999	-2.685456
74	1	0	-2.409305	-4.423539	-2.677869
75	1	0	-6.165266	-2.343691	-2.390788
76	1	0	-4.571359	-3.737312	-3.699904

TS$_{SPh}$-Cc(S-en)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2652.955644 hartree

Sum of electronic and thermal Free Energies = -2652.435186 hartree

The number of imaginary frequency = 1

Imaginary frequency = -351.66

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.156130	-0.089761	3.816338
2	1	0	0.940357	0.184836	3.117726
3	1	0	0.496185	-0.216656	4.841242
4	6	0	-1.153946	0.331424	3.624449
5	1	0	-1.815338	0.305988	4.488834
6	6	0	-1.000605	0.687477	1.226732
7	1	0	0.073909	0.768529	1.355396

8	1	0	-0.494479	1.104606	-0.661286
9	7	0	-1.319664	0.842327	-0.081890
10	6	0	-2.493967	0.513601	-0.743893
11	8	0	-2.456933	1.053925	-1.977888
12	8	0	-3.392342	-0.180533	-0.315062
13	1	0	0.032284	-1.902434	-0.800064
14	6	0	-3.853405	-3.243344	-3.170318
15	6	0	-4.093119	-3.407749	-1.817420
16	6	0	-3.098671	-3.087107	-0.870756
17	6	0	-1.852167	-2.597808	-1.337367
18	6	0	-1.607732	-2.427360	-2.713986
19	6	0	-2.606629	-2.752252	-3.614721
20	1	0	-4.224502	-3.565980	0.923184
21	1	0	-4.624380	-3.490649	-3.893933
22	1	0	-5.052767	-3.777365	-1.465810
23	6	0	-3.273042	-3.203689	0.543322
24	1	0	-0.644502	-2.040067	-3.033343
25	1	0	-2.427989	-2.624464	-4.678559
26	6	0	-1.024224	-2.368208	0.918390
27	6	0	-2.278657	-2.855613	1.408378
28	1	0	-2.423036	-2.935486	2.478646
29	7	0	-0.881915	-2.268068	-0.426993
30	6	0	0.109418	-2.038960	1.709143
31	1	0	0.991626	-1.743755	1.152898
32	6	0	0.195240	-2.079520	3.096169
33	1	0	-0.606880	-2.507228	3.689956
34	1	0	1.181171	-2.192624	3.537517
35	6	0	-3.619048	0.788055	-2.778426
36	1	0	-4.500821	1.240787	-2.316095
37	1	0	-3.412945	1.250044	-3.744434
38	1	0	-3.774858	-0.287870	-2.890090
39	6	0	5.141000	-0.210968	0.296214
40	6	0	6.334704	-0.864812	0.641923
41	6	0	6.335440	-2.028418	1.407782
42	6	0	5.124516	-2.572164	1.840227
43	6	0	3.925126	-1.944262	1.509416
44	6	0	3.931165	-0.773878	0.750007
45	6	0	5.166857	1.031430	-0.508626
46	6	0	6.111318	2.041093	-0.261801
47	6	0	6.150081	3.200381	-1.033413
48	6	0	5.233350	3.376603	-2.073229
49	6	0	4.285048	2.390293	-2.337743
50	6	0	4.261338	1.231760	-1.565254
51	1	0	7.273496	-0.454508	0.280425
52	1	0	7.275098	-2.514931	1.653557
53	1	0	5.110590	-3.485207	2.429255
54	1	0	2.974165	-2.354509	1.830561
55	1	0	6.807737	1.914378	0.562578
56	1	0	6.886582	3.969187	-0.816968
57	1	0	5.252842	4.281608	-2.674146
58	1	0	3.557443	2.493177	-3.135504
59	8	0	2.730182	-0.120050	0.541283
60	8	0	3.370829	0.224991	-1.903148
61	15	0	2.034853	0.003460	-0.975367
62	8	0	1.452337	-1.330606	-1.372321
63	8	0	1.183550	1.240355	-0.918283
64	6	0	-1.774588	0.638784	2.383397
65	16	0	-3.539476	0.907915	2.491130
66	6	0	-3.821931	2.306852	1.408227
67	6	0	-5.000032	2.316733	0.649619
68	6	0	-2.930206	3.382284	1.320141
69	6	0	-5.285985	3.401757	-0.179277
70	1	0	-5.669568	1.463343	0.688236
71	6	0	-3.209834	4.449965	0.467374
72	1	0	-2.014467	3.374388	1.902907
73	6	0	-4.389006	4.467597	-0.280178
74	1	0	-6.204110	3.403729	-0.761259
75	1	0	-2.503109	5.271841	0.391923
76	1	0	-4.604455	5.303004	-0.940436

TS_{SPh}-Ct(R-en)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2652.952557 hartree

Sum of electronic and thermal Free Energies = -2652.430757 hartree

The number of imaginary frequency = 1

Imaginary frequency = -374.96

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.097473	-2.888111	1.721025
2	1	0	0.999478	-2.462803	1.293001
3	1	0	0.283798	-3.648208	2.476062
4	6	0	-1.045406	-3.048480	0.938252
5	1	0	-1.775289	-3.787632	1.262130
6	6	0	-0.605779	-1.235266	-0.637719
7	1	0	0.430201	-1.252219	-0.314568
8	1	0	0.063097	0.125176	-1.968557
9	7	0	-0.814150	-0.262013	-1.555438
10	6	0	-1.980999	0.403321	-1.938448
11	8	0	-2.961246	0.264888	-1.029167
12	8	0	-2.042472	1.087349	-2.935162
13	1	0	0.267842	1.820453	0.454656
14	6	0	-3.367843	4.721660	-0.533723
15	6	0	-3.779182	3.827194	0.438169
16	6	0	-2.900154	2.828023	0.906685
17	6	0	-1.585581	2.773875	0.374367
18	6	0	-1.168669	3.685762	-0.615040
19	6	0	-2.060891	4.643676	-1.060988
20	1	0	-4.251143	1.871062	2.313524
21	1	0	-4.051007	5.483071	-0.897512
22	1	0	-4.786168	3.873509	0.845076
23	6	0	-3.253193	1.846523	1.883676
24	1	0	-0.161541	3.607705	-1.013324
25	1	0	-1.751001	5.341797	-1.832680
26	6	0	-1.042557	0.844370	1.722483
27	6	0	-2.365051	0.888648	2.273564
28	1	0	-2.636096	0.163354	3.030210
29	7	0	-0.723825	1.803744	0.817494
30	6	0	-0.018652	-0.061952	2.106176
31	1	0	0.978209	0.169570	1.743108
32	6	0	-0.172517	-1.194320	2.906535

33	1	0	-1.130138	-1.414940	3.370960
34	1	0	0.682791	-1.511122	3.496121
35	6	0	-4.230794	0.817810	-1.419175
36	1	0	-4.130374	1.883133	-1.633821
37	1	0	-4.609000	0.295336	-2.301466
38	1	0	-4.887793	0.644794	-0.567869
39	6	0	4.957204	-1.268253	-0.125232
40	6	0	5.838181	-2.326537	-0.397974
41	6	0	5.372035	-3.571702	-0.815573
42	6	0	4.001525	-3.779950	-0.983224
43	6	0	3.105177	-2.745077	-0.719903
44	6	0	3.578926	-1.508697	-0.282893
45	6	0	5.459928	0.052421	0.316124
46	6	0	6.488185	0.161190	1.266146
47	6	0	6.973528	1.403178	1.669961
48	6	0	6.430988	2.572082	1.129967
49	6	0	5.409453	2.491968	0.185225
50	6	0	4.937858	1.245076	-0.217807
51	1	0	6.906115	-2.152473	-0.299955
52	1	0	6.077354	-4.370515	-1.026351
53	1	0	3.628904	-4.741417	-1.325322
54	1	0	2.037609	-2.881982	-0.856225
55	1	0	6.893009	-0.747891	1.702602
56	1	0	7.765859	1.458962	2.411177
57	1	0	6.799690	3.544411	1.444756
58	1	0	4.967373	3.377905	-0.257693
59	8	0	2.663916	-0.536449	0.085771
60	8	0	3.991853	1.191745	-1.229701
61	15	0	2.435078	0.823390	-0.873335
62	8	0	1.740916	0.428946	-2.142258
63	8	0	1.830097	1.845958	0.059637
64	6	0	-1.434472	-2.254308	-0.171345
65	16	0	-2.879821	-2.777766	-1.096177
66	6	0	-4.299733	-2.233477	-0.153965
67	6	0	-5.555213	-2.357073	-0.767360
68	6	0	-4.214603	-1.697445	1.133643
69	6	0	-6.704362	-1.937061	-0.099007
70	1	0	-5.631460	-2.767260	-1.771208
71	6	0	-5.368015	-1.271481	1.792723
72	1	0	-3.246289	-1.591604	1.604533
73	6	0	-6.618482	-1.385955	1.182441
74	1	0	-7.670515	-2.033736	-0.587130
75	1	0	-5.286051	-0.849413	2.791867
76	1	0	-7.515039	-1.054996	1.698680

TS_{SPh}-Ct(S-en)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2652.951717 hartree

Sum of electronic and thermal Free Energies = -2652.430539 hartree

The number of imaginary frequency = 1

Imaginary frequency = -344.06

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.122091	0.418773	3.814990
2	1	0	0.691202	0.727416	3.165955
3	1	0	0.137100	0.387347	4.870255
4	6	0	-1.444394	0.688573	3.487730
5	1	0	-2.171018	0.650529	4.297359
6	6	0	-1.121212	0.895589	1.092828
7	1	0	-0.074132	1.060672	1.325948
8	1	0	-0.388842	1.220015	-0.725022
9	7	0	-1.276818	0.951019	-0.251560
10	6	0	-2.299352	0.609223	-1.134250
11	8	0	-3.255361	-0.134837	-0.557985
12	8	0	-2.263934	0.916013	-2.306337
13	1	0	0.130573	-1.722196	-0.671676
14	6	0	-3.480372	-3.738288	-3.006467
15	6	0	-3.741401	-3.824480	-1.650320
16	6	0	-2.839714	-3.277435	-0.713401
17	6	0	-1.655439	-2.658362	-1.191387
18	6	0	-1.398220	-2.556545	-2.572502
19	6	0	-2.309883	-3.095228	-3.463303
20	1	0	-3.966155	-3.727991	1.089014
21	1	0	-4.179603	-4.157900	-3.723385
22	1	0	-4.647358	-4.304751	-1.289195
23	6	0	-3.054376	-3.281270	0.700547
24	1	0	-0.493743	-2.055256	-2.903834
25	1	0	-2.120689	-3.018703	-4.529844
26	6	0	-0.927323	-2.162088	1.055762
27	6	0	-2.142498	-2.735404	1.554865
28	1	0	-2.315517	-2.738940	2.623837
29	7	0	-0.759395	-2.143770	-0.289712
30	6	0	0.144214	-1.673512	1.850845
31	1	0	1.020033	-1.341131	1.306426
32	6	0	0.178162	-1.605827	3.238566
33	1	0	-0.596852	-2.071445	3.839472
34	1	0	1.153110	-1.575244	3.715890
35	6	0	-4.383206	-0.412490	-1.405441
36	1	0	-4.863666	0.522548	-1.702620
37	1	0	-4.065616	-0.968119	-2.289327
38	1	0	-5.054883	-1.013721	-0.793209
39	6	0	5.259321	-0.240777	0.304738
40	6	0	6.417157	-0.984552	0.583655
41	6	0	6.364228	-2.171462	1.311327
42	6	0	5.135230	-2.646790	1.773201
43	6	0	3.970104	-1.929043	1.508619
44	6	0	4.031970	-0.737444	0.786292
45	6	0	5.336432	1.027585	-0.455423
46	6	0	6.352151	1.964950	-0.206617
47	6	0	6.436528	3.151415	-0.931980
48	6	0	5.494505	3.429032	-1.925949
49	6	0	4.475845	2.515929	-2.192027
50	6	0	4.406489	1.329182	-1.466439
51	1	0	7.368708	-0.626159	0.200900
52	1	0	7.276326	-2.728641	1.505657
53	1	0	5.080813	-3.575991	2.333961
54	1	0	3.003985	-2.280721	1.855019
55	1	0	7.069185	1.759986	0.583657
56	1	0	7.228562	3.862573	-0.714513
57	1	0	5.549399	4.355754	-2.490443

58	1	0	3.727972	2.697322	-2.956417
59	8	0	2.873040	0.003587	0.638430
60	8	0	3.444376	0.394678	-1.814706
61	15	0	2.135099	0.185227	-0.848477
62	8	0	1.506783	-1.122957	-1.263187
63	8	0	1.310277	1.435893	-0.725142
64	6	0	-1.989166	0.850610	2.182844
65	16	0	-3.775532	0.933144	2.161746
66	6	0	-4.162353	2.263852	1.030680
67	6	0	-5.432502	2.238985	0.436056
68	6	0	-3.288490	3.320546	0.748426
69	6	0	-5.819365	3.259493	-0.431878
70	1	0	-6.111469	1.416686	0.646117
71	6	0	-3.675565	4.324006	-0.140274
72	1	0	-2.309274	3.357070	1.213161
73	6	0	-4.939074	4.301000	-0.732364
74	1	0	-6.806643	3.230216	-0.885424
75	1	0	-2.981591	5.128874	-0.366062
76	1	0	-5.233888	5.084937	-1.423798

TS$_{SPh}$-Tc(R-ex)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2652.966873 hartree

Sum of electronic and thermal Free Energies = -2652.445841 hartree

The number of imaginary frequency = 1

Imaginary frequency = -356.49

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.498796	-0.264619	0.181387
2	1	0	5.218478	-1.312007	0.251807
3	1	0	6.530839	-0.098770	-0.118338
4	6	0	4.899315	0.680638	1.008108
5	1	0	5.390807	1.646500	1.102583
6	6	0	2.878223	-0.586312	1.467143
7	1	0	3.407840	-1.507666	1.250463
8	1	0	0.873755	-0.000376	1.768861
9	7	0	1.565859	-0.787265	1.736408
10	6	0	1.078622	-2.092819	1.739596
11	8	0	-0.252414	-2.088248	1.910279
12	8	0	1.764793	-3.088945	1.599859
13	1	0	0.583090	-0.785425	-1.298731
14	6	0	-1.007195	-5.244370	-1.461123
15	6	0	0.374359	-5.279964	-1.518492
16	6	0	1.120063	-4.081674	-1.511372
17	6	0	0.425629	-2.846557	-1.429808
18	6	0	-0.982702	-2.811378	-1.375083
19	6	0	-1.680219	-4.005466	-1.394911
20	1	0	3.097720	-4.965417	-1.655991
21	1	0	-1.576453	-6.169053	-1.468992
22	1	0	0.903953	-6.227495	-1.573119
23	6	0	2.545247	-4.031360	-1.594277
24	1	0	-1.491252	-1.857416	-1.300222
25	1	0	-2.765282	-3.984506	-1.349905
26	6	0	2.495622	-1.601992	-1.490149
27	6	0	3.209950	-2.840437	-1.599144
28	1	0	4.291053	-2.813505	-1.663425
29	7	0	1.144281	-1.675717	-1.400836
30	6	0	3.097332	-0.317411	-1.457844
31	1	0	2.427714	0.519830	-1.296459
32	6	0	4.457143	-0.057318	-1.637635
33	1	0	5.095412	-0.791773	-2.122364
34	1	0	4.738733	0.970925	-1.836974
35	6	0	-0.867697	-3.386999	1.984835
36	1	0	-0.689333	-3.823035	2.972724
37	1	0	-1.930821	-3.209720	1.828057
38	1	0	-0.472750	-4.049240	1.214276
39	6	0	-4.355567	1.431409	-0.657835
40	6	0	-5.432075	1.475216	-1.557764
41	6	0	-5.330394	2.137325	-2.779649
42	6	0	-4.135539	2.771005	-3.130204
43	6	0	-3.051593	2.742892	-2.254491
44	6	0	-3.164938	2.086137	-1.030956
45	6	0	-4.468708	0.745968	0.649295
46	6	0	-5.610022	0.881643	1.455037
47	6	0	-5.694123	0.261297	2.700455
48	6	0	-4.620233	-0.495148	3.176811
49	6	0	-3.477110	-0.649556	2.393717
50	6	0	-3.419469	-0.055178	1.135289
51	1	0	-6.353181	0.962999	-1.292783
52	1	0	-6.177469	2.150730	-3.459854
53	1	0	-4.046101	3.284310	-4.083734
54	1	0	-2.111098	3.229139	-2.491264
55	1	0	-6.425608	1.507987	1.104032
56	1	0	-6.585487	0.388942	3.308328
57	1	0	-4.667769	-0.956021	4.159725
58	1	0	-2.611654	-1.202003	2.740686
59	8	0	-2.105742	2.163159	-0.143597
60	8	0	-2.330973	-0.316447	0.320343
61	15	0	-1.159391	0.844112	0.134897
62	8	0	-0.411678	0.463543	-1.125071
63	8	0	-0.413248	1.084346	1.412930
64	6	0	3.590179	0.600017	1.542235
65	16	0	2.855714	2.081117	2.248084
66	6	0	2.859719	3.145211	0.792626
67	6	0	3.783820	4.191343	0.691707
68	6	0	1.939144	2.920260	-0.238486
69	6	0	3.795790	4.999746	-0.448243
70	1	0	4.488255	4.367654	1.499551
71	6	0	1.968604	3.719460	-1.380823
72	1	0	1.206261	2.130834	-0.140488
73	6	0	2.895634	4.760069	-1.488441
74	1	0	4.513502	5.812569	-0.523796
75	1	0	1.253938	3.529813	-2.177202
76	1	0	2.911836	5.386803	-2.376245

TS$_{SPh}$-Tc(S-ex)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2652.965521 hartree

Sum of electronic and thermal Free Energies = -2652.445256

hartree
The number of imaginary frequency = 1
Imaginary frequency = -350.96

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.794843	3.654420	-0.415986
2	1	0	-4.488324	2.881790	-0.096938
3	1	0	-4.269953	4.516280	-0.878171
4	6	0	-2.599783	3.856187	0.267809
5	1	0	-2.077149	4.793520	0.091420
6	6	0	-2.470405	1.640544	1.251335
7	1	0	-3.543232	1.536716	1.134077
8	1	0	-0.851959	0.391478	1.820828
9	7	0	-1.892015	0.533669	1.770945
10	6	0	-2.698694	-0.556585	2.094773
11	8	0	-1.941007	-1.565388	2.543870
12	8	0	-3.911186	-0.583587	1.980984
13	1	0	-1.238419	-0.665547	-0.942350
14	6	0	-3.461915	-4.786035	-0.131312
15	6	0	-4.412992	-3.842464	-0.477831
16	6	0	-4.029587	-2.518078	-0.779039
17	6	0	-2.653640	-2.177554	-0.717210
18	6	0	-1.687024	-3.136385	-0.349732
19	6	0	-2.098438	-4.426254	-0.067091
20	1	0	-6.006025	-1.720539	-1.196547
21	1	0	-3.762962	-5.803896	0.097448
22	1	0	-5.466176	-4.107263	-0.522755
23	6	0	-4.945840	-1.485114	-1.152177
24	1	0	-0.643865	-2.846220	-0.281418
25	1	0	-1.358510	-5.168796	0.217344
26	6	0	-3.115412	0.098401	-1.385747
27	6	0	-4.510780	-0.227106	-1.448717
28	1	0	-5.213958	0.546937	-1.732113
29	7	0	-2.270009	-0.894141	-1.009666
30	6	0	-2.543881	1.359729	-1.693214
31	1	0	-1.466009	1.420593	-1.591336
32	6	0	-3.234552	2.498759	-2.104558
33	1	0	-4.259135	2.424897	-2.460437
34	1	0	-2.656685	3.283911	-2.579430
35	6	0	-2.669482	-2.725196	2.977783
36	1	0	-3.317567	-3.096336	2.181964
37	1	0	-1.906766	-3.462587	3.226652
38	1	0	-3.273712	-2.483485	3.857304
39	6	0	4.033794	-2.022696	-0.612331
40	6	0	4.931347	-2.572991	-1.541634
41	6	0	4.522576	-3.518558	-2.479775
42	6	0	3.189010	-3.931983	-2.512431
43	6	0	2.276897	-3.400845	-1.602437
44	6	0	2.695823	-2.461933	-0.660716
45	6	0	4.488869	-1.023585	0.382103
46	6	0	5.708736	-1.170604	1.061876
47	6	0	6.145739	-0.216658	1.978766
48	6	0	5.362647	0.911032	2.239946
49	6	0	4.146955	1.080496	1.579950
50	6	0	3.724587	0.123733	0.660557
51	1	0	5.962434	-2.230523	-1.532130
52	1	0	5.239348	-3.921453	-3.189828
53	1	0	2.857674	-4.662861	-3.245107
54	1	0	1.235600	-3.706760	-1.601966
55	1	0	6.306016	-2.059252	0.876729
56	1	0	7.090228	-0.358466	2.496682
57	1	0	5.694680	1.654595	2.959246
58	1	0	3.511866	1.942706	1.753828
59	8	0	1.784975	-2.044369	0.292830
60	8	0	2.561451	0.358190	-0.051872
61	15	0	1.200632	-0.492769	0.309553
62	8	0	0.295959	-0.275773	-0.886260
63	8	0	0.708571	-0.236871	1.701328
64	6	0	-1.878701	2.863351	0.974632
65	16	0	-0.187243	3.182877	1.492508
66	6	0	0.518320	3.887504	-0.007304
67	6	0	0.753045	5.266990	-0.071468
68	6	0	0.862555	3.064650	-1.088563
69	6	0	1.316554	5.825560	-1.221028
70	1	0	0.493523	5.895275	0.775715
71	6	0	1.414194	3.633757	-2.236992
72	1	0	0.719311	1.991923	-1.029702
73	6	0	1.641304	5.010728	-2.307057
74	1	0	1.497767	6.896265	-1.266659
75	1	0	1.682059	2.990889	-3.071030
76	1	0	2.078505	5.446119	-3.201788

TS$_{SPh}$-Tt(R-ex)
B3LYP-D3/6-31g(d) in gas phase
SCF Done: E(RB3LYP) = -2652.964546 hartree
Sum of electronic and thermal Free Energies = -2652.441962 hartree
The number of imaginary frequency = 1
Imaginary frequency = -358.19

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.153116	1.863456	-0.063051
2	1	0	-5.278538	0.784180	-0.064870
3	1	0	-6.044450	2.411394	0.234025
4	6	0	-4.282338	2.474845	-0.963961
5	1	0	-4.409869	3.539904	-1.141979
6	6	0	-2.897935	0.523874	-1.410495
7	1	0	-3.731913	-0.110706	-1.136536
8	1	0	-0.838009	0.336089	-1.830317
9	7	0	-1.768888	-0.147970	-1.725544
10	6	0	-1.672201	-1.535660	-1.779240
11	8	0	-2.865006	-2.140635	-1.564850
12	8	0	-0.636923	-2.126747	-1.996475
13	1	0	-0.846201	-0.499086	1.168697
14	6	0	-1.266536	-5.243246	1.475972
15	6	0	-2.501650	-4.680703	1.741575
16	6	0	-2.668919	-3.279676	1.706209
17	6	0	-1.546581	-2.461397	1.405085
18	6	0	-0.290700	-3.038469	1.127064

19	6	0	-0.166086	-4.415807	1.164910
20	1	0	-4.791379	-3.230837	2.161820
21	1	0	-1.141880	-6.321651	1.500929
22	1	0	-3.359518	-5.306395	1.974783
23	6	0	-3.917303	-2.624743	1.935757
24	1	0	0.549823	-2.403137	0.868994
25	1	0	0.797923	-4.863867	0.943059
26	6	0	-2.877247	-0.452684	1.582143
27	6	0	-4.023469	-1.266321	1.872054
28	1	0	-4.977212	-0.782772	2.044538
29	7	0	-1.703093	-1.097265	1.365028
30	6	0	-2.892714	0.964153	1.496620
31	1	0	-1.952223	1.444045	1.242670
32	6	0	-4.026301	1.752740	1.709967
33	1	0	-4.873147	1.359953	2.266916
34	1	0	-3.869229	2.815906	1.853124
35	6	0	-2.839815	-3.573001	-1.702910
36	1	0	-2.078463	-4.010489	-1.055917
37	1	0	-3.834438	-3.906815	-1.406513
38	1	0	-2.636003	-3.846181	-2.742129
39	6	0	4.334738	-0.864431	-0.543446
40	6	0	5.442668	-1.266201	-1.306611
41	6	0	5.292034	-2.100900	-2.412742
42	6	0	4.020501	-2.545617	-2.787071
43	6	0	2.902267	-2.163187	-2.047516
44	6	0	3.071602	-1.342625	-0.935491
45	6	0	4.479749	0.013677	0.641173
46	6	0	5.521089	-0.178303	1.563532
47	6	0	5.663374	0.639978	2.682635
48	6	0	4.750473	1.672766	2.910378
49	6	0	3.707261	1.886578	2.011219
50	6	0	3.582381	1.072257	0.887118
51	1	0	6.427661	-0.896163	-1.035014
52	1	0	6.164499	-2.390754	-2.991968
53	1	0	3.898910	-3.183419	-3.658506
54	1	0	1.894627	-2.471621	-2.306165
55	1	0	6.213708	-0.999828	1.401513
56	1	0	6.476283	0.463298	3.381547
57	1	0	4.847898	2.308359	3.786402
58	1	0	2.978472	2.678070	2.152395
59	8	0	1.968499	-1.051083	-0.151996
60	8	0	2.608094	1.393404	-0.039654
61	15	0	1.275314	0.451280	-0.253185
62	8	0	0.770536	0.741254	-1.636930
63	8	0	0.350488	0.513001	0.940994
64	6	0	-3.108560	1.894850	-1.503005
65	16	0	-1.894514	2.962444	-2.285270
66	6	0	-0.976269	3.640043	-0.885821
67	6	0	0.417558	3.682433	-0.987931
68	6	0	-1.608057	4.162874	0.249780
69	6	0	1.172244	4.232268	0.050513
70	1	0	0.909898	3.234744	-1.842467
71	6	0	-0.845766	4.687771	1.292651
72	1	0	-2.690356	4.162093	0.320677
73	6	0	0.547409	4.727003	1.194681
74	1	0	2.254740	4.232424	-0.028001
75	1	0	-1.343151	5.077515	2.177392
76	1	0	1.139706	5.138987	2.007454

TS$_{SPh}$-Tt(S-ex)

B3LYP-D3/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -2652.958291 hartree

Sum of electronic and thermal Free Energies = -2652.437919 hartree

The number of imaginary frequency = 1

Imaginary frequency = -351.89

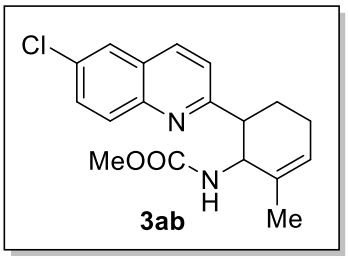
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.107205	1.711784	3.743691
2	1	0	2.899902	1.056676	3.394245
3	1	0	2.203117	2.019055	4.782131
4	6	0	1.464490	2.571960	2.862858
5	1	0	0.898471	3.397791	3.290127
6	6	0	1.992135	1.350984	0.817792
7	1	0	2.883353	0.945782	1.280737
8	1	0	0.798920	1.000079	-0.869161
9	7	0	1.742964	0.887023	-0.432275
10	6	0	2.620557	0.104269	-1.172354
11	8	0	3.798812	-0.077727	-0.524278
12	8	0	2.359328	-0.349263	-2.263749
13	1	0	0.567123	-1.800099	0.332092
14	6	0	4.107497	-4.608934	-1.070240
15	6	0	4.418684	-4.136147	0.191306
16	6	0	3.538795	-3.256602	0.858605
17	6	0	2.332437	-2.874837	0.213166
18	6	0	2.022809	-3.348929	-1.078963
19	6	0	2.909361	-4.208662	-1.701735
20	1	0	4.707204	-2.984496	2.668357
21	1	0	4.786441	-5.285179	-1.581002
22	1	0	5.341309	-4.431577	0.684397
23	6	0	3.789733	-2.709834	2.153470
24	1	0	1.106039	-3.016220	-1.553704
25	1	0	2.681080	-4.574738	-2.698288
26	6	0	1.686693	-1.485602	2.078238
27	6	0	2.902545	-1.856376	2.743186
28	1	0	3.106761	-1.446804	3.724814
29	7	0	1.469387	-2.019414	0.852835
30	6	0	0.720333	-0.585534	2.607906
31	1	0	-0.134408	-0.357959	1.979257
32	6	0	0.801406	0.005304	3.865323
33	1	0	1.424871	-0.423527	4.644908
34	1	0	-0.076488	0.522419	4.236081
35	6	0	4.788491	-0.795730	-1.280712
36	1	0	5.638942	-0.907743	-0.607452
37	1	0	4.409717	-1.771868	-1.586566
38	1	0	5.073121	-0.222867	-2.167812
39	6	0	-4.564423	0.068369	0.402256
40	6	0	-5.703671	0.843443	0.674654
41	6	0	-5.612779	2.062203	1.343469
42	6	0	-4.365186	2.536490	1.755608
43	6	0	-3.218776	1.788911	1.494611

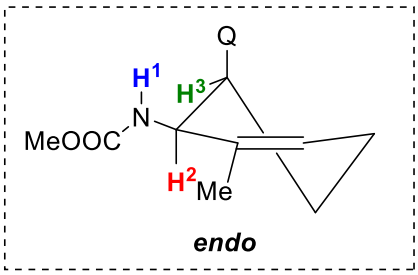
44	6	0	-3.318273	0.571555	0.823787
45	6	0	-4.680701	-1.242613	-0.276842
46	6	0	-5.703088	-2.144872	0.060247
47	6	0	-5.826123	-3.375861	-0.580507
48	6	0	-4.915689	-3.736099	-1.577278
49	6	0	-3.890983	-2.859948	-1.929767
50	6	0	-3.782872	-1.627707	-1.288989
51	1	0	-6.670809	0.482414	0.335730
52	1	0	-6.510753	2.643672	1.532910
53	1	0	-4.281954	3.488612	2.272599
54	1	0	-2.235580	2.129751	1.796422
55	1	0	-6.394911	-1.875208	0.853520
56	1	0	-6.623445	-4.056479	-0.295006
57	1	0	-5.000664	-4.697137	-2.077177
58	1	0	-3.168069	-3.103150	-2.701133
59	8	0	-2.173709	-0.188258	0.672260
60	8	0	-2.817977	-0.739232	-1.731440
61	15	0	-1.484698	-0.450349	-0.820527
62	8	0	-0.845318	0.797641	-1.353700
63	8	0	-0.678245	-1.713738	-0.623899
64	6	0	1.302561	2.366496	1.469950
65	16	0	0.083328	3.388136	0.648009
66	6	0	0.946944	3.865897	-0.856392
67	6	0	0.380211	3.546782	-2.094773
68	6	0	2.153219	4.575290	-0.789363
69	6	0	1.026266	3.948213	-3.266975
70	1	0	-0.523046	2.948208	-2.133437
71	6	0	2.797672	4.955369	-1.965188
72	1	0	2.582648	4.818116	0.178359
73	6	0	2.231941	4.647335	-3.206341
74	1	0	0.591629	3.691007	-4.228917
75	1	0	3.736325	5.501220	-1.913092
76	1	0	2.734243	4.948461	-4.121875

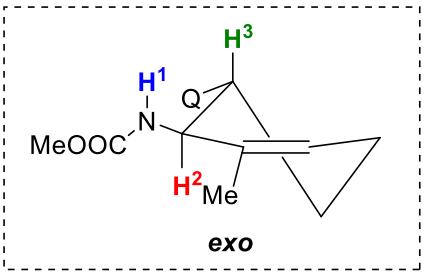
---

5. Determination of relative configurations

The coupling constants of ^{1}H NMR determined the relative configuration of **3ab** and **3ai**[6]. Quinoline moiety and amide group were in the opposite direction.





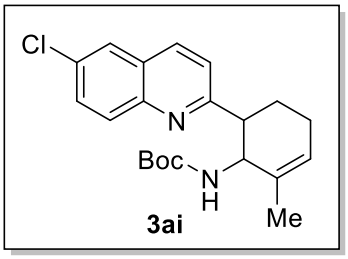


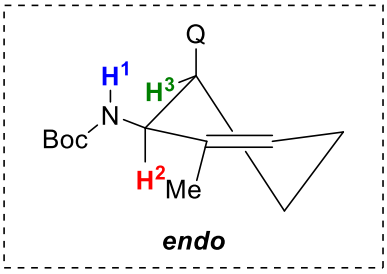
H^1 : 4.97 (d, *J* = 10.2 Hz, 1H)
H^2 : 4.50 (dd, *J* = 10.2, 4.2 Hz, 1H)
H^3 : 3.37 (ddd, *J* = 12.6, 4.2, 3.0 Hz, 1H)

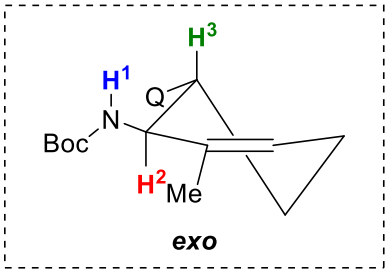
$J(H^2/H^3)$ = 4.2 Hz

H^1 : 4.64 (d, *J* = 9.0 Hz, 1H)
H^2 : 4.69 (dd, *J* = 9.0, 9.0 Hz, 1H)
H^3 : 3.20 (ddd, *J* = 10.2, 9.0, 3.6 Hz, 1H)

$J(H^2/H^3)$ = 9.0 Hz







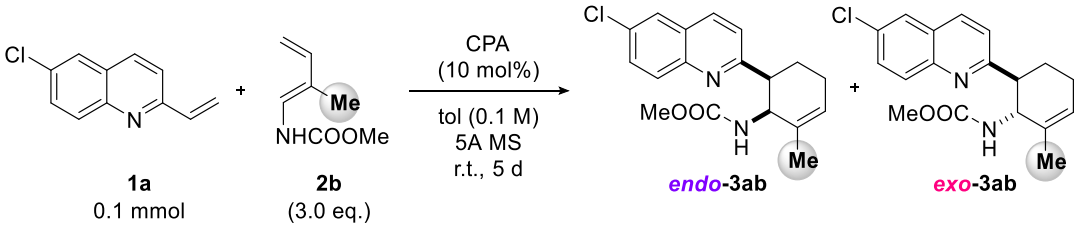
H^1 : 4.69 (d, *J* = 10.2 Hz, 1H)
H^2 : 4.43 (dd, *J* = 10.2, 4.2 Hz, 1H)
H^3 : 3.34 (ddd, *J* = 12.6, 4.2, 3.0 Hz, 1H)

$J(H^2/H^3)$ = 4.2 Hz

H^1 : 4.51 (d, *J* = 9.0 Hz, 1H)
H^2 : 4.60 (dd, *J* = 9.0, 9.0 Hz, 1H)
H^3 : 3.20 (ddd, *J* = 10.2, 9.0, 3.0 Hz, 1H)

$J(H^2/H^3)$ = 9.0 Hz

6. Catalyst screening for enantioselective reaction

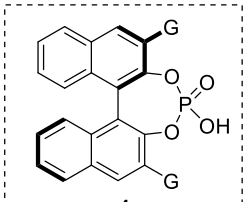


1a 0.1 mmol

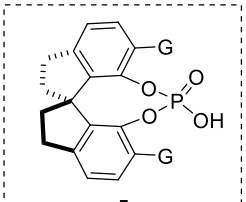
2b (3.0 eq.)

***endo*-3ab**

***exo*-3ab**



4



5

Entry	CPA (G)	Yield (%)[a]	***endo/exo*[b]**	Ee (%)
1	(*R*)-**4a** (G = H)	52	15/85	5/31
2	(*R*)-**4b** (G = Me)	60	16/84	rac/75
3	(*R*)-**4c** (G = 2,4,6-(*i*Pr)$_3$-C$_6$H$_2$)	50	17/83	67/69
4	(*R*)-**4d** (G = Bn)	**90**	**3/97**	16/**81**
5	(*S*)-**5c** (G = 2,4,6-(*i*Pr)$_3$-C$_6$H$_2$)	trace	-	-

[a] Isolated yield. [b] Determined by ^{1}H NMR of crude materials.

7. References

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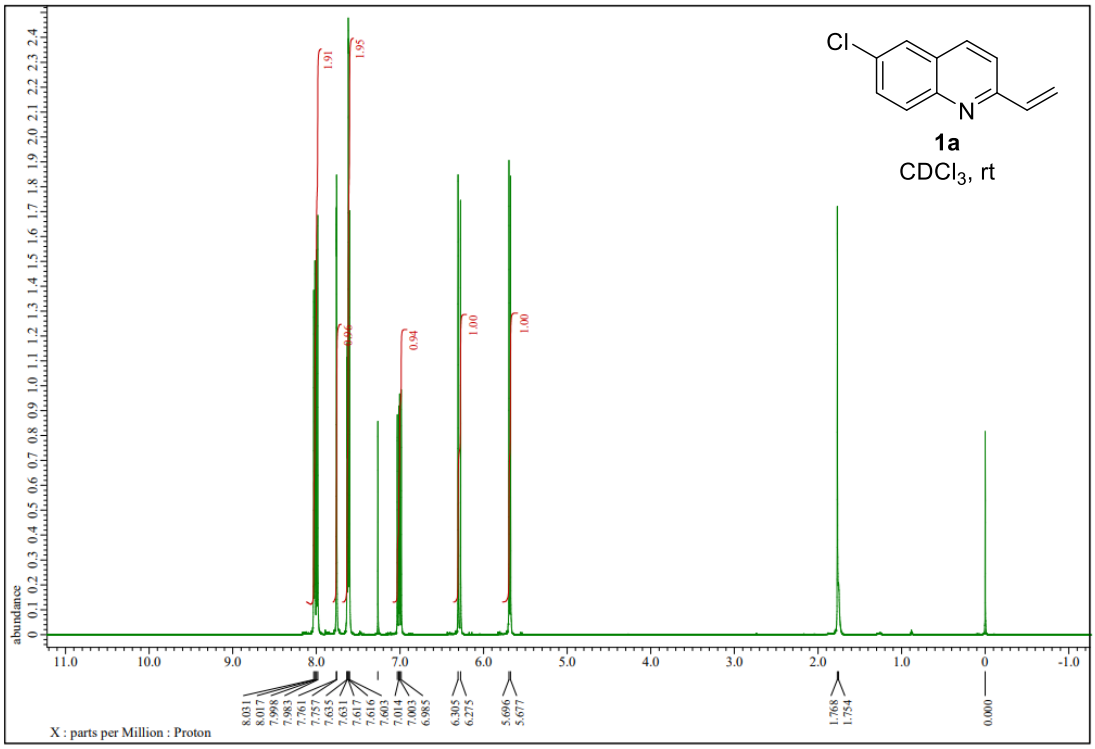
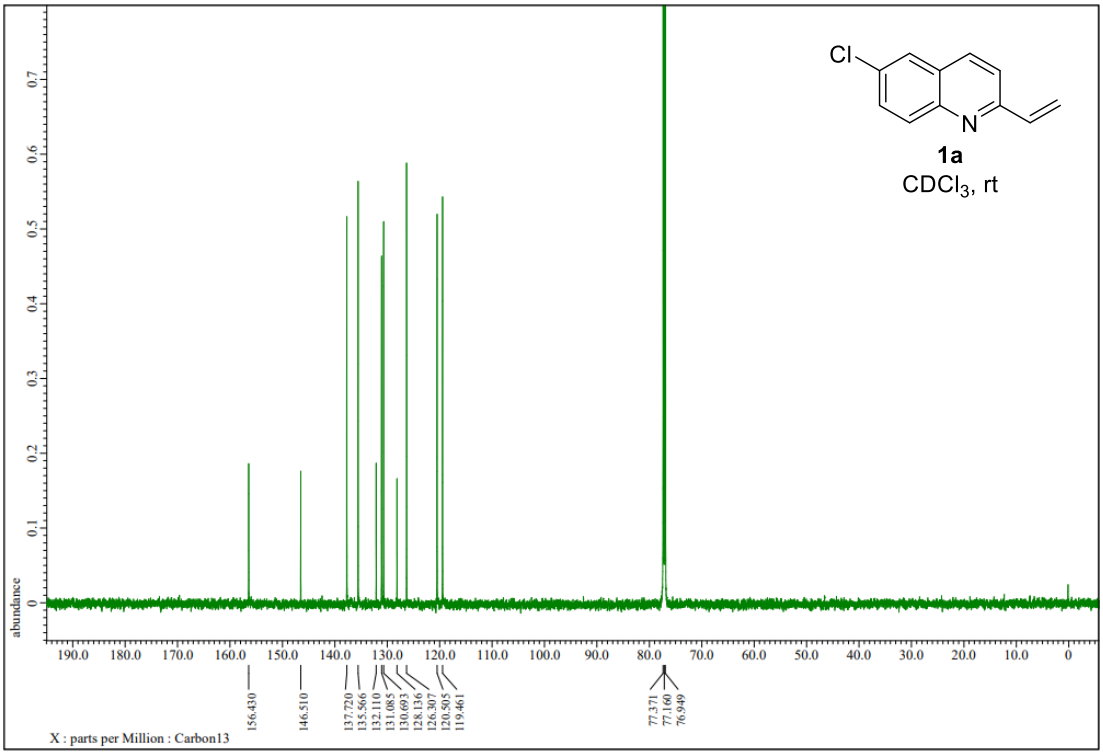
[6] (a) Lam,Y.-H.; Cheong, P. H.-Y.; Mata, J. M. B.; Stanway, S. J.; Gouverneur, V.; Houk, K. N. Diels−Alder Exo Selectivity in Terminal-Substituted Dienes and Dienophiles: Experimental Discoveries and Computational Explanations. *J. Am. Chem. Soc.* **2009**, *131*, 1947-1957. (b) Liu, Z.; Lin, X.; Yang, N.; Su, Z.; Hu, C.; Xiao, P.; He, Y.; Song, Z. Unique Steric Effect of Geminal Bis(silane) To Control the High *Exo*-selectivity in Intermolecular Diels–Alder Reaction *J. Am. Chem. Soc.* **2016**, *138*, 1877-1883.

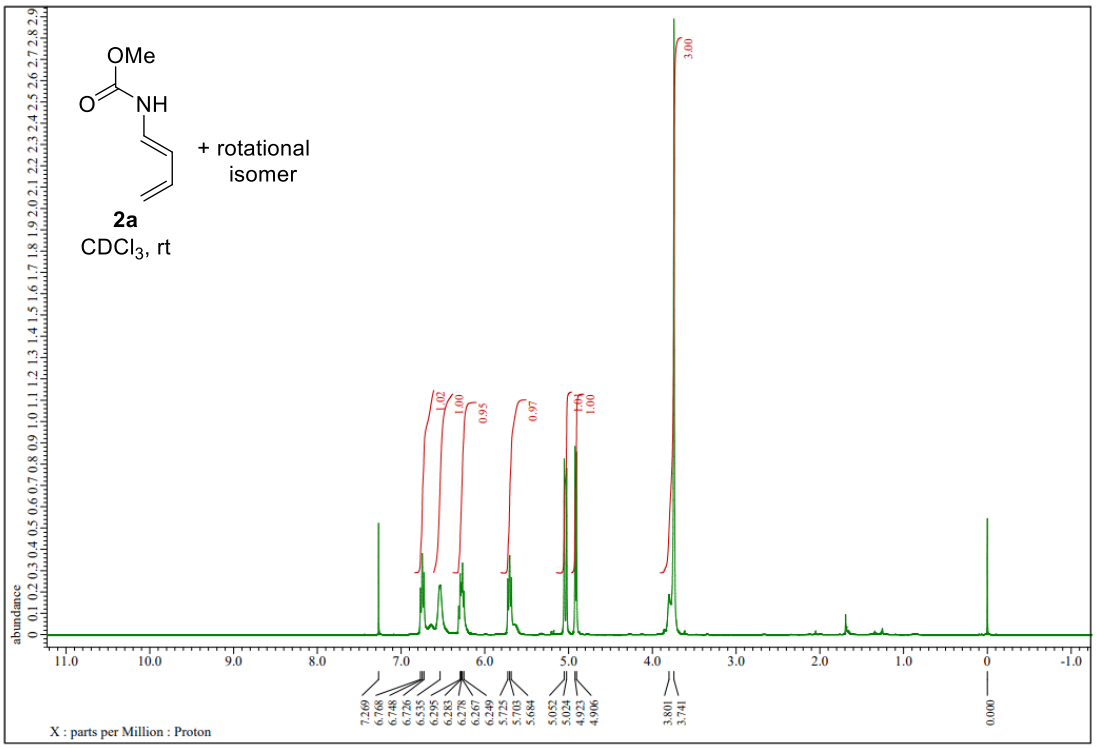
8. NMR spectra

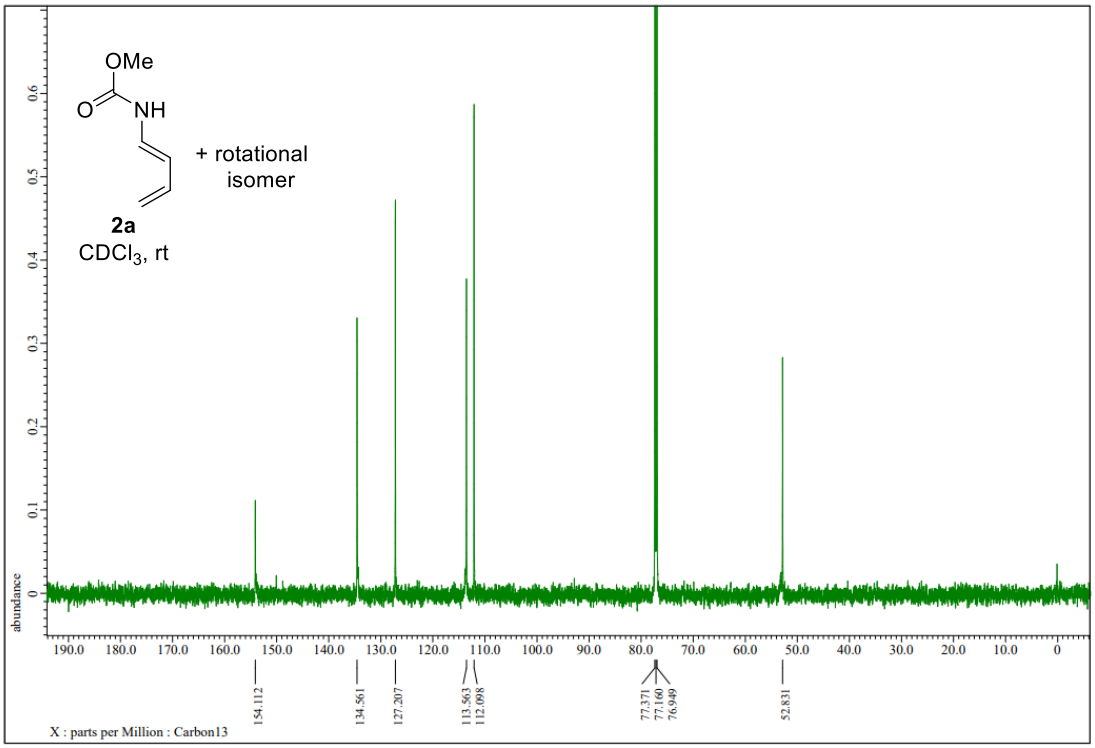
^{1}H and ^{13}C NMR charts of **1a**.



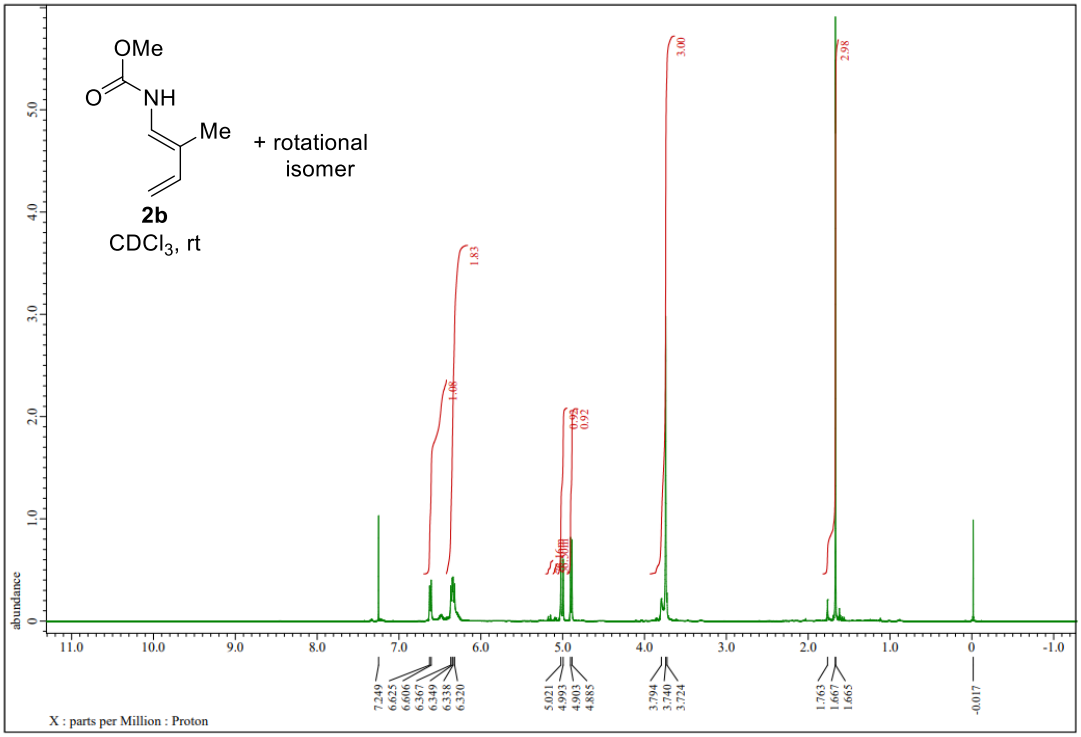


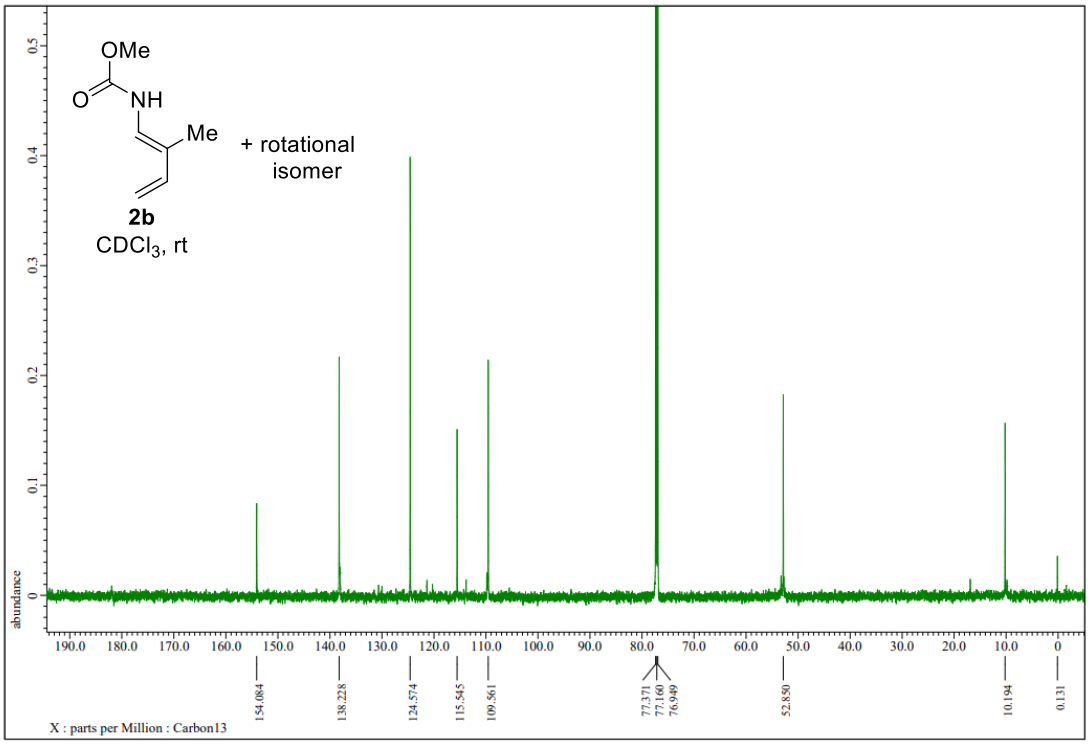
^{1}H and ^{13}C NMR charts of **2a**.



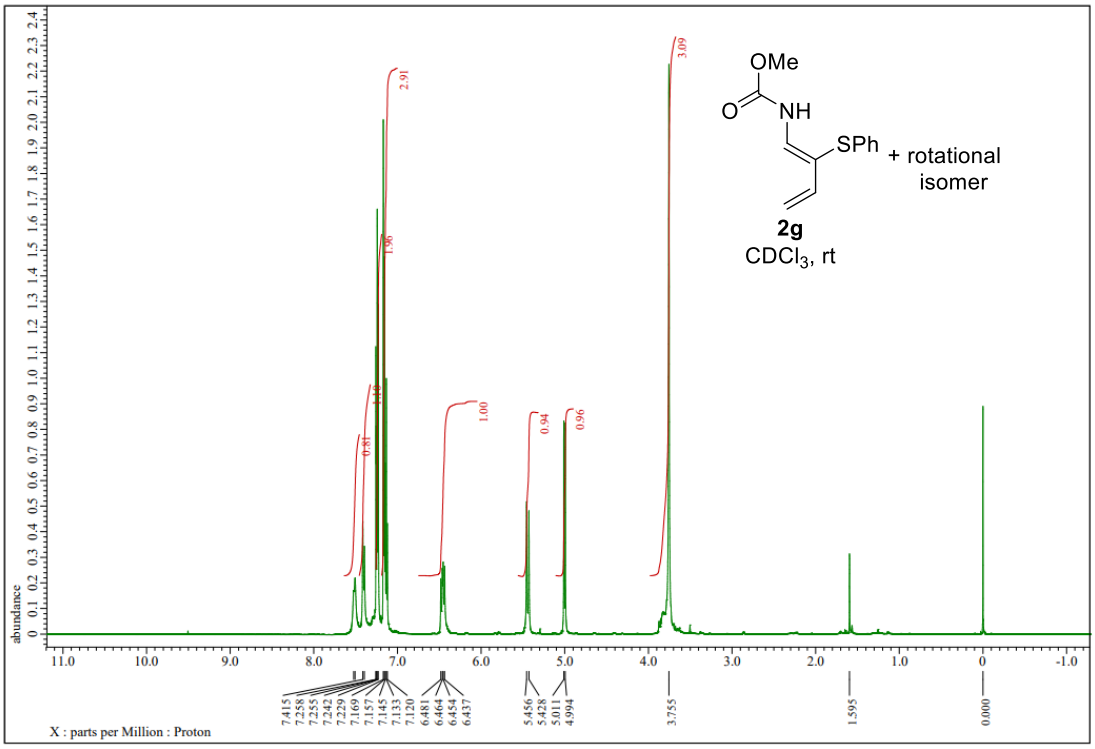


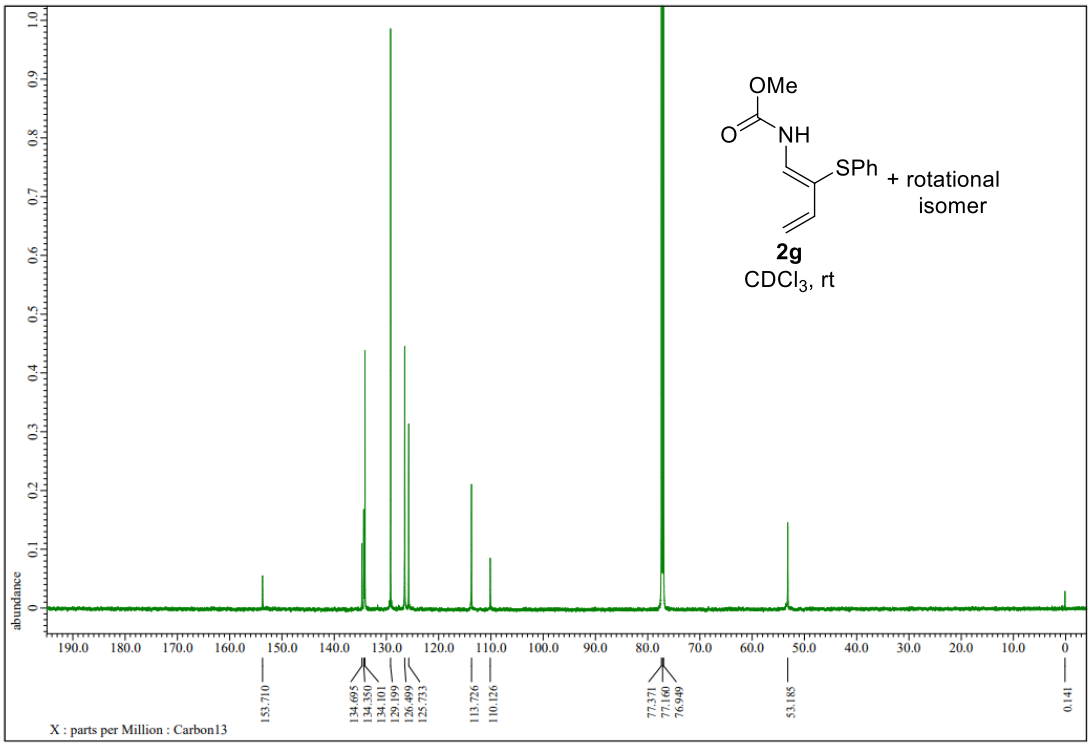
^{1}H and ^{13}C NMR charts of **2b**.



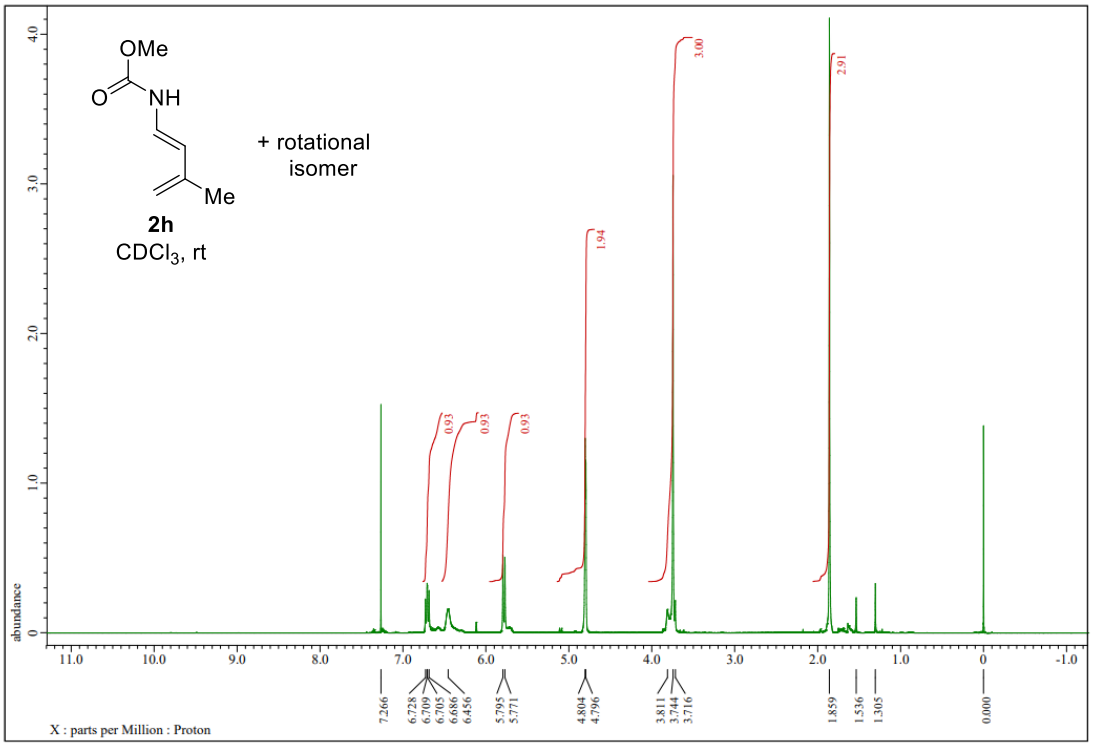


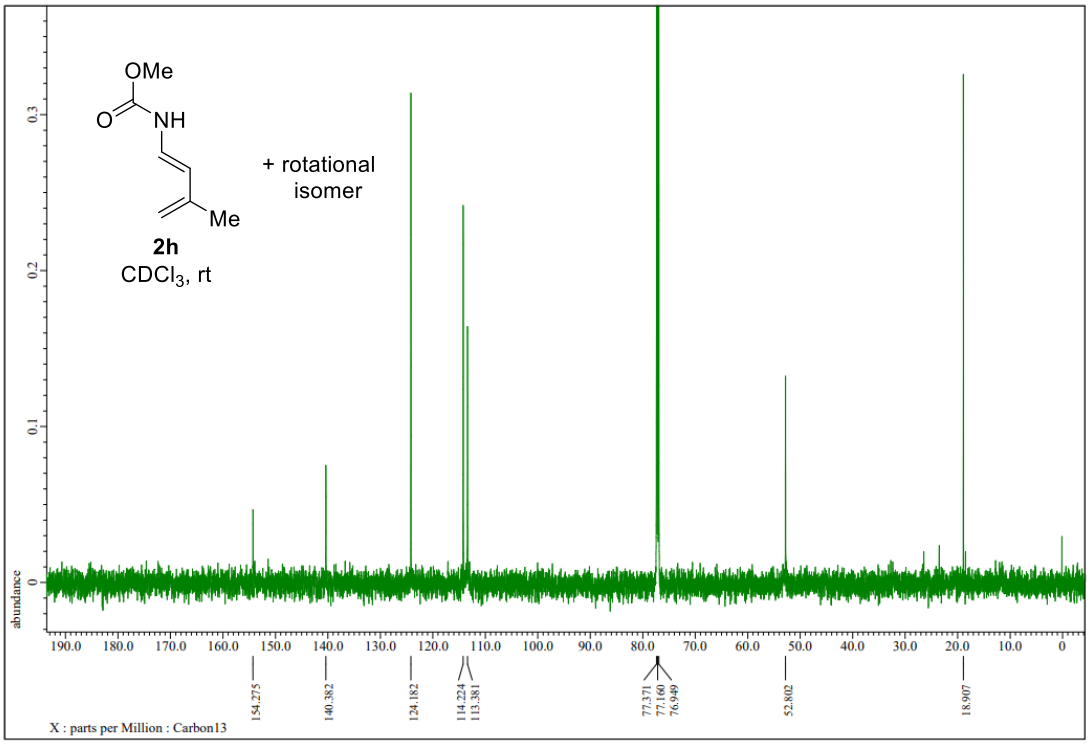
^{1}H and ^{13}C NMR charts of **2g**.



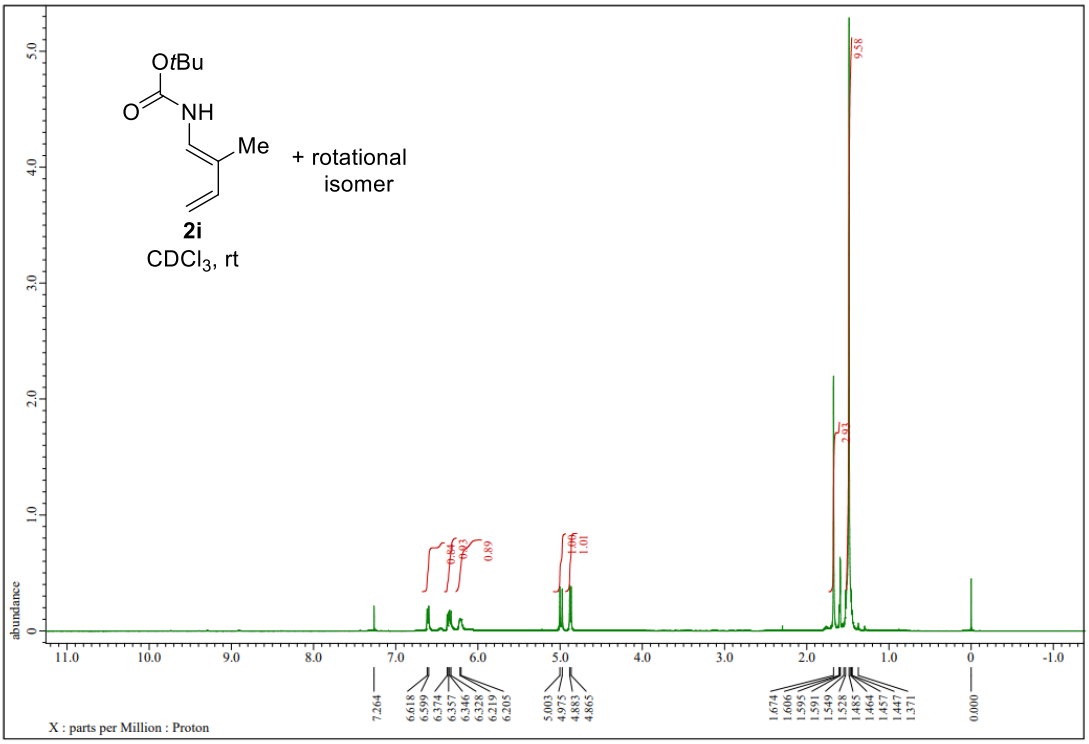


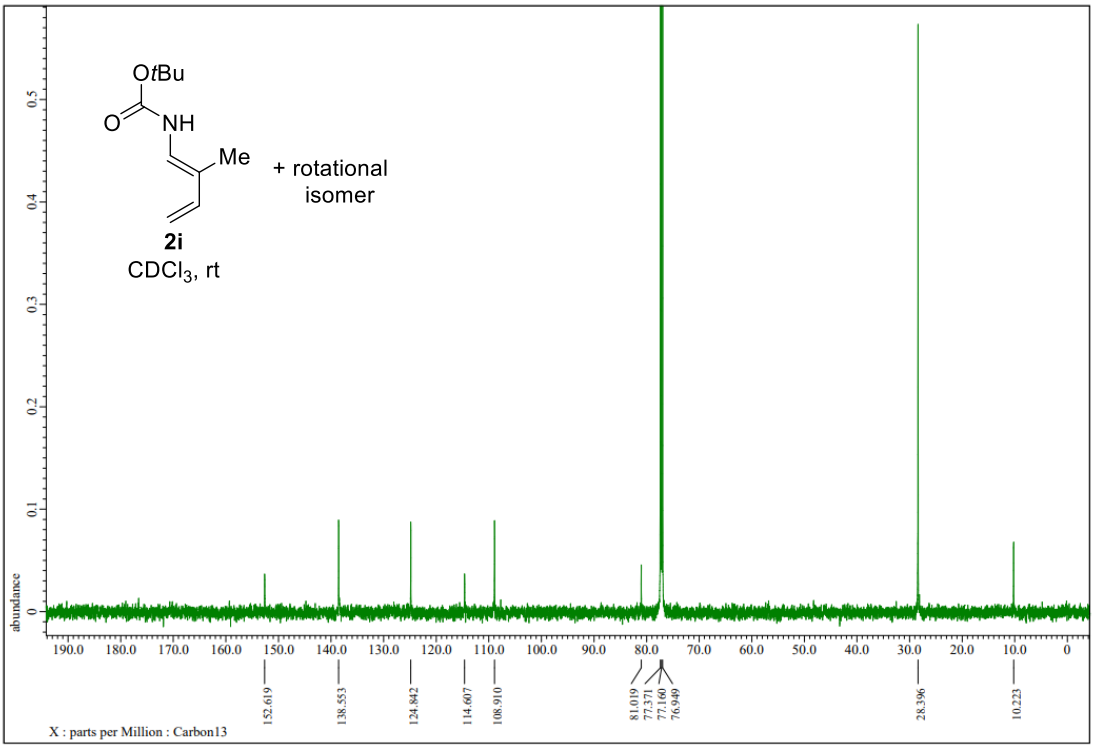
^{1}H and ^{13}C NMR charts of **2h**.



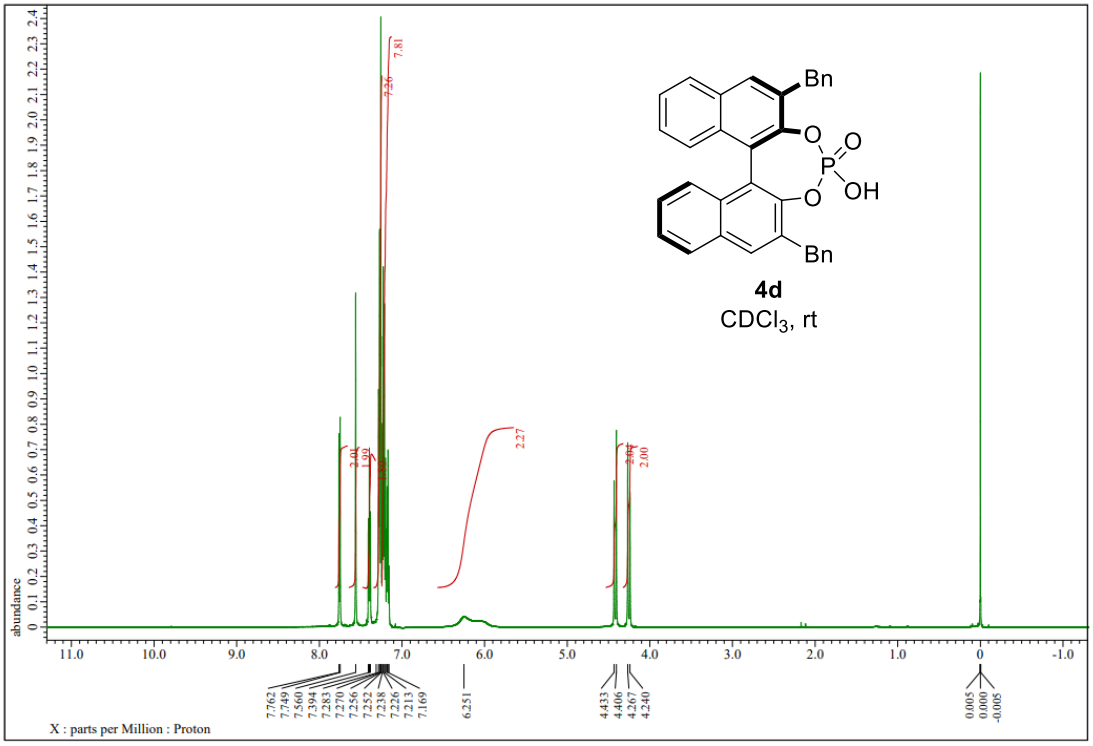


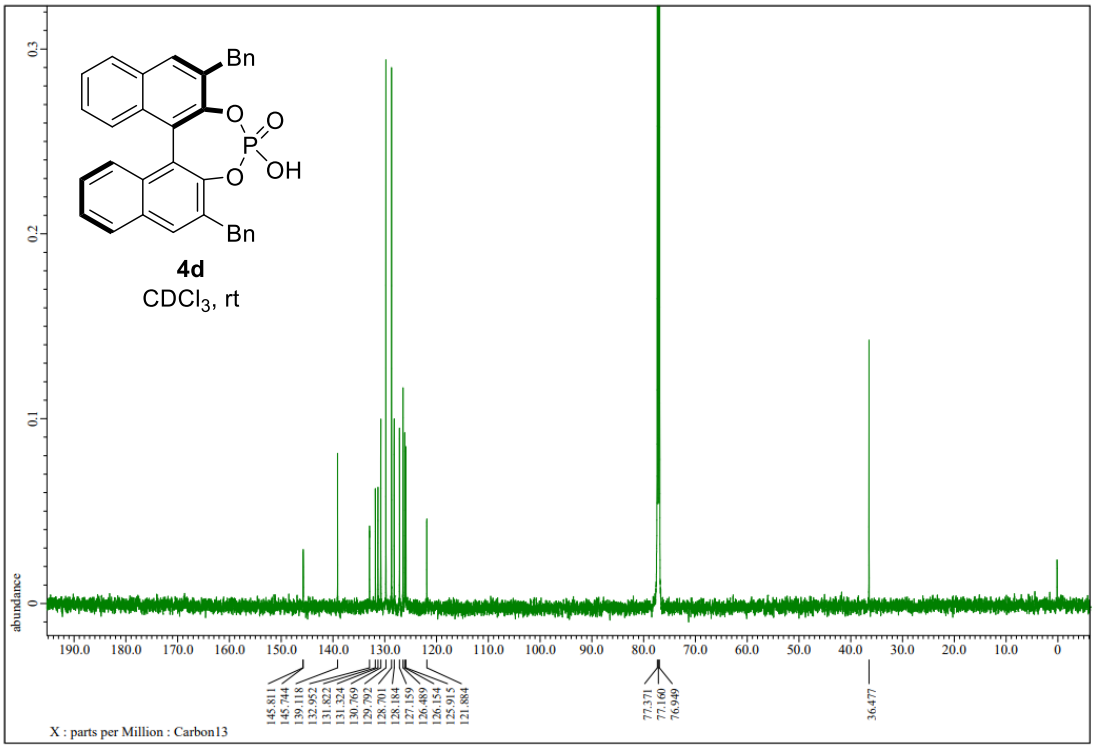
^{1}H and ^{13}C NMR charts of **2i**.

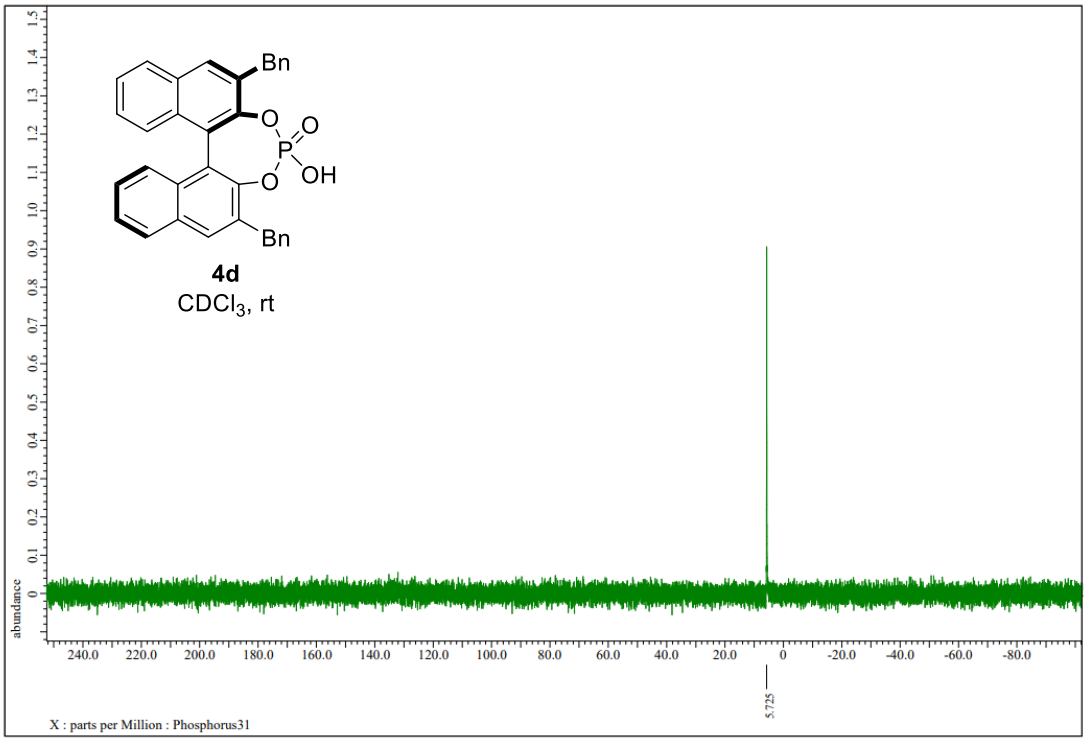




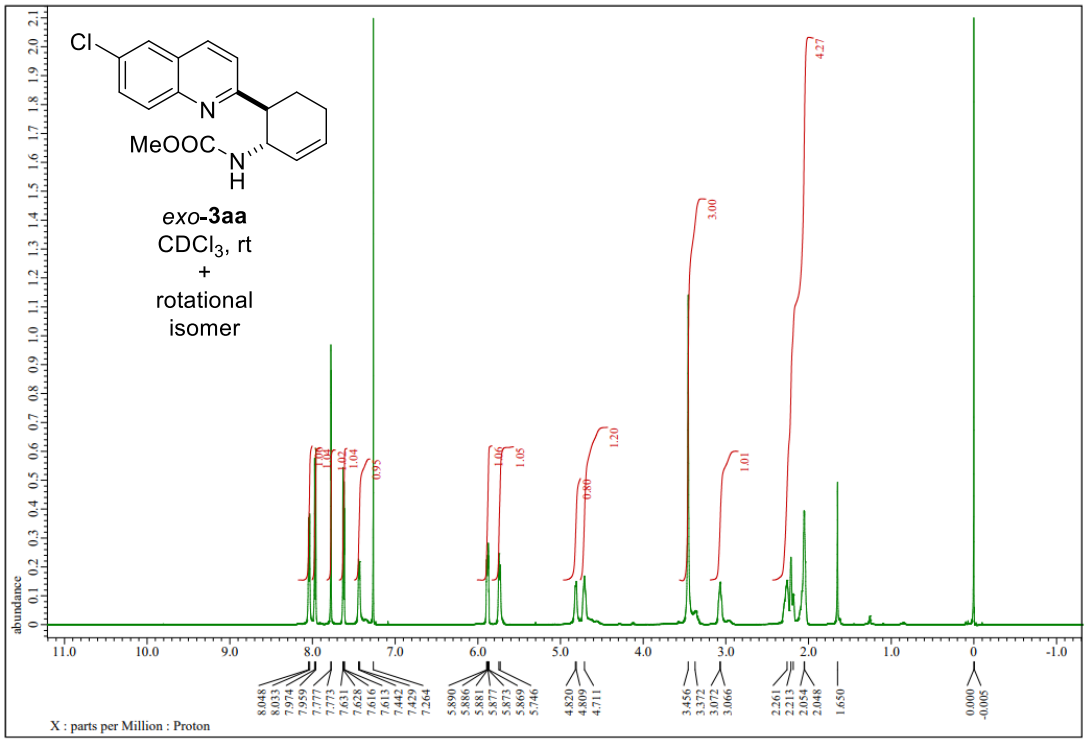
^{1}H, ^{13}C and ^{31}P NMR charts of **4d**.

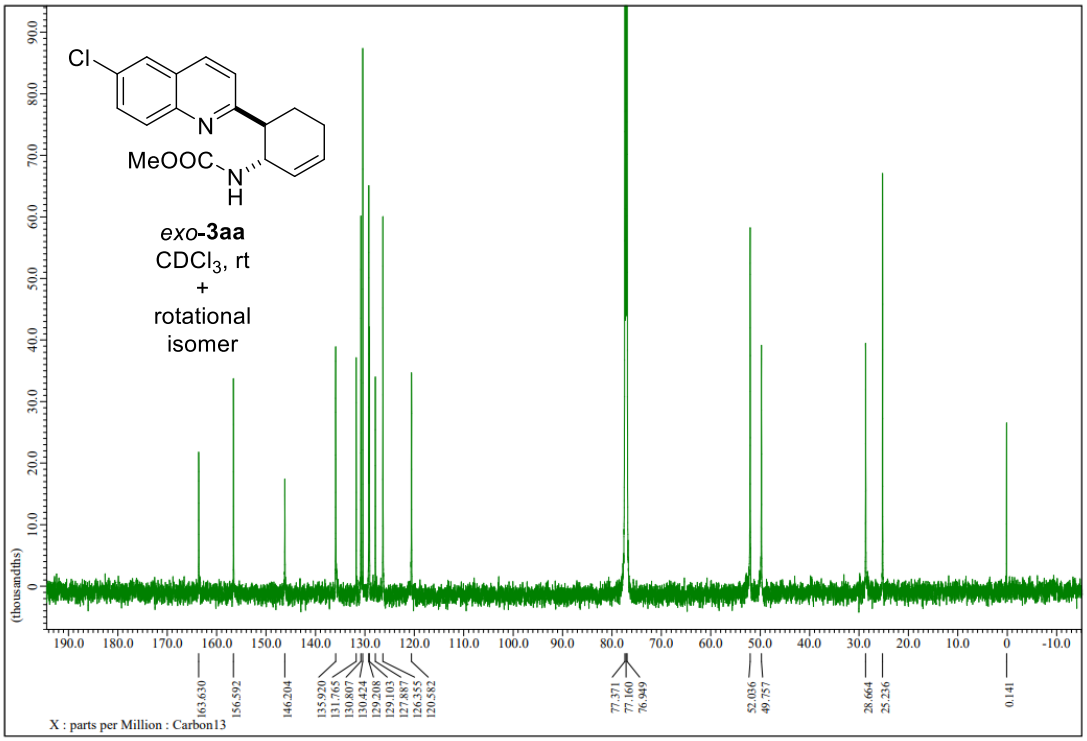




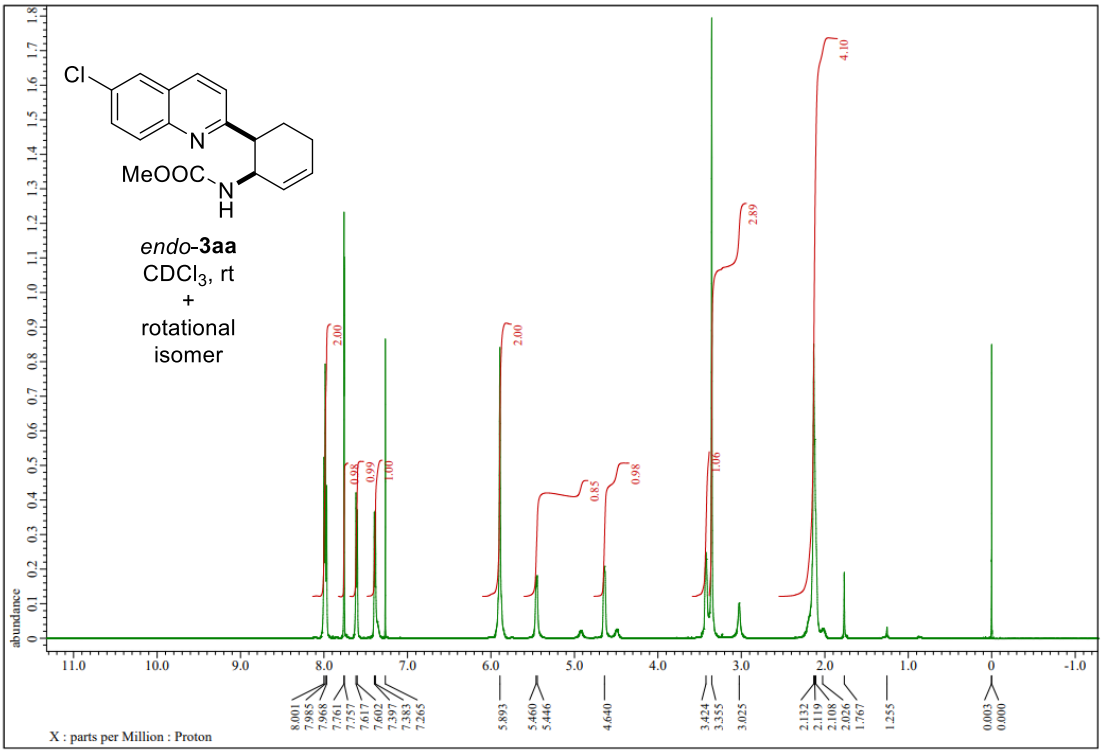

Bn
O
O
P
O
OH
Bn
4d
CDCl3, rt
abundance
1.5
1.4
1.3
1.2
1.1
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
240.0
220.0
200.0
180.0
160.0
140.0
120.0
100.0
80.0
60.0
40.0
20.0
0
-20.0
-40.0
-60.0
-80.0
5.725
X : parts per Million : Phosphorus31

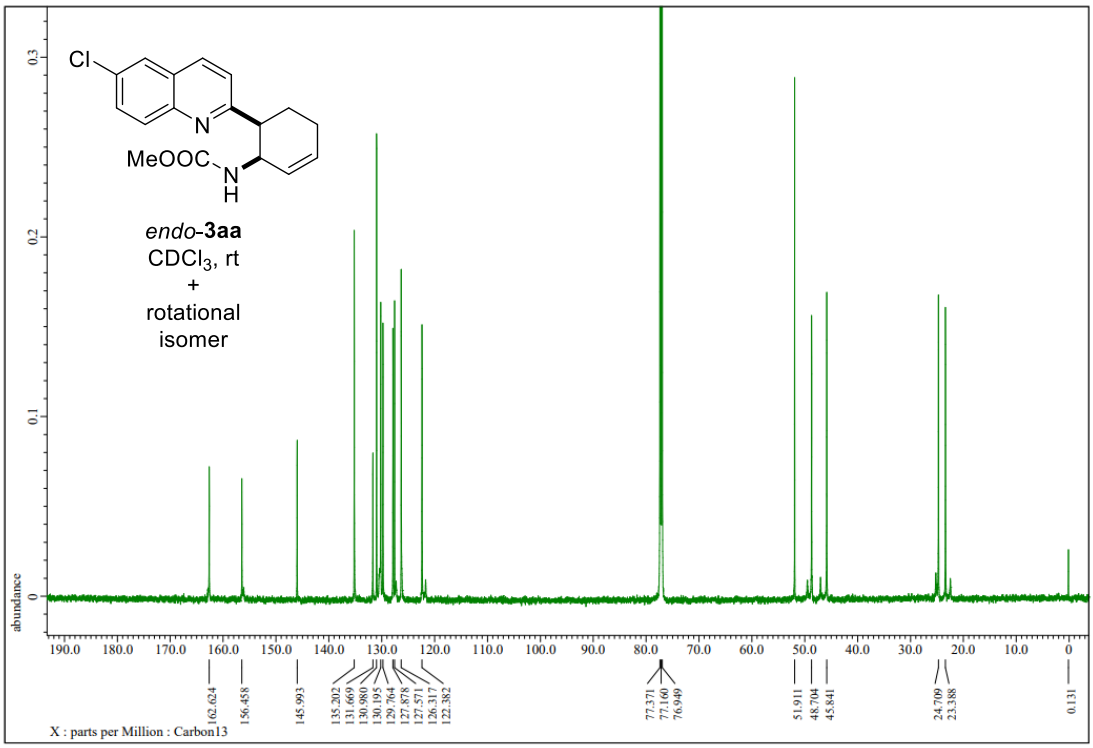
^{1}H and ^{13}C NMR charts of *exo*-**3aa**.



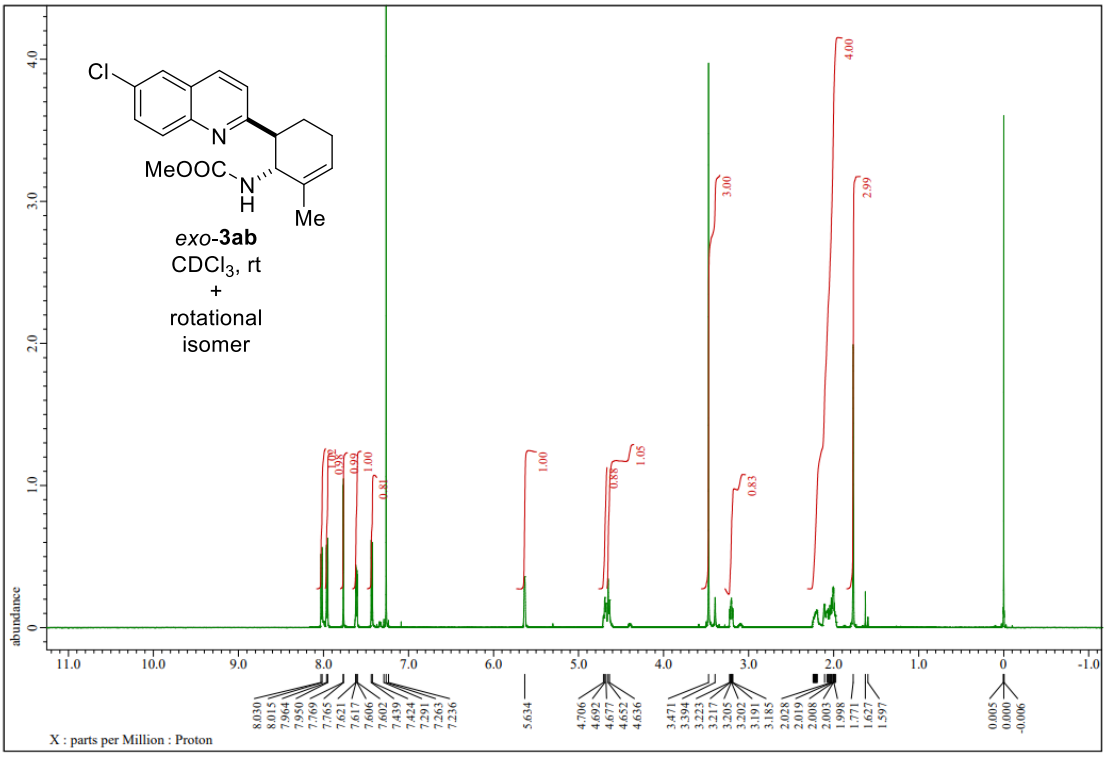


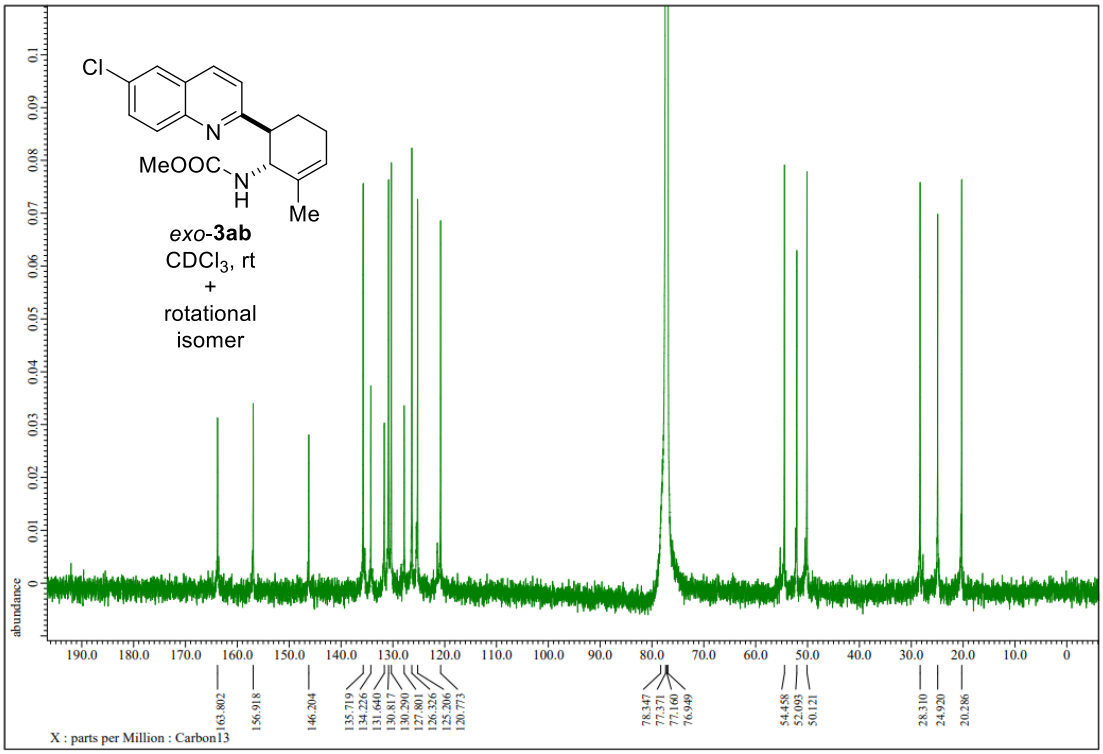
^{1}H and ^{13}C NMR charts of *endo*-**3aa**.



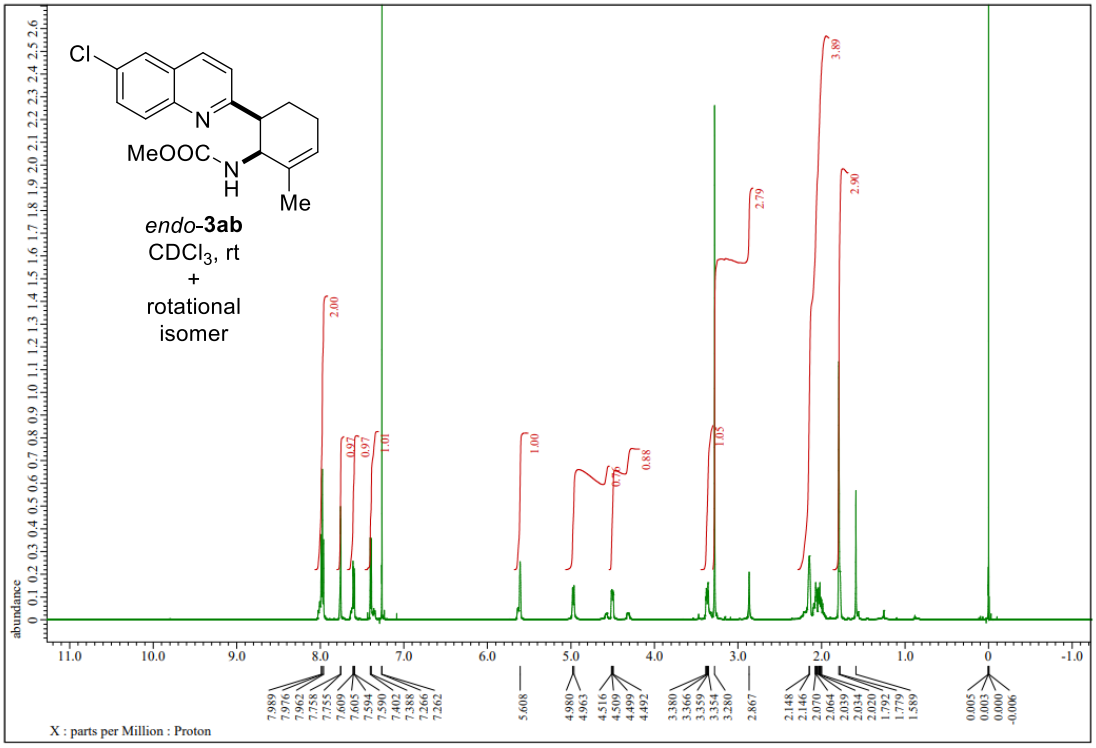


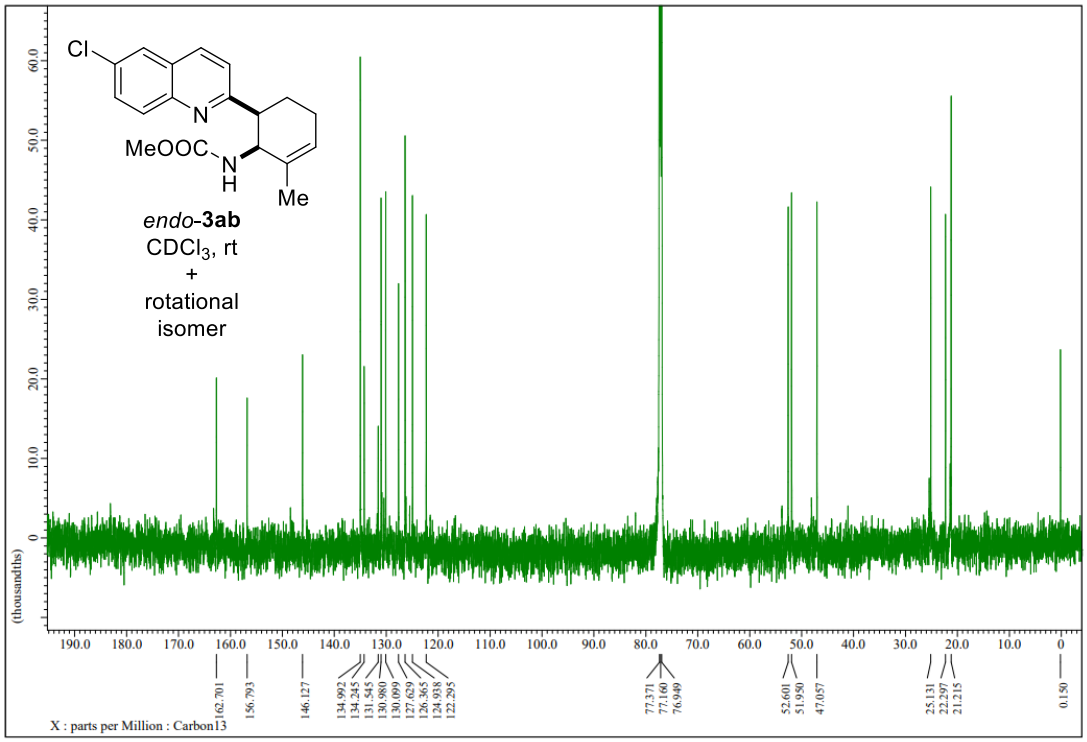
^{1}H and ^{13}C NMR charts of *exo*-**3ab**.



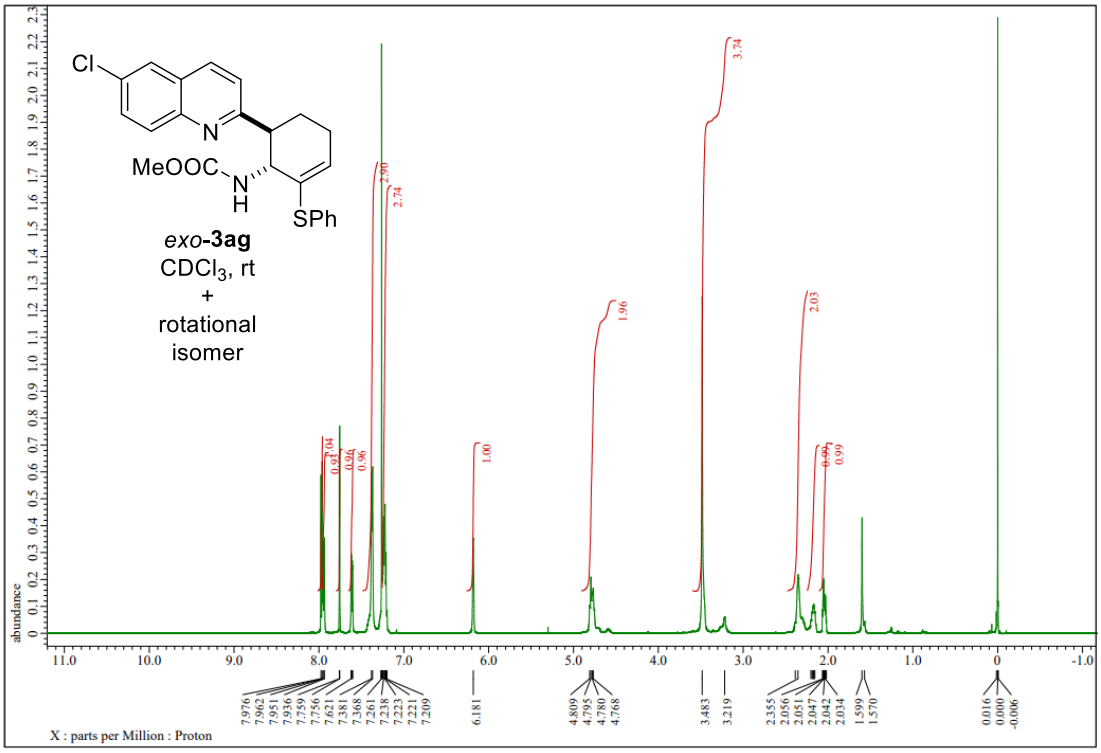


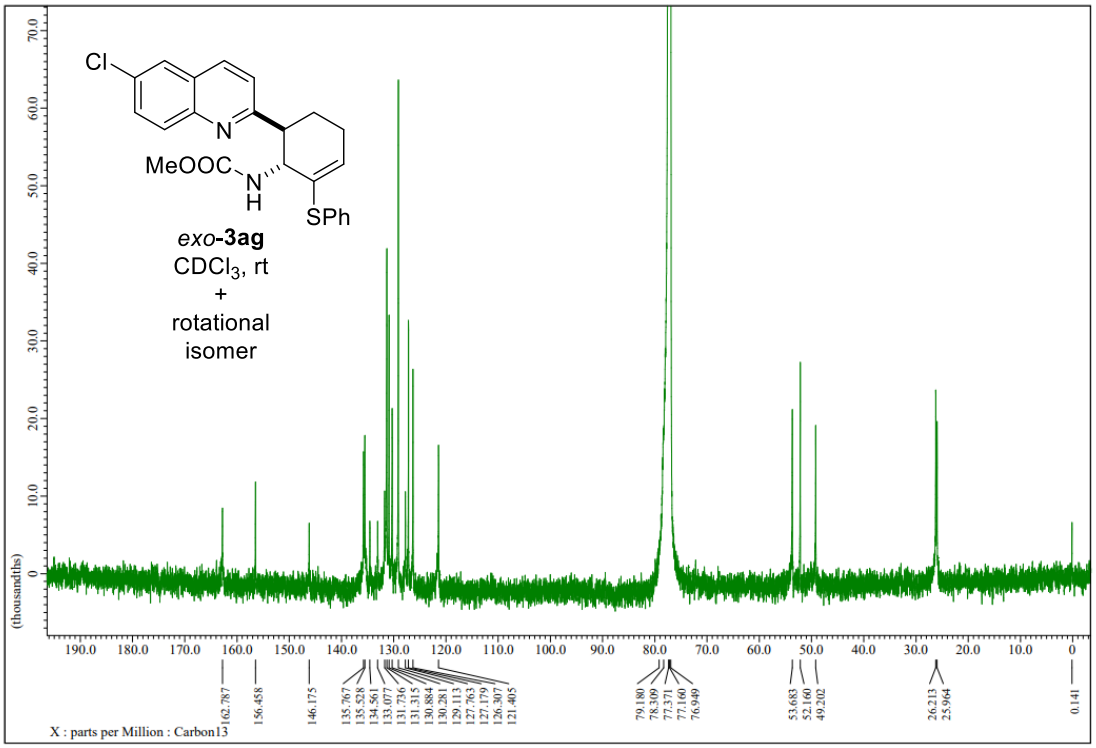
^{1}H and ^{13}C NMR charts of *endo*-**3ab**.



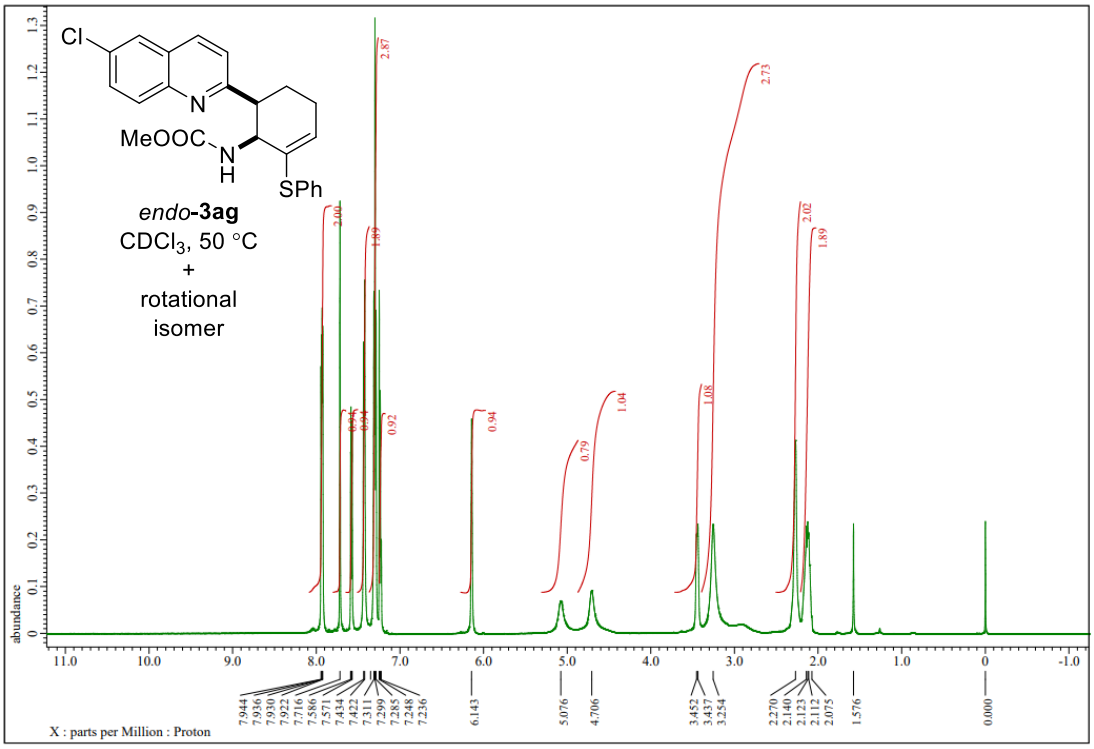


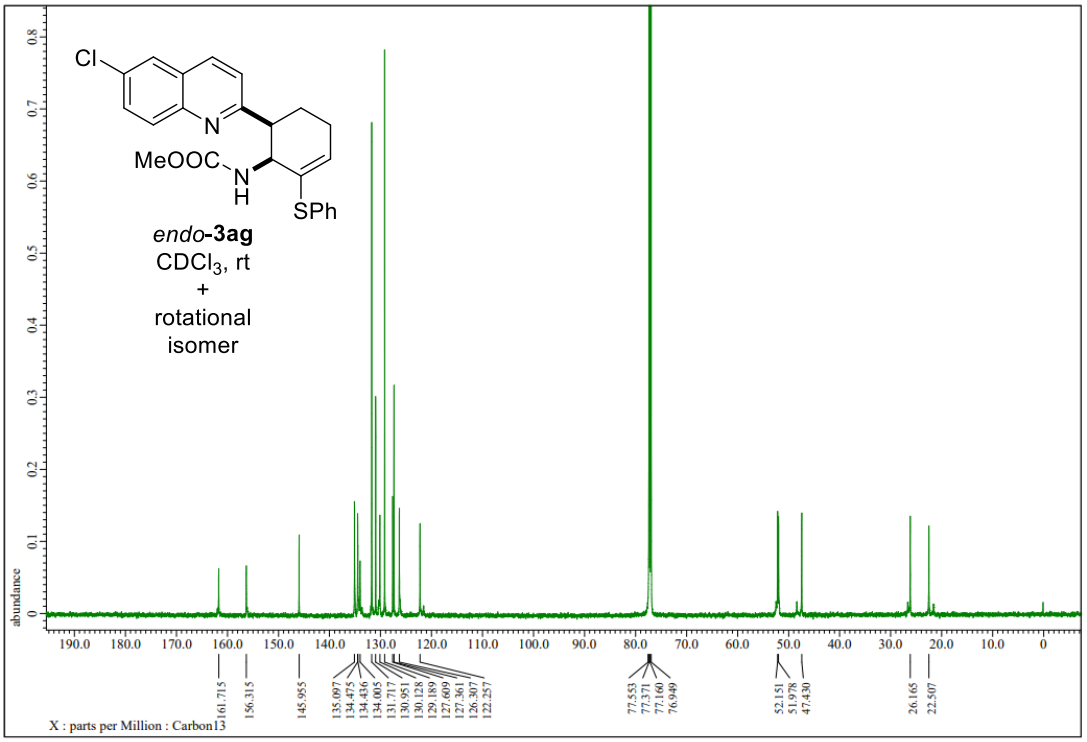
^{1}H and ^{13}C NMR charts of *exo*-**3ag**.



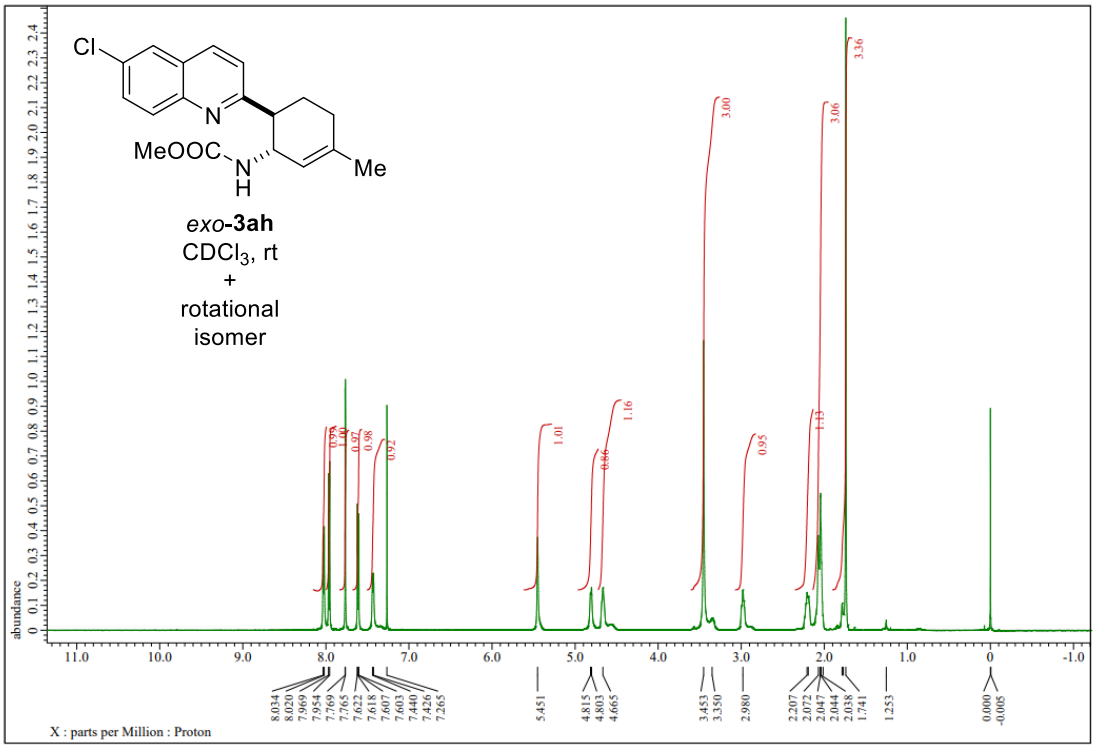


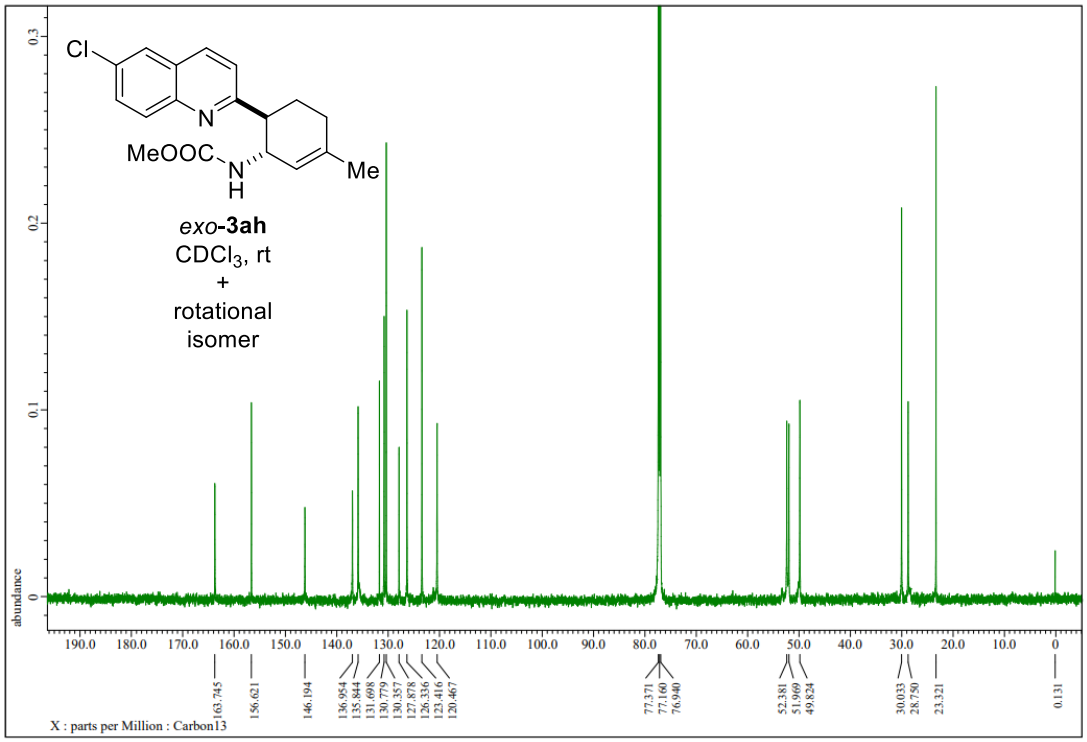
^{1}H and ^{13}C NMR charts of *endo*-**3ag**.



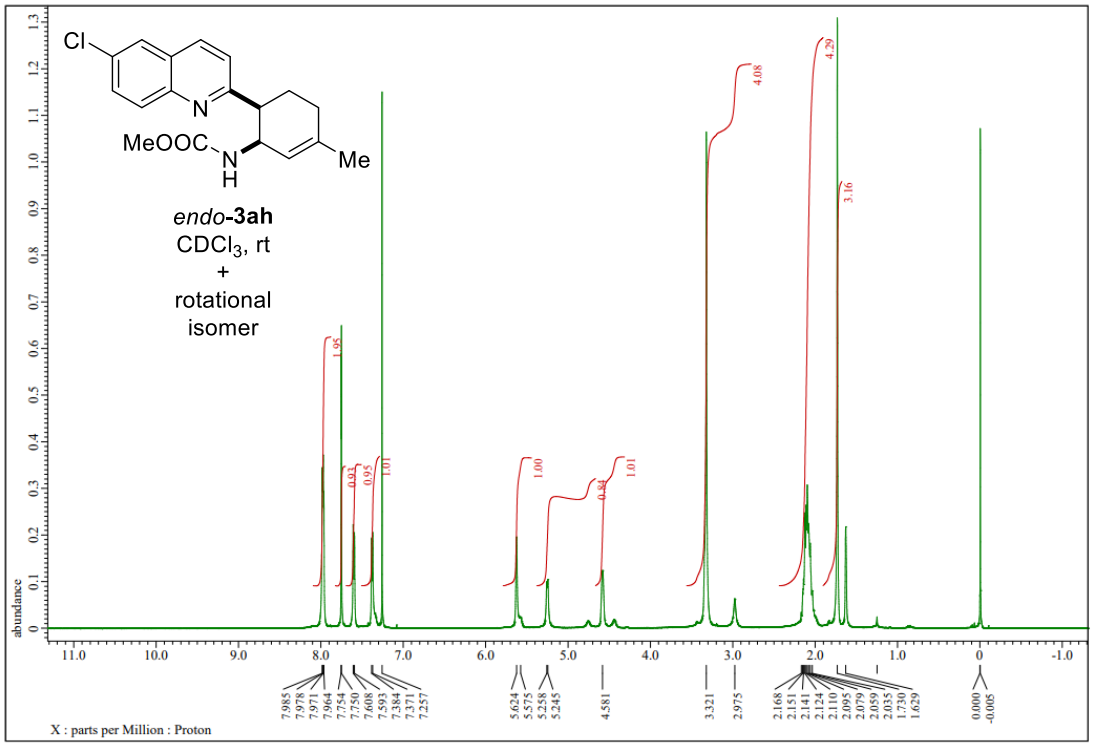


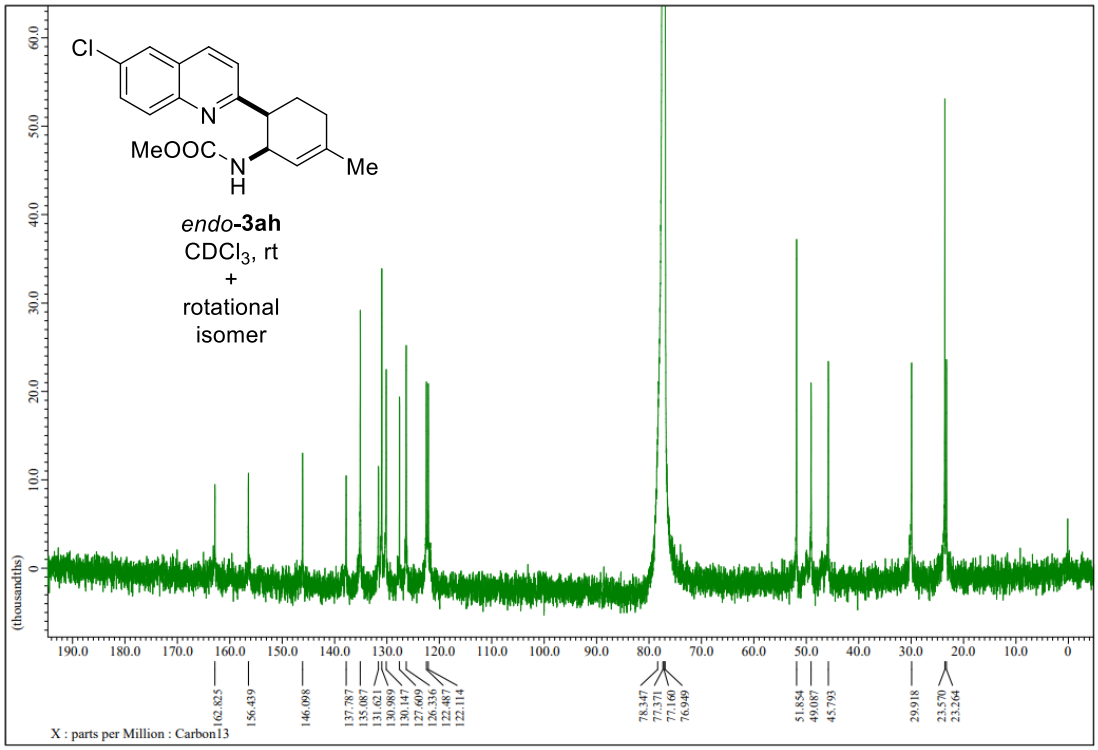
^{1}H and ^{13}C NMR charts of *exo*-**3ah**.



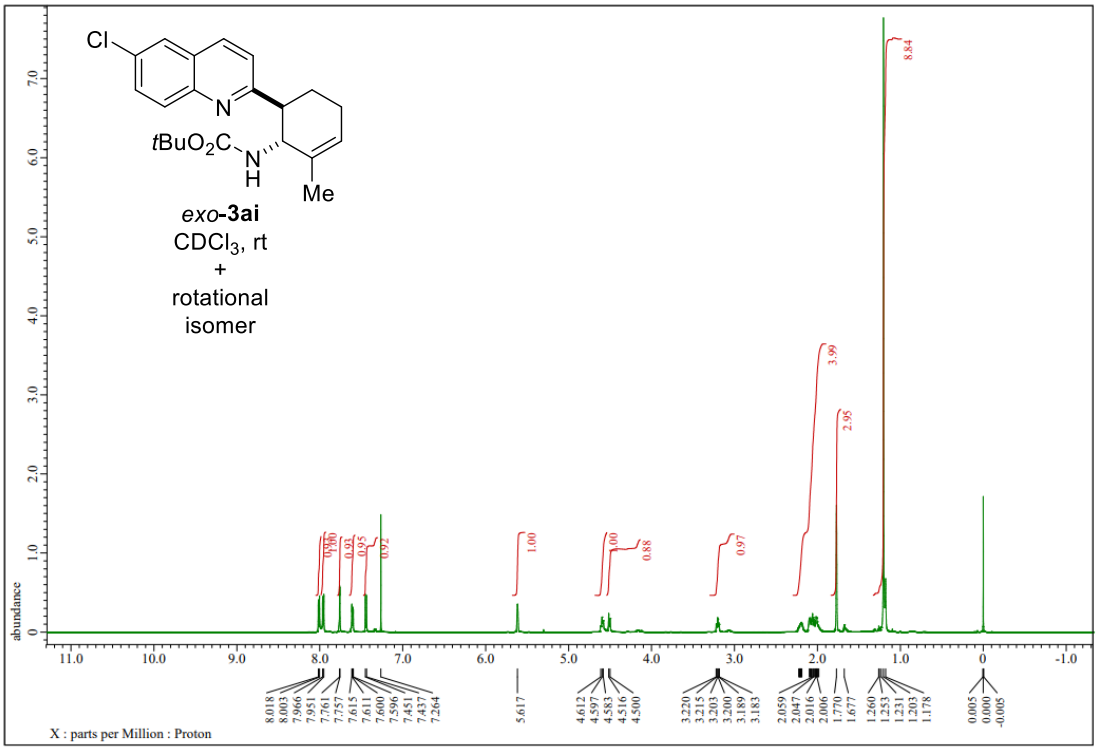


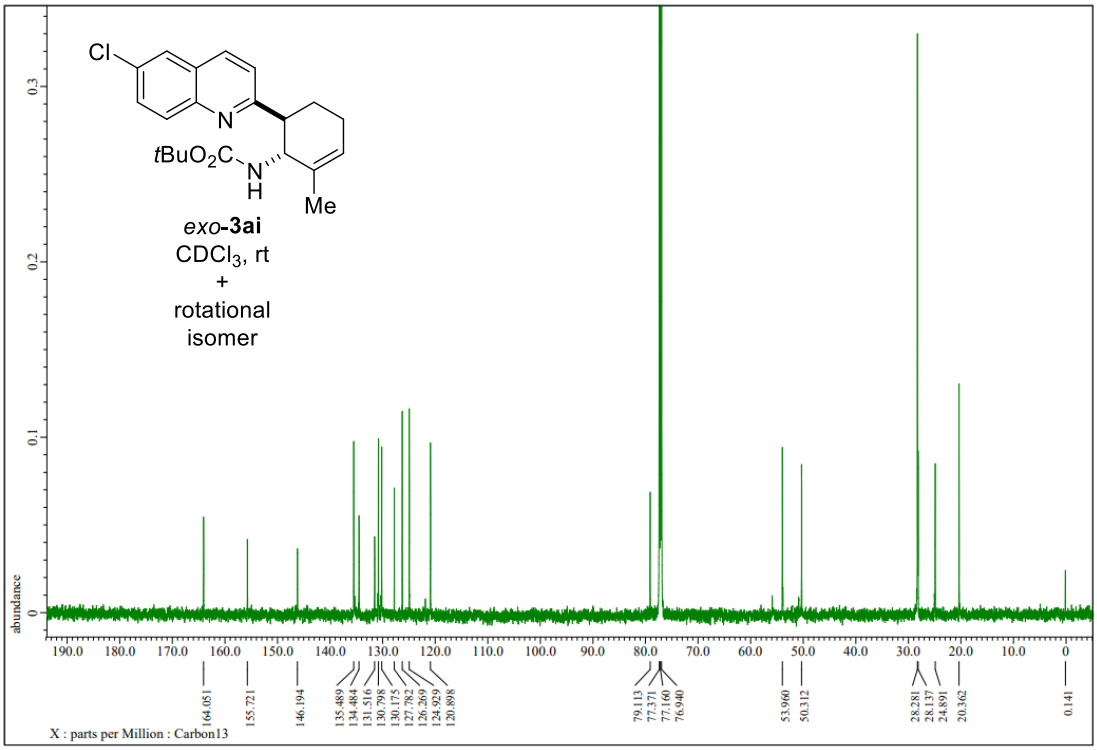
^{1}H and ^{13}C NMR charts of *endo*-**3ah**.



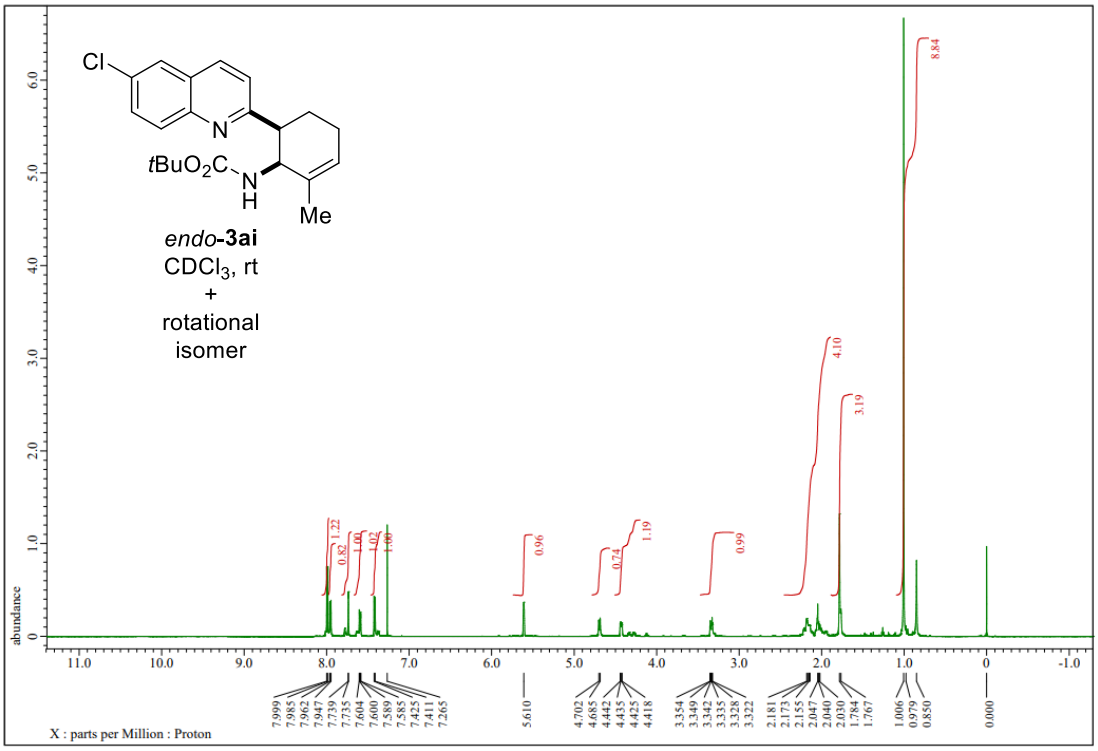


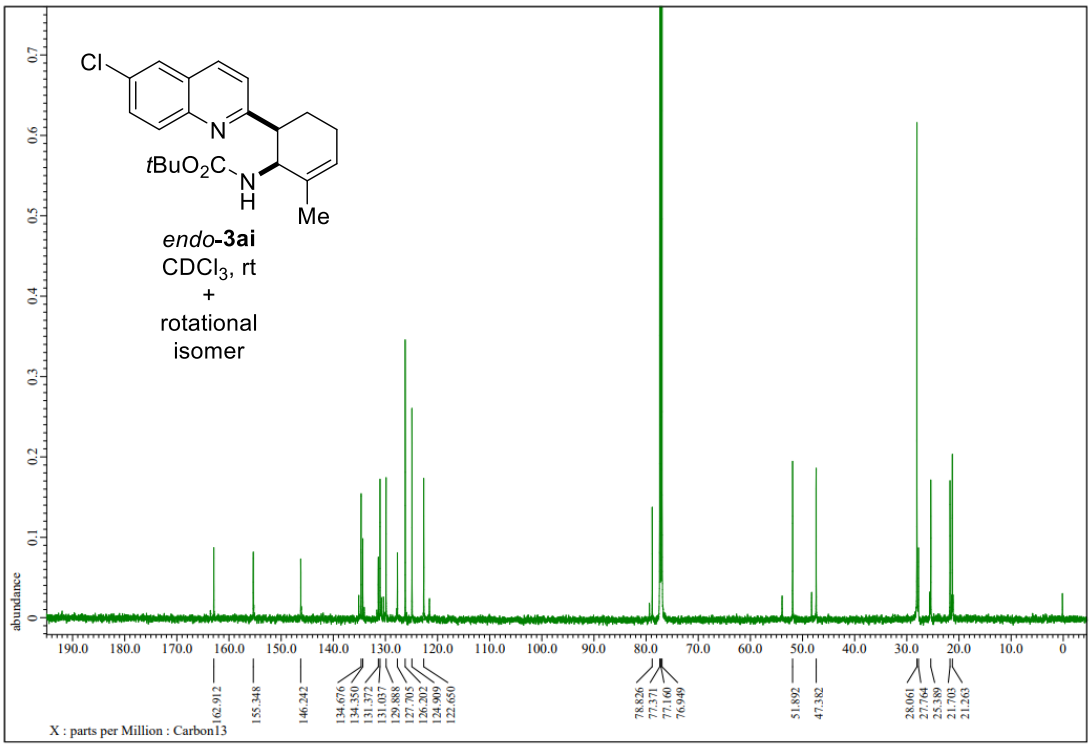
^{1}H and ^{13}C NMR charts of *exo*-**3ai**.



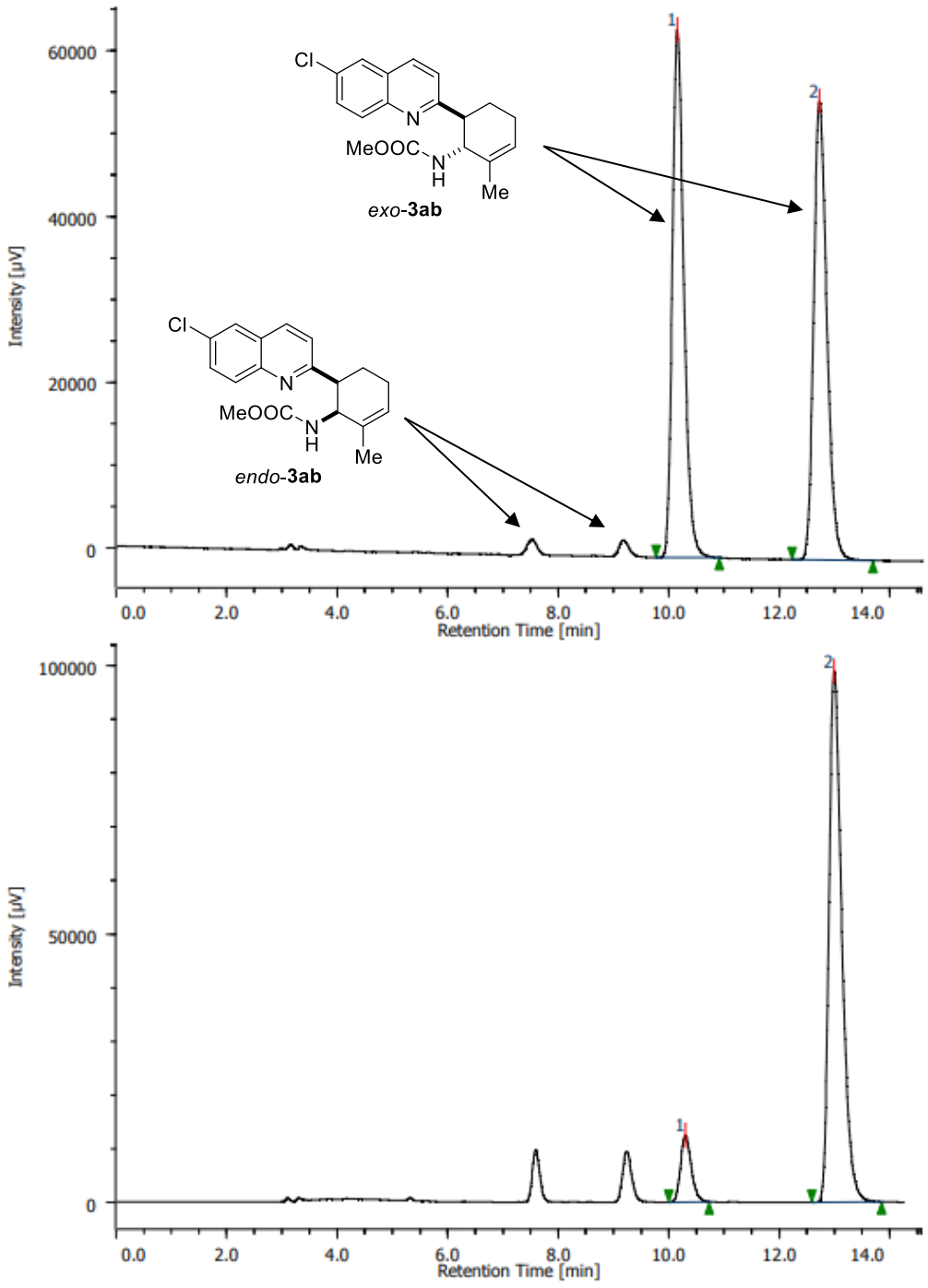


^{1}H and ^{13}C NMR charts of *endo*-**3ai**.





9. HPLC charts



exo-3ab

Peak	1 (*exo*)	2 (*exo*)
Retention Time (min)	10.3	13.0
Area (%)	9.5	90.5-