Supplementary Information

Rhodium/Diene-Catalyzed Tandem 1,4-Shift/1,4-Addition of (*E*)-1,2-Diphenylethenylboronic Acid to Enones: Density Functional Theory Modeling and Asymmetric Catalysis

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Contents of Supplementary Information:

1. General.

All anaerobic and moisture-sensitive manipulations were carried out with standard Schlenk techniques under predried nitrogen or glovebox techniques under argon. NMR spectra were recorded on a JEOL JNM LA-500 spectrometer (500 MHz for ^{1}H NMR and 125 MHz for ^{13}C NMR). Chemical shifts are reported in δ ppm referenced to chloroform-*d* (δ 7.26 for ^{1}H NMR and δ 77.16 for ^{13}C NMR) and benzene-d_6 (δ 7.16 for ^{1}H NMR): the following abbreviations are used; d: doublet, t: triplet, q: quartet, quint: quintet, sept: septet, oct: octet, m: multiplet, br: broad. Optical rotations were measured on a JASCO P-2200 polarimeter. High-resolution mass spectra were obtained with a Bruker micrOTOF spectrometer.

Dioxane, CH_2Cl_2, and toluene were purified by passing through a neutral alumina column under nitrogen atmosphere. MeOH was distilled over magnesium turnings under nitrogen. 1,2-Dimethoxyethane was distilled over benzophenone ketyl under nitrogen.

Rhodium complexes, $[RhCl(bod)]_2$,[1] $[RhCl(nbd)]_2$,[2] $[RhCl(tfb)]_2$,[3] $[RhCl(cod)]_2$,[4] $[Rh(OH)(cod)]_2$,[5] $[RhCl(C_2H_4)_2]_2$,[6] $[RhCl((R,R)$-Ph-bod*$)]_2$,[7] $[RhCl((R,R)$-Bn-bod*$)]_2$,[8] $[RhCl((R)$-**L1**$)]_2$,[9] and $[RhCl((R)$-**L2**$)]_2$[10] were prepared following the literature procedures. (*E*)-1,2-diphenylethenylboronic acid (**1**)[11] were prepared following the literature procedures. The starting enone **2d** was purchased and purified by column chromatography on silica gel (hexane/EtOAc = 20/1). All other materials were purchased and used without purification.

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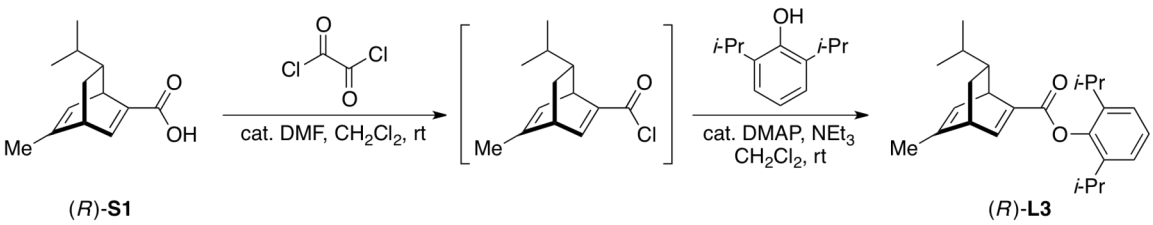
[11] (*a*) J. Cotter, A.-M. L. Hogan and D. F. O'Shea, *Org. Lett.*, 2007, **9**, 1493; (*b*) T. Tricotet, P. Fleming, J. Cotter, A.-M. L. Hogan, C. Strohmann, V. H. Gessner and D. F. O'Shea, *J. Am. Chem. Soc.*, 2009, **131**, 3142.

2. Preparation of ligand L3.



(*R*)-**S1** (*R*)-**L3**

To a solution of (*R*)-**S1**[12] (619 mg, 3.0 mmol) and DMF (10 μL) in CH_2Cl_2 (6.0 mL) was added oxalyl chloride (515 μL, 6.0 mmol) at room temperature, and the mixture was stirred at room temperature for 1 h, then the solvent was removed under reduced pressure. To a solution of 2,6-diisopropylphenol (1.07 g, 6.0 mmol), DMAP (36.7 mg, 0.30 mmol), and triethylamine (0.83 mL, 6.0 mmol) in CH_2Cl_2 (6.0 mL) was added a solution of the acid chloride in CH_2Cl_2 (6.0 mL) dropwise at 0 °C, and the mixture was stirred at room temperature overnight. Aqueous NH_4Cl was added, the organic layer was separated, washed with brine, dried over Na_2SO_4, filtered, and concentrated on a rotary evaporator. The residue was subjected to flash column chromatography on silica gel ($CHCl_3$/hexane = 1/5~EtOAc/hexane = 5/95) to give (*R*)-**L3** (1.06 g, 2.90 mmol, 97% yield). $[\alpha]^{20}_D$ +7.1 (*c* 2.51, $CHCl_3$). ^{1}H NMR ($CDCl_3$): δ 0.86 (d, *J* = 6.5 Hz, 3H), 1.00 (d, *J* = 6.5 Hz, 3H), 1.04 (ddd, *J* = 11.7, 4.9, 2.4 Hz, 1H), 1.10-1.28 (m, 2H), 1.19 (d, *J* = 6.9 Hz, 12H), 1.66 (ddd, *J* = 11.6, 8.7, 3.0 Hz, 1H), 1.88 (d, *J* = 1.7 Hz, 3H), 2.89 (sept, *J* = 6.9 Hz, 2H), 3.46-3.50 (m, 1H), 4.22 (dt, *J* = 6.1, 2.0 Hz, 1H), 5.88 (dt, *J* = 6.0, 1.6 Hz, 1H), 7.151 (d, *J* = 8.6 Hz, 1H), 7.153 (d, *J* = 6.6 Hz, 1H), 7.20 (dd, *J* = 8.8, 6.1 Hz, 1H), 7.56 (dd, *J* = 6.2, 1.8 Hz, 1H). ^{13}C NMR ($CDCl_3$): δ 19.2, 21.5, 22.1, 22.67, 22.74, 23.9, 24.1, 27.70, 27.74, 31.6, 33.9, 40.0, 44.4, 48.3, 123.9, 124.2, 126.3, 140.6, 140.7, 143.5, 146.1, 148.1, 163.6. HRMS (ESI) calcd for $C_{25}H_{34}NaO_2$ $(M+Na)^+$ 389.2451, found 389.2459.

3. Preparation of [RhCl((*R*)-L3)]$_2$.

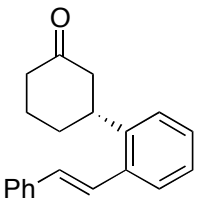
A mixture of (*R*)-**L3** (183 mg, 0.50 mmol) and $[RhCl(C_2H_4)_2]_2$ (107 mg, 0.55 mmol of Rh) in CH_2Cl_2 (10 mL) was stirred at room temperature for 21 h. The mixture was subjected to column chromatography on silica gel under air (hexane/EtOAc = 15/1~2/1)

[12] (*a*) K. Okamoto, T. Hayashi and V. H. Rawal, *Chem. Commun.*, 2009, 4815; (*b*) K. Okamoto, T. Hayashi and V. H. Rawal, *Org. Lett.*, 2008, **10**, 4387; (*c*) G. Pattison, G. Piraux and H. W. Lam, *J. Am. Chem. Soc.*, 2010, **132**, 14373.

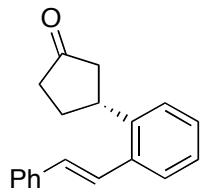
to give [RhCl((*R*)-**L3**)]$_2$ (240 mg, 0.48 mmol of Rh, 95% yield). $[\alpha]^{20}_D$ +179.2 (*c* 0.11, $CHCl_3$). ^{1}H NMR ($CDCl_3$): δ 0.77-0.91 (m, 4H), 0.84 (d, *J* = 6.6 Hz, 6H), 0.93 (d, *J* = 6.6 Hz, 6H), 1.17 (br s, 18H), 1.24-1.32 (m, 2H), 1.34-1.39 (m, 8H), 1.57 (s, 6H), 2.98 (br s, 2H), 3.14 (br s, 2H), 3.39 (d, *J* = 5.5 Hz, 2H), 4.14-4.24 (m, 4H), 4.75 (t, *J* = 5.1 Hz, 2H), 7.13 (d, *J* = 7.2 Hz, 4H), 7.18 (t, *J* = 7.5 Hz, 2H). ^{13}C NMR ($CDCl_3$): δ 20.9 (2C), 21.0 (4C), 23.1 (4C), 24.2 (2C), 24.3 (2C), 27.4 (2C), 27.6 (2C), 30.7 (2C), 31.0 (2C), 43.9 (d, *J* = 3.1 Hz, 2C), 46.9 (2C), 48.1 (d, *J* = 2.6 Hz, 2C), 49.8 (d, *J* = 11.9 Hz, 2C), 51.0 (d, *J* = 10.3 Hz, 2C), 52.6 (d, *J* = 10.1 Hz, 2C), 73.0 (d, *J* = 9.8 Hz, 2C), 123.9 (4C), 126.4 (2C), 140.7 (4C), 146.2 (2C), 168.8 (2C). HRMS (ESI) calcd for $C_{50}H_{68}Cl_3O_4Rh_2$ $(M+Cl)^-$ 1043.2299, found 1043.2300.

4. A typical procedure for the catalytic reactions (entry 5 in Table 3).

To a solution of [RhCl((*R*)-**L3**)]$_2$ (5.0 mg, 10 μmol of Rh, 5 mol % Rh), Cs_2CO_3 (97.7 mg, 0.30 mmol), and (*E*)-1,2-diphenylethenylboronic acid (**1**) (89.6 mg, 0.40 mmol) in dioxane (1.0 mL) was added 2-cyclohexenone (**2a**) (19.2 mg, 0.20 mmol) and H_2O (50 μL). After stirring at 70 °C for 4 h, the reaction mixture was diluted with Et_2O (1.0 mL), and filtered through a pad of silica gel. The plug was washed with Et_2O (30 mL) and the combined filtrates were concentrated on a rotary evaporator. The residue was purified by preparative TLC on silica gel with hexane/EtOAc (3/1) to give **3a** (54.5 mg, 99% yield).

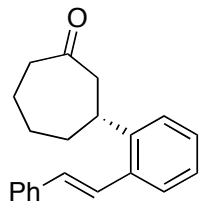


Compound 3a: 99% yield, 99% ee (entry 5 in Table 3). The ee was determined on a Daicel Chiralcel OD-H column with hexane/2-propanol = 80/20, flow = 0.5 mL/min, wavelength = 254 nm. Retention times: 11.9 min [(*S*)-enantiomer], 13.3 min [(*R*)-enantiomer]. $[\alpha]^{20}_D$ +116.4 (*c* 0.90, $CHCl_3$). ^{1}H NMR ($CDCl_3$): δ 1.82 (qdd, *J* = 12.4, 4.6, 3.4 Hz, 1H), 1.88 (qd, *J* = 12.2, 3.0 Hz, 1H), 2.05-2.11 (m, 1H), 2.16 (tt, *J* = 9.7, 3.3 Hz, 1H), 2.41 (td, *J* = 13.2 Hz, 1H), 2.48-2.52 (m, 1H), 2.58 (q, *J* = 13.1 Hz, 1H), 2.60-2.65 (m, 1H), 3.44 (tt, *J* = 11.3, 4.0 Hz, 1H), 6.97 (d, *J* = 16.0 Hz, 1H), 7.25-7.33 (m, 4H), 7.37 (d, *J* = 16.1 Hz, 1H), 7.38 (t, *J* = 7.6 Hz, 2H), 7.51 (d, *J* = 7.8 Hz, 2H), 7.59 (d, *J* = 7.6 Hz, 1H). ^{13}C NMR ($CDCl_3$): δ 25.7, 32.4, 40.3, 41.4, 48.5, 125.5, 125.7, 126.8, 126.96, 126.97, 128.0, 128.2, 128.9, 131.9, 136.0, 137.5, 141.8, 211.0. HRMS (ESI) calcd for $C_{20}H_{20}NaO$ $(M+Na)^+$ 299.1406, found 299.1413.

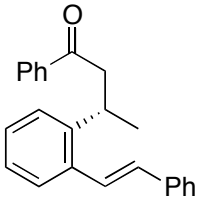


Compound 3b: 95% yield, 96% ee (entry 6 in Table 3). The ee was determined on a Daicel Chiralcel OJ-H column with hexane/2-propanol = 80/20, flow = 0.5 mL/min, wavelength = 254 nm. Retention times: 32.0 min [(*S*)-enantiomer], 35.6 min [(*R*)-enantiomer]. $[\alpha]^{20}_D$ +65.3 (*c* 0.83, $CHCl_3$). ^{1}H NMR ($CDCl_3$): δ 2.03-2.11 (m, 1H), 2.30-2.51 (m, 4H), 2.68 (dd, *J* = 18.5, 7.9 Hz, 1H), 3.81 (tt, *J* = 10.1, 6.7 Hz, 1H), 6.99 (d, *J* = 16.0 Hz, 1H), 7.26-7.33 (m, 4H), 7.38 (t, *J* = 6.8 Hz, 2H), 7.41 (d, *J* = 16.0 Hz, 1H), 7.52 (d, *J* = 7.5 Hz, 2H), 7.60 (d, *J* = 7.8 Hz, 1H). ^{13}C NMR ($CDCl_3$): δ 30.5, 38.5, 38.6, 45.7, 125.2, 126.2, 126.7, 127.0, 127.1, 128.0, 128.2, 128.9, 131.8, 136.9, 137.5, 140.4, 218.4. HRMS (ESI) calcd for $C_{19}H_{18}NaO$ $(M+Na)^+$

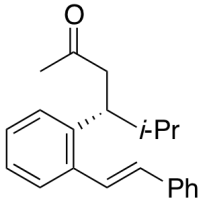
285.1250, found 285. 1251.



Compound 3c: 83% yield, 95% ee (entry 7 in Table 3). The ee was determined on a Daicel Chiralpak AD-H column with hexane/2-propanol = 98/2, flow = 0.5 mL/min, wavelength = 254 nm. Retention times: 37.3 min [(*S*)-enantiomer], 49.1 min [(*R*)-enantiomer]. $[\alpha]^{20}_{D}$ +112.4 (*c* 0.61, $CHCl_3$). ^{1}H NMR ($CDCl_3$): δ 1.47-1.56 (m, 1H), 1.71-1.80 (m, 2H), 2.00-2.13 (m, 3H), 2.63 (dd, *J* = 9.4, 4.3 Hz, 2H), 2.68 (dt, *J* = 14.0, 2.1 Hz, 1H), 2.97 (dd, *J* = 14.1, 11.7 Hz, 1H), 3.30 (tt, *J* = 11.5, 2.2 Hz, 1H), 6.96 (d, *J* = 16.0 Hz, 1H), 7.20-7.30 (m, 4H), 7.39 (t, *J* = 7.7 Hz, 2H), 7.41 (d, *J* = 16.0 Hz, 1H), 7.54 (d, *J* = 7.2 Hz, 2H), 7.57 (dd, *J* = 7.4, 1.4 Hz, 1H). ^{13}C NMR ($CDCl_3$): δ 24.4, 29.5, 38.2, 38.7, 44.1, 50.8, 125.5, 126.0, 126.6, 126.80, 126.83, 127.9, 128.2, 128.9, 131.8, 135.5, 137.6, 144.3, 213.5. HRMS (ESI) calcd for $C_{21}H_{22}NaO$ $(M+Na)^+$ 313.1563, found 313.1572.



Compound 3d: 93% yield, 95% ee (entry 8 in Table 3). The ee was determined on a Daicel Chiralpak AD-H column with hexane/2-propanol = 2/1, flow = 0.5 mL/min, wavelength = 254 nm. Retention times: 10.6 min [(*R*)-enantiomer], 12.6 min [(*S*)-enantiomer]. $[\alpha]^{20}_{D}$ –82.7 (*c* 0.77, $CHCl_3$). ^{1}H NMR ($CDCl_3$): δ 1.36 (d, *J* = 6.8 Hz, 3H), 3.18 (dd, *J* = 16.2, 8.8 Hz, 1H), 3.32 (dd, *J* = 16.3, 5.0 Hz, 1H), 3.97 (dqd, *J* = 8.6, 6.8, 5.2 Hz, 1H), 6.96 (d, *J* = 16.0 Hz, 1H), 7.22-7.42 (m, 8H), 7.51-7.53 (m, 3H), 7.56 (d, *J* = 16.1 Hz, 1H), 7.58 (d, *J* = 8.0 Hz, 1H), 7.94 (d, *J* = 8.4 Hz, 2H). ^{13}C NMR ($CDCl_3$): δ 21.3, 30.9, 46.9, 125.7, 126.5, 126.6, 126.7, 126.8, 127.8, 128.1, 128.3, 128.7, 128.8, 131.5, 133.1, 136.1, 137.3, 137.7, 144.2, 199.2. HRMS (ESI) calcd for $C_{24}H_{22}NaO$ $(M+Na)^+$ 349.1563, found 349.1565.

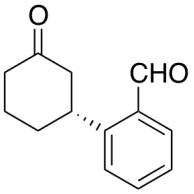


Compound 3e: 73% yield, 99% ee (entry 9 in Table 3). The ee was determined on a Daicel Chiralcel OJ-H column with hexane/2-propanol = 80/20, flow = 0.5 mL/min, wavelength = 254 nm. Retention times: 11.2 min [(*R*)-enantiomer], 14.5 min [(*S*)-enantiomer]. $[\alpha]^{20}_{D}$ –118.4 (*c* 0.57, $CHCl_3$). ^{1}H NMR ($CDCl_3$): δ 0.76 (d, *J* = 6.7 Hz, 3H), 0.96 (d, *J* = 6.6 Hz, 3H), 1.89 (oct, *J* = 6.9 Hz, 1H),

2.00 (s, 3H), 2.86 (d, J = 7.1 Hz, 2H), 3.44 (q, J = 7.4 Hz, 1H), 6.92 (d, J = 16.1 Hz, 1H), 7.14-7.29 (m, 4H), 7.38 (t, J = 7.7 Hz, 2H), 7.54-7.57 (m, 3H), 7.62 (d, J = 16.0 Hz, 1H). ^{13}C NMR ($CDCl_3$): δ 20.5, 21.1, 30.7, 34.0, 42.6, 47.7, 126.4, 126.77, 126.79, 127.5, 127.66, 127.72, 128.8, 131.1, 137.5, 137.9, 142.2, 208.2. HRMS (ESI) calcd for $C_{21}H_{24}NaO$ $(M+Na)^+$ 315.1719, found 315.1720.

5. A procedure for the ozone oxidation in eq 2.

A solution of **3a** (99% ee, 276.4 mg, 1.0 mmol) in CH_2Cl_2 (10 mL) was cooled to –78 °C and ozone was bubbled into the reaction mixture for 10 min. The excess ozone was discharged by nitrogen stream for 10 min, and then dimethyl sulfide (0.37 mL, 5.0 mmol) and CH_2Cl_2 (2 mL) were added. The mixture was allowed to warm to room temperature overnight, and then concentrated on a rotary evaporator. The residue was purified by column chromatography on silica gel (hexane/EtOAc = 2/1) to give aldehyde **18** (162.0 mg, 80% yield).



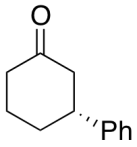
Compound 18: 80% yield. $[\alpha]^{20}_D$ –2.4 (c 0.62, $CHCl_3$). ^{1}H NMR ($CDCl_3$): δ 1.79-1.94 (m, 2H), 2.06-2.16 (m, 2H), 2.39 (ddd, J = 14.6, 12.2, 6.2 Hz, 1H), 2.51 (dt, J = 14.9, 4.0 Hz, 1H), 2.59 (d, J = 8.4 Hz, 2H), 4.18 (dtd, J = 11.1, 8.1, 3.4 Hz, 1H), 7.43-7.46 (m, 2H), 7.60 (td, J = 7.6, 1.5 Hz, 1H), 7.24 (dd, J = 7.8, 1.5 Hz, 1H), 10.22 (s, 1H). ^{13}C NMR ($CDCl_3$): δ 25.4, 33.0, 38.5, 41.3, 48.0, 126.7, 127.2, 133.3, 134.2, 134.3, 146.6, 192.7, 210.6. HRMS (ESI) calcd for $C_{13}H_{14}NaO_2$ $(M+Na)^+$ 225.0886, found 225.0884.

6. A procedure for the decarbonylation in eq 2.

According to a procedure reported by Tsuji,[13] a solution of $[IrCl(cod)]_2$ (6.7 mg, 20 μmol of Ir, 10 mol % Ir) and PPh_3 (5.2 mg, 20 μmol, 10 mol %) in dioxane (2.0 mL) was stirred at room temperature for 10 min. A solution of **18** (99% ee, 40.4 mg, 0.20 mmol) in dioxane (2.0 mL) was added and the mixture was heated for 48 h under reflux. After cooling to room temperature, the mixture was diluted with Et_2O (1.0 mL), and filtered through a pad of silica gel. The plug was washed with Et_2O (30 mL) and the

[13] T. Iwai, T. Fujihara and Y. Tsuji, *Chem. Commun.*, 2008, 6215.

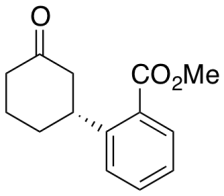
combined filtrates were concentrated on a rotary evaporator. The residue was purified by preparative TLC on silica gel with hexane/EtOAc (3/1) to give **19** (6.1 mg, 18% yield).



Compound 19 [CAS: 34993-51-6 for the (*R*)-enantiomer]: 18% yield, 99% ee. The ee was determined on a Daicel Chiralpak AD-H column with hexane/2-propanol = 100/1, flow = 0.5 mL/min, wavelength = 224 nm. Retention times: 25.6 min [(*S*)-enantiomer], 31.6 min [(*R*)-enantiomer]. $[\alpha]^{20}_{D}$ +18.6 (*c* 0.19, $CHCl_3$); cf. $[\alpha]^{20}_{D}$ +20.3 (*c* 1.04, $CHCl_3$) for the (*R*)-enantiomer.[14]

7. A procedure for the transformation of compound 18 into 21 in eq 2.

To a solution of **18** (100.5 mg, 0.50 mmol) in *t*-BuOH (5.0 mL) were added 2-methyl-2-butene (526 μL, 5.0 mmol), $NaH_2PO_4 \cdot 2H_2O$ (387.6 mg, 2.5 mmol) in H_2O (1.0 mL), and $NaClO_2$ (134.8 mg, 1.5 mmol) in H_2O (1.5 mL) and the mixture was stirred at room temperature for 1 h. The mixture was diluted with H_2O. The aqueous layer was extracted with Et_2O. The combined organic layer was dried over $MgSO_4$, filtered, and concentrated under vacuum. The residue was used directly for the next step without further purification. To the crude carboxylic acid in toluene/MeOH (1.0 mL/2.0 mL) was added dropwise Me_3SiCHN_2 (2.0 M in Et_2O, 0.75 mL, 1.5 mmol), and the mixture was stirred at room temperature for 1 h. The volatiles were removed under reduced pressure. The residue was subjected to preparative TLC on silica gel with hexane/EtOAc (2/1) to give methyl ester **20** (73.8 mg, 64% yield).

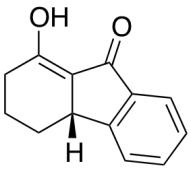


Compound 20 [CAS: 61698-12-2 for racemate]: 64% yield. $[\alpha]^{20}_{D}$ +31.1 (*c* 0.53, $CHCl_3$). ^{1}H NMR ($CDCl_3$): δ 1.77-1.88 (m, 2H), 2.08-2.16 (m, 2H), 2.35-2.41 (m, 1H), 2.46-2.55 (m, 2H), 2.60 (ddt, *J* = 13.8, 4.1, 2.0 Hz, 1H), 3.85-3.95 (m, 1H), 3.89 (s, 3H), 7.28 (td, *J* = 7.6, 1.1 Hz, 1H), 7.40 (d, *J* = 7.9 Hz, 1H), 7.50 (td, *J* = 7.6, 1.4 Hz, 1H), 7.82 (dd, *J* = 7.8, 1.3 Hz, 1H). ^{13}C NMR ($CDCl_3$): δ 25.6, 33.0, 40.2, 41.4, 48.6, 52.3, 126.5, 126.6, 129.8, 130.7, 132.3, 145.4, 168.3, 210.9. HRMS (ESI) calcd

[14] (*a*) A. G. Schultz and R. E. Harrington, *J. Am. Chem. Soc.*, 1991, **113**, 4926; (*b*) R. Shintani, Y. Ichikawa, K. Takatsu, F.-X. Chen and T. Hayashi, *J. Org. Chem.*, 2009, **74**, 869.

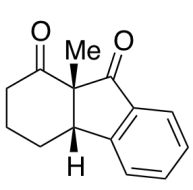
for $C_{14}H_{16}NaO_3$ $(M+Na)^+$ 225.0992, found 225.0994.

To a solution of **20** (14.0 mg, 0.060 mmol) in 1,2-dimethoxyethane (1.0 mL) was added $NaN(SiMe_3)_2$ (1.9 M in THF, 48 μL, 0.090 mmol), and the mixture was stirred at room temperature for 1 h. The mixture was diluted with H_2O. The aqueous layer was washed with Et_2O, acidified with 3.6*N* H_2SO_4, and extracted with Et_2O. The combined organic layer was dried over $MgSO_4$, filtered, and concentrated under vacuum to give diketone **21** (10.2 mg, 85% yield).



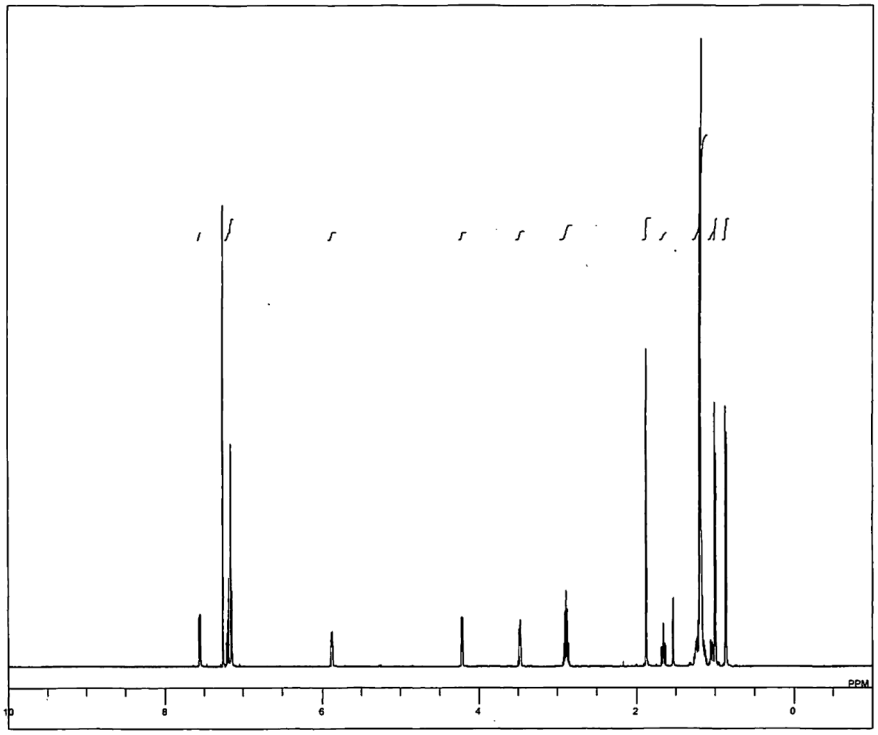
Compound 21: 85% yield, 99% ee. The ee of **21** was determined by HPLC analysis of compound **S2**, which was obtained by methylation of **21** with MeI. $[\alpha]^{20}_D$ –7.8 (*c* 0.72, benzene). Compound **21** exists as an equilibrium mixture of keto and enol forms (keto form/enol form = 9/91 in benzene). ^{1}H NMR (C_6D_6): enol tautomer δ 0.52 (qd, *J* = 12.5, 2.9 Hz, 1H), 1.12-1.22 (m, 1H), 1.39-1.44 (m, 1H), 1.76-1.81 (m, 1H), 1.84-1.91 (m, 1H), 2.07 (dd, *J* = 19.4, 7.0 Hz, 1H), 3.05 (dd, *J* = 11.6, 4.7 Hz, 1H), 7.03 (t, *J* = 7.4 Hz, 1H), 7.09 (dd, *J* = 7.6, 0.9 Hz, 1H), 7.15-7.19 (overlapped with solvent signal, 1H), 7.91 (d, *J* = 7.7 Hz, 1H). HRMS (ESI) calcd for $C_{13}H_{12}NaO_2$ $(M+Na)^+$ 223.0730, found 223.0730.

To a solution of compound **21** (11.9 mg, 0.059 mmol) in acetone (3 mL) were added K_2CO_3 (7.4 mg. 0.053 mmol) and MeI (4.4 μL, 0.071 mmol). The mixture was heated for 3 h under reflux, then filtered, and concentrated under vacuum. The residue was subjected to preparative TLC on silica gel with hexane/EtOAc (1/1) to give **S2** (8.5 mg, 67% yield).



Compound S2: 67% yield, 99% ee. The ee was determined on a Daicel Chiralpak AD-H column with hexane/2-propanol = 90/10, flow = 0.5 mL/min, wavelength = 210 nm. Retention times: 21.4 min [(*S*)-enantiomer], 23.4 min [(*R*)-enantiomer]. $[\alpha]^{20}_D$ –274 (*c* 0.42, $CHCl_3$). ^{1}H NMR ($CDCl_3$): δ 1.40 (s, 3H), 1.47-1.56 (m, 1H), 1.72-1.79 (m, 1H), 2.01-2.06 (m, 1H), 2.11 (dddd, *J* = 14.1, 12.0, 5.9, 3.3 Hz, 1H), 2.32 (dddd, *J* = 17.7, 7.4, 4.4, 0.9 Hz, 1H), 2.38 (ddd, *J* = 17.8, 9.4, 7.0 Hz, 1H), 3.51 (dd, *J* = 5.3, 4.2 Hz, 1H), 7.44 (t, *J* = 7.4 Hz, 1H), 7.53 (dd, *J* = 7.7, 0.6 Hz, 1H), 7.68 (td, *J* = 7.4, 1.0 Hz, 1H),

7.79 (d, J = 7.7 Hz, 1H). ^{13}C NMR ($CDCl_3$): δ 19.1, 21.6, 28.5, 38.6, 49.2, 64.3, 124.8, 125.4, 128.4, 135.6, 135.7, 155.8, 202.4, 207.5. HRMS (ESI) calcd for $C_{14}H_{14}NaO_2$ $(M+Na)^+$ 237.0886, found 237.0892.



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OBSET	0.00 KHz
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IWT	1000.0000 sec
POINT	65536
SPO	65536
TIMES	8
DUMMY	0
FREQU	8000.00 Hz
FLT	4000 Hz
DELAY	50.00 usec
ACQTM	8.1920 sec
PD	1.0000 sec
ADBIT	16
RGAIN	24
BF	0.12 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	non
EXPCM	single pulse nondecoupling & nonpresaturation
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IFR	499.10 MHz
IRSET	0.00 KHz
IRFIN	128250.00 Hz
IRRPW	50 usec
IRATN	511
DFILE	2,6-diisopropylphenylester.als
SF	th5at
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LKFIN	26934.0 Hz
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LGAIN	20
LKPHS	353
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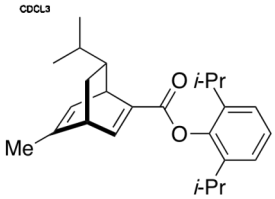
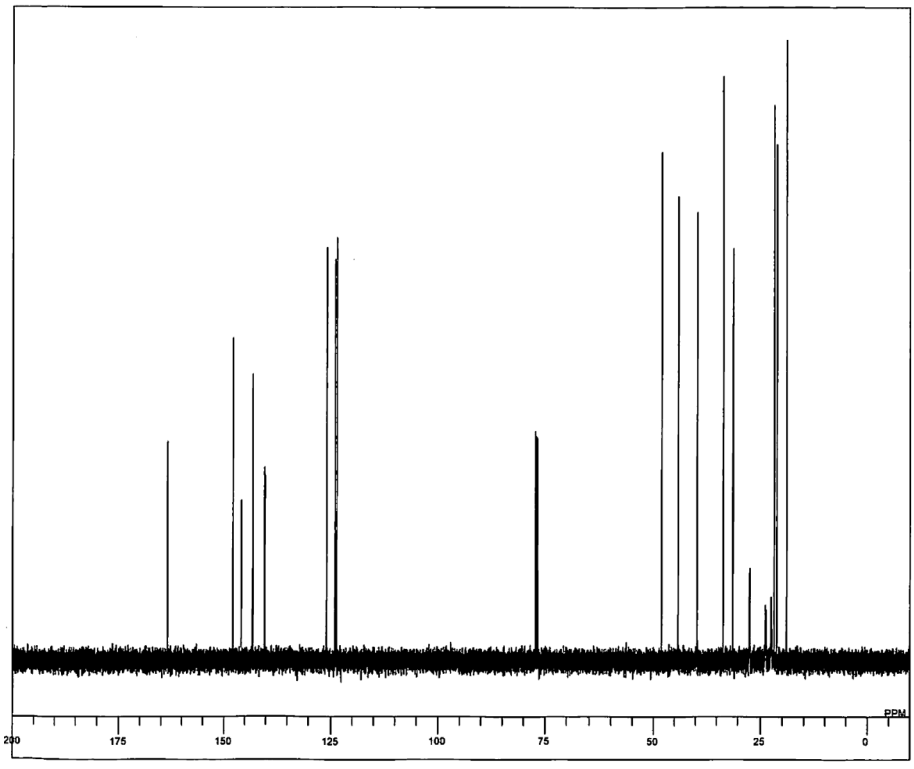
FILDC	
FILDF	
SLVNT	CDCL3



(*R*)-**L3**



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PREDL	0.01000 msec
IWT	1000.0000 sec
POINT	65536
SPO	65536
TIMES	64
DUMMY	2
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	1.9333 sec
PD	1.0670 sec
ADBIT	16
RGAIN	30
BF	0.12 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	single pulse with bilevel decoupling
IRNUC	1H
IFR	499.10 MHz
IRSET	0.00 KHz
IRFIN	128250.00 Hz
IRRPW	50 usec
IRATN	511
DFILE	2,6-diisopropylphenylester_13C.als
SF	th5at
LKSET	0.00 KHz
LKFIN	26934.0 Hz
LKLEV	200
LGAIN	25
LKPHS	353
LKSIG	907
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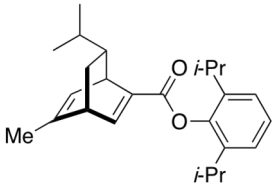
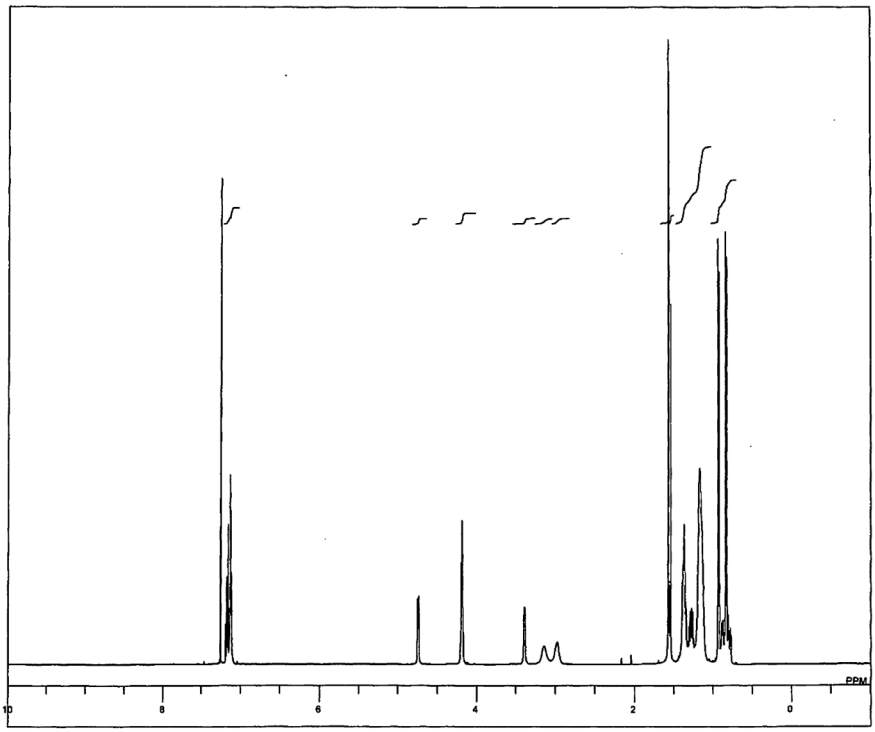
FILDF	
SLVNT	CDCL3



(*R*)-**L3**



MENUF	1H
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PW1	5.50 usec
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POINT	65536
SPO	65536
TIMES	64
DUMMY	0
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FLT	4000 Hz
DELAY	50.00 usec
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PD	1.0000 sec
ADBIT	16
RGAIN	15
BF	0.12 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	non
EXPCM	single pulse nondecoupling & nonpresaturation
IRNUC	1H
IFR	499.10 MHz
IRSET	0.00 KHz
IRFIN	128250.00 Hz
IRRPW	50 usec
IRATN	511
DFILE	RhCl(2,6-diisopropylphenylester-DA-diene).als
SF	th5at
LKSET	0.00 KHz
LKFIN	26934.0 Hz
LKLEV	200
LGAIN	20
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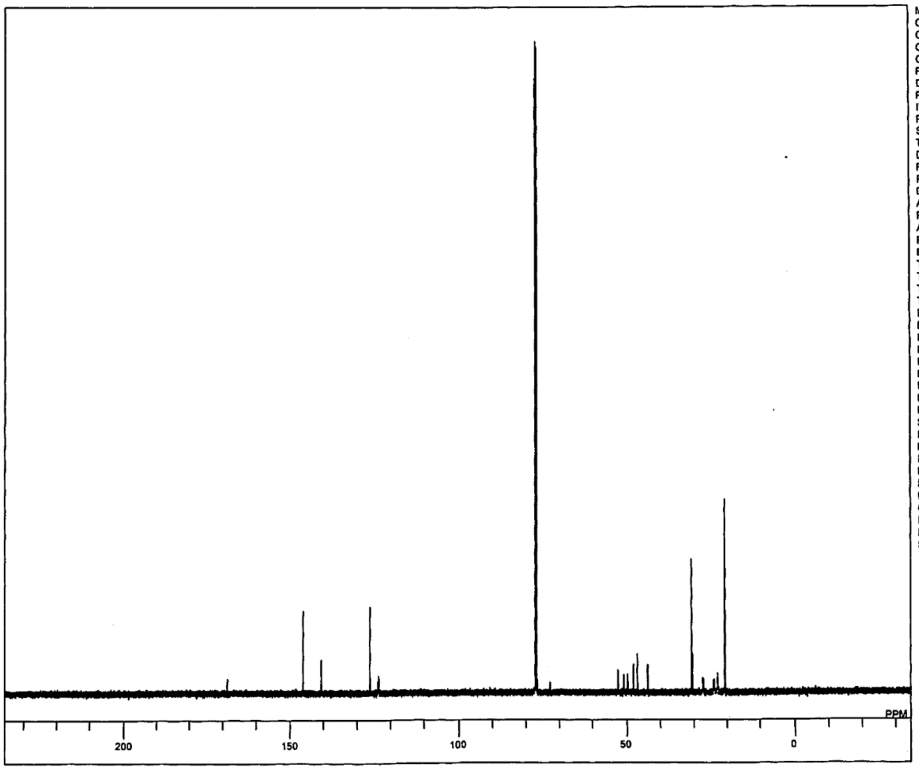
FILDC	
FILDF	
SLVNT	CDCL3

[RhCl((*R*)-**L3**)]$_2$



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OBFIN	143041.00 Hz
PW1	6.25 usec
DEADT	10.00 usec
PREDL	0.01000 msec
IWT	1000.0000 sec
POINT	65536
SPO	65536
TIMES	10000
DUMMY	2
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	1.9333 sec
PD	1.0570 sec
ADBIT	16
RGAIN	24
BF	0.12 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	single pulse with bilevel decoupling
IRNUC	1H
IFR	499.10 MHz
IRSET	0.00 KHz
IRFIN	128250.00 Hz
IRRPW	50 usec
IRATN	511
DFILE	Rh-diene-complex-13C.als
SF	th5at
LKSET	0.00 KHz
LKFIN	26934.0 Hz
LKLEV	200
LGAIN	20
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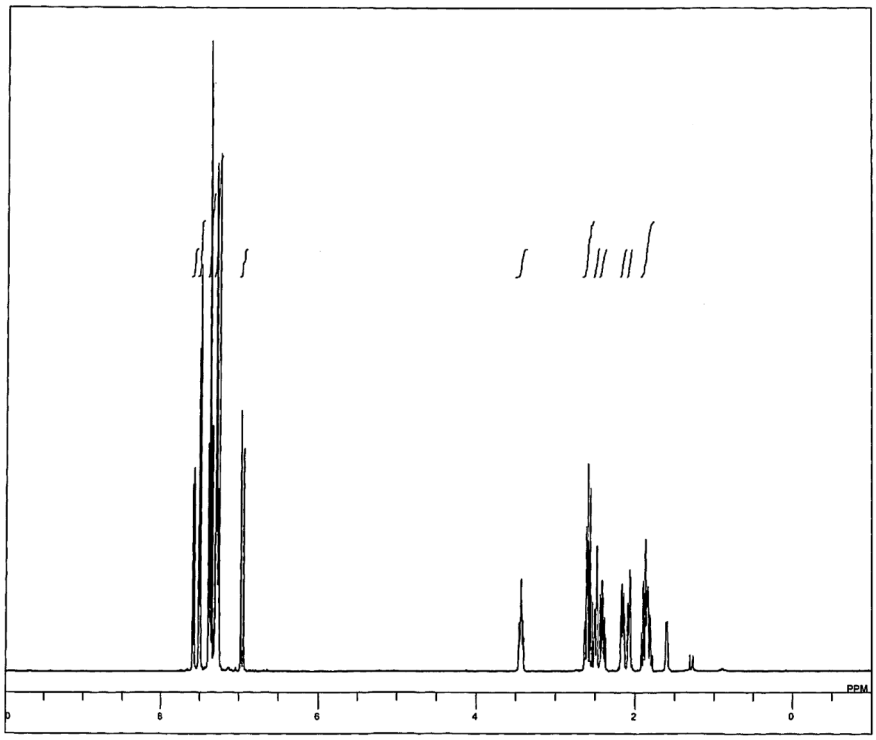
FILDC	
FILDF	
SLVNT	CDCL3

[RhCl((*R*)-**L3**)]$_2$



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OBFIN	128885.00 Hz
PW1	5.50 usec
DEADT	72.30 usec
PREDL	0.01000 msec
IWT	1000.0000 sec
POINT	65536
SPO	65536
TIMES	8
DUMMY	0
FREQU	8000.00 Hz
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DELAY	50.00 usec
ACQTM	8.1920 sec
PD	1.0000 sec
ADBIT	16
RGAIN	13
BF	0.12 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	non
EXPCM	single pulse nondecoupling & nonpresaturation
IRNUC	1H
IFR	499.10 MHz
IRSET	0.00 KHz
IRFIN	128250.00 Hz
IRRPW	50 usec
IRATN	511
DFILE	cyclohexenone-pdt.als
SF	th5at
LKSET	0.00 KHz
LKFIN	26934.0 Hz
LKLEV	200
LGAIN	20
LKPHS	359
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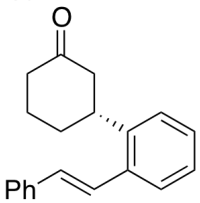
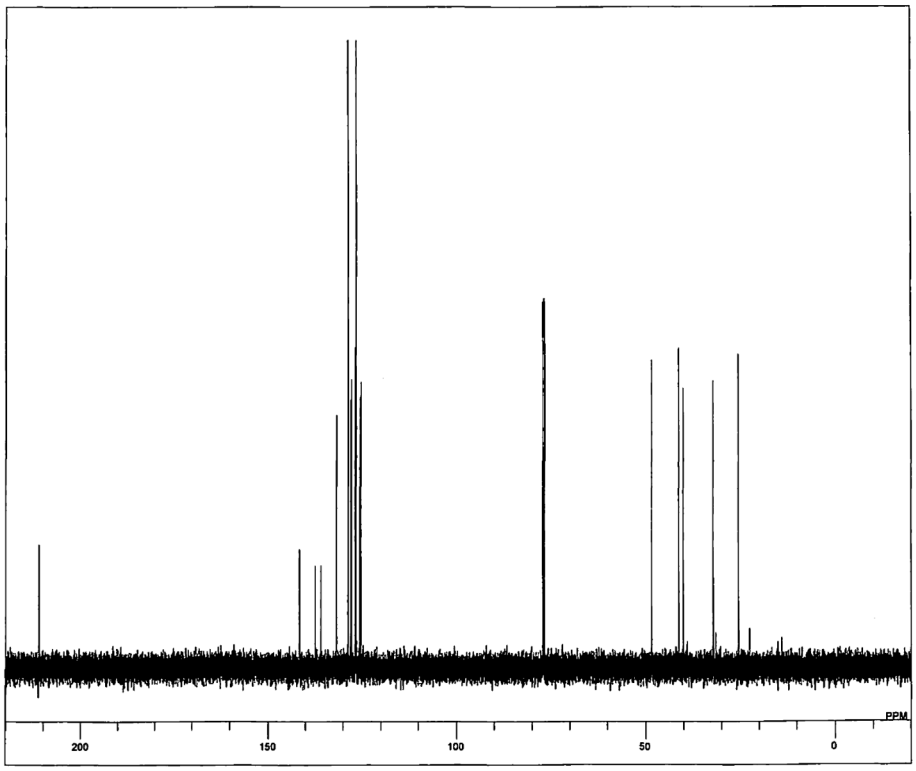
FILDC	
FILDF	
SLVNT	CDCL3



3a



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OBSET	0.00 KHz
OBFIN	143041.00 Hz
PW1	6.25 usec
DEADT	10.00 usec
PREDL	0.01000 msec
IWT	1000.0000 sec
POINT	65536
SPO	65536
TIMES	10000
DUMMY	2
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	1.9333 sec
PD	1.0670 sec
ADBIT	16
RGAIN	24
BF	0.12 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	single pulse with bilevel decoupling
IRNUC	1H
IFR	499.10 MHz
IRSET	0.00 KHz
IRFIN	128250.00 Hz
IRRPW	50 usec
IRATN	511
DFILE	cyclohexenone-pdt-13C.als
SF	th5at
LKSET	0.00 KHz
LKFIN	26934.0 Hz
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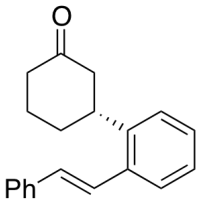
FILDC	
FILDF	
SLVNT	CDCL3



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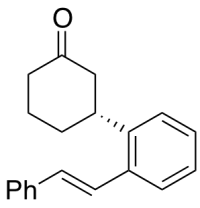

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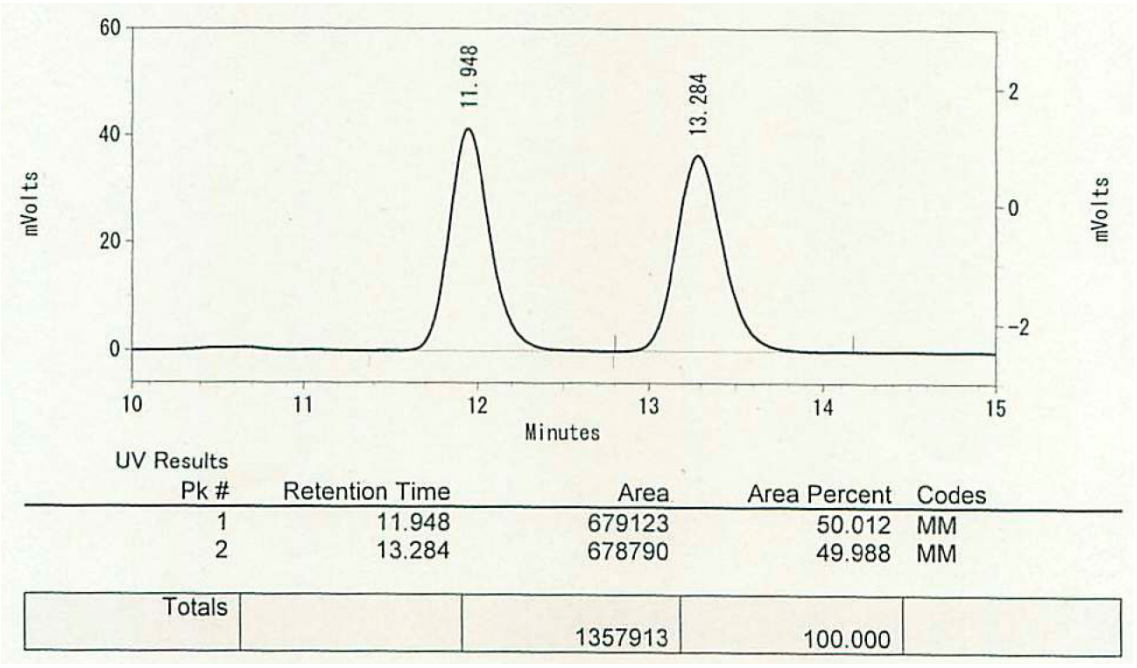

UV Results

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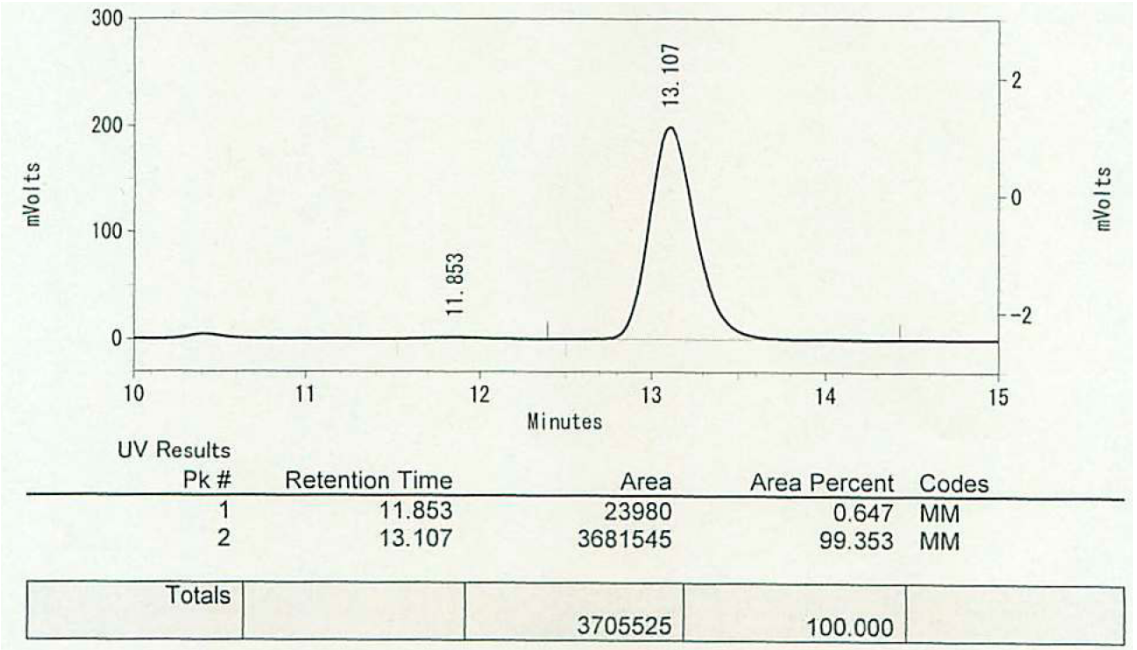

UV Results

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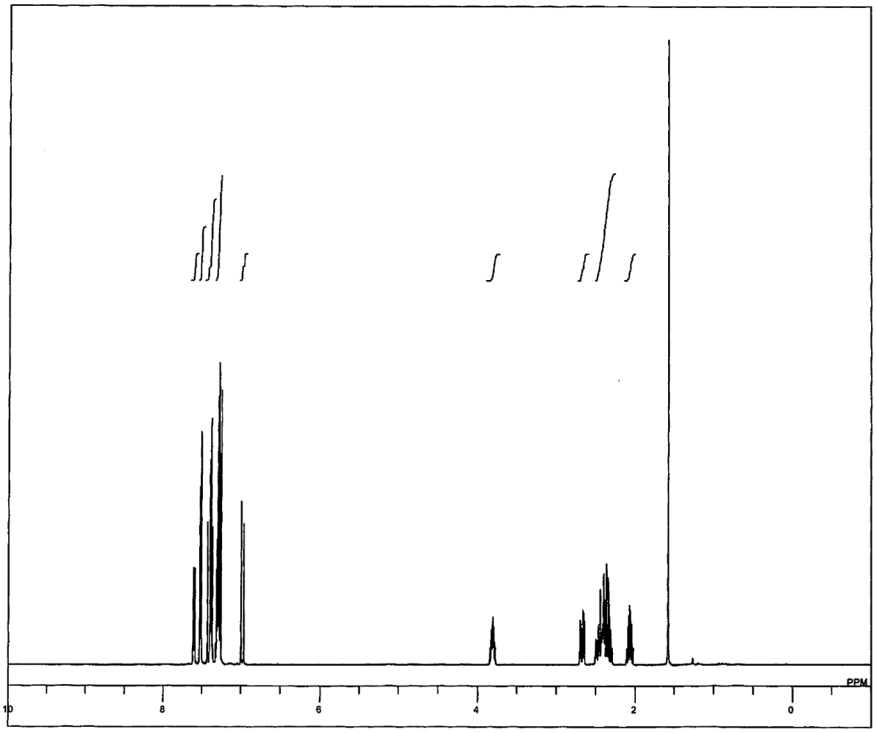

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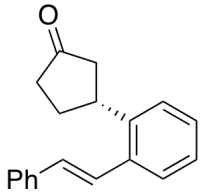
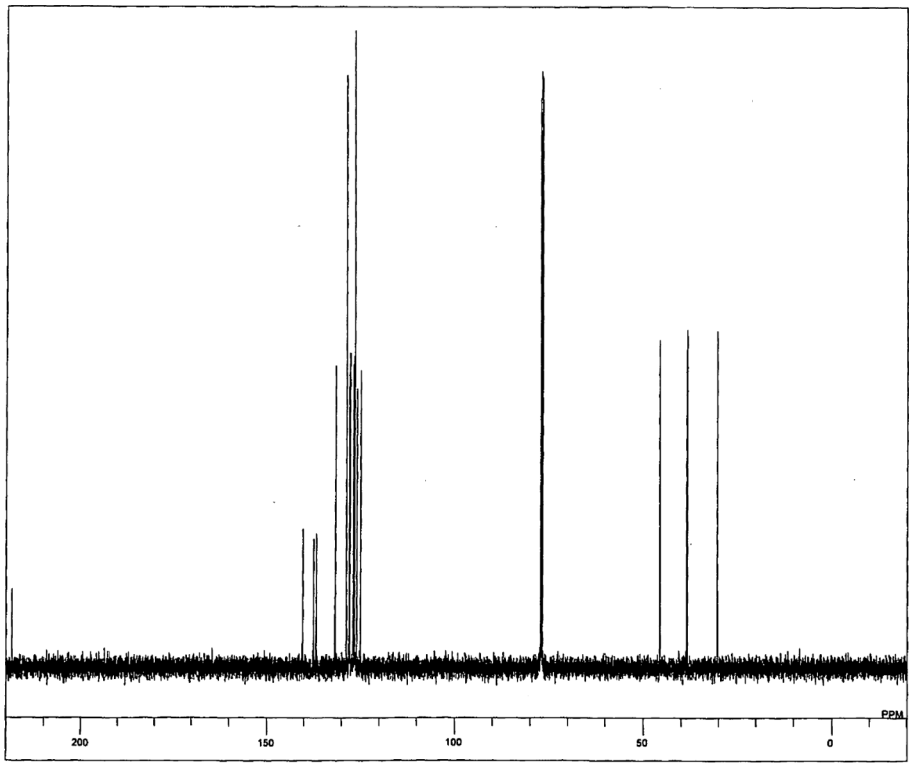
OBSET	0.00 KHz
OBFIN	128885.00 Hz
PW1	5.50 usec
DEADT	72.30 usec
PREDL	0.01000 msec
IWT	1000.0000 sec
POINT	65536
SPO	65536
TIMES	8
DUMMY	0
FREQU	8000.00 Hz
FLT	4000 Hz
DELAY	50.00 usec
ACQTM	8.1920 sec
PD	1.0000 sec
ADBIT	16
RGAIN	15
BF	0.12 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	non
EXPCM	single pulse nondecoupling & nonpresaturation
IRNUC	1H
IFR	499.10 MHz
IRSET	0.00 KHz
IRFIN	128250.00 Hz
IRRPW	50 usec
IRATN	511
DFILE	cyclopentenone-pdt.als
SF	th5at_8
LKSET	0.00 KHz
LKFIN	26934.0 Hz
LKLEV	200
LGAIN	20
LKPHS	359
LKSIG	537
CSPED	15 Hz
FILDC	
FILDF	
SLVNT	CDCL3



3b



MENUF	13C
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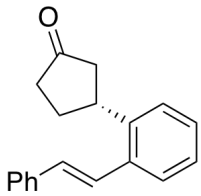
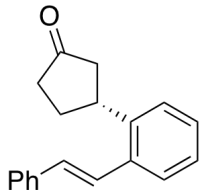
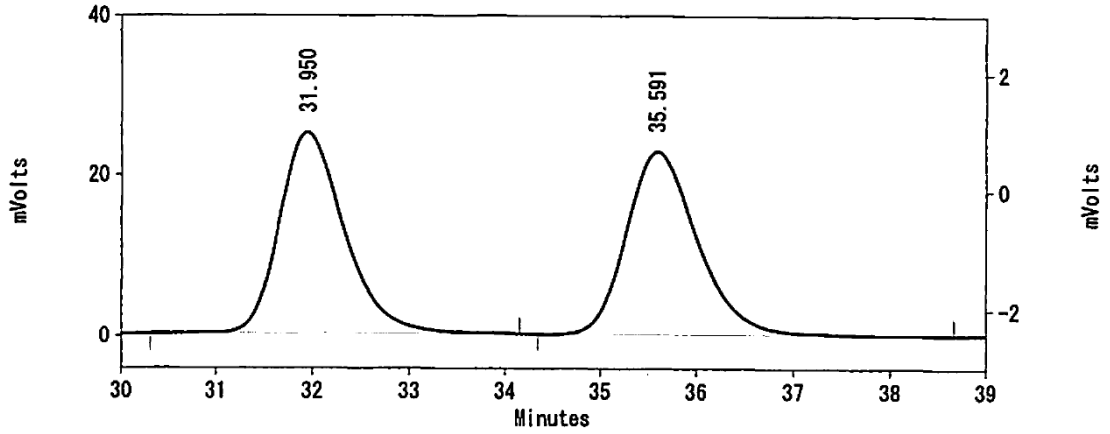
OBSET	0.00 KHz
OBFIN	143041.00 Hz
PW1	6.25 usec
DEADT	10.00 usec
PREDL	0.01000 msec
IWT	1000.0000 sec
POINT	65536
SPO	65536
TIMES	10000
DUMMY	2
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	1.9333 sec
PD	1.0570 sec
ADBIT	16
RGAIN	24
BF	1.20 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	single pulse with bilevel decoupling
IRNUC	1H
IFR	499.10 MHz
IRSET	0.00 KHz
IRFIN	128250.00 Hz
IRRPW	50 usec
IRATN	511
DFILE	cyclopentenona-pdt-13C.als
SF	th5at_8
LKSET	0.00 KHz
LKFIN	26934.0 Hz
LKLEV	200
LGAIN	25
LKPHS	359
LKSIG	1723
CSPED	16 Hz
FILDC	
FILDF	
SLVNT	CDCL3



3b



3b



UV Results

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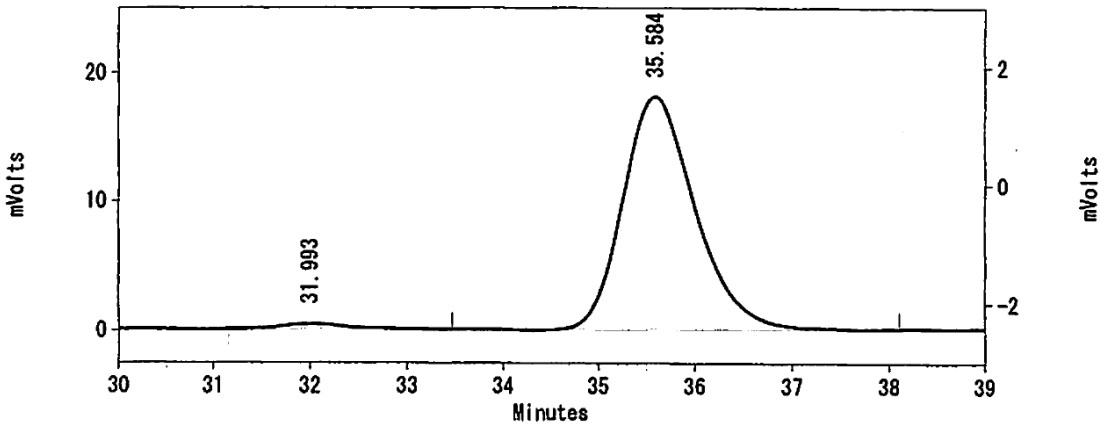

UV Results

Pk #	Retention Time	Area	Area Percent	Codes
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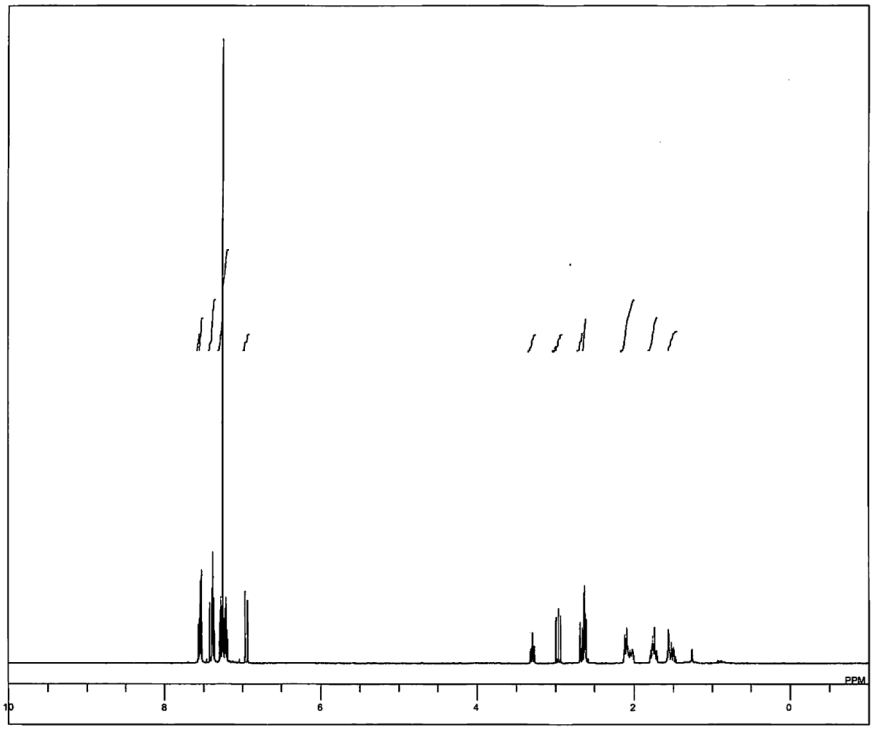
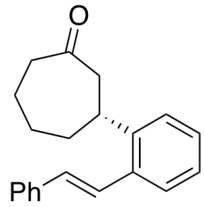
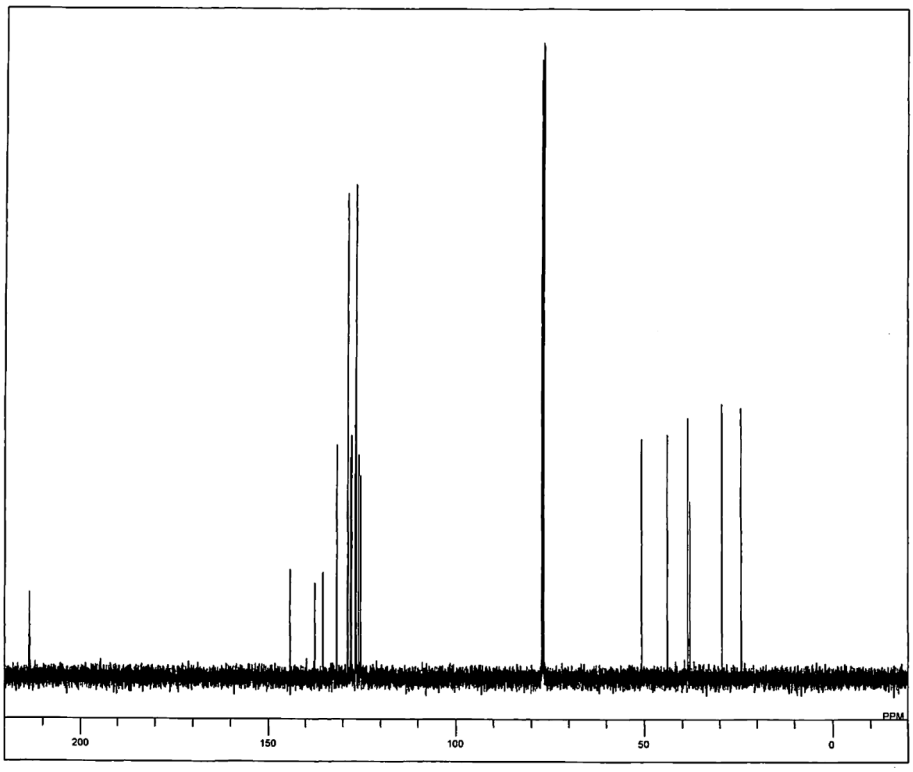
2	35.584	938415	97.898	MM
Totals		958568	100.000	



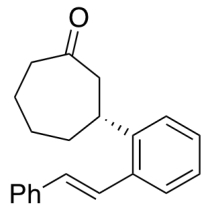
MENUF	1H
OBNUC	1H
OFR	499.10 MHz
OBSET	0.00 KHz
OBFIN	128885.00 Hz
PW1	5.50 usec
DEADT	72.30 usec
PREDL	0.01000 msec
IWT	1000.0000 sec
POINT	65536
SPO	65536
TIMES	8
DUMMY	0
FREQU	8000.00 Hz
FLT	4000 Hz
DELAY	50.00 usec
ACQTM	8.1920 sec
PD	1.0000 sec
ADBIT	16
RGAIN	16
BF	0.12 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	non
EXPCM	single pulse nondecoupling & nonpresaturation
IRNUC	1H
IFR	499.10 MHz
IRSET	0.00 KHz
IRFIN	128250.00 Hz
IRRPW	50 usec
IRATN	511
DFILE	cycloheptenone-pdt-1H.als
SF	th5at
LKSET	0.00 KHz
LKFIN	26934.0 Hz
LKLEV	200
LGAIN	21
LKPHS	359
LKSIG	676
CSPED	15 Hz
FILDC	
FILDF	
SLVNT	CDCL3



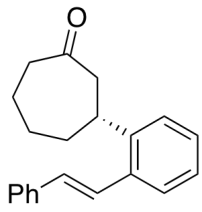
3c



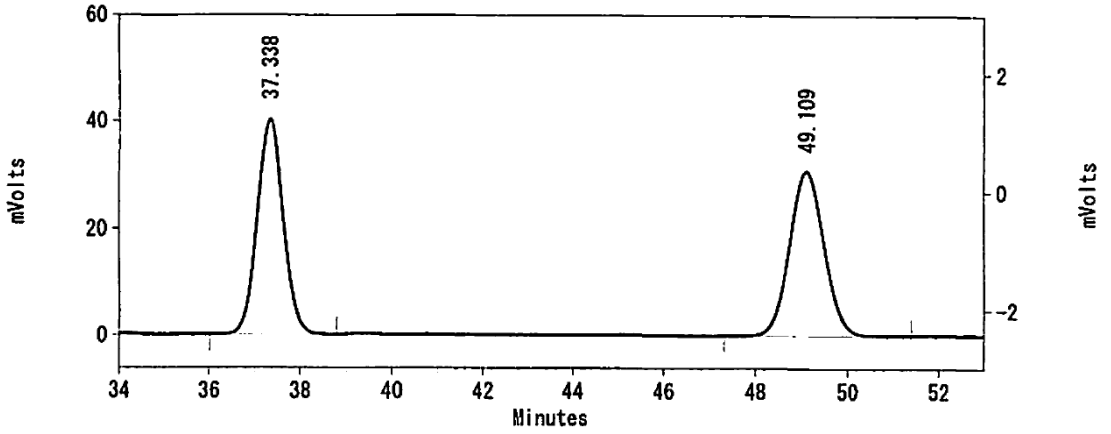
MENUF	13C
OBNUC	13C
OFR	125.40 MHz
OBSET	0.00 KHz
OBFIN	143041.00 Hz
PW1	6.25 usec
DEADT	10.00 usec
PREDL	0.01000 msec
IWT	1000.0000 sec
POINT	65536
SPO	65536
TIMES	10000
DUMMY	2
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	1.9333 sec
PD	1.0670 sec
ADBIT	16
RGAIN	25
BF	1.20 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	single pulse with bilevel decoupling
IRNUC	1H
IFR	499.10 MHz
IRSET	0.00 KHz
IRFIN	128250.00 Hz
IRRPW	50 usec
IRATN	511
DFILE	cycloheptenone-pdt-13C.als
SF	th5at_8
LKSET	0.00 KHz
LKFIN	26934.0 Hz
LKLEV	200
LGAIN	25
LKPHS	359
LKSIG	788
CSPED	16 Hz
FILDC	
FILDF	
SLVNT	CDCL3



3c

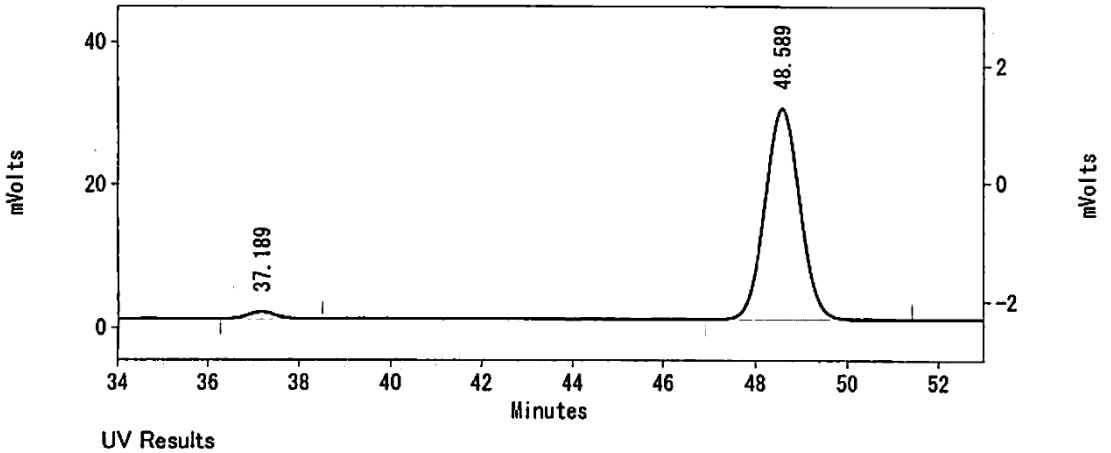


3c



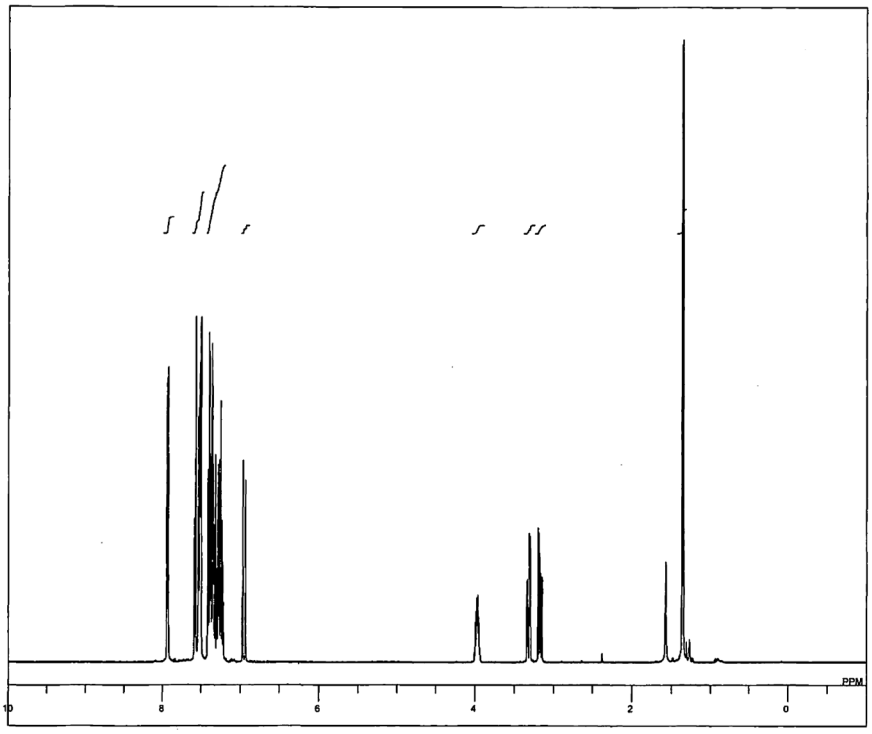
UV Results

Pk #	Retention Time	Area	Area Percent	Codes
1	37.338	1601361	50.124	MM
2	49.109	1593417	49.876	MM
Totals		3194778	100.000	

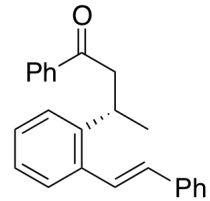


UV Results

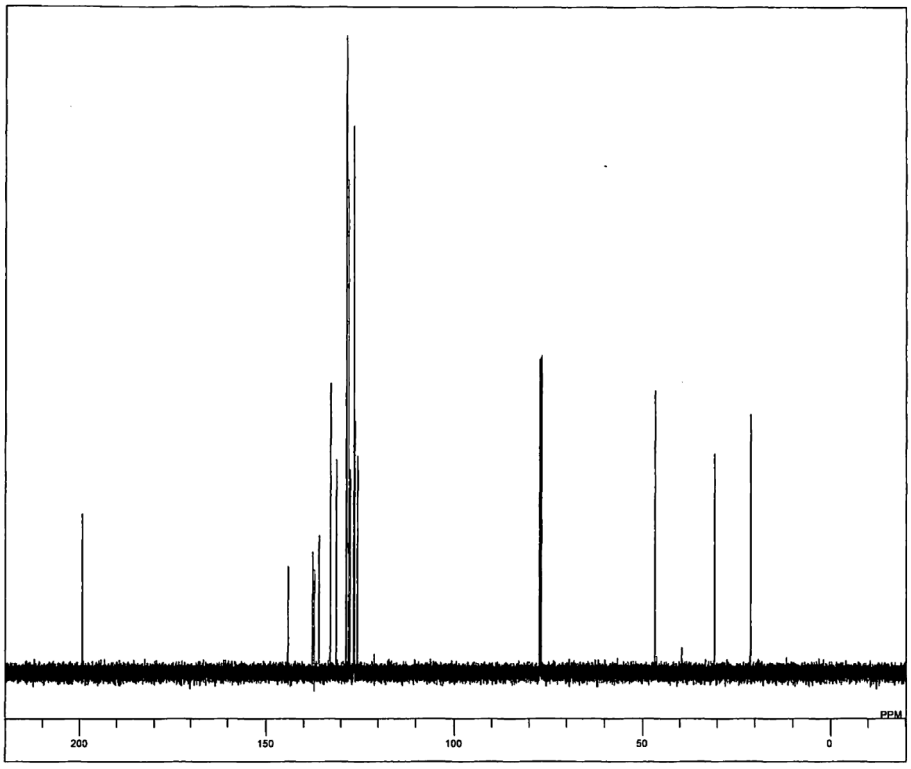
Pk #	Retention Time	Area	Area Percent	Codes
1	37.189	39673	2.498	MM
2	48.589	1548336	97.502	MM
Totals		1588009	100.000	



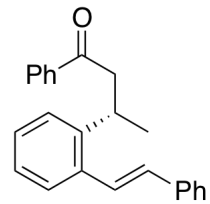
MENUF	1H
OBNUC	1H
OFR	499.10 MHz
OBSET	0.00 KHz
OBFIN	128885.00 Hz
PW1	5.50 usec
DEADT	72.30 usec
PREDL	0.01000 msec
IWT	1000.0000 sec
POINT	65536
SPO	65536
TIMES	8
DUMMY	0
FREQU	8000.00 Hz
FLT	4000 Hz
DELAY	50.00 usec
ACQTM	8.1920 sec
PD	1.0000 sec
ADBIT	16
RGAIN	15
BF	0.12 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	non
EXPCM	single pulse nondecoupling & nonpresaturation
IRNUC	1H
IFR	499.10 MHz
IRSET	0.00 KHz
IRFIN	128250.00 Hz
IRRPW	50 usec
IRATN	511
DFILE	Ph-Me-enone-pdt-1H.als
SF	th5at
LKSET	0.00 KHz
LKFIN	26934.0 Hz
LKLEV	200
LGAIN	21
LKPHS	359
LKSIG	1148
CSPED	17 Hz
FILDC	
FILDF	
SLVNT	CDCL3



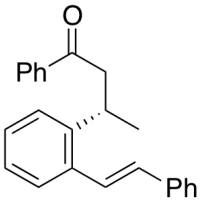
3d



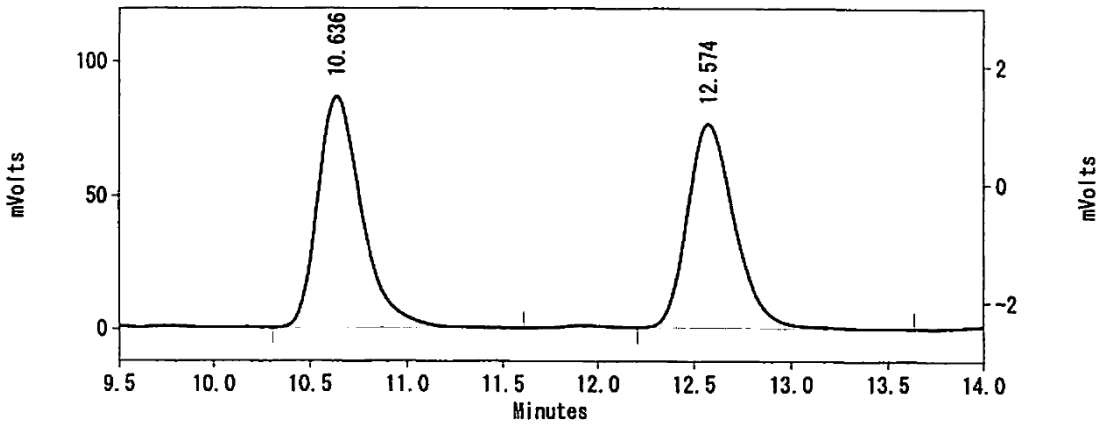
MENUF	13C
OBNUC	13C
OFR	125.40 MHz
OBSET	0.00 KHz
OBFIN	143041.00 Hz
PW1	6.25 usec
DEADT	10.00 usec
PREDL	0.01000 msec
IWT	1000.0000 sec
POINT	65536
SPO	65536
TIMES	10000
DUMMY	2
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	1.9333 sec
PD	1.0870 sec
ADBIT	16
RGAIN	24
BF	0.12 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	single pulse with bilevel decoupling
IRNUC	1H
IFR	499.10 MHz
IRSET	0.00 KHz
IRFIN	128250.00 Hz
IRRPW	50 usec
IRATN	511
DFILE	Ph-Me-enone-pdt-13C.als
SF	th5at
LKSET	0.00 KHz
LKFIN	26934.0 Hz
LKLEV	200
LGAIN	20
LKPHS	359
LKSIG	533
CSPED	16 Hz
FILDC	
FILDF	
SLVNT	CDCL3



3d

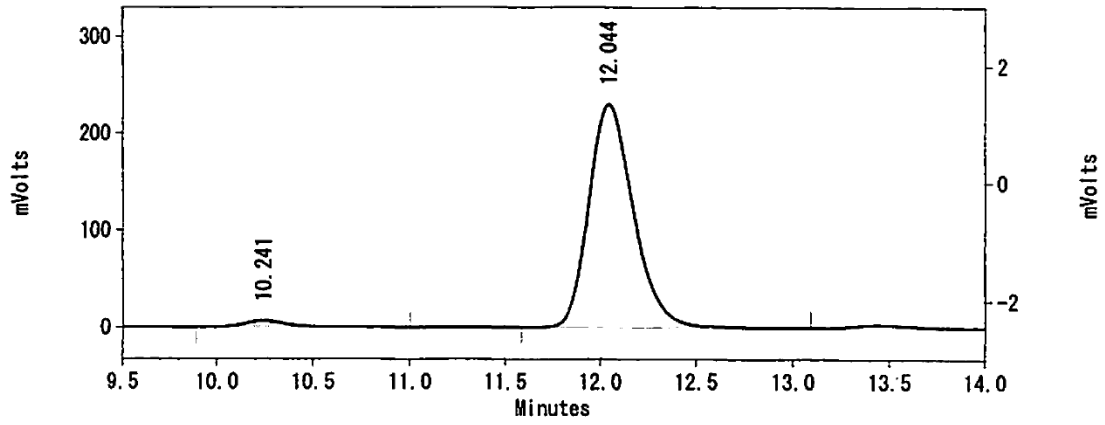


3d



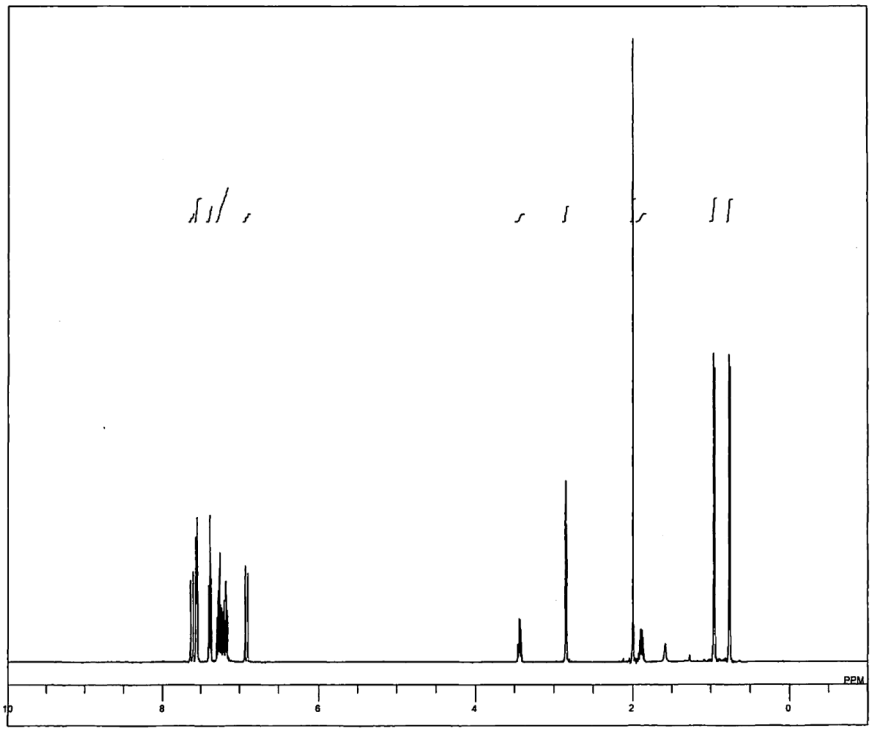
UV Results

Pk #	Retention Time	Area	Area Percent	Codes
1	10.636	1362417	51.476	MM
2	12.574	1284307	48.524	MM
Totals		2646724	100.000	

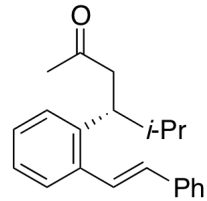


UV Results

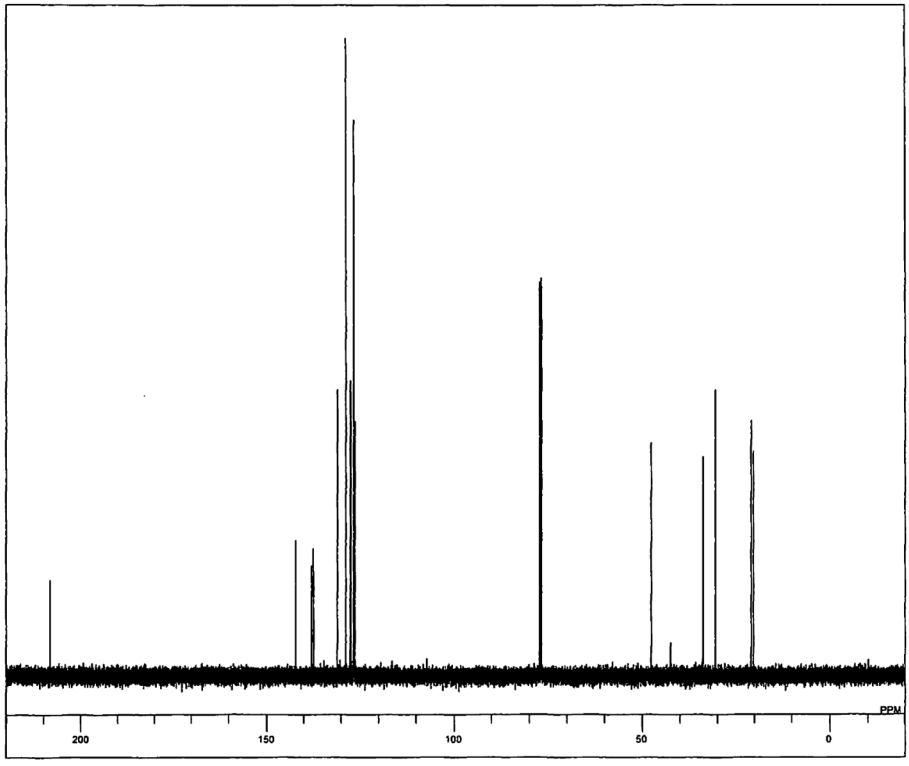
Pk #	Retention Time	Area	Area Percent	Codes
1	10.241	95708	2.514	MM
2	12.044	3711726	97.486	MM
Totals		3807434	100.000	



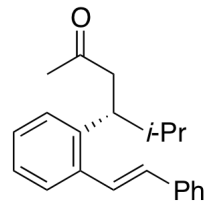
MENUF	1H
OBNUC	1H
OFR	499.10 MHz
OBSET	0.00 KHz
OBFIN	128885.00 Hz
PW1	5.50 usec
DEADT	72.30 usec
PREDL	0.01000 msec
IWT	1000.0000 sec
POINT	65536
SPO	65536
TIMES	8
DUMMY	0
FREQU	8000.00 Hz
FLT	4000 Hz
DELAY	50.00 usec
ACQTM	8.1920 sec
PD	1.0000 sec
ADBIT	16
RGAIN	14
BF	0.12 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	non
EXPCM	single pulse nondecoupling & nonpresaturation
IRNUC	1H
IFR	499.10 MHz
IRSET	0.00 KHz
IRFIN	128250.00 Hz
IRRPW	50 usec
IRATN	511
DFILE	Me-iPr-enone-pdt-1H.als
SF	th5at_9
LKSET	0.00 KHz
LKFIN	26934.0 Hz
LKLEV	200
LGAIN	21
LKPHS	359
LKSIG	934
CSPED	15 Hz
FILDC	
FILDF	
SLVNT	CDCL3



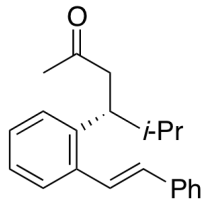
3e



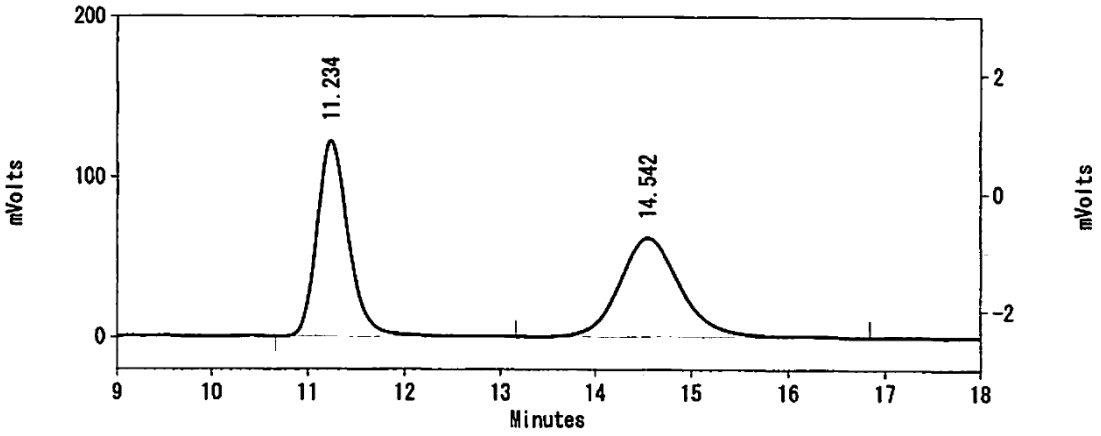
MENUF	13C
OBNUC	13C
OFR	125.40 MHz
OBSET	0.00 KHz
OBFIN	143041.00 Hz
PW1	6.25 usec
DEADT	10.00 usec
PREDL	0.01000 msec
IWT	1000.0000 sec
POINT	65536
SPO	65536
TIMES	10000
DUMMY	2
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	1.9333 sec
PD	1.0670 sec
ADBIT	16
RGAIN	24
BF	0.12 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	single pulse with bilevel decoupling
IRNUC	1H
IFR	499.10 MHz
IRSET	0.00 KHz
IRFIN	128250.00 Hz
IRRPW	50 usec
IRATN	511
DFILE	Me-iPr-enone-pdt-13C.als
SF	th5at_9
LKSET	0.00 KHz
LKFIN	26934.0 Hz
LKLEV	200
LGAIN	21
LKPHS	359
LKSIG	984
CSPED	13 Hz
FILDC	
FILDF	
SLVNT	CDCL3



3e

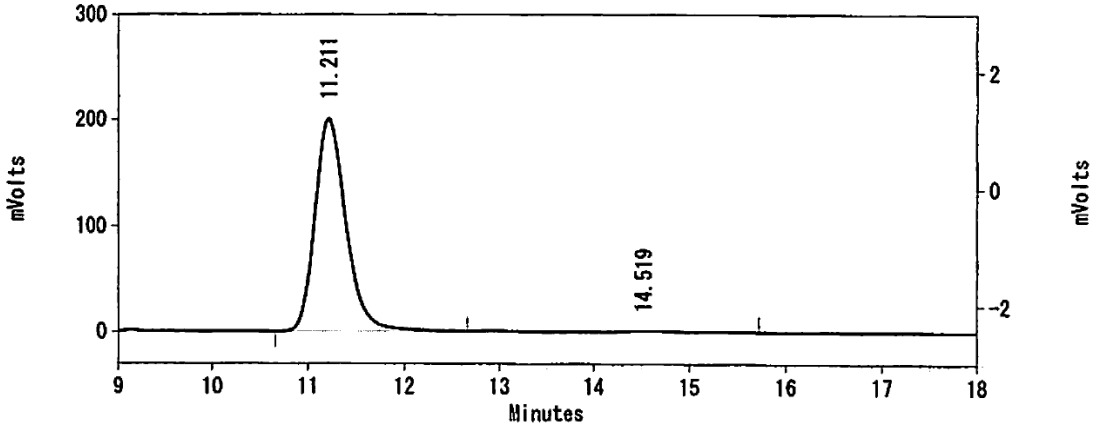


3e



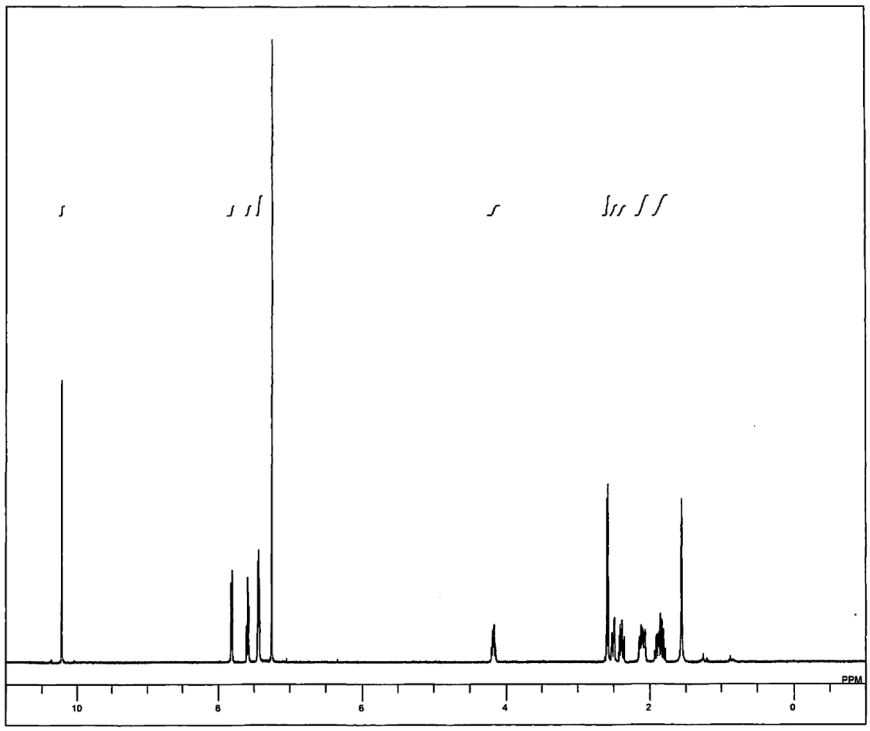
UV Results

Pk #	Retention Time	Area	Area Percent	Codes
1	11.234	2719991	49.953	MM
2	14.542	2725108	50.047	MM
Totals		5445099	100.000	

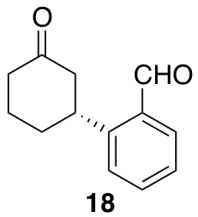


UV Results

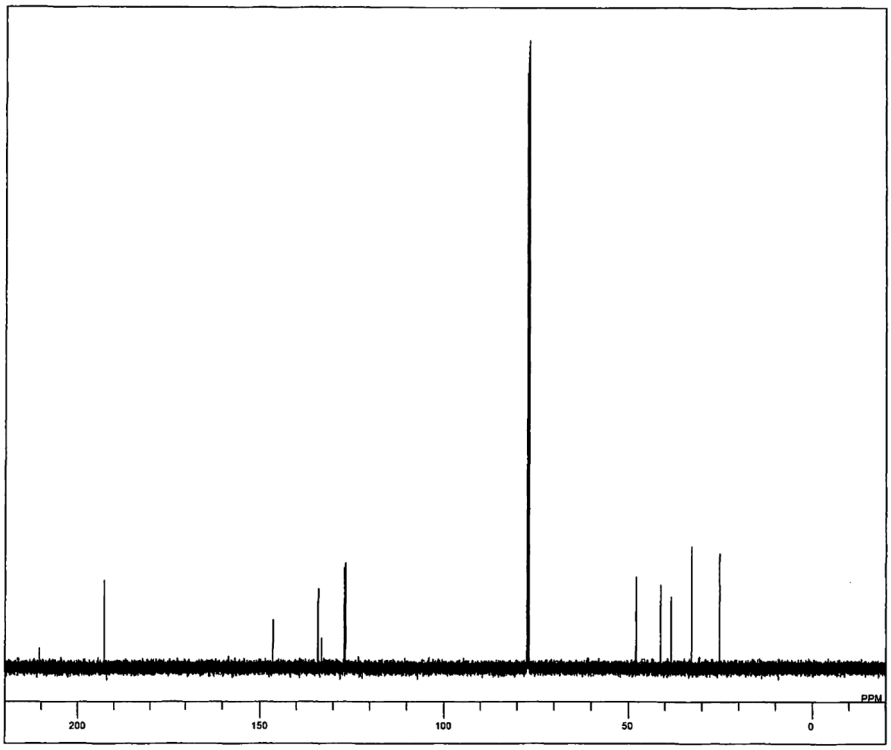
Pk #	Retention Time	Area	Area Percent	Codes
1	11.211	4455055	99.326	MM
2	14.519	30215	0.674	MM
Totals		4485270	100.000	



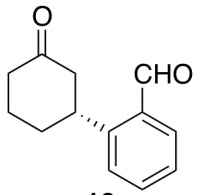
MENUF	1H
OBNUC	1H
OFR	499.10 MHz
OBSET	0.00 KHz
OBFIN	128885.00 Hz
PW1	5.50 usec
DEADT	72.30 usec
PREDL	0.01000 msec
IWT	1000.0000 sec
POINT	65536
SPO	65536
TIMES	8
DUMMY	0
FREQU	8000.00 Hz
FLT	4000 Hz
DELAY	50.00 usec
ACQTM	8.1920 sec
PD	1.0000 sec
ADBIT	16
RGAIN	19
BF	0.12 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	non
EXPCM	single pulse nondecoupling & nonpresaturation
IRNUC	1H
IFR	499.10 MHz
IRSET	0.00 KHz
IRFIN	128250.00 Hz
IRRPW	50 usec
IRATN	511
DFILE	cyclohexenone-ozonolysis-pdt.als
SF	th5at_9
LKSET	0.00 KHz
LKFIN	26934.0 Hz
LKLEV	200
LGAIN	20
LKPHS	359
LKSIG	514
CSPED	17 Hz
FILDC	
FILDF	
SLVNT	CDCL3



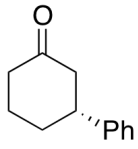
18



MENUF	13C
OBNUC	13C
OFR	125.40 MHz
OBSET	0.00 KHz
OBFIN	143041.00 Hz
PW1	6.25 usec
DEADT	10.00 usec
PREDL	0.01000 msec
IWT	1000.0000 sec
POINT	65536
SPO	65536
TIMES	10000
DUMMY	2
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	1.9333 sec
PD	1.0670 sec
ADBIT	16
RGAIN	24
BF	0.12 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	single pulse with bilevel decoupling
IRNUC	1H
IFR	499.10 MHz
IRSET	0.00 KHz
IRFIN	128250.00 Hz
IRRPW	50 usec
IRATN	511
DFILE	cyclohexenone-ozonolysis-pdt-13C.als
SF	th5at_9
LKSET	0.00 KHz
LKFIN	26934.0 Hz
LKLEV	200
LGAIN	22
LKPHS	359
LKSIG	865
CSPED	17 Hz
FILDC	
FILDF	
SLVNT	CDCL3



18



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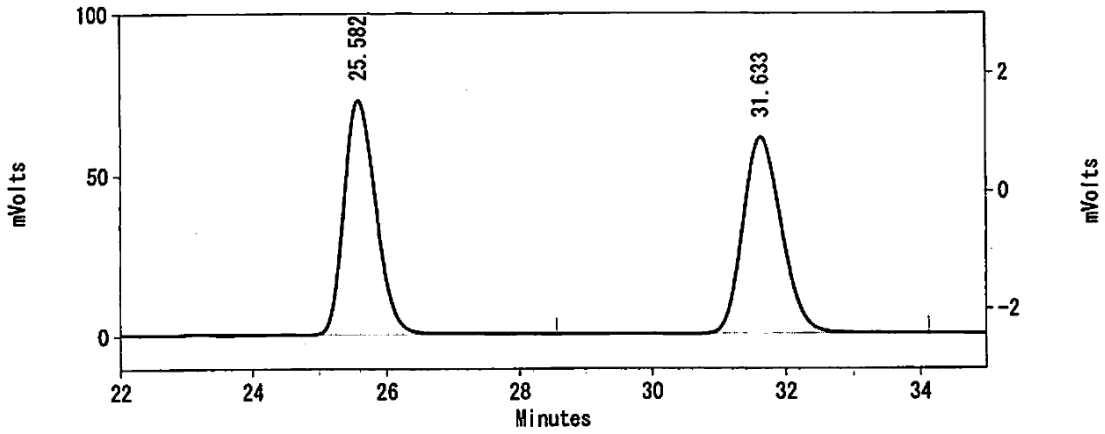
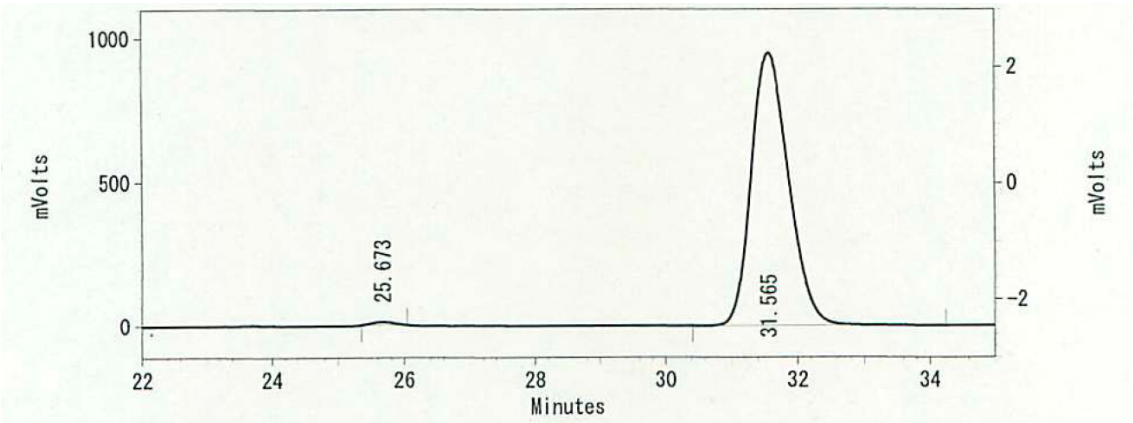


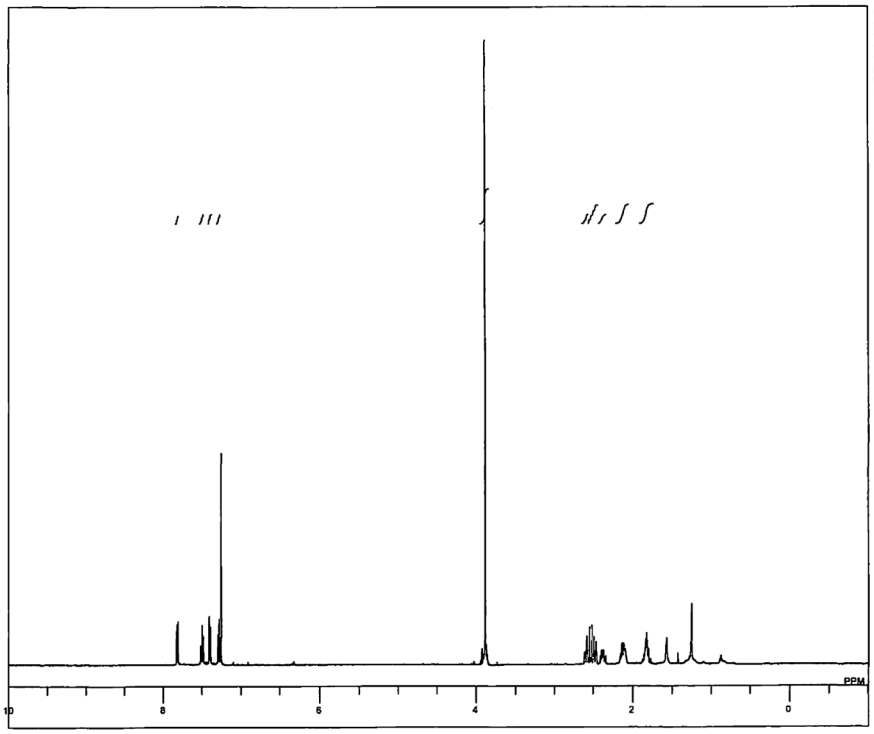
UV Results

Pk #	Retention Time	Area	Area Percent	Codes
1	25.582	2418222	49.683	MM
2	31.633	2449057	50.317	MM
Totals		4867279	100.000	

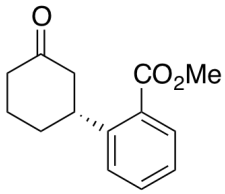


UV Results

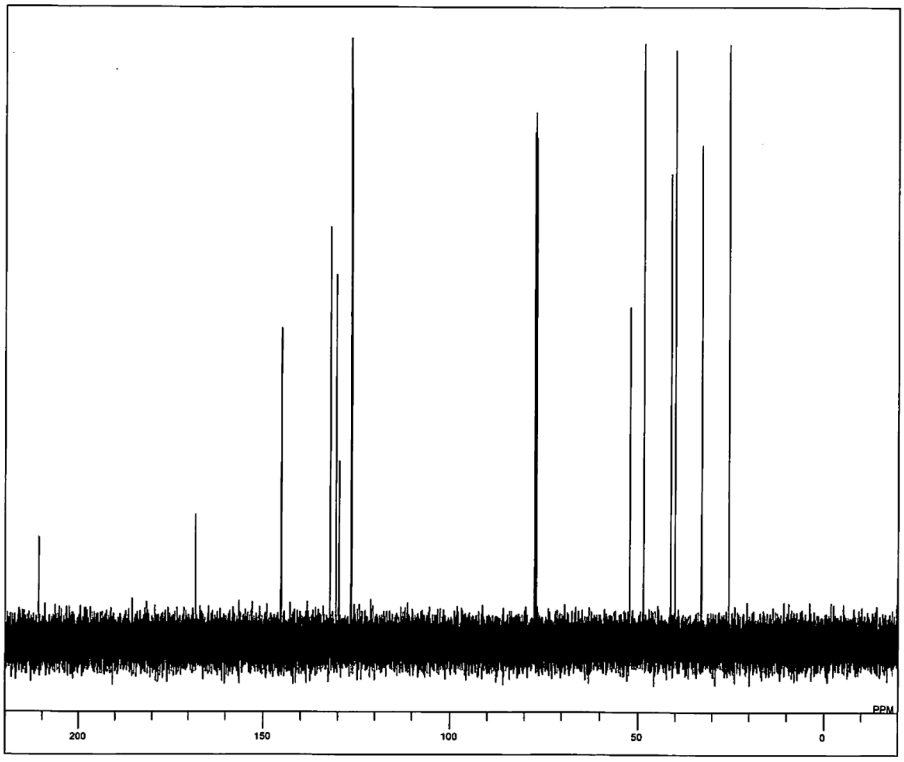
Pk #	Retention Time	Area	Area Percent	Codes
1	25.673	263660	0.702	MM
2	31.565	37315028	99.298	MM
Totals		37578688	100.000	



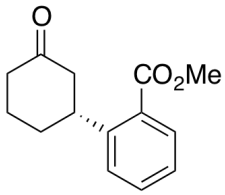
MENUF	1H
OBNUC	1H
OFR	499.10 MHz
OBSET	0.00 KHz
OBFIN	128885.00 Hz
PW1	5.50 usec
DEADT	72.30 usec
PREDL	0.01000 msec
IWT	1000.0000 sec
POINT	65536
SPO	65536
TIMES	8
DUMMY	0
FREQU	8000.00 Hz
FLT	4000 Hz
DELAY	50.00 usec
ACQTM	8.1920 sec
PD	1.0000 sec
ADBIT	16
RGAIN	17
BF	0.12 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	non
EXPCM	single pulse nondecoupling & nonpresaturation
IRNUC	1H
IFR	499.10 MHz
IRSET	0.00 KHz
IRFIN	128250.00 Hz
IRRPW	50 usec
IRATN	511
DFILE	cyclohexenone-ester-pdt.als
SF	th5at_9
LKSET	0.00 KHz
LKFIN	26934.0 Hz
LKLEV	200
LGAIN	21
LKPHS	359
LKSIG	545
CSPED	16 Hz
FILDC	
FILDF	
SLVNT	CDCL3



20



MENUF	13C
OBNUC	13C
OFR	125.40 MHz
OBSET	0.00 KHz
OBFIN	143041.00 Hz
PW1	6.25 usec
DEADT	10.00 usec
PREDL	0.01000 msec
IWT	1000.0000 sec
POINT	65536
SPO	65536
TIMES	10000
DUMMY	2
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	1.9333 sec
PD	1.0670 sec
ADBIT	16
RGAIN	24
BF	0.12 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	single pulse with bilevel decoupling
IRNUC	1H
IFR	499.10 MHz
IRSET	0.00 KHz
IRFIN	128250.00 Hz
IRRPW	50 usec
IRATN	511
DFILE	cyclohexenone-ester-pdt-13C.als
SF	th5at
LKSET	0.00 KHz
LKFIN	26934.0 Hz
LKLEV	200
LGAIN	23
LKPHS	359
LKSIG	636
CSPED	17 Hz
FILDC	
FILDF	
SLVNT	CDCL3



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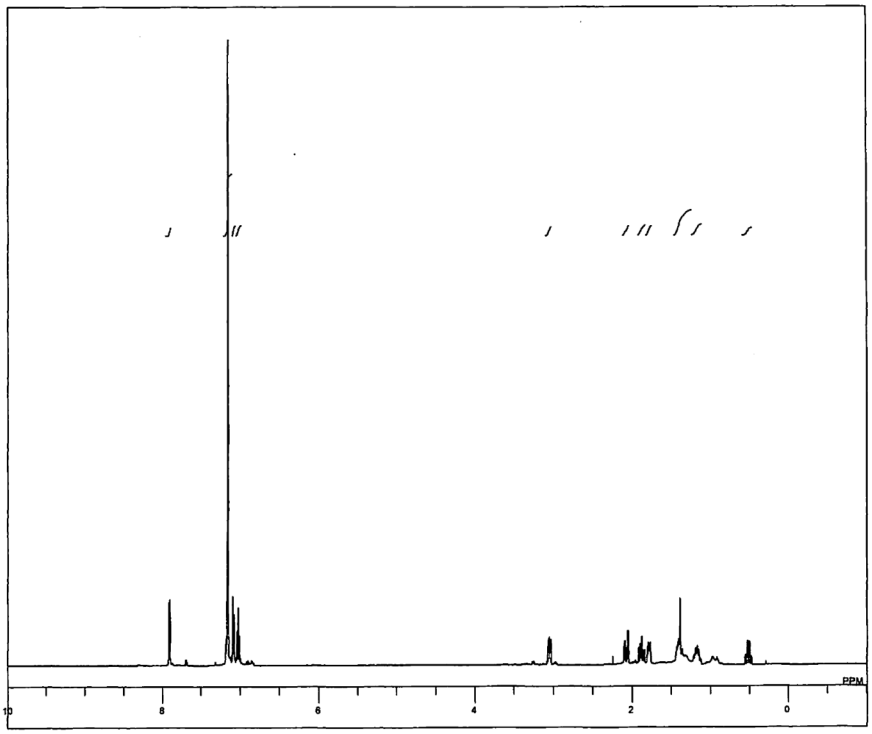
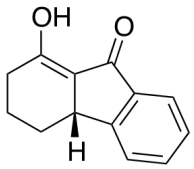
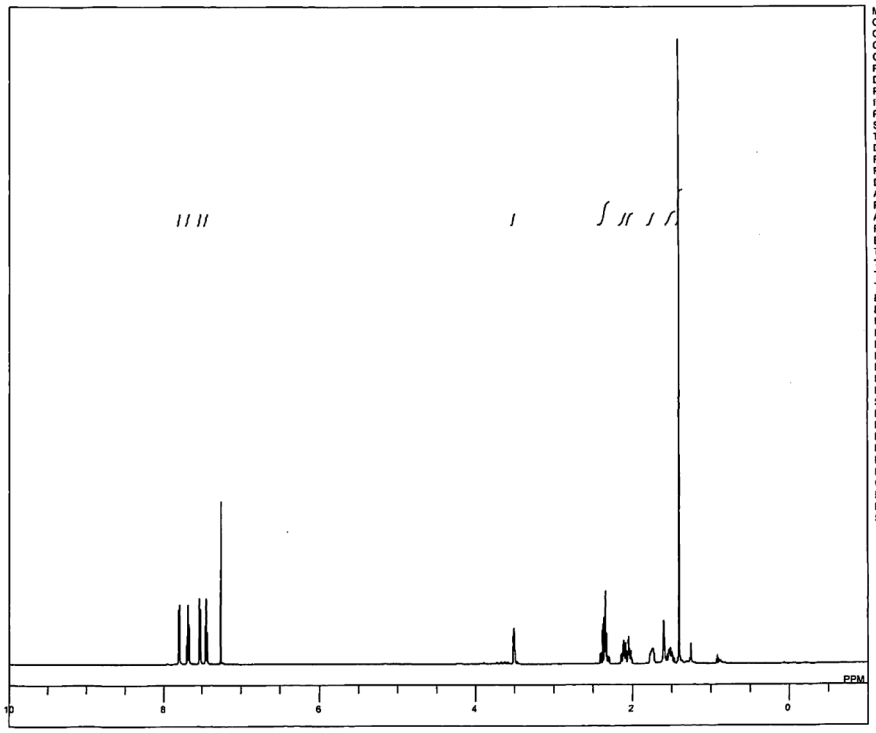


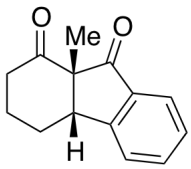
MENUF	1H
OBNUC	1H
OFR	499.10 MHz
OBSET	0.00 KHz
OBFIN	128885.00 Hz
PW1	5.50 usec
DEADT	72.30 usec
PREDL	0.01000 msec
IWT	1000.0000 sec
POINT	65536
SPO	65536
TIMES	8
DUMMY	0
FREQU	8000.00 Hz
FLT	4000 Hz
DELAY	50.00 usec
ACQTM	8.1920 sec
PD	1.0000 sec
ADBIT	16
RGAIN	15
BF	0.12 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	non
EXPCM	single pulse nondecoupling & nonpresaturation
IRNUC	1H
IFR	499.10 MHz
IRSET	0.00 KHz
IRFIN	128250.00 Hz
IRRPW	50 usec
IRATN	511
DFILE	diketone-enol-C6D6.als
SF	th5at_9
LKSET	0.00 KHz
LKFIN	26928.0 Hz
LKLEV	180
LGAIN	18
LKPHS	359
LKSIG	816
CSPED	16 Hz
FILDC	
FILDF	
SLVNT	C6D6



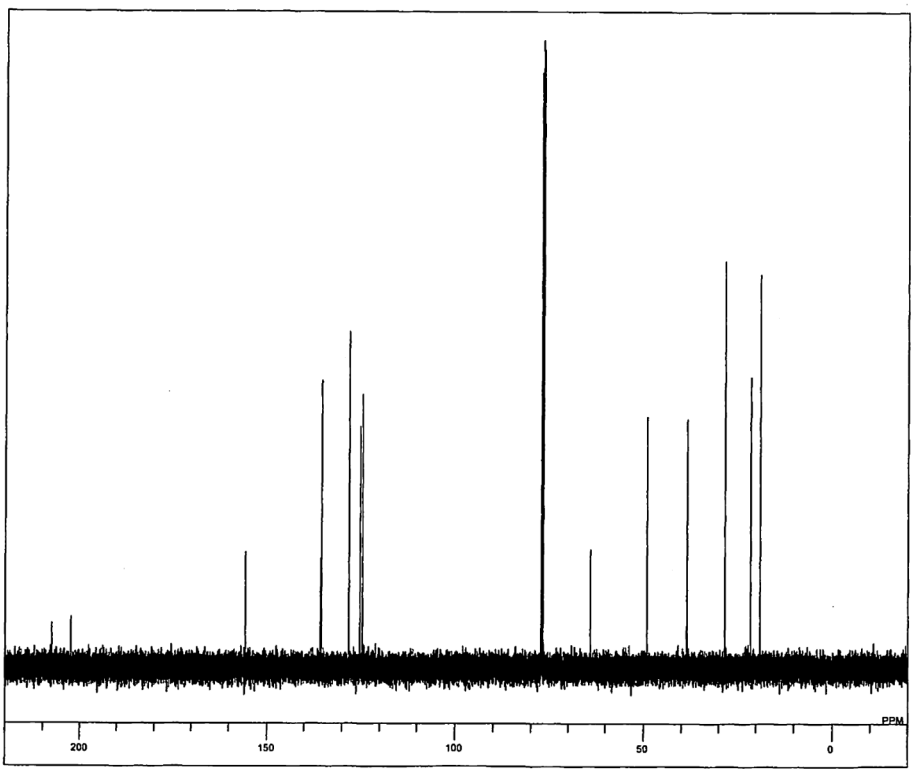
21



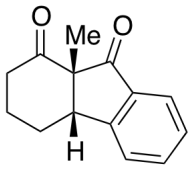
MENUF	1H
OBNUC	1H
OFR	499.10 MHz
OBSET	0.00 KHz
OBFIN	128885.00 Hz
PW1	5.50 usec
DEADT	72.30 usec
PREDL	0.01000 msec
IWT	1000.0000 sec
POINT	65536
SPO	65536
TIMES	8
DUMMY	0
FREQU	8000.00 Hz
FLT	4000 Hz
DELAY	50.00 usec
ACQTM	8.1920 sec
PD	1.0000 sec
ADBIT	16
RGAIN	16
BF	0.12 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	non
EXPCM	single pulse nondecoupling & nonpresaturation
IRNUC	1H
IFR	499.10 MHz
IRSET	0.00 KHz
IRFIN	128250.00 Hz
IRRPW	50 usec
IRATN	511
DFILE	diketone-Me.als
SF	th5at_9
LKSET	0.00 KHz
LKFIN	26934.0 Hz
LKLEV	200
LGAIN	21
LKPHS	359
LKSIG	683
CSPED	15 Hz
FILDC	
FILDF	
SLVNT	CDCL3



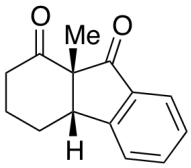
S2



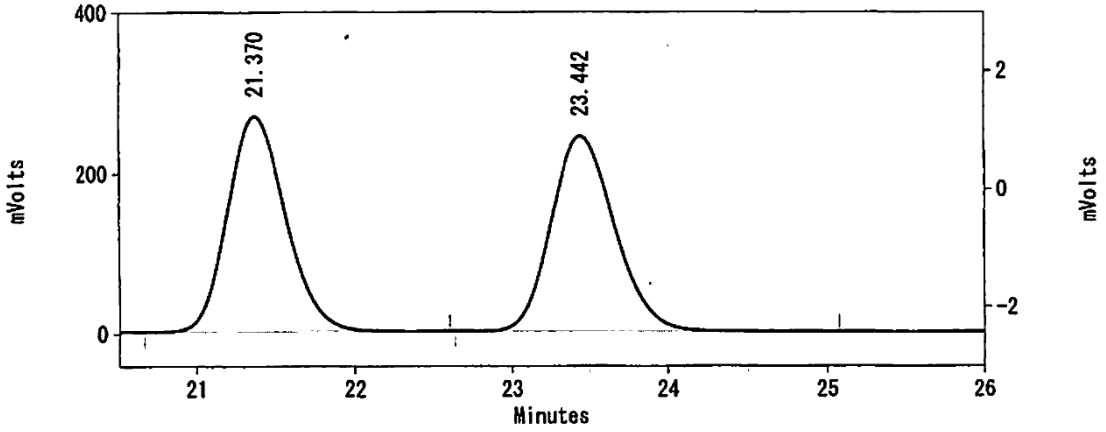
MENUF	13C
OBNUC	13C
OFR	125.40 MHz
OBSET	0.00 KHz
OBFIN	143041.00 Hz
PW1	6.25 usec
DEADT	10.00 usec
PREDL	0.01000 msec
IWT	1000.0000 sec
POINT	65536
SPO	65536
TIMES	10000
DUMMY	2
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	1.9333 sec
PD	1.0670 sec
ADBIT	16
RGAIN	25
BF	0.12 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	single pulse with bilevel decoupling
IRNUC	1H
IFR	499.10 MHz
IRSET	0.00 KHz
IRFIN	128250.00 Hz
IRRPW	50 usec
IRATN	511
DFILE	diketone-Me-13C.als
SF	th5at_9
LKSET	0.00 KHz
LKFIN	26934.0 Hz
LKLEV	200
LGAIN	21
LKPHS	359
LKSIG	681
CSPED	16 Hz
FILDC	
FILDF	
SLVNT	CDCL3



S2

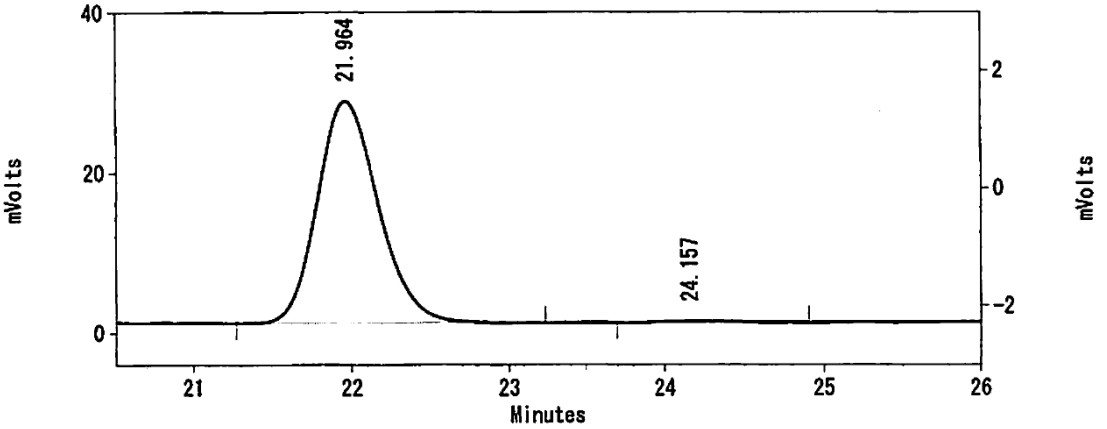


S2



UV Results

Pk #	Retention Time	Area	Area Percent	Codes
1	21.370	6881448	49.943	MM
2	23.442	6897265	50.057	MM
Totals		13778713	100.000	



UV Results

Pk #	Retention Time	Area	Area Percent	Codes
1	21.964	737845	99.303	MM
2	24.157	5176	0.697	MM
Totals		743021	100.000	

7. Computational details:

All computations were executed on Gaussian 09 (AM64L-G09RevA.02)[1] and Gaussview 5.1W as GUI using default PBE0 functionals and DGDZVP basis set. Optimizations were performed in gas phase followed by implicit solvent (1,4-dioxane) by IEFPCM treatment at 343.15K starting from structures built in Gaussview and subjected to pre-optimization at HF/3-21g or PBE0/SDD. For the PBE0/DGDZVP optimizations, cutoff values for Maximum Force = 0.0001500, RMS Force = 0.0001000, Maximum Displacement = 0.001800, RMS Displacement = 0.001200 were employed. In all cases, the predicted change in energy was confirmed to be less than 1×10^{-6}. All stationary points were confirmed to reside in their respective PEHS minima/saddle points by having only positive vibrational frequencies for intermediates or one negative frequency for transition states. Transition state search was performed by a relaxed PEHS scan of the key bonds broken or formed with step of 0.10 Å. The highest energy structure at the fine scan was further reoptimized with key transition state bonds frozen, followed by transition state optimization by the default Gaussian 09 algorithm The chemical correctness of the transition states found was confirmed by visual inspection of the normal mode having the negative vibrational frequency. In addition IRC were performed for key transition states in gas phase - the forward and reverse pathways were followed independently over up to 100 steps with the default Gaussian step size and convergence criteria as stated above; this number of steps arrived either at a minimum structure or a structure that was very close to the minimum for all cases. Analytical calculation of force constants was performed on the starting TS structure and thereafter the Hessian was updated analytically every 5th step. Atoms-in-molecules wavefunction analyzes were performed on AIM2000[2] and AIMAll[3] software packages.

8. Computational results

Cartesian coordinates for structures **1** - **16**, SCF energies and convergencies, thermodynamic quantities (DG, DH and DS) and the 3 lowest normal mode frequencies are listed below. Colour still images taken from two different angles are also shown.

1,4-Rhodium shift pathway

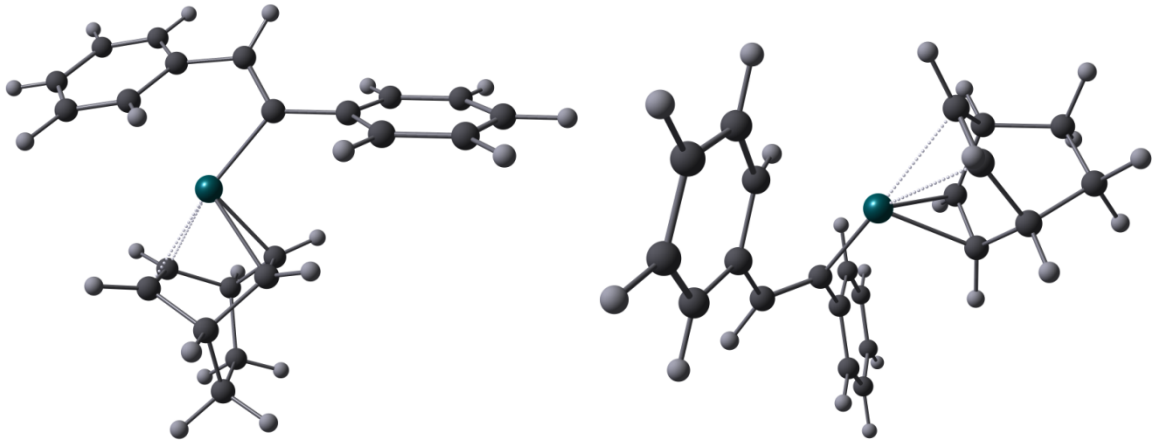
Structure 5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.499242	0.231423	-0.216025
2	6	0	0.579258	1.647460	0.927079
3	1	0	1.361297	1.250698	1.570602
4	6	0	-0.601447	2.417321	1.497700
5	1	0	-0.776249	2.181763	2.549197
6	6	0	-1.746789	1.957266	0.612514
7	1	0	-2.699122	1.628785	1.020712
8	6	0	-1.541669	2.209913	-0.722462
9	1	0	-2.317168	2.107979	-1.477218
10	6	0	-0.216295	2.889176	-1.015689
11	1	0	-0.066663	3.052721	-2.084730
12	6	0	0.788585	1.905369	-0.441143
13	1	0	1.745619	1.726880	-0.924488
14	6	0	0.817170	-1.315348	-0.173336
15	6	0	0.133644	-2.463714	0.040617

16	6	0	2.283784	-1.250508	-0.090398
17	6	0	3.038948	-0.721931	-1.150254
18	6	0	2.973685	-1.702997	1.046842
19	6	0	4.428958	-0.672186	-1.088043
20	1	0	2.519586	-0.369091	-2.038473
21	6	0	4.364362	-1.639179	1.116765
22	1	0	2.405817	-2.099570	1.885234
23	6	0	5.099869	-1.126963	0.048425
24	1	0	4.992473	-0.274348	-1.928741
25	1	0	4.875875	-1.991776	2.009358
26	1	0	6.184448	-1.079273	0.101411
27	6	0	-1.331753	-2.404452	-0.029339
28	6	0	-2.159882	-3.184072	0.799492
29	6	0	-1.953207	-1.499194	-0.922211
30	6	0	-3.540056	-3.041332	0.762152
31	1	0	-1.705170	-3.891149	1.489480
32	6	0	-3.346973	-1.349386	-0.940941
33	1	0	-1.351270	-1.057726	-1.736000
34	6	0	-4.142959	-2.112601	-0.097555
35	1	0	-4.160602	-3.652500	1.413062
36	1	0	-3.800384	-0.651339	-1.640372
37	1	0	-5.224216	-2.008015	-0.117064
38	1	0	0.605905	-3.419397	0.288760
39	6	0	-0.372847	3.934337	1.281436
40	1	0	-1.243359	4.484101	1.654342
41	1	0	0.487863	4.252199	1.879061
42	6	0	-0.141585	4.216529	-0.218265
43	1	0	0.837890	4.676396	-0.385929
44	1	0	-0.893039	4.911360	-0.607654

SCF Done: E(RPBE1PBE) = -5537.25502027 A.U. after 1 cycles
Convg = 0.4952D-08 -V/T = 2.0039
Zero-point correction= 0.365855 (Hartree/Particle)
Thermal correction to Energy= 0.391367
Thermal correction to Enthalpy= 0.392453
Thermal correction to Gibbs Free Energy= 0.305226
Sum of electronic and zero-point Energies= -5536.889165
Sum of electronic and thermal Energies= -5536.863654
Sum of electronic and thermal Enthalpies= -5536.862567
Sum of electronic and thermal Free Energies= -5536.949794

	1	2	3
	A	A	A
Frequencies --	22.9436	35.8873	43.6279
Red. masses --	4.4291	4.2954	4.5907
Frc consts --	0.0014	0.0033	0.0051
IR Inten --	0.0999	0.0336	0.6057



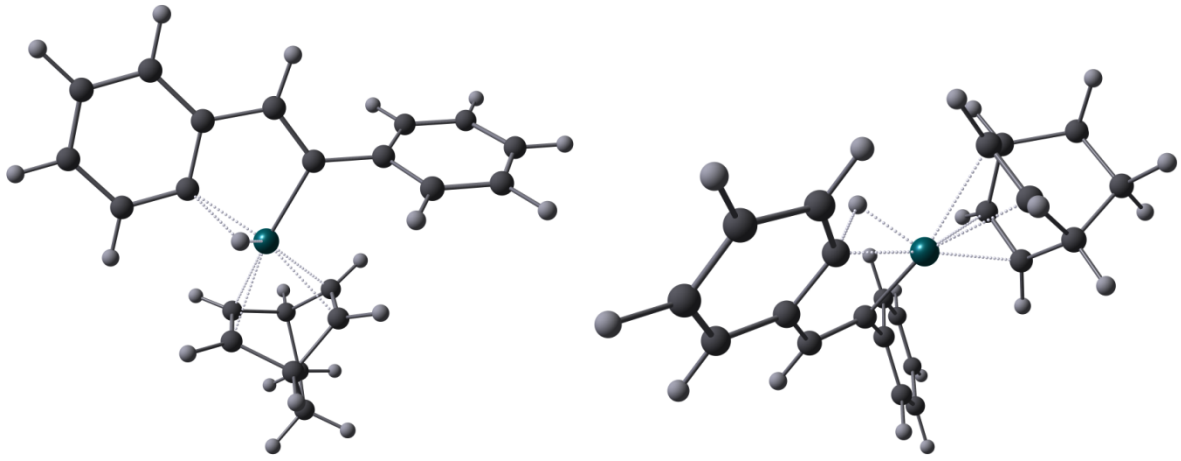
Structure 6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.429634	0.317858	-0.005157
2	6	0	1.285296	1.640384	0.730478
3	1	0	2.012928	1.060144	1.292027
4	6	0	0.369095	2.662853	1.388925
5	1	0	0.348022	2.560698	2.475385
6	6	0	-0.996505	2.428712	0.761641
7	1	0	-1.908520	2.391765	1.351280
8	6	0	-0.978190	2.497570	-0.605362
9	1	0	-1.874123	2.522529	-1.218532
10	6	0	0.388715	2.811976	-1.182213
11	1	0	0.378741	2.835364	-2.273015
12	6	0	1.291225	1.722891	-0.640113
13	1	0	2.023702	1.217335	-1.261217
14	6	0	0.355915	-1.559648	-0.083326
15	6	0	-0.573326	-2.532674	0.032945
16	6	0	1.803933	-1.813957	-0.068295
17	6	0	2.431567	-2.364165	1.061072
18	6	0	2.603000	-1.506407	-1.181953
19	6	0	3.804566	-2.604890	1.073250
20	1	0	1.828240	-2.601610	1.934039
21	6	0	3.972057	-1.755602	-1.173703
22	1	0	2.126604	-1.096121	-2.069562
23	6	0	4.581866	-2.301927	-0.043146
24	1	0	4.268654	-3.032966	1.958680
25	1	0	4.567274	-1.527337	-2.054807
26	1	0	5.652036	-2.491495	-0.034705
27	6	0	-1.973895	-2.117087	-0.004997
28	6	0	-3.073947	-2.958483	0.160472
29	6	0	-2.173513	-0.730513	-0.204686
30	6	0	-4.370738	-2.438927	0.096169
31	1	0	-2.922376	-4.020855	0.342389
32	6	0	-3.467489	-0.225822	-0.273676
33	6	0	-4.570021	-1.079173	-0.121933
34	1	0	-5.225456	-3.100744	0.212673
35	1	0	-3.636942	0.835873	-0.445319
36	1	0	-5.579103	-0.678122	-0.180906
37	1	0	-0.312783	-3.589924	0.123188
38	1	0	-1.022071	-0.127226	-1.392753
39	6	0	0.859754	4.165784	-0.580161

40	1	0	0.196215	4.961327	-0.933521
41	1	0	1.862517	4.391229	-0.956199
42	6	0	0.850200	4.076845	0.958502
43	1	0	0.183575	4.828489	1.393015
44	1	0	1.849022	4.251597	1.370575

SCF Done: E(RPBE1PBE) = -5537.22052407 A.U. after 12 cycles
Convg = 0.9429D-08 -V/T = 2.0039
Zero-point correction= 0.361421 (Hartree/Particle)
Thermal correction to Energy= 0.386640
Thermal correction to Enthalpy= 0.387727
Thermal correction to Gibbs Free Energy= 0.301881
Sum of electronic and zero-point Energies= -5536.859103
Sum of electronic and thermal Energies= -5536.833884
Sum of electronic and thermal Enthalpies= -5536.832797
Sum of electronic and thermal Free Energies= -5536.918643

	1	2	3
	A	A	A
Frequencies --	-672.1760	24.9323	35.1032
Red. masses --	1.1105	4.2803	3.8819
Frc consts --	0.2956	0.0016	0.0028
IR Inten --	286.9270	0.3031	0.1105



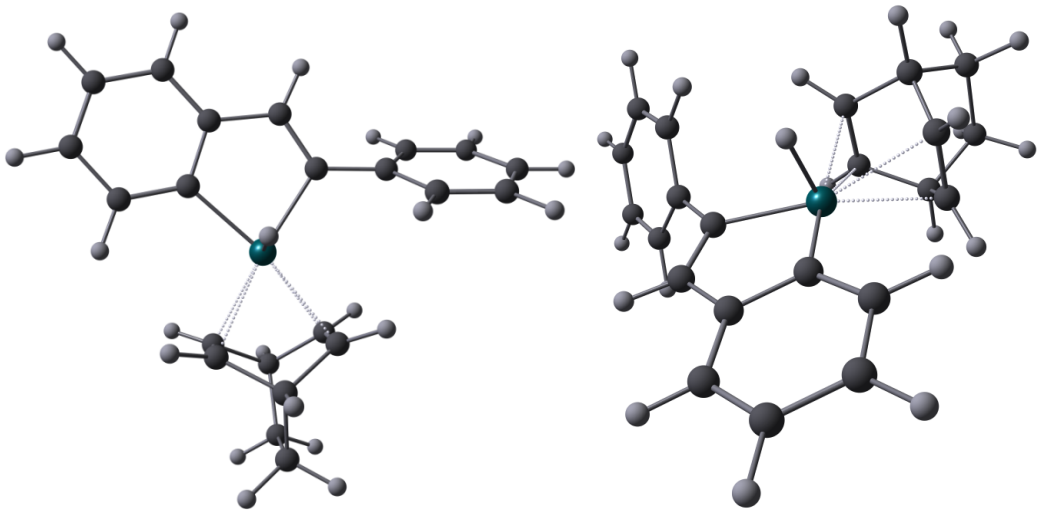
Structure 7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.040089	1.191904	0.247614
2	6	0	-1.045733	2.541853	0.323824
3	6	0	-2.251138	0.371936	0.398985
4	6	0	-3.043228	0.458129	1.556464
5	6	0	-2.656745	-0.517306	-0.610479
6	6	0	-4.200274	-0.307420	1.694278
7	1	0	-2.739365	1.132506	2.353496
8	6	0	-3.816293	-1.275423	-0.477456
9	1	0	-2.063740	-0.582566	-1.519936
10	6	0	-4.593055	-1.178257	0.678826
11	1	0	-4.796659	-0.223801	2.599756
12	1	0	-4.119588	-1.942718	-1.280808
13	1	0	-5.494929	-1.775303	0.785661
14	6	0	0.237275	3.213516	0.133532

15	6	0	0.444971	4.592542	0.162606
16	6	0	1.322049	2.330500	-0.085219
17	6	0	1.729177	5.111051	-0.042826
18	1	0	-0.390110	5.266193	0.347401
19	6	0	2.591706	2.859627	-0.285291
20	6	0	2.798336	4.250151	-0.267113
21	1	0	1.889439	6.186431	-0.028910
22	1	0	3.444397	2.204469	-0.460951
23	1	0	3.795468	4.652003	-0.433498
24	1	0	-1.958759	3.117986	0.493811
25	45	0	0.825975	0.385912	0.113087
26	6	0	0.739547	-1.830278	0.960610
27	6	0	0.591359	-1.943249	-0.389264
28	1	0	-0.085311	-1.918221	1.662679
29	6	0	2.192162	-1.802180	1.406568
30	6	0	1.903955	-2.018562	-1.141642
31	1	0	-0.361765	-2.136532	-0.870257
32	1	0	2.294555	-1.674469	2.485317
33	6	0	2.838087	-0.668302	0.625874
34	6	0	2.850310	-3.127532	0.923537
35	6	0	2.676452	-0.781685	-0.726824
36	1	0	1.759507	-2.071132	-2.221522
37	6	0	2.679858	-3.254512	-0.602269
38	1	0	3.509982	0.045271	1.095277
39	1	0	3.907844	-3.119359	1.204472
40	1	0	2.380920	-3.966817	1.445622
41	1	0	3.207271	-0.171679	-1.451575
42	1	0	2.126124	-4.161183	-0.863917
43	1	0	3.649971	-3.311063	-1.105268
44	1	0	0.501403	0.595471	-1.377427

SCF Done: E(RPBE1PBE) = -5537.22494786 A.U. after 1 cycles
Convg = 0.5703D-08 -V/T = 2.0039
Zero-point correction= 0.362942 (Hartree/Particle)
Thermal correction to Energy= 0.388479
Thermal correction to Enthalpy= 0.389566
Thermal correction to Gibbs Free Energy= 0.303740
Sum of electronic and zero-point Energies= -5536.862006
Sum of electronic and thermal Energies= -5536.836468
Sum of electronic and thermal Enthalpies= -5536.835382
Sum of electronic and thermal Free Energies= -5536.921208

	1	2	3
	A	A	A
Frequencies --	32.1314	40.9864	48.8370
Red. masses --	4.3988	4.0213	5.3600
Frc consts --	0.0027	0.0040	0.0075
IR Inten --	0.7487	0.0372	0.7365



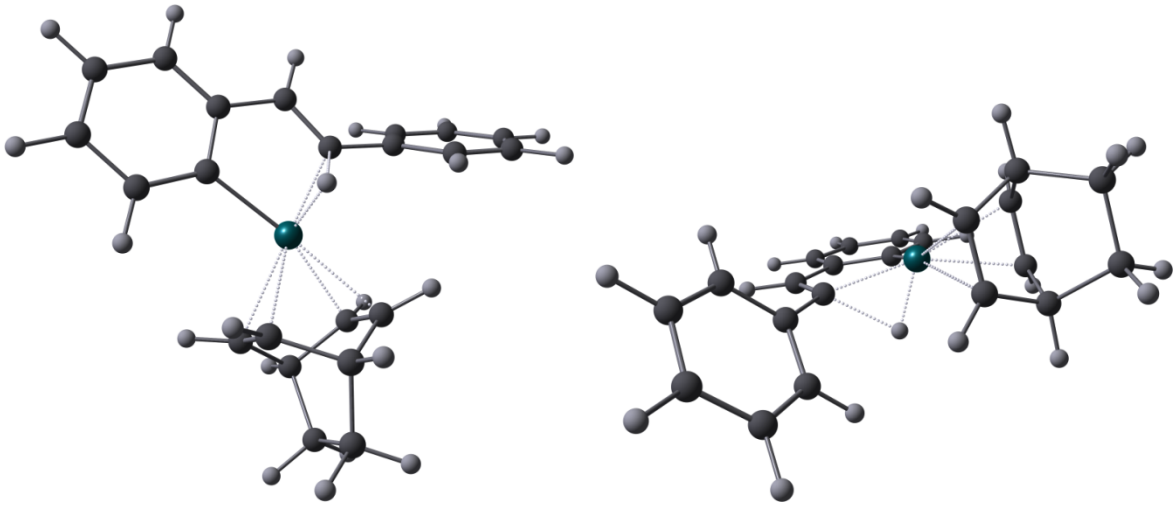
Structure 8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.471210	0.196011	0.041564
2	6	0	0.667695	2.084727	0.870939
3	1	0	1.472884	1.783119	1.535424
4	6	0	-0.620677	2.716010	1.372847
5	1	0	-0.722447	2.645625	2.457317
6	6	0	-1.731910	1.974340	0.641491
7	1	0	-2.644034	1.664473	1.144799
8	6	0	-1.594755	2.008458	-0.729042
9	1	0	-2.384299	1.727217	-1.419858
10	6	0	-0.376818	2.786022	-1.190021
11	1	0	-0.267010	2.772156	-2.275535
12	6	0	0.790876	2.122174	-0.487935
13	1	0	1.706581	1.859078	-1.007562
14	6	0	0.824156	-1.400699	-0.077330
15	6	0	0.180821	-2.581578	0.076943
16	6	0	2.286033	-1.256057	-0.070746
17	6	0	3.050984	-1.752240	0.997496
18	6	0	2.961899	-0.627963	-1.129032
19	6	0	4.439416	-1.635534	0.999782
20	1	0	2.542735	-2.225894	1.833790
21	6	0	4.348718	-0.516310	-1.129962
22	1	0	2.385002	-0.254755	-1.972559
23	6	0	5.095834	-1.016745	-0.062775
24	1	0	5.010811	-2.026630	1.838178
25	1	0	4.850970	-0.041196	-1.969291
26	1	0	6.178676	-0.924192	-0.060055
27	6	0	-1.277053	-2.566542	0.008787
28	6	0	-2.093339	-3.696107	0.067210
29	6	0	-1.840354	-1.276589	-0.127918
30	6	0	-3.480797	-3.558750	-0.038277
31	1	0	-1.651652	-4.682653	0.197495
32	6	0	-3.221629	-1.155919	-0.222290
33	6	0	-4.042671	-2.294982	-0.187237
34	1	0	-4.118838	-4.438393	-0.006135
35	1	0	-3.687369	-0.177263	-0.333617
36	1	0	-5.121192	-2.187754	-0.280975

37	1	0	0.721782	-3.518792	0.227418
38	1	0	-0.034264	-0.427630	-1.337183
39	6	0	-0.501051	4.235309	-0.641414
40	1	0	-1.368108	4.717191	-1.103971
41	1	0	0.383356	4.805932	-0.941612
42	6	0	-0.640322	4.194386	0.893183
43	1	0	-1.576497	4.659664	1.217527
44	1	0	0.177038	4.737729	1.377863

SCF Done: E(RPBE1PBE) = -5537.22139739 A.U. after 12 cycles
Convg = 0.7689D-08 -V/T = 2.0039
Zero-point correction= 0.361622 (Hartree/Particle)
Thermal correction to Energy= 0.386702
Thermal correction to Enthalpy= 0.387789
Thermal correction to Gibbs Free Energy= 0.302914
Sum of electronic and zero-point Energies= -5536.859776
Sum of electronic and thermal Energies= -5536.834696
Sum of electronic and thermal Enthalpies= -5536.833609
Sum of electronic and thermal Free Energies= -5536.918484

	1	2	3
	A	A	A
Frequencies --	-635.3114	31.4571	45.3099
Red. masses --	1.1093	4.4087	4.1261
Frc consts --	0.2638	0.0026	0.0050
IR Inten --	250.3082	0.6328	0.0815



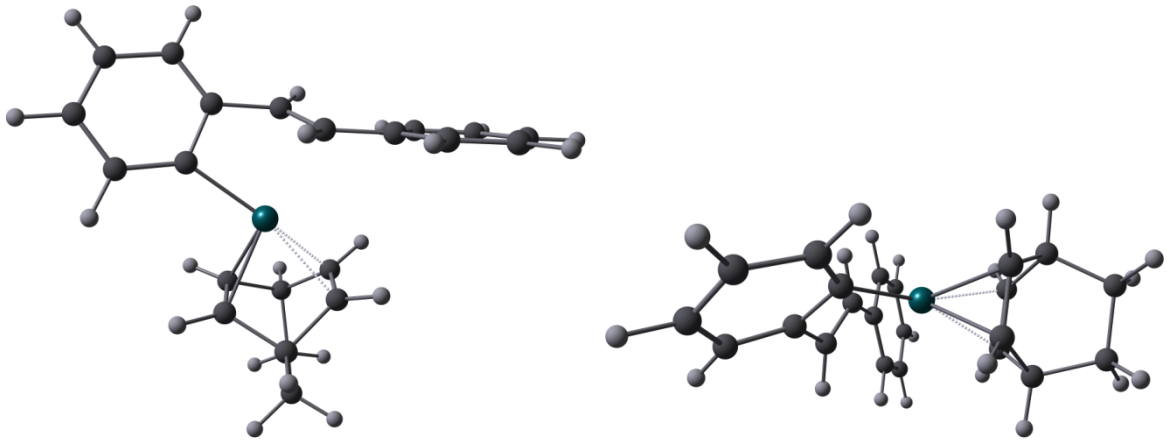
Structure 9

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.499253	0.247802	-0.210425
2	6	0	0.926879	1.742619	0.797386
3	1	0	1.693743	1.260296	1.396895
4	6	0	-0.225784	2.509715	1.419507
5	1	0	-0.307438	2.331990	2.493347
6	6	0	-1.433446	1.989103	0.661161
7	1	0	-2.378198	1.796606	1.163427
8	6	0	-1.332126	2.165818	-0.721665
9	1	0	-2.194374	2.144739	-1.383471

10	6	0	-0.030801	2.837733	-1.134970
11	1	0	0.053662	2.937395	-2.218696
12	6	0	1.032548	1.917257	-0.560012
13	1	0	1.892384	1.589737	-1.138798
14	6	0	0.711406	-1.664493	-0.353736
15	6	0	-0.201166	-1.995268	0.627967
16	6	0	2.170280	-1.581531	-0.172799
17	6	0	2.779390	-1.472085	1.087485
18	6	0	2.998023	-1.615100	-1.304680
19	6	0	4.163763	-1.414513	1.208190
20	1	0	2.166308	-1.421975	1.983790
21	6	0	4.384258	-1.554183	-1.185581
22	1	0	2.545717	-1.696903	-2.290823
23	6	0	4.975386	-1.455790	0.072913
24	1	0	4.614122	-1.330495	2.194093
25	1	0	5.003990	-1.585788	-2.078027
26	1	0	6.056623	-1.408044	0.169954
27	6	0	-1.645037	-2.102917	0.341141
28	6	0	-2.505056	-3.126556	0.748298
29	6	0	-2.097888	-0.966111	-0.347536
30	6	0	-3.844821	-3.047431	0.371814
31	1	0	-2.140585	-3.970831	1.331526
32	6	0	-3.454306	-0.888311	-0.682728
33	6	0	-4.310815	-1.942050	-0.352307
34	1	0	-4.534285	-3.842755	0.644173
35	1	0	-3.856333	-0.015387	-1.195929
36	1	0	-5.359230	-1.898829	-0.641206
37	1	0	0.151162	-2.227452	1.633360
38	1	0	0.368499	-1.720780	-1.392463
39	6	0	0.068996	4.213325	-0.425191
40	1	0	-0.724861	4.866019	-0.802903
41	1	0	1.023319	4.681946	-0.686812
42	6	0	-0.052287	4.017756	1.100252
43	1	0	-0.910341	4.567106	1.501271
44	1	0	0.838116	4.390419	1.616925

SCF Done: E(RPBE1PBE) = -5537.26105611 A.U. after 1 cycles
Convg = 0.3098D-08 -V/T = 2.0039
Zero-point correction= 0.366096 (Hartree/Particle)
Thermal correction to Energy= 0.391606
Thermal correction to Enthalpy= 0.392693
Thermal correction to Gibbs Free Energy= 0.306415
Sum of electronic and zero-point Energies= -5536.894960
Sum of electronic and thermal Energies= -5536.869450
Sum of electronic and thermal Enthalpies= -5536.868363
Sum of electronic and thermal Free Energies= -5536.954641

	1	2	3
	A	A	A
Frequencies --	33.5539	39.0685	49.4608
Red. masses --	4.6420	5.3989	3.8491
Frc consts --	0.0031	0.0049	0.0055
IR Inten --	0.1944	0.5800	0.2275



Carborhodation pathways

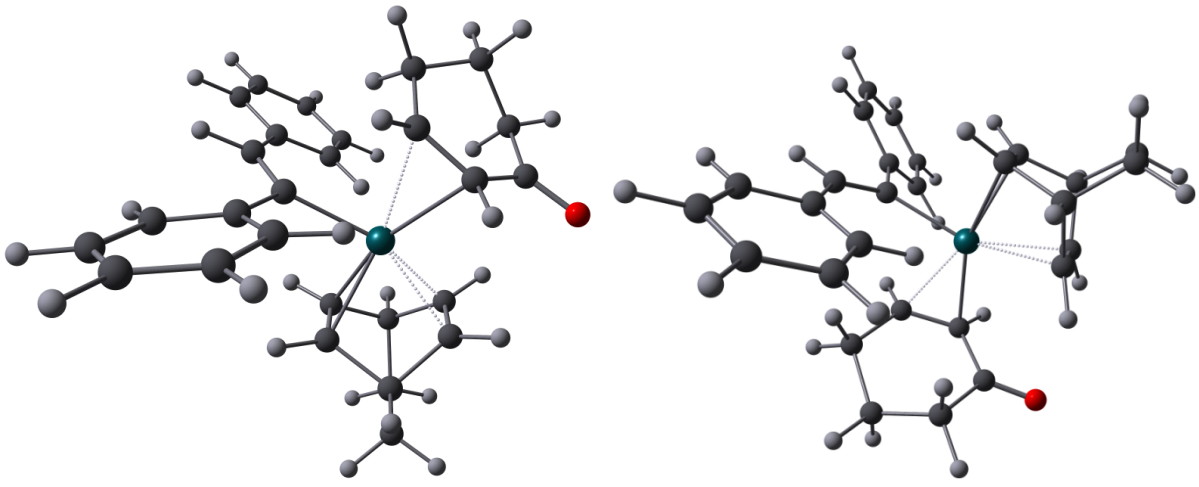
Structure 10a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.255352	-0.620942	0.163075
2	6	0	-1.617737	-0.951865	-1.501930
3	1	0	-2.405417	-0.207042	-1.570682
4	6	0	-1.921855	-2.405983	-1.196032
5	1	0	-2.911130	-2.534346	-0.753959
6	6	0	-0.809841	-2.788800	-0.237515
7	1	0	-0.988253	-3.358019	0.670503
8	6	0	0.451270	-2.595336	-0.755402
9	1	0	1.345229	-3.009047	-0.296776
10	6	0	0.445739	-2.044363	-2.169047
11	1	0	1.453740	-1.869584	-2.549651
12	6	0	-0.340999	-0.756287	-2.022359
13	1	0	-0.046861	0.158798	-2.528341
14	6	0	-0.656747	1.411125	0.052975
15	6	0	0.191694	2.381889	-0.374390
16	6	0	-2.068161	1.791003	0.320764
17	6	0	-2.697977	2.838136	-0.382606
18	6	0	-2.863719	1.085121	1.243249
19	6	0	-4.024010	3.187323	-0.142785
20	1	0	-2.147882	3.368985	-1.154534
21	6	0	-4.187898	1.435402	1.491618
22	1	0	-2.440363	0.233430	1.768395
23	6	0	-4.778187	2.495190	0.804743
24	1	0	-4.475679	3.996443	-0.711978
25	1	0	-4.764551	0.869935	2.219802
26	1	0	-5.814769	2.764579	0.989348
27	6	0	1.583863	2.311368	-0.826735
28	6	0	2.243381	3.517517	-1.133038
29	6	0	2.317456	1.121557	-0.995770
30	6	0	3.561847	3.538860	-1.576599
31	1	0	1.704997	4.456204	-1.016475
32	6	0	3.635943	1.139624	-1.437174
33	1	0	1.833114	0.170803	-0.770126
34	6	0	4.270692	2.347422	-1.732070
35	1	0	4.038820	4.489611	-1.801846
36	1	0	4.175405	0.202122	-1.554426
37	1	0	5.300512	2.359054	-2.079141

38	1	0	-0.192035	3.406373	-0.390832
39	6	0	0.328215	0.182069	2.312898
40	6	0	0.182149	-1.195955	2.285178
41	6	0	1.673531	0.851310	2.449623
42	1	0	1.967681	1.319023	1.506664
43	1	0	1.568536	1.674982	3.164418
44	6	0	2.753162	-0.118199	2.926537
45	1	0	3.740876	0.342682	2.826290
46	1	0	2.607465	-0.327723	3.993580
47	6	0	2.709083	-1.436496	2.157560
48	1	0	3.464744	-2.145207	2.506658
49	1	0	2.899188	-1.252843	1.091500
50	6	0	1.353735	-2.096426	2.281442
51	8	0	1.225540	-3.312052	2.389344
52	1	0	-0.533273	0.785171	2.579380
53	1	0	-0.769720	-1.661260	2.538623
54	6	0	-0.348735	-3.017166	-3.078754
55	1	0	0.196555	-3.963735	-3.148840
56	1	0	-0.396255	-2.596883	-4.088433
57	6	0	-1.761515	-3.231946	-2.499070
58	1	0	-1.938236	-4.288075	-2.272010
59	1	0	-2.532215	-2.922196	-3.212086

SCF Done: E(RPBE1PBE) = -5845.60293062 A.U. after 1 cycles
Convg = 0.2384D-08 -V/T = 2.0045
Zero-point correction= 0.497751 (Hartree/Particle)
Thermal correction to Energy= 0.532537
Thermal correction to Enthalpy= 0.533624
Thermal correction to Gibbs Free Energy= 0.426690
Sum of electronic and zero-point Energies= -5845.105179
Sum of electronic and thermal Energies= -5845.070394
Sum of electronic and thermal Enthalpies= -5845.069307
Sum of electronic and thermal Free Energies= -5845.176241

	1	2	3
	A	A	A
Frequencies --	23.6206	28.1961	41.0967
Red. masses --	4.4391	4.7911	4.8839
Frc consts --	0.0015	0.0022	0.0049
IR Inten --	0.1339	0.6389	0.4651



Structure 11a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.560581	-0.521293	0.210532
2	6	0	-1.912470	-0.494686	-1.558175
3	1	0	-2.254426	0.504085	-1.817088
4	6	0	-2.852902	-1.536429	-0.975252
5	1	0	-3.787727	-1.094426	-0.626523
6	6	0	-2.036352	-2.124159	0.161992
7	1	0	-2.469478	-2.353696	1.132030
8	6	0	-0.816541	-2.643518	-0.255536
9	1	0	-0.225291	-3.313518	0.363914
10	6	0	-0.590303	-2.513250	-1.752481
11	1	0	0.382669	-2.903699	-2.057711
12	6	0	-0.704842	-1.016378	-1.979634
13	1	0	-0.008416	-0.472650	-2.612281
14	6	0	0.174430	1.498530	0.140548
15	6	0	1.219339	1.951004	-0.619710
16	6	0	-1.041162	2.360499	0.210304
17	6	0	-1.407302	3.122737	-0.917972
18	6	0	-1.917644	2.402987	1.310958
19	6	0	-2.548319	3.919117	-0.926830
20	1	0	-0.800770	3.066047	-1.817360
21	6	0	-3.061473	3.196658	1.302627
22	1	0	-1.723613	1.810389	2.198834
23	6	0	-3.383417	3.968600	0.188105
24	1	0	-2.793128	4.491758	-1.818108
25	1	0	-3.707793	3.206255	2.176711
26	1	0	-4.278356	4.584932	0.182382
27	6	0	2.410485	1.270716	-1.110734
28	6	0	3.472529	2.050948	-1.609245
29	6	0	2.554145	-0.130050	-1.161852
30	6	0	4.631688	1.465469	-2.104787
31	1	0	3.383453	3.135365	-1.594086
32	6	0	3.716139	-0.716075	-1.652065
33	1	0	1.730140	-0.755065	-0.816066
34	6	0	4.762956	0.075659	-2.125883
35	1	0	5.436763	2.093698	-2.477353
36	1	0	3.801854	-1.799903	-1.675803
37	1	0	5.666021	-0.384546	-2.517896
38	1	0	1.161455	2.991387	-0.948666
39	6	0	0.636718	0.735988	1.877477
40	6	0	-0.104720	-0.451491	2.263321
41	6	0	2.150364	0.699395	2.015816
42	1	0	2.629623	0.356433	1.099531
43	1	0	2.515393	1.717038	2.187739
44	6	0	2.579772	-0.248557	3.131483
45	1	0	3.672473	-0.249880	3.207991
46	1	0	2.191940	0.090610	4.100632
47	6	0	2.065691	-1.654443	2.836667
48	1	0	2.362503	-2.380281	3.598695
49	1	0	2.473395	-2.005694	1.878993
50	6	0	0.551926	-1.669496	2.753680
51	8	0	-0.095195	-2.643105	3.141100
52	1	0	0.226121	1.652177	2.296157
53	1	0	-1.108446	-0.319741	2.676365
54	6	0	-1.748948	-3.224568	-2.498739
55	1	0	-1.696557	-4.298749	-2.293795
56	1	0	-1.609985	-3.095181	-3.576993
57	6	0	-3.099185	-2.637463	-2.038770
58	1	0	-3.737818	-3.413038	-1.603842
59	1	0	-3.647927	-2.203546	-2.881020

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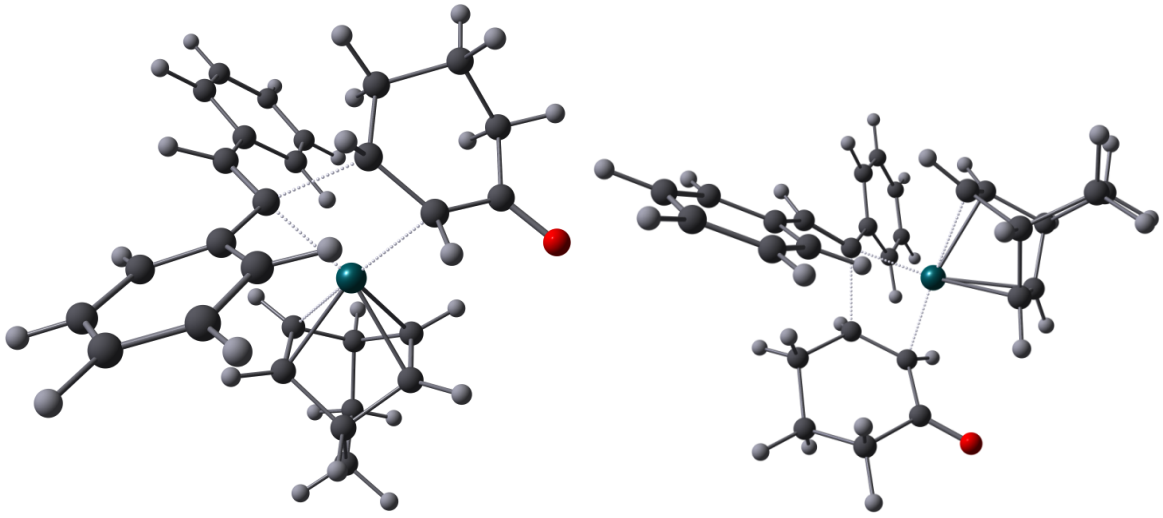
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5845.58121660     A.U. after    1 cycles
             Convg  =    0.3483D-08             -V/T =  2.0044
Zero-point correction=                           0.496968 (Hartree/Particle)
 Thermal correction to Energy=                    0.530772
 Thermal correction to Enthalpy=                  0.531859
 Thermal correction to Gibbs Free Energy=         0.427363
 Sum of electronic and zero-point Energies=          -5845.084249
 Sum of electronic and thermal Energies=             -5845.050445
 Sum of electronic and thermal Enthalpies=           -5845.049358
 Sum of electronic and thermal Free Energies=        -5845.153853

                     1                      2                      3
                     A                      A                      A
 Frequencies --  -298.3968               24.1144                31.7131
 Red. masses --     7.3146                4.8397                 4.8020
 Frc consts  --     0.3837                0.0017                 0.0028
 IR Inten    --   133.0463                0.9493                 0.2017
```



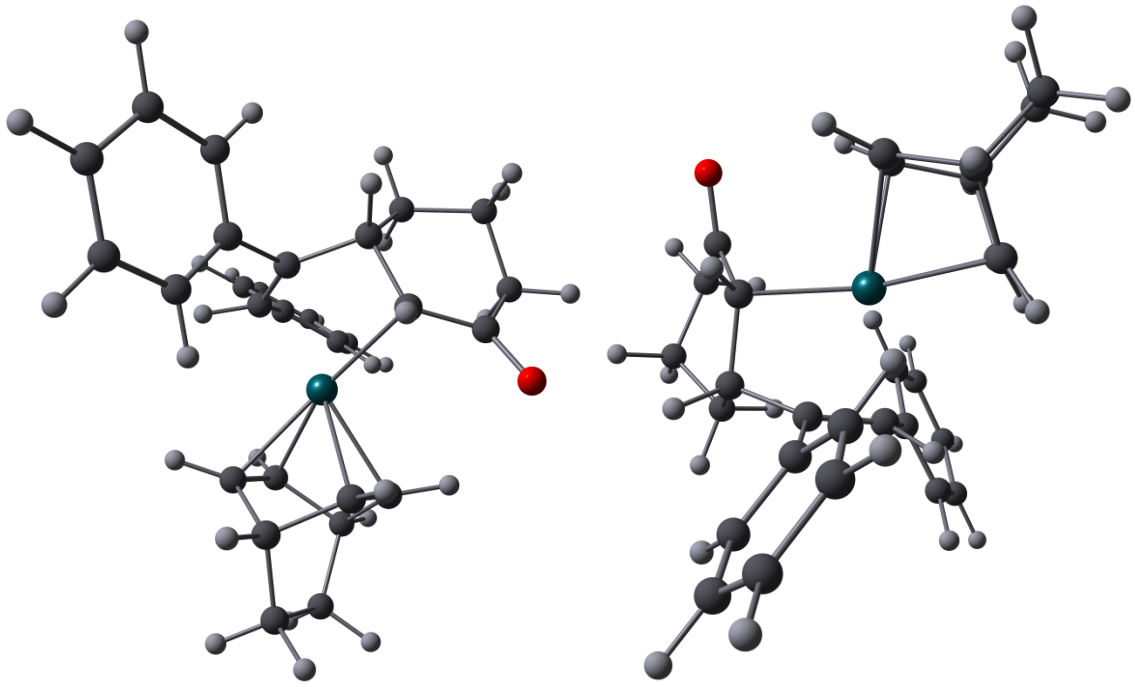
Structure 12a

```
---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1         45           0        0.572433   -0.477162    0.134045
      2          6           0        1.531974   -1.708809   -1.474990
      3          1           0        0.883049   -2.009758   -2.293539
      4          6           0        2.111858   -2.716787   -0.496912
      5          1           0        1.581352   -3.670650   -0.520918
      6          6           0        1.972119   -2.016612    0.841554
      7          1           0        1.632920   -2.534760    1.734517
      8          6           0        2.604725   -0.784072    0.891062
      9          1           0        2.792449   -0.264496    1.826524
     10          6           0        3.290858   -0.418668   -0.415120
     11          1           0        3.754077    0.568819   -0.374550
     12          6           0        2.162370   -0.479186   -1.429806
     13          1           0        2.034302    0.286338   -2.190293
     14          6           0       -1.644488    0.083039   -0.039981
     15          6           0       -0.949871    0.584313   -1.141499
     16          6           0       -2.545874   -1.087067   -0.292571
     17          6           0       -2.102848   -2.329408   -0.756856
```

18	6	0	-3.922523	-0.905051	-0.092909
19	6	0	-3.006121	-3.356775	-1.025949
20	1	0	-1.035494	-2.490817	-0.882580
21	6	0	-4.826868	-1.926742	-0.368625
22	1	0	-4.292167	0.052913	0.266453
23	6	0	-4.372239	-3.159930	-0.836587
24	1	0	-2.638084	-4.318040	-1.375953
25	1	0	-5.890161	-1.759037	-0.217259
26	1	0	-5.076720	-3.960896	-1.044272
27	6	0	-0.425016	1.943496	-1.466970
28	6	0	-0.997846	2.590471	-2.571994
29	6	0	0.626345	2.590722	-0.802202
30	6	0	-0.564940	3.851454	-2.975877
31	1	0	-1.801952	2.100288	-3.116690
32	6	0	1.067601	3.847269	-1.208682
33	1	0	1.110644	2.091165	0.034325
34	6	0	0.470386	4.488224	-2.293580
35	1	0	-1.035468	4.334429	-3.828453
36	1	0	1.885577	4.325732	-0.675791
37	1	0	0.814305	5.469648	-2.608992
38	1	0	-1.145230	0.014567	-2.051742
39	6	0	-1.705277	0.635244	1.388418
40	6	0	-0.456896	-0.030219	1.966245
41	6	0	-1.786490	2.153124	1.555153
42	1	0	-1.183045	2.673205	0.809685
43	1	0	-2.821651	2.475388	1.391450
44	6	0	-1.300726	2.564103	2.938833
45	1	0	-1.418943	3.644655	3.076972
46	1	0	-1.908322	2.079538	3.714772
47	6	0	0.163505	2.168962	3.116604
48	1	0	0.547732	2.435771	4.105347
49	1	0	0.779248	2.705768	2.382284
50	6	0	0.383285	0.675797	2.933460
51	8	0	1.233955	0.096682	3.621823
52	1	0	-2.594303	0.213763	1.873479
53	1	0	-0.644622	-1.053470	2.309628
54	6	0	4.324846	-1.523194	-0.759618
55	1	0	5.117203	-1.512498	-0.004374
56	1	0	4.791327	-1.285768	-1.721191
57	6	0	3.622341	-2.895044	-0.806814
58	1	0	4.055755	-3.585139	-0.075972
59	1	0	3.729965	-3.359755	-1.792206

SCF Done: E(RPBE1PBE) = -5845.62086559 A.U. after 1 cycles
Convg = 0.3146D-08 -V/T = 2.0044
Zero-point correction= 0.499289 (Hartree/Particle)
Thermal correction to Energy= 0.533242
Thermal correction to Enthalpy= 0.534328
Thermal correction to Gibbs Free Energy= 0.429340
Sum of electronic and zero-point Energies= -5845.121577
Sum of electronic and thermal Energies= -5845.087624
Sum of electronic and thermal Enthalpies= -5845.086537
Sum of electronic and thermal Free Energies= -5845.191525

	1	2	3
	A	A	A
Frequencies --	24.6611	33.5683	37.9621
Red. masses --	4.9371	5.0948	4.0516
Frc consts --	0.0018	0.0034	0.0034
IR Inten --	0.8115	0.8851	0.0968



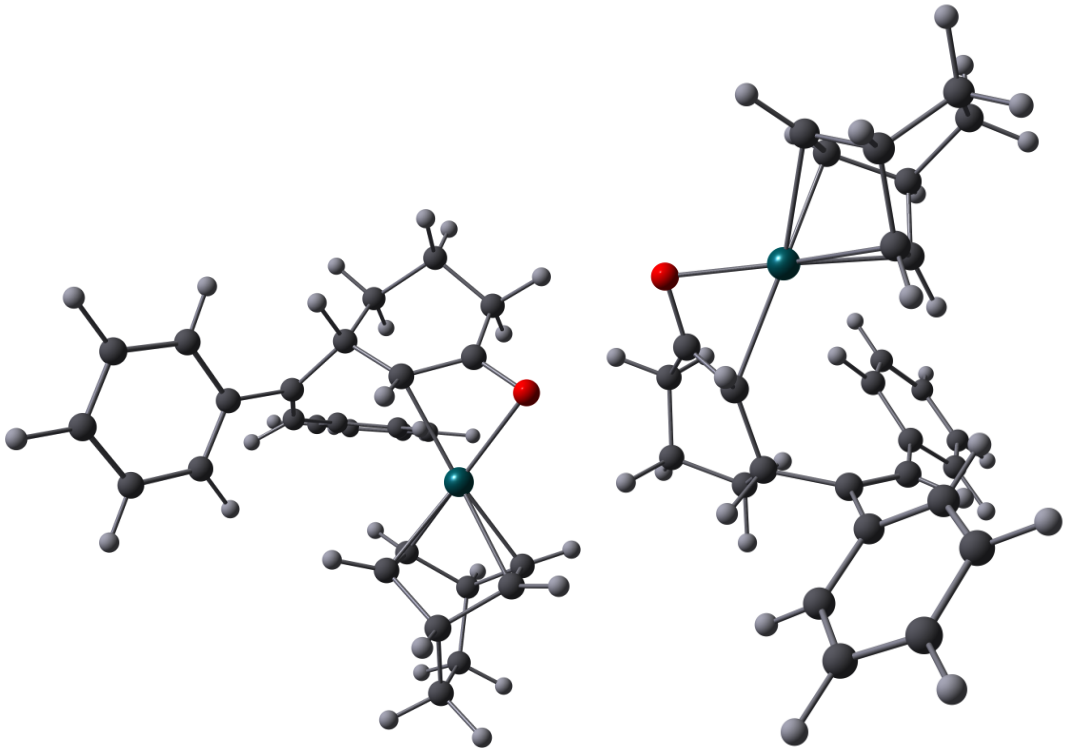
Structure 13a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	1.513729	-0.423303	0.908020
2	6	0	3.527966	-0.084708	0.159461
3	6	0	2.872473	-2.312341	-0.564232
4	6	0	3.405805	-1.418435	0.542198
5	6	0	3.104549	0.166245	-1.277357
6	6	0	3.788224	-2.208770	-1.807641
7	6	0	1.663930	-0.312363	-1.244769
8	6	0	1.538241	-1.647555	-0.857359
9	6	0	3.931269	-0.731246	-2.229388
10	1	0	2.753676	-3.346087	-0.234413
11	1	0	3.178568	1.220753	-1.550597
12	1	0	4.763418	-2.645271	-1.567970
13	1	0	3.359383	-2.809390	-2.616611
14	1	0	3.579550	-0.578747	-3.255085
15	1	0	4.978911	-0.413949	-2.199673
16	1	0	0.872704	0.232274	-1.751750
17	1	0	3.874429	-1.823694	1.435571
18	8	0	1.392406	0.060742	2.953441
19	6	0	0.225250	0.526302	2.638456
20	6	0	-0.575486	-0.211181	1.748210
21	6	0	-1.939994	0.289181	1.291523
22	1	0	-2.649594	-0.317603	1.869018
23	6	0	-2.239378	1.737235	1.709149
24	1	0	-3.324591	1.885193	1.669315
25	1	0	-2.158831	1.350861	3.836565
26	6	0	-1.708602	2.035979	3.106312
27	1	0	-1.808829	2.459656	1.014346
28	1	0	-1.992730	3.050001	3.407516
29	6	0	-0.191365	1.884323	3.140634
30	1	0	0.207994	1.991640	4.154421

31	1	0	0.289484	2.662553	2.534889
32	1	0	-0.470103	-1.300704	1.810767
33	1	0	4.102919	0.642562	0.727734
34	1	0	0.635884	-2.230375	-1.024004
35	6	0	-2.240147	-0.038534	-0.166325
36	6	0	-2.055100	0.742619	-1.258542
37	6	0	-2.849771	-1.377334	-0.407710
38	6	0	-1.428016	2.058387	-1.461633
39	1	0	-2.475863	0.341408	-2.181267
40	6	0	-2.395234	-2.188100	-1.459952
41	6	0	-3.902948	-1.865691	0.381906
42	6	0	-1.967198	2.900596	-2.449187
43	6	0	-0.278049	2.497550	-0.784841
44	6	0	-2.970616	-3.430122	-1.717821
45	1	0	-1.568523	-1.841402	-2.074927
46	6	0	-4.484292	-3.104035	0.122846
47	1	0	-4.302684	-1.260502	1.191292
48	6	0	-1.411931	4.147781	-2.719024
49	1	0	-2.844563	2.572269	-3.002670
50	6	0	0.286860	3.739100	-1.062860
51	1	0	0.192463	1.844047	-0.053940
52	6	0	-4.019333	-3.895799	-0.926580
53	1	0	-2.590923	-4.039650	-2.534042
54	1	0	-5.309192	-3.449176	0.740925
55	6	0	-0.280888	4.575738	-2.023537
56	1	0	-1.859350	4.784724	-3.477781
57	1	0	1.180405	4.052003	-0.527982
58	1	0	-4.468043	-4.865821	-1.123296
59	1	0	0.159653	5.546203	-2.236394

SCF Done: E(RPBE1PBE) = -5845.62336065 A.U. after 1 cycles
Convg = 0.4514D-08 -V/T = 2.0044
Zero-point correction= 0.500009 (Hartree/Particle)
Thermal correction to Energy= 0.533642
Thermal correction to Enthalpy= 0.534729
Thermal correction to Gibbs Free Energy= 0.429994
Sum of electronic and zero-point Energies= -5845.123352
Sum of electronic and thermal Energies= -5845.089719
Sum of electronic and thermal Enthalpies= -5845.088632
Sum of electronic and thermal Free Energies= -5845.193367

	1	2	3
	A	A	A
Frequencies --	16.7953	29.2069	35.5267
Red. masses --	5.3608	5.1252	5.3287
Frc consts --	0.0009	0.0026	0.0040
IR Inten --	0.1305	0.4155	0.1461



Structure 10b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.261592	-0.460617	-0.049397
2	6	0	-1.920598	0.085267	-1.393048
3	1	0	-2.282604	1.099863	-1.258118
4	6	0	-2.800210	-1.115568	-1.113126
5	1	0	-3.663033	-0.858393	-0.496166
6	6	0	-1.853351	-2.064909	-0.410199
7	1	0	-2.147051	-2.619815	0.475664
8	6	0	-0.733010	-2.374049	-1.150740
9	1	0	-0.063184	-3.188177	-0.886903
10	6	0	-0.701845	-1.691949	-2.507767
11	1	0	0.206587	-1.925042	-3.066274
12	6	0	-0.793592	-0.218619	-2.149697
13	1	0	-0.207469	0.537422	-2.664685
14	6	0	0.448972	1.502877	-0.027209
15	6	0	1.731611	1.885691	-0.254867
16	6	0	-0.555953	2.586472	0.110008
17	6	0	-0.482785	3.755570	-0.672008
18	6	0	-1.640296	2.483309	0.999086
19	6	0	-1.418919	4.779265	-0.541603
20	1	0	0.307454	3.849906	-1.412186
21	6	0	-2.572494	3.506969	1.139573
22	1	0	-1.755277	1.573485	1.580025
23	6	0	-2.465928	4.667381	0.372390
24	1	0	-1.336083	5.664408	-1.168002
25	1	0	-3.392024	3.394835	1.845720
26	1	0	-3.197947	5.464473	0.472594
27	6	0	2.920421	1.058987	-0.480742
28	6	0	4.188464	1.597590	-0.191705

29	6	0	2.875275	-0.248439	-0.995756
30	6	0	5.351082	0.855320	-0.371529
31	1	0	4.254317	2.613861	0.192239
32	6	0	4.037081	-0.994179	-1.175632
33	1	0	1.909868	-0.668937	-1.273362
34	6	0	5.282409	-0.450367	-0.860228
35	1	0	6.315320	1.295933	-0.130250
36	1	0	3.972605	-2.002846	-1.577601
37	1	0	6.189151	-1.031678	-1.005411
38	1	0	1.956433	2.955890	-0.212822
39	6	0	0.894755	-0.355647	1.984545
40	6	0	0.801126	-1.655790	1.513939
41	1	0	1.594895	-2.072979	0.896098
42	6	0	0.065149	0.119651	3.143613
43	6	0	-1.225793	-0.676110	3.294005
44	1	0	-1.896805	-0.437631	2.458728
45	1	0	-1.745753	-0.389384	4.214233
46	1	0	1.787893	0.214094	1.752007
47	6	0	-0.097857	-2.646959	2.138102
48	6	0	-0.949459	-2.175774	3.297435
49	1	0	-1.867261	-2.770385	3.317647
50	1	0	-0.386826	-2.447684	4.202219
51	8	0	-0.097190	-3.821550	1.782084
52	1	0	0.680615	-0.000988	4.049085
53	1	0	-0.130026	1.192211	3.056660
54	6	0	-3.229606	-1.745306	-2.463944
55	1	0	-3.831327	-2.637901	-2.265456
56	1	0	-3.871128	-1.035865	-2.996419
57	6	0	-1.977349	-2.093260	-3.293973
58	1	0	-1.981501	-1.568023	-4.254393
59	1	0	-1.934465	-3.165040	-3.512196

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SCF Done:  E(RPBE1PBE) =  -5845.60643039     A.U. after    1 cycles
             Convg  =    0.3471D-08             -V/T =  2.0045
Zero-point correction=                           0.497439 (Hartree/Particle)
 Thermal correction to Energy=                    0.532215
 Thermal correction to Enthalpy=                  0.533301
 Thermal correction to Gibbs Free Energy=         0.426514
 Sum of electronic and zero-point Energies=          -5845.108992
 Sum of electronic and thermal Energies=             -5845.074216
 Sum of electronic and thermal Enthalpies=           -5845.073129
 Sum of electronic and thermal Free Energies=        -5845.179916

                     1                      2                      3
                     A                      A                      A
 Frequencies --    25.3479                30.1519                41.3845
 Red. masses --     4.6103                 4.7458                 4.6405
 Frc consts  --     0.0017                 0.0025                 0.0047
 IR Inten    --     0.0879                 0.4174                 1.749
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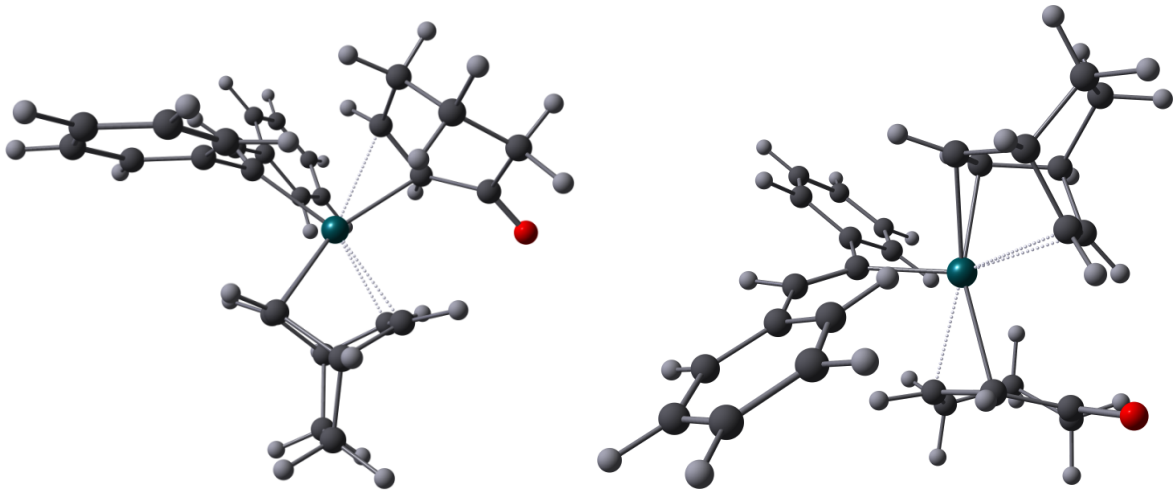


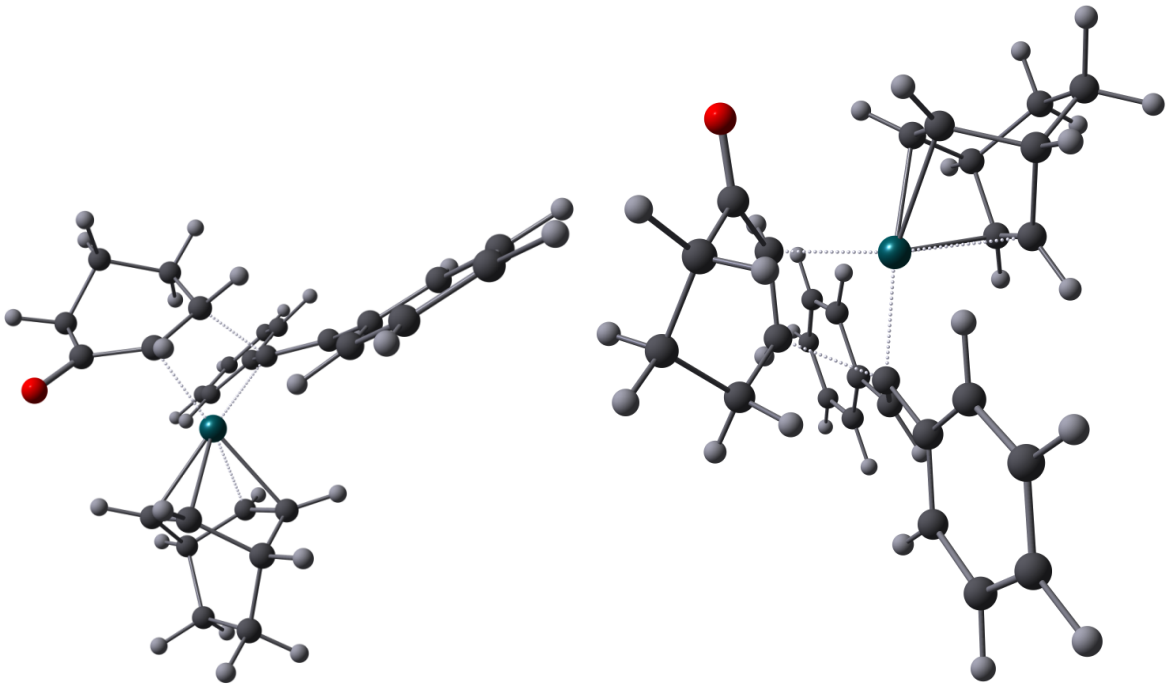
Structure 11b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.283225	0.711615	0.158672
2	6	0	1.038684	1.545376	-1.796181
3	1	0	1.382125	0.797227	-2.505020
4	6	0	1.988728	2.516206	-1.116235
5	1	0	3.031602	2.205318	-1.206434
6	6	0	1.509333	2.504244	0.326164
7	1	0	2.196680	2.493935	1.168532
8	6	0	0.173250	2.867056	0.458529
9	1	0	-0.260262	3.167929	1.409001
10	6	0	-0.497284	3.176222	-0.868286
11	1	0	-1.555064	3.419279	-0.750777
12	6	0	-0.289751	1.892138	-1.653034
13	1	0	-1.088578	1.437080	-2.232555
14	6	0	-0.313703	-1.282683	-0.485889
15	6	0	-1.567264	-1.468060	-0.993651
16	6	0	0.796140	-2.057777	-1.110475
17	6	0	0.585544	-3.335902	-1.658030
18	6	0	2.111421	-1.563657	-1.129509
19	6	0	1.623742	-4.058014	-2.239188
20	1	0	-0.400932	-3.788733	-1.605797
21	6	0	3.154382	-2.283762	-1.706219
22	1	0	2.313834	-0.594536	-0.675321
23	6	0	2.916079	-3.534263	-2.273345
24	1	0	1.424940	-5.043534	-2.653161
25	1	0	4.158697	-1.867101	-1.706525
26	1	0	3.728438	-4.101521	-2.719805
27	6	0	-2.857081	-0.961433	-0.535354
28	6	0	-4.015696	-1.664953	-0.921105
29	6	0	-3.027237	0.180231	0.269314
30	6	0	-5.278105	-1.272064	-0.493080
31	1	0	-3.914420	-2.542880	-1.555939
32	6	0	-4.290562	0.570997	0.702709
33	1	0	-2.155695	0.784202	0.520659
34	6	0	-5.422419	-0.153075	0.329084
35	1	0	-6.153136	-1.838503	-0.801255
36	1	0	-4.394312	1.458034	1.322871
37	1	0	-6.408611	0.159978	0.661377

38	1	0	-1.656215	-2.121582	-1.863596
39	6	0	-0.278609	-1.230964	1.500180
40	6	0	0.048164	0.034234	2.135021
41	6	0	0.278572	4.321249	-1.569689
42	1	0	0.164012	5.238566	-0.983242
43	1	0	-0.171860	4.507537	-2.550033
44	6	0	1.764783	3.932758	-1.706642
45	1	0	2.407595	4.642697	-1.176218
46	1	0	2.077541	3.936092	-2.755852
47	6	0	0.583667	-2.446552	1.842166
48	6	0	1.262972	0.224263	2.936559
49	8	0	1.497886	1.278807	3.528497
50	6	0	2.176850	-0.976187	3.078614
51	1	0	2.793849	-0.823945	3.968181
52	1	0	2.851747	-1.020760	2.213109
53	6	0	1.346525	-2.255324	3.149537
54	1	0	-0.061111	-3.330567	1.882352
55	1	0	1.321054	-2.647428	1.062954
56	1	0	0.654056	-2.195649	3.998618
57	1	0	1.992175	-3.122893	3.324360
58	1	0	-1.346337	-1.434442	1.535139
59	1	0	-0.786785	0.651231	2.474346

SCF Done: E(RPBE1PBE) = -5845.58201967 A.U. after 1 cycles
Convg = 0.2095D-08 -V/T = 2.0044
Zero-point correction= 0.496907 (Hartree/Particle)
Thermal correction to Energy= 0.530727
Thermal correction to Enthalpy= 0.531814
Thermal correction to Gibbs Free Energy= 0.427534
Sum of electronic and zero-point Energies= -5845.085113
Sum of electronic and thermal Energies= -5845.051292
Sum of electronic and thermal Enthalpies= -5845.050206
Sum of electronic and thermal Free Energies= -5845.154486

	1	2	3
	A	A	A
Frequencies --	-322.1999	28.0387	34.9744
Red. masses --	6.9577	5.2292	4.6857
Frc consts --	0.4256	0.0024	0.0034
IR Inten --	128.4479	1.2578	0.2955



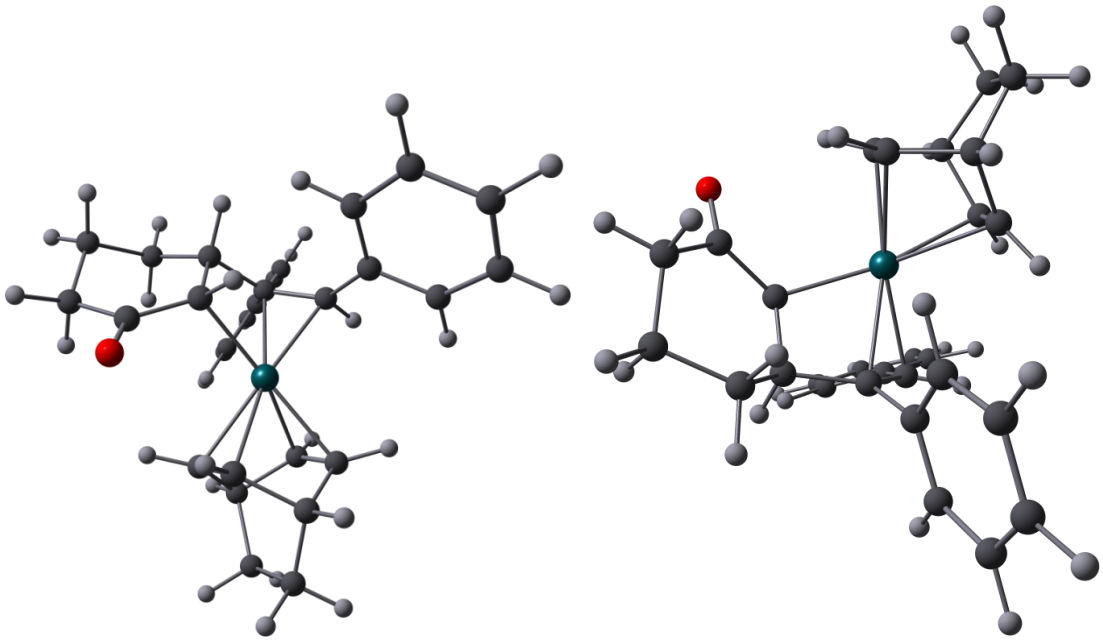
Structure 12b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.513229	0.466278	0.028362
2	6	0	-0.292564	1.942377	-1.651885
3	1	0	0.396097	1.632752	-2.433656
4	6	0	0.013173	3.116371	-0.737678
5	1	0	1.062408	3.414453	-0.785050
6	6	0	-0.376570	2.592918	0.630865
7	1	0	0.232821	2.774802	1.512398
8	6	0	-1.697095	2.176652	0.708474
9	1	0	-2.192986	1.976495	1.654461
10	6	0	-2.445628	2.336540	-0.607361
11	1	0	-3.471019	1.969465	-0.541834
12	6	0	-1.610628	1.533509	-1.591702
13	1	0	-2.067956	0.873603	-2.323720
14	6	0	1.044870	-1.152987	-0.174034
15	6	0	-0.035862	-1.462912	-1.001941
16	6	0	2.314529	-0.795104	-0.883749
17	6	0	2.981030	-1.807280	-1.588126
18	6	0	2.877384	0.487062	-0.876994
19	6	0	4.176256	-1.549207	-2.258309
20	1	0	2.556138	-2.808270	-1.607871
21	6	0	4.070213	0.748330	-1.547255
22	1	0	2.360358	1.285362	-0.350718
23	6	0	4.726693	-0.269161	-2.239503
24	1	0	4.674853	-2.350342	-2.798112
25	1	0	4.486238	1.752793	-1.533489
26	1	0	5.656175	-0.064289	-2.764161
27	6	0	-1.259494	-2.271784	-0.807924
28	6	0	-2.223059	-2.213598	-1.832741
29	6	0	-1.512185	-3.143935	0.264946
30	6	0	-3.395464	-2.958343	-1.777787

31	1	0	-2.037648	-1.573124	-2.692318
32	6	0	-2.681732	-3.896385	0.317468
33	1	0	-0.789703	-3.255568	1.064805
34	6	0	-3.635343	-3.804199	-0.695659
35	1	0	-4.120033	-2.884006	-2.584695
36	1	0	-2.847084	-4.563769	1.159393
37	1	0	-4.548591	-4.390904	-0.646272
38	1	0	0.144352	-1.251010	-2.056165
39	6	0	1.061968	-1.393966	1.349205
40	6	0	-0.143596	-0.580391	1.829447
41	6	0	-2.395808	3.830512	-1.022726
42	1	0	-2.954664	4.419765	-0.288795
43	1	0	-2.901548	3.949733	-1.986376
44	6	0	-0.927938	4.294579	-1.105044
45	1	0	-0.738654	5.127162	-0.419955
46	1	0	-0.680090	4.643513	-2.112693
47	6	0	2.374681	-0.965226	2.010113
48	6	0	-0.085911	0.227654	3.049244
49	8	0	-1.094809	0.753380	3.535071
50	6	0	1.250921	0.407307	3.747964
51	1	0	1.044859	0.573287	4.809467
52	1	0	1.711514	1.330426	3.369612
53	6	0	2.193555	-0.766175	3.507511
54	1	0	3.152263	-1.706434	1.794877
55	1	0	2.726634	-0.018887	1.587278
56	1	0	1.784775	-1.675188	3.968622
57	1	0	3.161378	-0.578688	3.985616
58	1	0	0.950841	-2.468957	1.558760
59	1	0	-1.096327	-1.122697	1.814785

SCF Done: E(RPBE1PBE) = -5845.62567977 A.U. after 1 cycles
Convg = 0.4378D-08 -V/T = 2.0044
Zero-point correction= 0.499183 (Hartree/Particle)
Thermal correction to Energy= 0.533002
Thermal correction to Enthalpy= 0.534089
Thermal correction to Gibbs Free Energy= 0.430010
Sum of electronic and zero-point Energies= -5845.126497
Sum of electronic and thermal Energies= -5845.092678
Sum of electronic and thermal Enthalpies= -5845.091591
Sum of electronic and thermal Free Energies= -5845.195669

	1	2	3
	A	A	A
Frequencies --	25.8329	32.6662	42.0779
Red. masses --	4.6307	4.6156	5.3212
Frc consts --	0.0018	0.0029	0.0056
IR Inten --	1.4257	0.1538	0.0541



Structure 13b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-1.671418	-0.643904	0.662083
2	6	0	-3.268281	-1.928805	-0.011286
3	6	0	-3.611718	0.205133	-1.122729
4	6	0	-3.775109	-0.637061	0.129516
5	6	0	-2.663992	-2.192091	-1.380271
6	6	0	-4.290894	-0.500066	-2.320893
7	6	0	-1.591345	-1.117118	-1.433670
8	6	0	-2.103359	0.173689	-1.296256
9	6	0	-3.721644	-1.925620	-2.477976
10	1	0	-3.988426	1.220953	-0.986797
11	1	0	-2.245204	-3.197186	-1.457296
12	1	0	-5.372736	-0.525337	-2.153051
13	1	0	-4.120731	0.093069	-3.225438
14	1	0	-3.255622	-2.057380	-3.459921
15	1	0	-4.514363	-2.676513	-2.396710
16	1	0	-0.595559	-1.316395	-1.822263
17	1	0	-4.447751	-0.351185	0.934701
18	6	0	1.637998	0.586374	1.300371
19	6	0	0.419071	-0.299279	1.520756
20	1	0	2.511646	-0.015995	1.585193
21	1	0	0.473930	-1.310309	1.098934
22	6	0	-0.423270	-0.165440	2.634908
23	8	0	-1.454129	-0.945108	2.731145
24	6	0	-0.219191	0.921119	3.657458
25	1	0	-0.906370	1.750270	3.447739
26	1	0	-0.515957	0.513509	4.629341
27	6	0	1.227551	1.404845	3.659807
28	1	0	1.337071	2.258986	4.336563
29	1	0	1.878339	0.609994	4.046211
30	6	0	1.658540	1.795018	2.251331
31	1	0	0.998946	2.591251	1.895576
32	1	0	2.670914	2.214542	2.258570

33	6	0	1.864073	0.953255	-0.160128
34	6	0	2.601581	0.204207	-1.014378
35	1	0	-1.541577	1.057965	-1.581907
36	1	0	-3.506177	-2.735329	0.678011
37	6	0	3.392893	-1.022304	-0.839671
38	6	0	4.430050	-1.232469	-1.769817
39	6	0	3.205162	-2.009605	0.144566
40	6	0	5.261985	-2.343925	-1.702618
41	1	0	4.589056	-0.496613	-2.555273
42	6	0	4.034907	-3.126539	0.210295
43	1	0	2.390661	-1.935276	0.854561
44	6	0	5.071925	-3.299399	-0.704522
45	1	0	6.057601	-2.466940	-2.432949
46	1	0	3.859875	-3.873708	0.980262
47	1	0	5.714865	-4.173670	-0.648415
48	6	0	1.307690	2.231862	-0.681388
49	6	0	0.018958	2.677097	-0.345008
50	6	0	2.081140	3.056585	-1.514444
51	6	0	-0.484387	3.875067	-0.844394
52	1	0	-0.603548	2.065148	0.302386
53	6	0	1.579715	4.255062	-2.017026
54	1	0	3.103162	2.769513	-1.747086
55	6	0	0.290709	4.670351	-1.687958
56	1	0	-1.489914	4.187676	-0.573090
57	1	0	2.206099	4.873477	-2.655054
58	1	0	-0.100772	5.607894	-2.073881
59	1	0	2.674835	0.594471	-2.029240

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SCF Done:  E(RPBE1PBE) =  -5845.62479480     A.U. after    1 cycles
            Convg  =    0.2275D-08             -V/T =  2.0044
Zero-point correction=                           0.500330 (Hartree/Particle)
 Thermal correction to Energy=                    0.533946
 Thermal correction to Enthalpy=                  0.535033
 Thermal correction to Gibbs Free Energy=         0.429676
 Sum of electronic and zero-point Energies=          -5845.124465
 Sum of electronic and thermal Energies=             -5845.090849
 Sum of electronic and thermal Enthalpies=           -5845.089762
 Sum of electronic and thermal Free Energies=        -5845.195119

                     1                      2                      3
                     A                      A                      A
 Frequencies --    10.7390                27.0411                37.1632
 Red. masses --     5.2470                 4.1821                 4.7281
 Frc consts  --     0.0004                 0.0018                 0.0038
 IR Inten    --     0.1523                 0.3154                 0.1583
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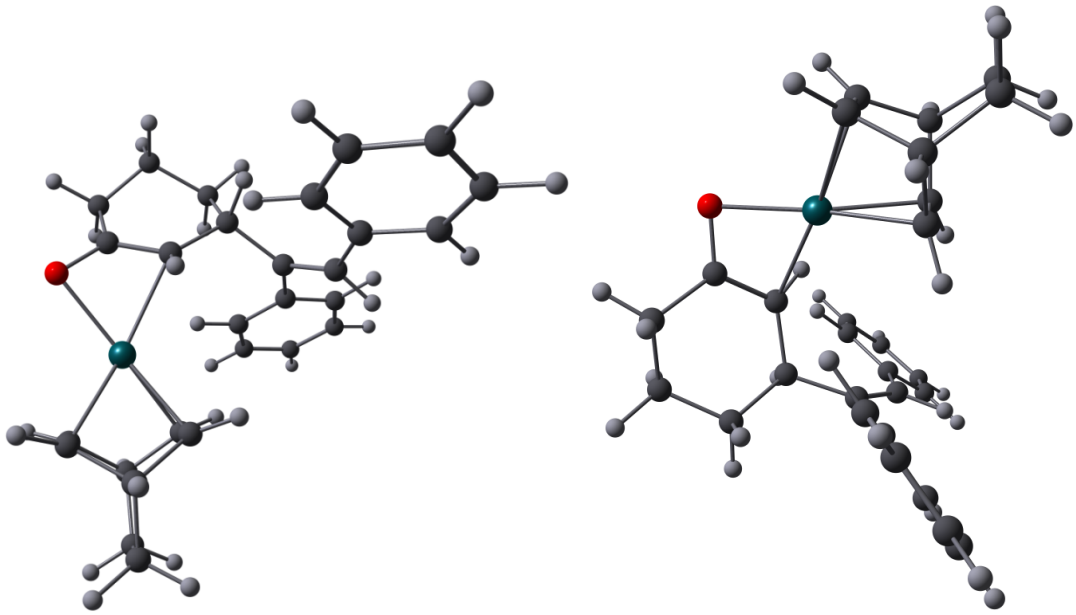


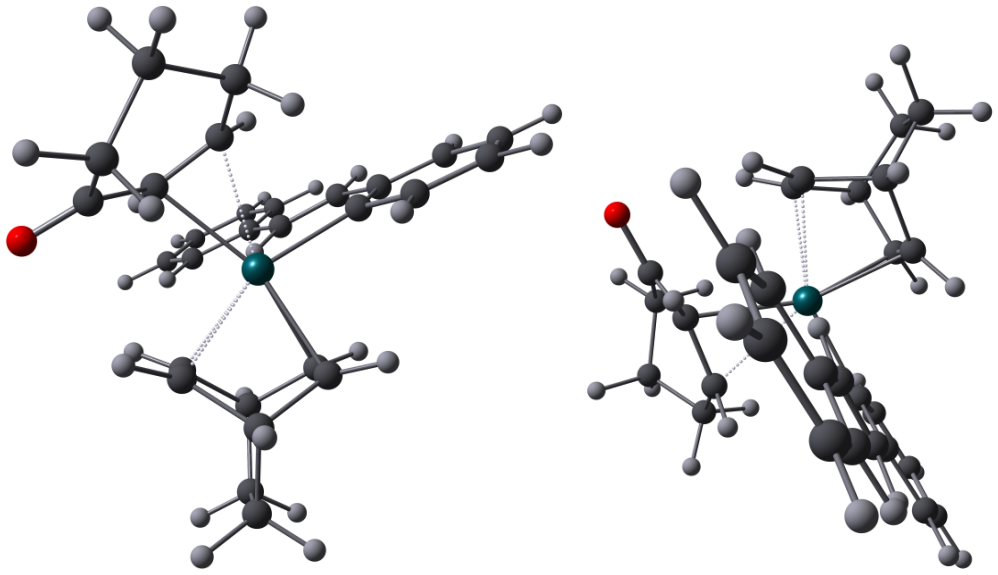
Structure 14a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.884278	-0.130819	-0.087303
2	6	0	0.417873	-0.715496	-2.130828
3	1	0	-0.253056	-0.026956	-2.636547
4	6	0	0.009550	-2.141982	-1.811950
5	1	0	-1.073236	-2.275247	-1.840232
6	6	0	0.580687	-2.355985	-0.421126
7	1	0	0.018707	-2.837320	0.375012
8	6	0	1.940553	-2.151889	-0.350675
9	1	0	2.537741	-2.464119	0.500566
10	6	0	2.563109	-1.761689	-1.675543
11	1	0	3.635241	-1.576586	-1.589426
12	6	0	1.792545	-0.511218	-2.047926
13	1	0	2.280748	0.357927	-2.479228
14	6	0	-2.285327	0.562094	-0.100729
15	6	0	-2.027655	1.834413	-0.464800
16	6	0	-3.592549	-0.014202	0.217585
17	6	0	-4.807487	0.684743	0.096621
18	6	0	-3.649161	-1.343541	0.669776
19	6	0	-6.016434	0.080140	0.419287
20	1	0	-4.812445	1.711796	-0.257626
21	6	0	-4.859237	-1.950382	0.995513
22	1	0	-2.723259	-1.906334	0.771273
23	6	0	-6.052251	-1.240763	0.872581
24	1	0	-6.941305	0.642145	0.315924
25	1	0	-4.869791	-2.979055	1.346733
26	1	0	-6.999804	-1.709025	1.124854
27	6	0	-0.738243	2.454449	-0.781772
28	6	0	-0.811015	3.779523	-1.262212
29	6	0	0.534847	1.842115	-0.623980
30	6	0	0.319816	4.509731	-1.600796
31	1	0	-1.791844	4.240677	-1.369647
32	6	0	1.658997	2.605814	-0.974315
33	6	0	1.570633	3.913420	-1.454500

34	1	0	0.226821	5.527805	-1.970025
35	1	0	2.652558	2.171594	-0.867305
36	1	0	2.476025	4.460519	-1.709405
37	1	0	-2.871482	2.520059	-0.547258
38	6	0	0.703281	1.011004	1.925211
39	6	0	0.646323	-0.364053	2.118563
40	6	0	1.914572	1.826477	2.318453
41	1	0	2.471083	2.140725	1.429563
42	1	0	1.566403	2.753875	2.786003
43	6	0	2.832191	1.068392	3.274530
44	1	0	3.776501	1.608855	3.397140
45	1	0	2.365532	1.018920	4.266168
46	6	0	3.098221	-0.352158	2.782711
47	1	0	3.750375	-0.911192	3.458918
48	1	0	3.588865	-0.321233	1.799840
49	6	0	1.804552	-1.122326	2.630838
50	8	0	1.712297	-2.308469	2.932989
51	1	0	-0.237494	1.543296	1.819152
52	1	0	-0.313016	-0.876274	2.175305
53	1	0	-1.440487	-0.129248	-0.030699
54	6	0	2.255627	-2.870478	-2.715686
55	1	0	2.661432	-2.568677	-3.686587
56	1	0	2.775814	-3.787165	-2.420118
57	6	0	0.732619	-3.098187	-2.796172
58	1	0	0.474281	-4.130979	-2.541781
59	1	0	0.358402	-2.911968	-3.807816

SCF Done: E(RPBE1PBE) = -5845.60481218 A.U. after 1 cycles
Convg = 0.6181D-08 -V/T = 2.0044
Zero-point correction= 0.497291 (Hartree/Particle)
Thermal correction to Energy= 0.532352
Thermal correction to Enthalpy= 0.533439
Thermal correction to Gibbs Free Energy= 0.424757
Sum of electronic and zero-point Energies= -5845.107521
Sum of electronic and thermal Energies= -5845.072460
Sum of electronic and thermal Enthalpies= -5845.071373
Sum of electronic and thermal Free Energies= -5845.180055

	1	2	3
	A	A	A
Frequencies --	17.2328	27.0905	29.4740
Red. masses --	3.8386	5.2752	4.6269
Frc consts --	0.0007	0.0023	0.0024
IR Inten --	0.1078	0.7331	1.1049



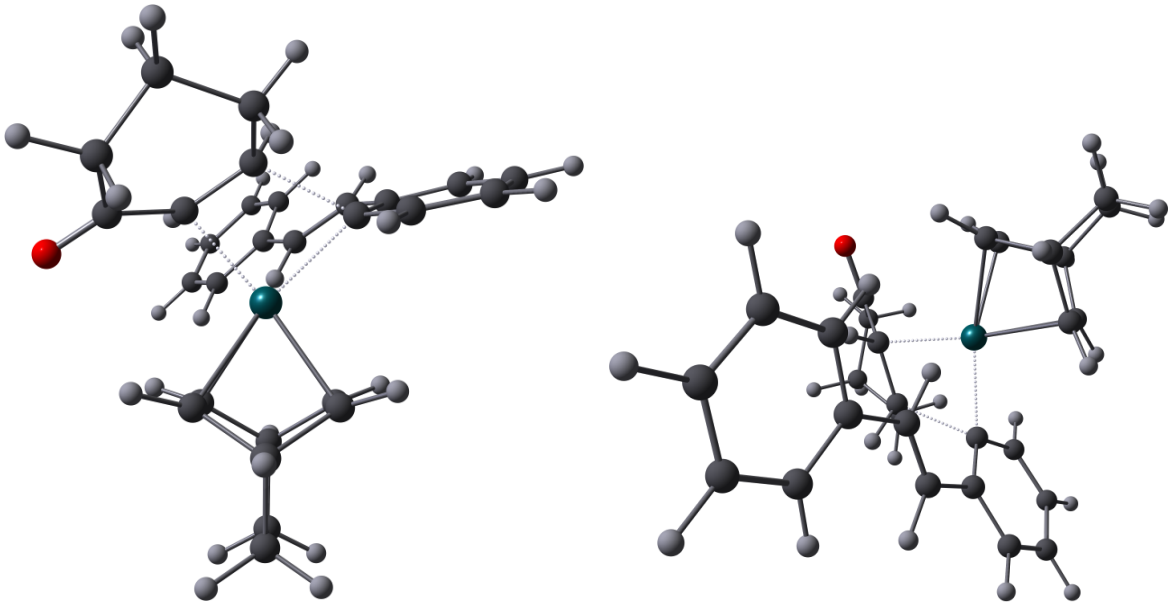
Structure 15a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.891827	-0.265749	0.013899
2	6	0	0.944177	-1.335484	-1.945770
3	1	0	0.366213	-0.847007	-2.725935
4	6	0	0.524873	-2.664743	-1.339365
5	1	0	-0.511065	-2.916114	-1.575616
6	6	0	0.736991	-2.435630	0.148278
7	1	0	0.034675	-2.791463	0.898058
8	6	0	2.040840	-2.070289	0.463587
9	1	0	2.428908	-2.113802	1.478077
10	6	0	2.949771	-1.991129	-0.749902
11	1	0	3.960826	-1.673882	-0.487559
12	6	0	2.240328	-0.977555	-1.629009
13	1	0	2.774830	-0.179196	-2.136150
14	6	0	-2.242992	0.407269	-0.516870
15	6	0	-1.947074	1.614332	-1.039649
16	6	0	-3.567645	-0.097510	-0.152682
17	6	0	-4.740375	0.675876	-0.216029
18	6	0	-3.680590	-1.425277	0.290938
19	6	0	-5.970631	0.136251	0.138860
20	1	0	-4.693993	1.712330	-0.538804
21	6	0	-4.912016	-1.966096	0.650552
22	1	0	-2.784097	-2.038176	0.356767
23	6	0	-6.065336	-1.187833	0.574048
24	1	0	-6.863964	0.753046	0.082512
25	1	0	-4.970083	-2.995800	0.993430
26	1	0	-7.028783	-1.604277	0.855293
27	6	0	-0.617931	2.121740	-1.381786
28	6	0	-0.562310	3.062812	-2.426531
29	6	0	0.583112	1.754073	-0.709429
30	6	0	0.636378	3.606213	-2.866467
31	1	0	-1.492091	3.354811	-2.911585
32	6	0	1.779099	2.342629	-1.163262
33	6	0	1.821671	3.230405	-2.231830
34	1	0	0.647280	4.320468	-3.685444

35	1	0	2.716112	2.091098	-0.672904
36	1	0	2.774892	3.642078	-2.555292
37	1	0	-2.765238	2.291727	-1.285056
38	6	0	0.381795	1.698322	1.256273
39	6	0	0.219843	0.401904	1.892427
40	6	0	1.509579	2.583448	1.776427
41	1	0	2.448205	2.362773	1.263925
42	1	0	1.278596	3.631353	1.561929
43	6	0	1.751180	2.347853	3.264193
44	1	0	2.542038	3.018217	3.618608
45	1	0	0.849575	2.582521	3.843649
46	6	0	2.146913	0.892244	3.489657
47	1	0	2.331756	0.663983	4.542987
48	1	0	3.075773	0.671303	2.945853
49	6	0	1.067727	-0.055284	3.000067
50	8	0	0.879044	-1.135853	3.560188
51	1	0	-0.565384	2.219277	1.133713
52	1	0	-0.793620	-0.000698	1.949562
53	1	0	-1.418274	-0.297211	-0.366481
54	6	0	2.950543	-3.366084	-1.467330
55	1	0	3.570760	-3.297800	-2.366999
56	1	0	3.416077	-4.108508	-0.810979
57	6	0	1.503631	-3.767178	-1.820488
58	1	0	1.231311	-4.715180	-1.345498
59	1	0	1.384912	-3.902043	-2.900443

SCF Done: E(RPBE1PBE) = -5845.58461202 A.U. after 1 cycles
Convg = 0.2330D-08 -V/T = 2.0044
Zero-point correction= 0.496870 (Hartree/Particle)
Thermal correction to Energy= 0.530844
Thermal correction to Enthalpy= 0.531931
Thermal correction to Gibbs Free Energy= 0.425741
Sum of electronic and zero-point Energies= -5845.087742
Sum of electronic and thermal Energies= -5845.053768
Sum of electronic and thermal Enthalpies= -5845.052681
Sum of electronic and thermal Free Energies= -5845.158871

	1	2	3
	A	A	A
Frequencies --	-295.1602	11.7606	27.8115
Red. masses --	7.8276	3.6636	5.3668
Frc consts --	0.4018	0.0003	0.0024
IR Inten --	103.5783	0.0491	0.9931



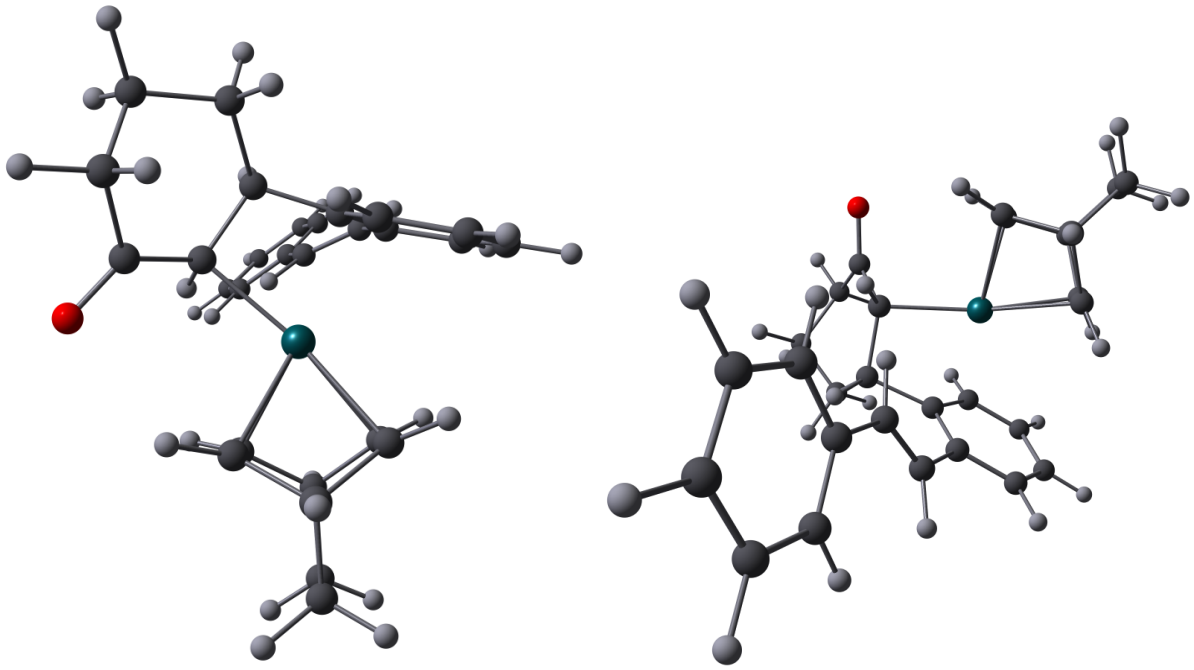
Structure 16a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-1.259752	-0.103839	0.016359
2	6	0	-1.610073	-2.169518	0.791656
3	1	0	-0.954609	-2.438318	1.616774
4	6	0	-1.472648	-2.794329	-0.588021
5	1	0	-0.525613	-3.324278	-0.706691
6	6	0	-1.573286	-1.585388	-1.502886
7	1	0	-0.948733	-1.469917	-2.385194
8	6	0	-2.759206	-0.864196	-1.333396
9	1	0	-3.105404	-0.140041	-2.067018
10	6	0	-3.669998	-1.464292	-0.277861
11	1	0	-4.577734	-0.875210	-0.133949
12	6	0	-2.784544	-1.463506	0.956769
13	1	0	-3.142203	-1.122587	1.924169
14	6	0	2.694583	-0.183491	0.307046
15	6	0	2.310743	0.137730	1.556371
16	6	0	4.040173	-0.570346	-0.123387
17	6	0	5.177570	-0.463416	0.695597
18	6	0	4.209207	-1.074127	-1.422862
19	6	0	6.426784	-0.861341	0.234963
20	1	0	5.091216	-0.055326	1.699013
21	6	0	5.460421	-1.472770	-1.885676
22	1	0	3.343522	-1.155977	-2.076636
23	6	0	6.576082	-1.370709	-1.057271
24	1	0	7.293609	-0.767983	0.884121
25	1	0	5.563791	-1.861227	-2.895387
26	1	0	7.555250	-1.677674	-1.414678
27	6	0	0.951373	0.485657	1.998338
28	6	0	0.556620	-0.020752	3.245547
29	6	0	0.052690	1.338138	1.284306
30	6	0	-0.706791	0.220292	3.783093
31	1	0	1.263974	-0.631270	3.802662
32	6	0	-1.241783	1.522872	1.828014
33	6	0	-1.616592	0.982574	3.065240

34	1	0	-0.972015	-0.190795	4.753415
35	1	0	-1.930499	2.205156	1.335666
36	1	0	-2.610050	1.180857	3.458786
37	1	0	3.040421	0.070201	2.362926
38	6	0	0.428250	2.125047	0.018003
39	6	0	-0.269643	1.383398	-1.129878
40	6	0	0.106588	3.630975	0.149713
41	1	0	-0.690656	3.795436	0.881619
42	1	0	0.987182	4.148087	0.547520
43	6	0	-0.336918	4.256010	-1.166006
44	1	0	-0.579784	5.313548	-1.012022
45	1	0	0.476465	4.224719	-1.902248
46	6	0	-1.547466	3.503512	-1.716137
47	1	0	-1.952033	3.966337	-2.620292
48	1	0	-2.349565	3.495565	-0.965328
49	6	0	-1.157281	2.077701	-2.059283
50	8	0	-1.545545	1.567190	-3.118297
51	1	0	1.509107	2.036786	-0.120757
52	1	0	0.406079	0.736344	-1.701180
53	1	0	1.935513	-0.209192	-0.473035
54	6	0	-3.995461	-2.930741	-0.664140
55	1	0	-4.622385	-3.373534	0.116782
56	1	0	-4.583510	-2.930768	-1.587647
57	6	0	-2.685741	-3.725781	-0.840667
58	1	0	-2.610419	-4.140314	-1.851186
59	1	0	-2.639621	-4.568585	-0.143108

SCF Done: E(RPBE1PBE) = -5845.62311941 A.U. after 1 cycles
Convg = 0.3065D-08 -V/T = 2.0044
Zero-point correction= 0.498750 (Hartree/Particle)
Thermal correction to Energy= 0.533054
Thermal correction to Enthalpy= 0.534141
Thermal correction to Gibbs Free Energy= 0.426453
Sum of electronic and zero-point Energies= -5845.124369
Sum of electronic and thermal Energies= -5845.090065
Sum of electronic and thermal Enthalpies= -5845.088979
Sum of electronic and thermal Free Energies= -5845.196666

	1	2	3
	A	A	A
Frequencies --	13.7942	22.5183	27.8049
Red. masses --	5.6100	3.7331	4.2928
Frc consts --	0.0006	0.0011	0.0020
IR Inten --	0.4305	0.0407	0.3374



Structure 17a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	1.912654	-0.960527	-0.154210
2	6	0	4.032857	-1.442878	-0.431078
3	6	0	3.417989	0.116374	-2.192837
4	6	0	3.433344	-1.313428	-1.677970
5	6	0	4.537133	-0.125809	0.128549
6	6	0	4.865831	0.661694	-2.251086
7	6	0	3.255599	0.687165	0.164933
8	6	0	2.649785	0.824245	-1.087840
9	6	0	5.532943	0.516446	-0.867694
10	1	0	2.916128	0.198110	-3.158680
11	1	0	4.977852	-0.242908	1.120448
12	1	0	5.423382	0.111817	-3.016355
13	1	0	4.837368	1.709841	-2.566396
14	1	0	5.847170	1.490408	-0.478166
15	1	0	6.429977	-0.108667	-0.927048
16	1	0	3.032124	1.340347	1.003785
17	1	0	3.219081	-2.162074	-2.322796
18	8	0	0.850100	-2.731006	0.342003
19	6	0	0.300706	-1.881954	1.154410
20	6	0	-0.172196	-0.661939	0.629217
21	6	0	-0.811190	0.388373	1.517930
22	1	0	-1.870744	0.120000	1.634857
23	6	0	-0.211583	0.300568	2.926326
24	1	0	-0.698611	1.030453	3.582201
25	1	0	-1.466558	-1.354987	3.473126
26	6	0	-0.396489	-1.113294	3.472018
27	1	0	0.859147	0.537831	2.906712
28	1	0	-0.065250	-1.166195	4.514550
29	6	0	-0.794021	1.773219	0.900514
30	6	0	0.314794	2.600981	1.105856
31	6	0	-1.882992	2.288704	0.152972

32	6	0	0.391522	3.892931	0.597040
33	6	0	-1.800519	3.610636	-0.328557
34	6	0	-0.680997	4.405273	-0.130306
35	1	0	1.275395	4.498775	0.780029
36	1	0	-2.645235	4.012740	-0.883950
37	1	0	-0.651071	5.416437	-0.527471
38	6	0	0.363814	-2.145383	2.639536
39	1	0	-0.021353	-3.156543	2.812280
40	1	0	1.423013	-2.175005	2.920772
41	1	0	-0.478754	-0.687695	-0.420700
42	1	0	4.328190	-2.401583	-0.012221
43	1	0	1.903576	1.585369	-1.300591
44	1	0	1.142123	2.224547	1.698202
45	6	0	-3.147850	1.598624	-0.144848
46	6	0	-3.390282	0.288326	-0.347357
47	1	0	-3.985504	2.284316	-0.273043
48	1	0	-2.568464	-0.422087	-0.323466
49	6	0	-4.692104	-0.304724	-0.669382
50	6	0	-4.729017	-1.625876	-1.143874
51	6	0	-5.913180	0.375586	-0.521164
52	6	0	-5.932869	-2.239420	-1.479784
53	1	0	-3.796665	-2.175359	-1.255498
54	6	0	-7.115802	-0.236244	-0.855339
55	1	0	-5.928396	1.387006	-0.124267
56	6	0	-7.133726	-1.545993	-1.339955
57	1	0	-5.932505	-3.261730	-1.848820
58	1	0	-8.048480	0.307583	-0.728749
59	1	0	-8.076151	-2.022186	-1.596699

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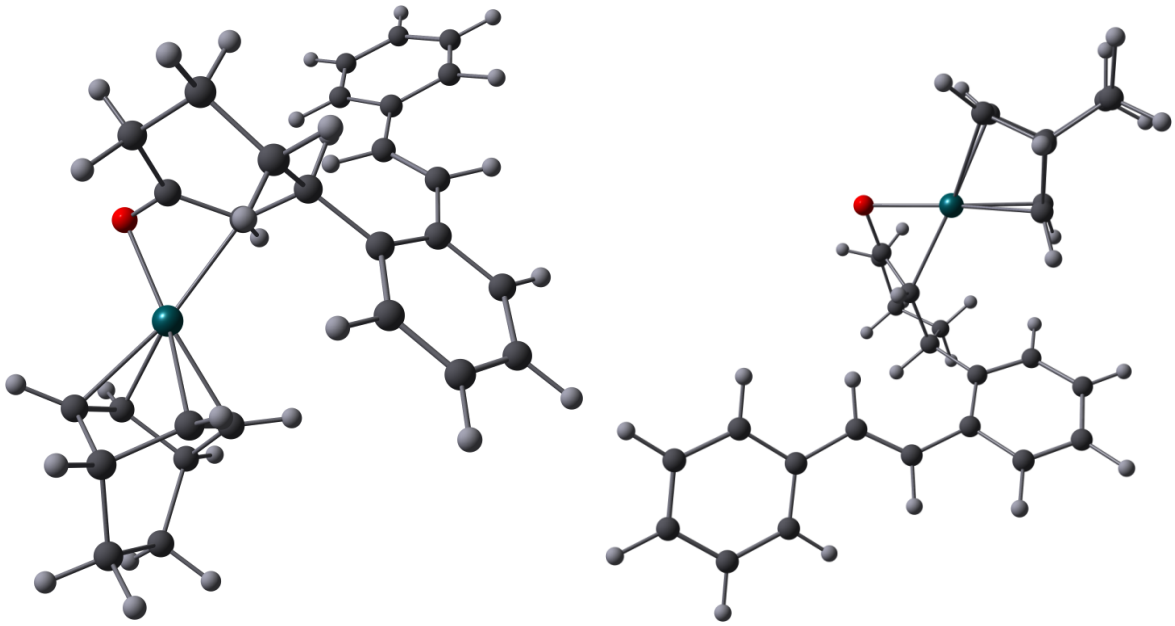
SCF Done:  E(RPBE1PBE) =  -5845.63322062     A.U. after    1 cycles
             Convg  =    0.2013D-08             -V/T =  2.0044
Zero-point correction=                           0.499718 (Hartree/Particle)
 Thermal correction to Energy=                    0.533724
 Thermal correction to Enthalpy=                  0.534811
 Thermal correction to Gibbs Free Energy=         0.427486
 Sum of electronic and zero-point Energies=          -5845.133502
 Sum of electronic and thermal Energies=             -5845.099496
 Sum of electronic and thermal Enthalpies=           -5845.098409
 Sum of electronic and thermal Free Energies=        -5845.205734

                    1                      2                      3
                    A                      A                      A
 Frequencies --    12.7544               19.1489               27.4557
 Red. masses --     4.8071                4.1024                5.2084
 Frc consts  --     0.0005                0.0009                0.0023
 IR Inten    --     0.1579                0.4954                0.2212
```



Structure 14b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	1.225442	-0.090640	0.179074
2	6	0	0.899512	-0.535384	-1.945335
3	1	0	0.257673	0.179326	-2.452034
4	6	0	0.501259	-1.989671	-1.773884
5	1	0	-0.570459	-2.140052	-1.915567
6	6	0	0.945728	-2.292356	-0.355224
7	1	0	0.323457	-2.839593	0.347643
8	6	0	2.288239	-2.073600	-0.142737
9	1	0	2.805558	-2.430817	0.743057
10	6	0	3.021329	-1.574412	-1.372843
11	1	0	4.075518	-1.375311	-1.172991
12	6	0	2.256771	-0.312755	-1.728428
13	1	0	2.762484	0.592443	-2.052445
14	6	0	-1.885407	0.678417	-0.499217
15	6	0	-1.522228	1.949787	-0.764254
16	6	0	-3.226330	0.104884	-0.620110
17	6	0	-4.370196	0.852413	-0.956009
18	6	0	-3.396363	-1.270215	-0.383467
19	6	0	-5.617732	0.248293	-1.054197
20	1	0	-4.289227	1.920501	-1.137671
21	6	0	-4.645677	-1.877322	-0.480866
22	1	0	-2.529357	-1.873493	-0.120708
23	6	0	-5.765935	-1.120753	-0.818146
24	1	0	-6.485311	0.849795	-1.313871
25	1	0	-4.743674	-2.943317	-0.291836
26	1	0	-6.743855	-1.588286	-0.894271
27	6	0	-0.201066	2.574589	-0.648500
28	6	0	-0.153254	3.938812	-1.012978
29	6	0	0.988408	1.934059	-0.206849
30	6	0	1.017727	4.680710	-0.965513
31	1	0	-1.072133	4.421105	-1.343652
32	6	0	2.156972	2.712958	-0.166858

33	6	0	2.189173	4.057073	-0.537412
34	1	0	1.017029	5.728220	-1.255627
35	1	0	3.086874	2.256167	0.171183
36	1	0	3.123692	4.612271	-0.488797
37	1	0	-2.295996	2.634422	-1.112478
38	6	0	1.024681	0.887268	2.292917
39	6	0	1.468237	-0.423819	2.379905
40	1	0	2.533248	-0.647065	2.410072
41	6	0	-0.363964	1.298237	2.728362
42	1	0	1.772486	1.672588	2.245672
43	6	0	0.570893	-1.522266	2.792328
44	6	0	-0.877544	-1.156633	3.033612
45	1	0	-1.316541	-1.922709	3.678524
46	8	0	0.990028	-2.665555	2.947290
47	1	0	-1.002659	1.497816	1.863056
48	1	0	-1.106343	-0.013317	-0.163700
49	6	0	2.837759	-2.606057	-2.516105
50	1	0	3.320625	-2.222513	-3.420625
51	1	0	3.354302	-3.531815	-2.243223
52	6	0	1.334658	-2.857261	-2.751620
53	1	0	1.082205	-3.910966	-2.595468
54	1	0	1.048536	-2.606339	-3.778019
55	6	0	-1.008457	0.244167	3.626793
56	1	0	-2.063767	0.484736	3.790083
57	1	0	-0.522855	0.258714	4.610577
58	1	0	-1.405428	-1.204320	2.071753
59	1	0	-0.284372	2.250066	3.264545

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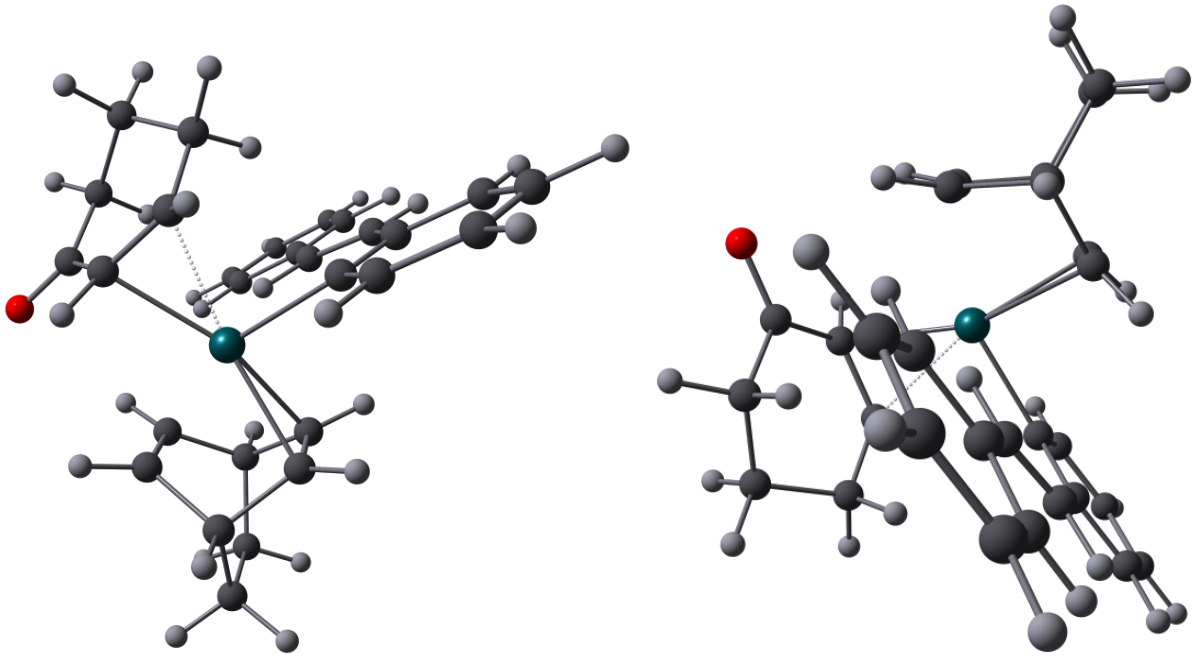
SCF Done:  E(RPBE1PBE) =  -5845.60325845     A.U. after    1 cycles
            Convg  =    0.2578D-08             -V/T =  2.0044
Zero-point correction=                           0.497566 (Hartree/Particle)
 Thermal correction to Energy=                    0.532484
 Thermal correction to Enthalpy=                  0.533571
 Thermal correction to Gibbs Free Energy=         0.426258
 Sum of electronic and zero-point Energies=          -5845.105692
 Sum of electronic and thermal Energies=             -5845.070774
 Sum of electronic and thermal Enthalpies=           -5845.069687
 Sum of electronic and thermal Free Energies=        -5845.177001
                    1                      2                      3
                    A                      A                      A
 Frequencies --    22.4212               26.5616               41.9870
 Red. masses --     4.5082                5.0835                4.1804
 Frc consts  --     0.0013                0.0021                0.0043
 IR Inten    --     0.1931                0.3303                0.1772
```



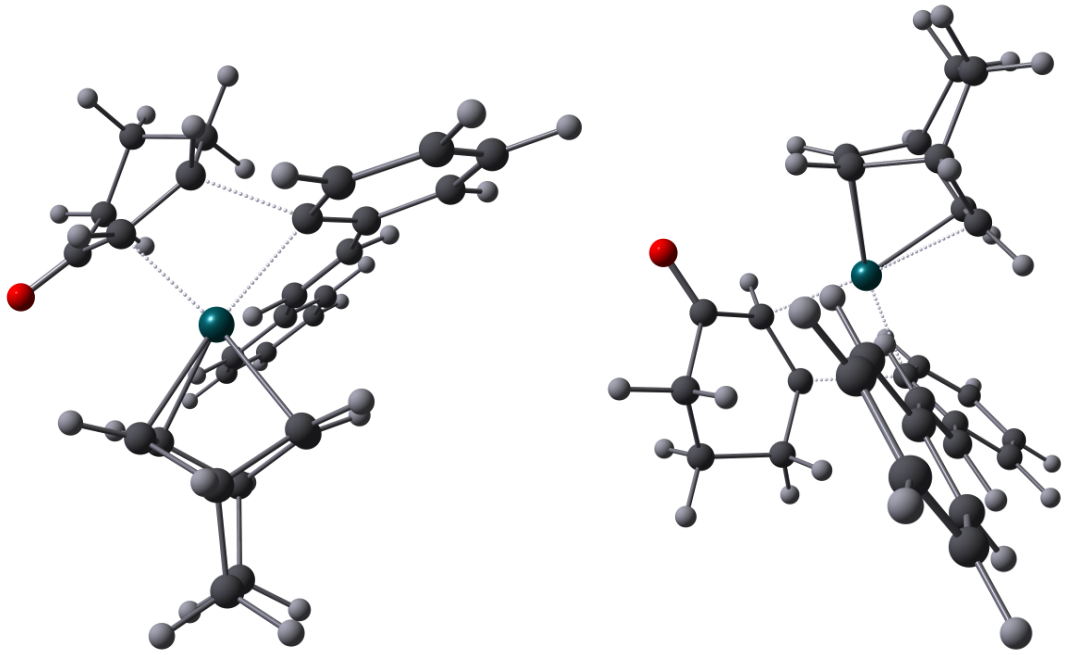
Structure 15b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	1.210839	-0.152070	0.345434
2	6	0	1.162802	-1.222487	-1.634779
3	1	0	0.542991	-0.737109	-2.383708
4	6	0	0.785201	-2.557723	-1.017288
5	1	0	-0.255204	-2.822573	-1.215795
6	6	0	1.049767	-2.327972	0.462047
7	1	0	0.375813	-2.682975	1.238190
8	6	0	2.362801	-1.956449	0.729477
9	1	0	2.795565	-2.007548	1.725249
10	6	0	3.221619	-1.855265	-0.518624
11	1	0	4.237428	-1.524371	-0.294506
12	6	0	2.463372	-0.845566	-1.364334
13	1	0	2.966659	-0.034834	-1.884228
14	6	0	-1.759503	0.392558	-0.779742
15	6	0	-1.367279	1.551642	-1.347512
16	6	0	-3.079956	-0.229242	-0.864872
17	6	0	-4.168632	0.340805	-1.549637
18	6	0	-3.282428	-1.464389	-0.225499
19	6	0	-5.398707	-0.303021	-1.596121
20	1	0	-4.057458	1.298459	-2.050458
21	6	0	-4.515923	-2.108733	-0.268708
22	1	0	-2.456725	-1.921882	0.315861
23	6	0	-5.581393	-1.531905	-0.956622
24	1	0	-6.225248	0.156431	-2.132220
25	1	0	-4.644355	-3.062143	0.237037
26	1	0	-6.546178	-2.030457	-0.993439
27	6	0	-0.054267	2.190431	-1.265017
28	6	0	0.206943	3.157239	-2.258765
29	6	0	0.965297	1.892522	-0.313763
30	6	0	1.438399	3.781923	-2.383966
31	1	0	-0.583458	3.395853	-2.968230

32	6	0	2.197718	2.561809	-0.456545
33	6	0	2.454138	3.466208	-1.478545
34	1	0	1.604280	4.511617	-3.172035
35	1	0	2.981384	2.373459	0.276265
36	1	0	3.428591	3.943033	-1.552075
37	1	0	-2.079950	2.088480	-1.973487
38	6	0	0.615480	1.800809	1.646487
39	6	0	0.870796	0.534146	2.305582
40	1	0	-1.017221	-0.163216	-0.192763
41	6	0	3.213366	-3.224501	-1.246393
42	1	0	3.792474	-3.139018	-2.171665
43	1	0	3.719210	-3.964241	-0.617403
44	6	0	1.758832	-3.645898	-1.538945
45	1	0	1.519695	-4.597610	-1.053434
46	1	0	1.597150	-3.782912	-2.613044
47	6	0	-0.178504	-0.203284	3.023048
48	8	0	0.057372	-1.251182	3.625775
49	6	0	-0.760967	2.437361	1.806407
50	1	0	-0.644973	3.525928	1.803346
51	1	0	-1.412382	2.194379	0.966512
52	6	0	-1.451724	1.954981	3.079743
53	1	0	-0.894849	2.280148	3.967786
54	1	0	-2.448963	2.403508	3.147203
55	6	0	-1.555201	0.431826	3.070845
56	1	0	-2.066704	0.041782	3.955138
57	1	0	-2.133116	0.105470	2.196171
58	1	0	1.422658	2.509522	1.803539
59	1	0	1.863839	0.388465	2.737722

SCF Done: E(RPBE1PBE) = -5845.58205541 A.U. after 1 cycles
Convg = 0.4315D-08 -V/T = 2.0044
Zero-point correction= 0.496568 (Hartree/Particle)
Thermal correction to Energy= 0.530615
Thermal correction to Enthalpy= 0.531702
Thermal correction to Gibbs Free Energy= 0.426036
Sum of electronic and zero-point Energies= -5845.085487
Sum of electronic and thermal Energies= -5845.051440
Sum of electronic and thermal Enthalpies= -5845.050354
Sum of electronic and thermal Free Energies= -5845.156020

	1	2	3
	A	A	A
Frequencies --	-298.1798	20.3776	24.9732
Red. masses --	7.7628	4.6905	4.9449
Frc consts --	0.4067	0.0011	0.0018
IR Inten --	97.8289	0.6149	0.9855



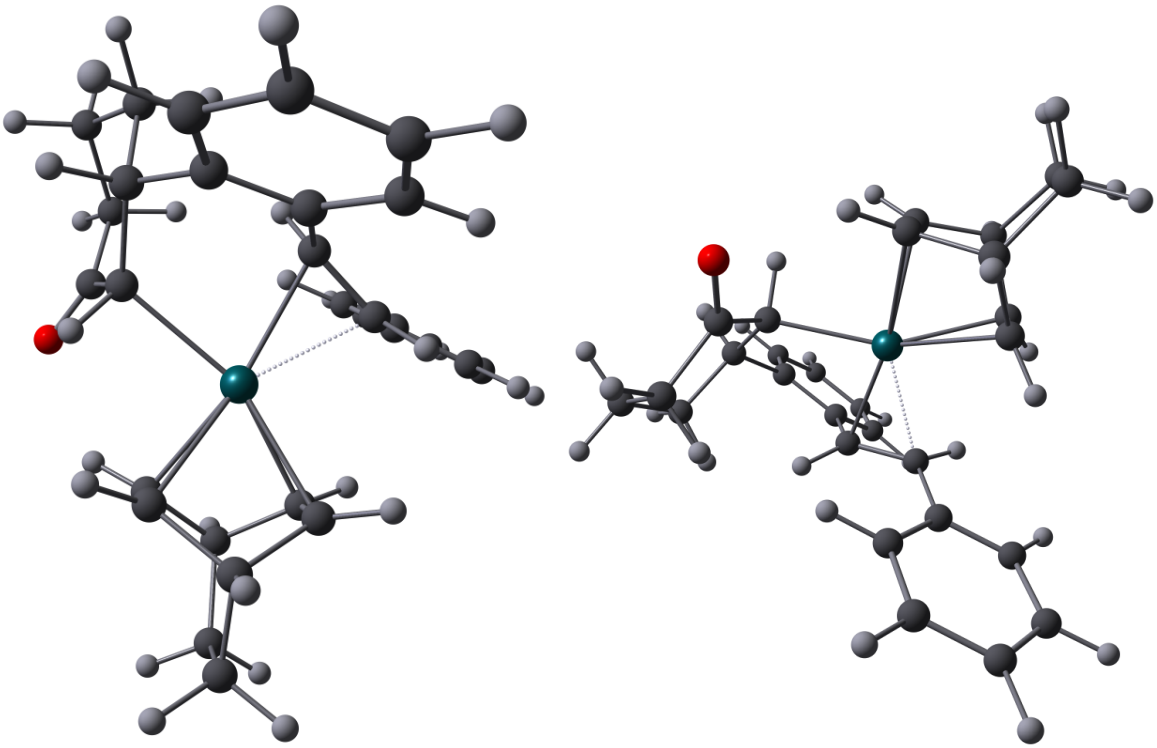
Structure 16b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.273593	-0.567599	0.039383
2	6	0	-2.433647	-0.933542	-0.377391
3	1	0	-3.007473	-0.024069	-0.530424
4	6	0	-2.653655	-1.818758	0.833550
5	1	0	-3.211458	-1.307905	1.619715
6	6	0	-1.234127	-2.137342	1.257421
7	1	0	-0.898123	-2.072832	2.289389
8	6	0	-0.495269	-2.750091	0.255768
9	1	0	0.446491	-3.258989	0.440284
10	6	0	-1.268162	-2.958942	-1.030136
11	1	0	-0.655286	-3.409565	-1.812417
12	6	0	-1.690681	-1.545214	-1.375452
13	1	0	-1.640911	-1.173522	-2.395155
14	6	0	-0.447013	1.292356	-1.233702
15	6	0	0.828086	1.209472	-0.698447
16	6	0	-1.512001	2.203140	-0.773491
17	6	0	-1.566028	2.731260	0.526333
18	6	0	-2.523844	2.565522	-1.674482
19	6	0	-2.584426	3.599189	0.901553
20	1	0	-0.819923	2.438252	1.259549
21	6	0	-3.545201	3.437023	-1.300282
22	1	0	-2.504299	2.165027	-2.686150
23	6	0	-3.579368	3.960570	-0.009969
24	1	0	-2.609243	3.990620	1.915294
25	1	0	-4.314726	3.705885	-2.019285
26	1	0	-4.375415	4.637671	0.287522
27	6	0	1.985350	0.632743	-1.417537
28	6	0	2.101045	0.713954	-2.809540
29	6	0	3.004790	0.003271	-0.674658
30	6	0	3.197334	0.162558	-3.470982
31	1	0	1.335878	1.233322	-3.381433

32	6	0	4.096283	-0.539907	-1.348323
33	6	0	4.198603	-0.470087	-2.739069
34	1	0	3.271212	0.236100	-4.553010
35	1	0	4.876295	-1.038524	-0.775645
36	1	0	5.055572	-0.907219	-3.245126
37	1	0	1.050951	1.826327	0.166610
38	6	0	2.895260	-0.057626	0.828664
39	6	0	1.534004	-0.612705	1.324635
40	1	0	-0.599762	0.894310	-2.235600
41	6	0	-2.531552	-3.804416	-0.728653
42	1	0	-3.117303	-3.907230	-1.647937
43	1	0	-2.221682	-4.811282	-0.430944
44	6	0	-3.356172	-3.124909	0.383555
45	1	0	-3.464570	-3.783085	1.251466
46	1	0	-4.365375	-2.883398	0.034482
47	6	0	1.114373	-0.181004	2.671282
48	8	0	0.505599	-0.917699	3.459267
49	6	0	3.335310	1.296004	1.431309
50	1	0	4.412882	1.405304	1.261785
51	1	0	2.868998	2.133910	0.902015
52	6	0	3.013451	1.412079	2.912493
53	1	0	3.571012	0.657865	3.482989
54	1	0	3.326594	2.390315	3.294541
55	6	0	1.515592	1.207680	3.133111
56	1	0	1.234645	1.306541	4.184816
57	1	0	0.962470	1.968889	2.567495
58	1	0	3.650467	-0.779992	1.170420
59	1	0	1.618972	-1.702854	1.353009

SCF Done: E(RPBE1PBE) = -5845.63560390 A.U. after 1 cycles
Convg = 0.1749D-08 -V/T = 2.0044
Zero-point correction= 0.501066 (Hartree/Particle)
Thermal correction to Energy= 0.534361
Thermal correction to Enthalpy= 0.535447
Thermal correction to Gibbs Free Energy= 0.432948
Sum of electronic and zero-point Energies= -5845.134538
Sum of electronic and thermal Energies= -5845.101243
Sum of electronic and thermal Enthalpies= -5845.100156
Sum of electronic and thermal Free Energies= -5845.202656

	1	2	3
	A	A	A
Frequencies --	21.3115	35.4300	42.8795
Red. masses --	4.8826	4.4122	5.0935
Frc consts --	0.0013	0.0033	0.0055
IR Inten --	1.1893	0.5533	0.0935



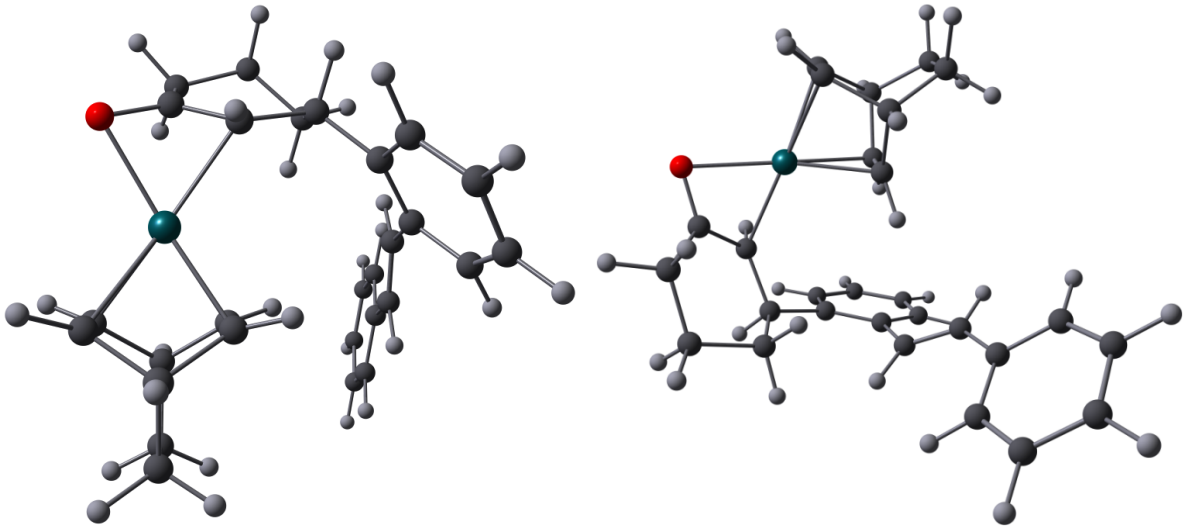
Structure 17b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	2.105612	0.459976	-0.514199
2	6	0	2.959101	2.370062	0.124753
3	6	0	0.613152	2.783055	-0.346296
4	6	0	2.027657	2.624675	-0.873435
5	6	0	2.347095	2.304801	1.515054
6	6	0	0.577380	3.917195	0.707387
7	6	0	1.332800	1.184657	1.347113
8	6	0	0.400840	1.443340	0.336837
9	6	0	1.609686	3.631713	1.817881
10	1	0	-0.108237	2.953476	-1.147667
11	1	0	3.091629	2.073670	2.279259
12	1	0	0.786819	4.870944	0.211786
13	1	0	-0.435111	3.986858	1.118931
14	1	0	1.124238	3.553560	2.796340
15	1	0	2.344467	4.440537	1.888417
16	1	0	1.177223	0.428982	2.113446
17	1	0	2.305720	2.918512	-1.882545
18	6	0	0.620530	-2.621979	-0.406678
19	6	0	1.837488	-1.735921	-0.633100
20	1	0	0.981638	-3.661814	-0.470499
21	1	0	2.647071	-1.822160	0.097807
22	6	0	2.233664	-1.316718	-1.922955
23	8	0	3.249803	-0.519625	-2.021342
24	6	0	1.417498	-1.627304	-3.152135
25	1	0	0.952074	-0.696343	-3.496153
26	1	0	2.114162	-1.929470	-3.941867
27	6	0	0.366718	-2.702679	-2.893938
28	1	0	-0.352802	-2.723208	-3.719117

29	1	0	0.844976	-3.690264	-2.870605
30	6	0	-0.357847	-2.466150	-1.570467
31	1	0	-0.789672	-1.458669	-1.579220
32	1	0	-1.178091	-3.185625	-1.471106
33	6	0	0.124275	-2.487876	1.034520
34	6	0	-1.071265	-1.891975	1.503175
35	6	0	1.022230	-2.987085	1.991720
36	6	0	-1.281066	-1.805758	2.895040
37	6	0	0.804032	-2.889308	3.359398
38	6	0	-0.362568	-2.280521	3.818901
39	1	0	-2.219126	-1.385981	3.248012
40	1	0	1.530974	-3.295452	4.057951
41	1	0	-0.568725	-2.203780	4.883232
42	1	0	-0.537013	0.903021	0.247834
43	1	0	4.032042	2.451699	-0.030574
44	6	0	-2.149760	-1.380580	0.637841
45	6	0	-2.867392	-0.270957	0.897709
46	1	0	-2.391568	-1.959445	-0.246077
47	1	0	-2.588733	0.334354	1.760816
48	6	0	-3.979063	0.261722	0.105440
49	6	0	-4.471535	1.540206	0.413080
50	6	0	-4.581381	-0.436238	-0.956021
51	6	0	-5.513192	2.109181	-0.314914
52	1	0	-4.025498	2.095973	1.235321
53	6	0	-5.620810	0.130608	-1.683982
54	1	0	-4.244311	-1.437412	-1.210569
55	6	0	-6.092537	1.407452	-1.370192
56	1	0	-5.873347	3.101675	-0.056812
57	1	0	-6.072826	-0.428679	-2.499152
58	1	0	-6.907158	1.845782	-1.940270
59	1	0	1.933840	-3.468365	1.642376

SCF Done: E(RPBE1PBE) = -5845.62985734 A.U. after 1 cycles
Convg = 0.1733D-08 -V/T = 2.0044
Zero-point correction= 0.499792 (Hartree/Particle)
Thermal correction to Energy= 0.533627
Thermal correction to Enthalpy= 0.534714
Thermal correction to Gibbs Free Energy= 0.428295
Sum of electronic and zero-point Energies= -5845.130065
Sum of electronic and thermal Energies= -5845.096230
Sum of electronic and thermal Enthalpies= -5845.095143
Sum of electronic and thermal Free Energies= -5845.201562

	1	2	3
	A	A	A
Frequencies --	13.5523	21.3829	26.9283
Red. masses --	5.1575	4.1066	5.0557
Frc consts --	0.0006	0.0011	0.0022
IR Inten --	0.1694	0.0222	0.3220



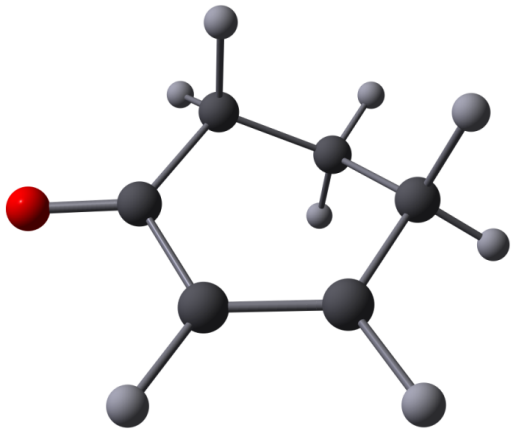
Additional structures:

Cyclohexenone

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.962786	1.316501	0.026452
2	1	0	-1.472304	2.279416	0.022905
3	6	0	0.378388	1.285575	-0.058478
4	1	0	0.965699	2.195826	-0.153244
5	6	0	1.134987	0.021818	0.015786
6	8	0	2.356376	0.001849	-0.074855
7	6	0	-1.810895	0.087597	0.133428
8	1	0	-2.735892	0.230605	-0.435904
9	1	0	-2.124409	-0.027400	1.181831
10	6	0	0.327111	-1.233624	0.267527
11	1	0	0.254269	-1.345523	1.358615
12	1	0	0.896279	-2.090369	-0.102278
13	6	0	-1.068843	-1.157153	-0.341705
14	1	0	-1.639526	-2.058480	-0.096773
15	1	0	-0.982898	-1.123150	-1.434372

SCF Done: E(RPBE1PBE) = -308.332694733 A.U. after 1 cycles
Convg = 0.2929D-08 -V/T = 2.0137
Zero-point correction= 0.128507 (Hartree/Particle)
Thermal correction to Energy= 0.136393
Thermal correction to Enthalpy= 0.137479
Thermal correction to Gibbs Free Energy= 0.092858
Sum of electronic and zero-point Energies= -308.204188
Sum of electronic and thermal Energies= -308.196302
Sum of electronic and thermal Enthalpies= -308.195215
Sum of electronic and thermal Free Energies= -308.239836

	1	2	3
	A	A	A
Frequencies --	103.2147	246.0749	307.9645
Red. masses --	3.2349	1.8126	2.4747
Frc consts --	0.0203	0.0647	0.1383
IR Inten --	3.8194	0.5517	1.2044



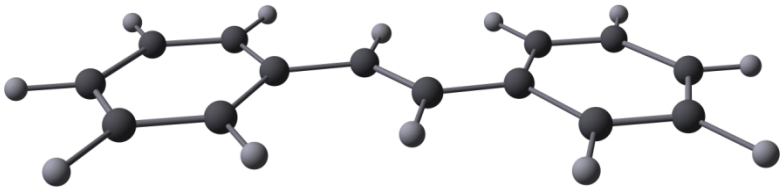
(*E*)-Stilbene

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.496682	0.455046	0.000005
2	6	0	-0.496684	-0.455053	-0.000061
3	6	0	1.935371	0.185975	-0.000013
4	6	0	2.486591	-1.108048	0.000430
5	6	0	2.821826	1.275437	-0.000428
6	6	0	3.862911	-1.297517	0.000450
7	1	0	1.836841	-1.978679	0.000793
8	6	0	4.201298	1.086923	-0.000422
9	1	0	2.419307	2.286233	-0.000768
10	6	0	4.730108	-0.202135	0.000025
11	1	0	4.265429	-2.307235	0.000819
12	1	0	4.863721	1.948606	-0.000762
13	1	0	5.805910	-0.354951	0.000060
14	6	0	-1.935372	-0.185982	-0.000051
15	6	0	-2.821830	-1.275438	-0.000442
16	6	0	-2.486587	1.108047	0.000389
17	6	0	-4.201305	-1.086917	-0.000400
18	1	0	-2.419319	-2.286236	-0.000788
19	6	0	-3.862903	1.297521	0.000445
20	6	0	-4.730107	0.202141	0.000054
21	1	0	-4.863727	-1.948600	-0.000718
22	1	0	-4.265422	2.307239	0.000808
23	1	0	-5.805908	0.354966	0.000115
24	1	0	-0.238347	-1.513229	-0.000179
25	1	0	0.238346	1.513222	0.000021
26	1	0	-1.836829	1.978671	0.000711

SCF Done: E(RPBE1PBE) = -540.078846524 A.U. after 12 cycles
Convg = 0.2894D-08 -V/T = 2.0149
Zero-point correction= 0.216164 (Hartree/Particle)
Thermal correction to Energy= 0.230970
Thermal correction to Enthalpy= 0.232056
Thermal correction to Gibbs Free Energy= 0.168059
Sum of electronic and zero-point Energies= -539.862682
Sum of electronic and thermal Energies= -539.847877
Sum of electronic and thermal Enthalpies= -539.846790
Sum of electronic and thermal Free Energies= -539.910788

1 2 3

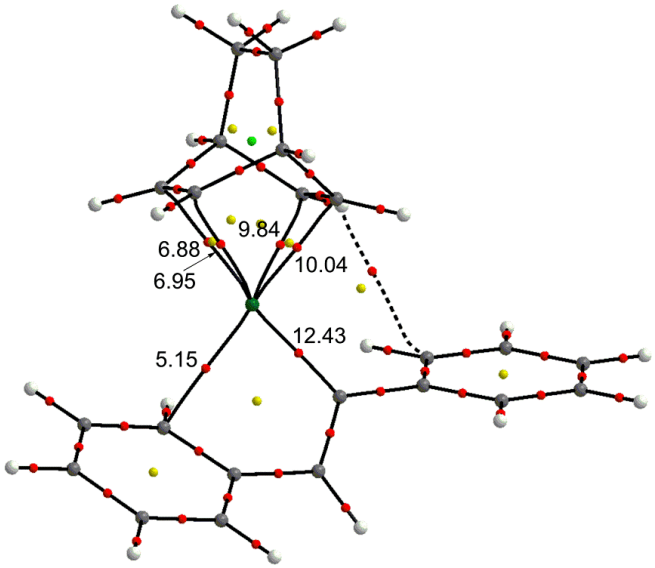
	A	A	A
Frequencies --	10.0166	58.1132	75.3665
Red. masses --	3.5613	4.8346	2.9297
Frc consts --	0.0002	0.0096	0.0098
IR Inten --	0.0001	0.8116	0.0001



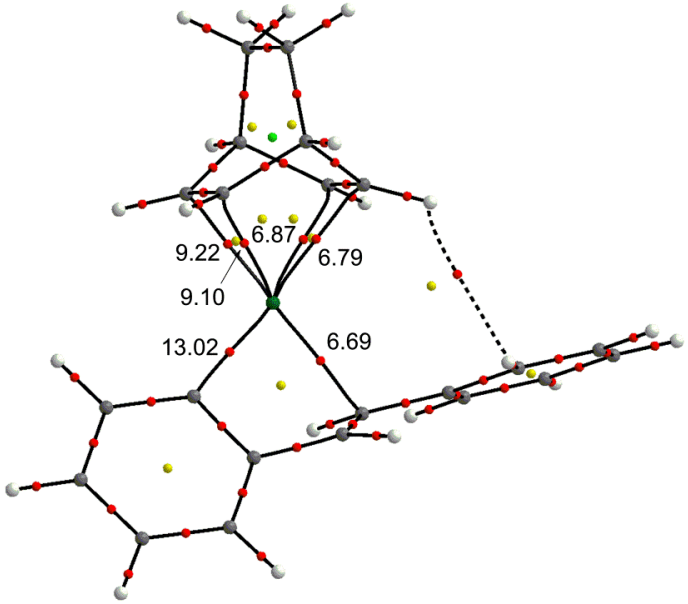
9. Atoms-in-molecules molecular graphs

The graphs were generated using AIMAll package. Bond critical points (BCP) are colored in red, ring critical points (RCP) – in yellow and cage critical points (CCP) – in green. The electron density at BCP ($\rho_b \times 10^2$ ē bohr^{-3}) for Rh are listed at their respective bond paths.

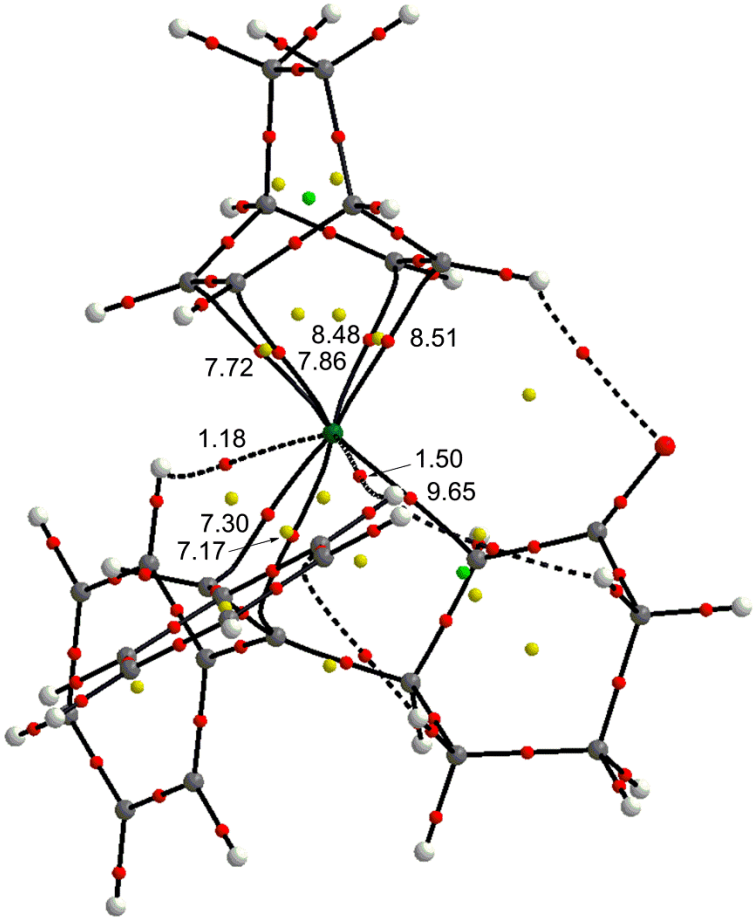
Structure 5



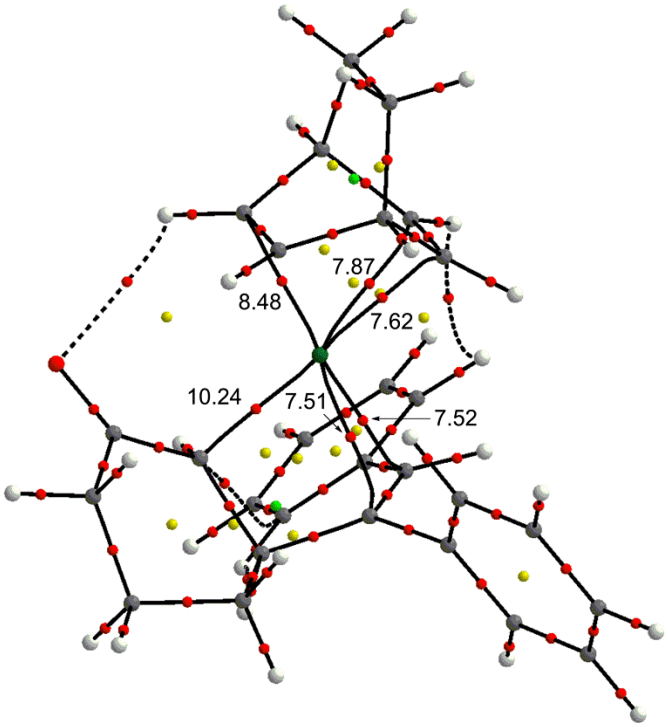
Structure 9



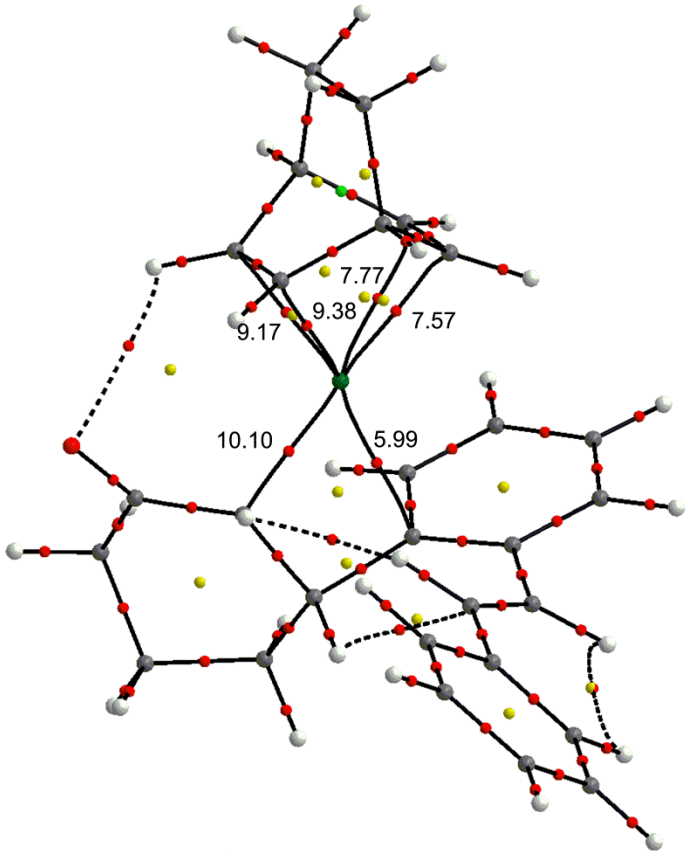
Structure 12a



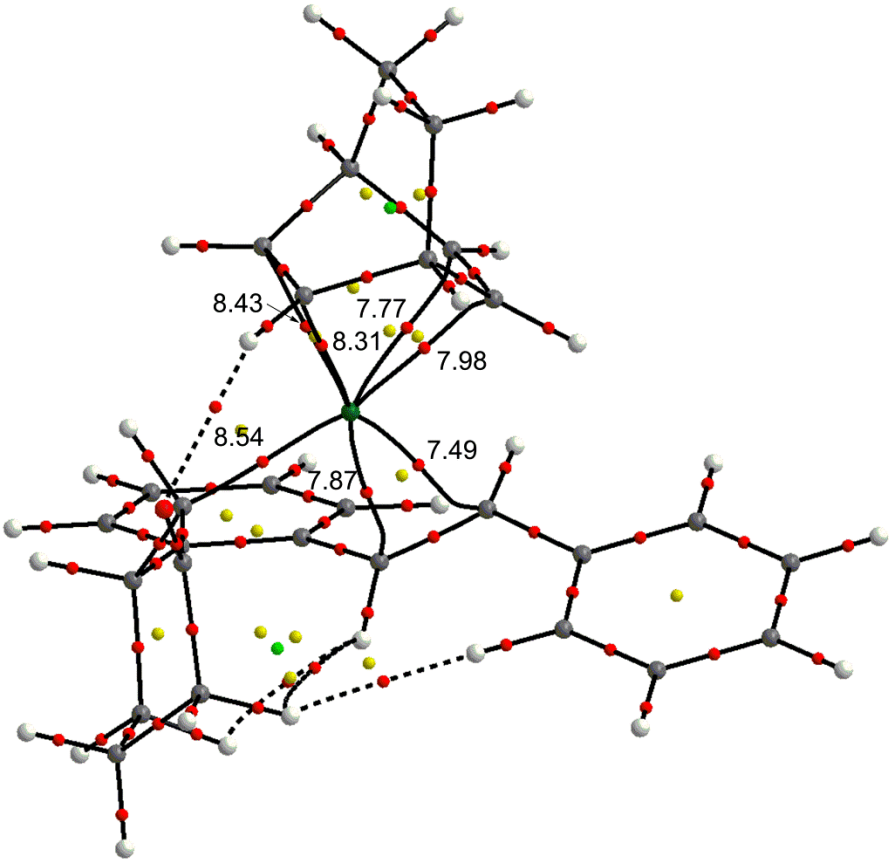
Structure 12b



Structure 16a



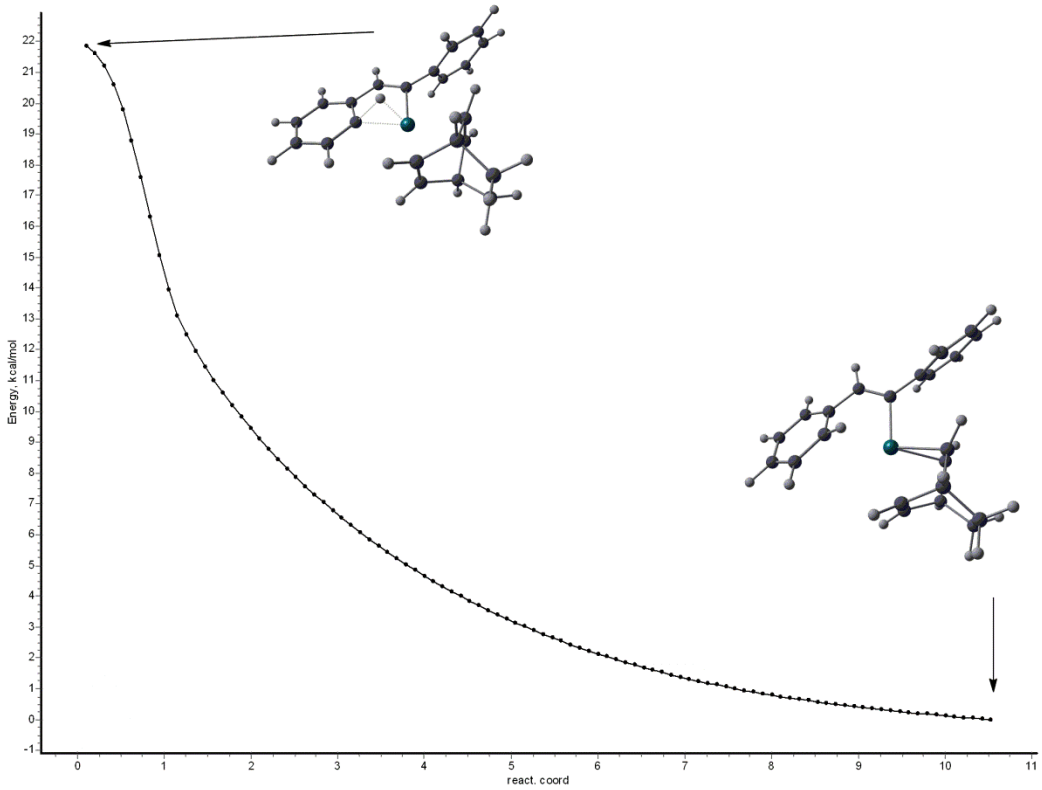
Structure 16b



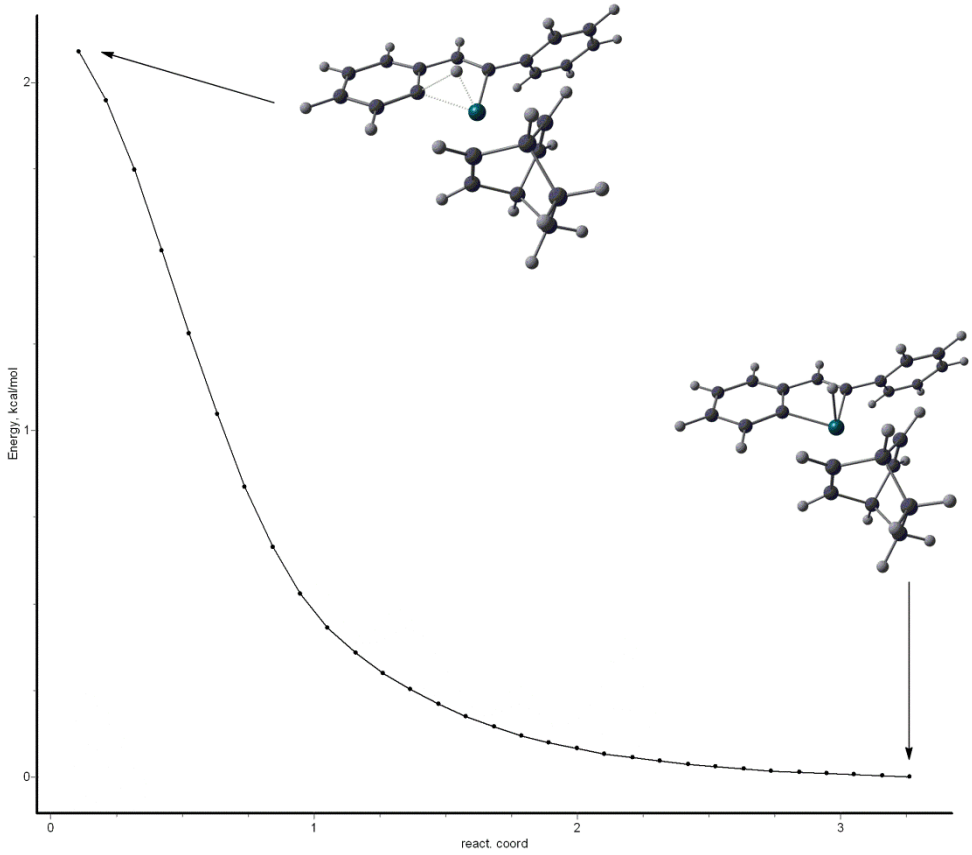
10. IRC plots for selected transition states

Rh-1,4-shift oxidative addition (structure 6)

Forward direction:

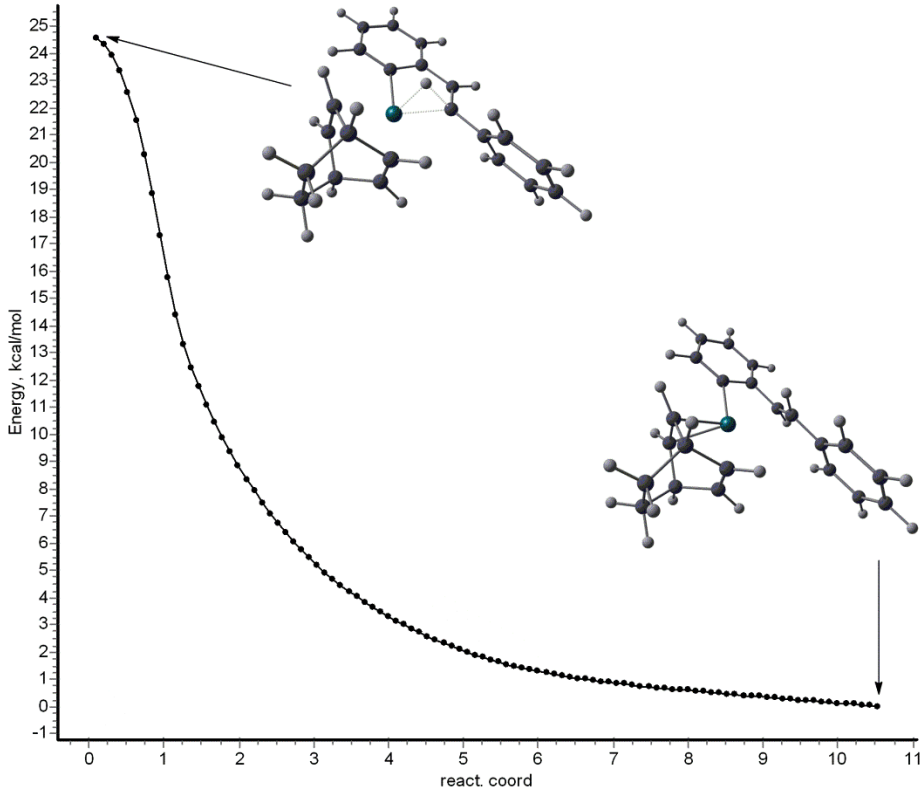


Reverse direction:

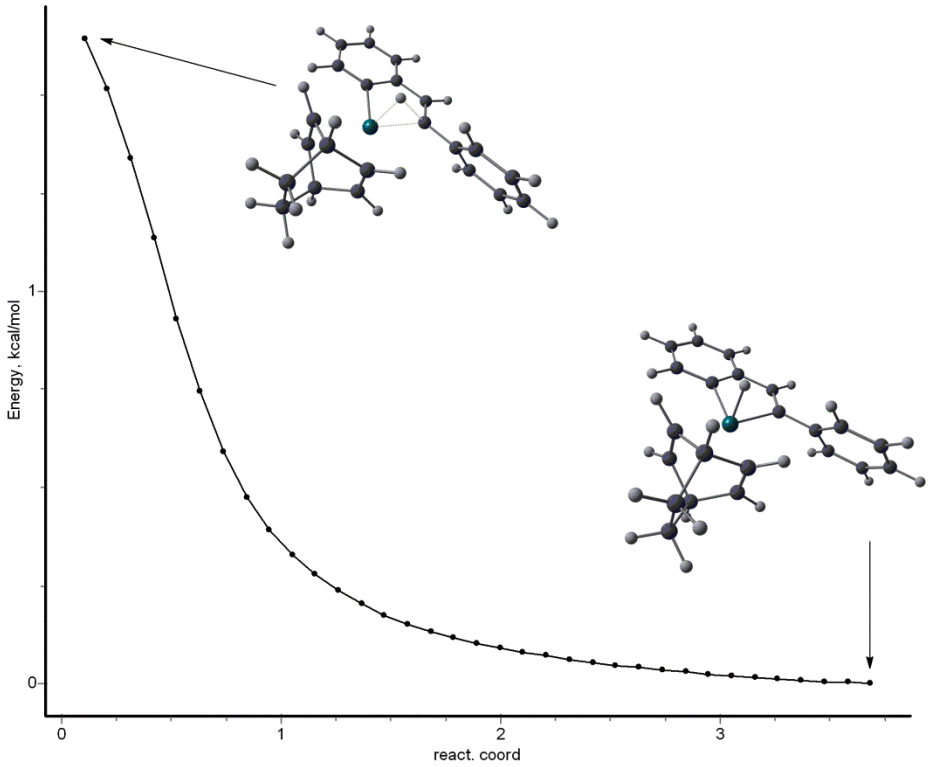


Rh-1,4-shift reductive elimination (structure 8)

Forward direction:

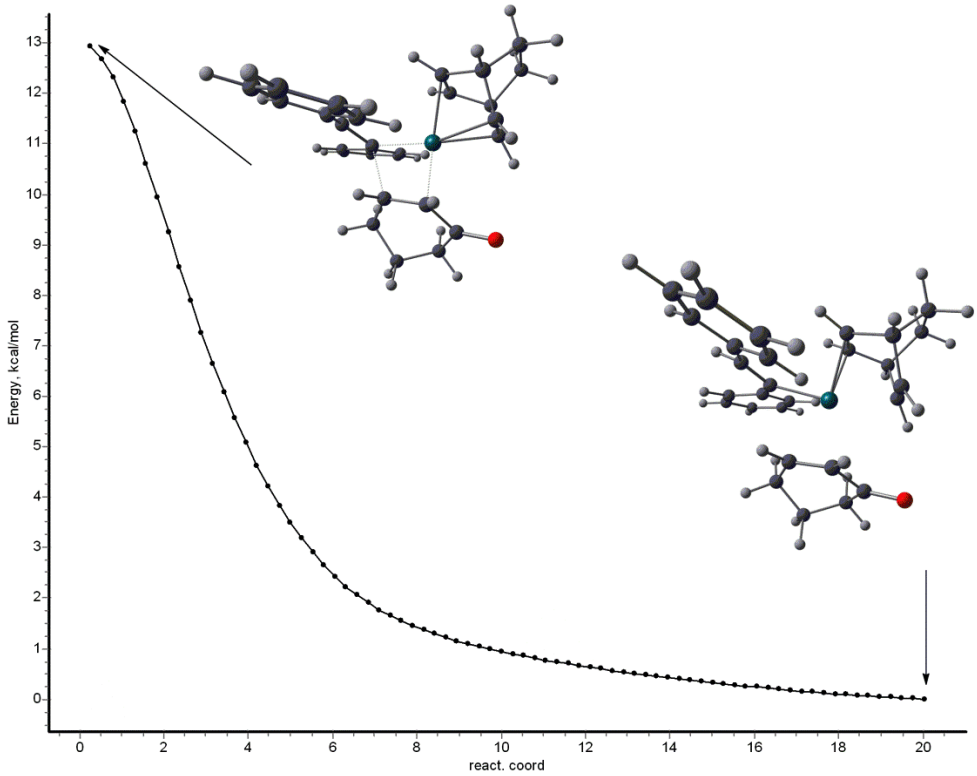


Reverse direction:

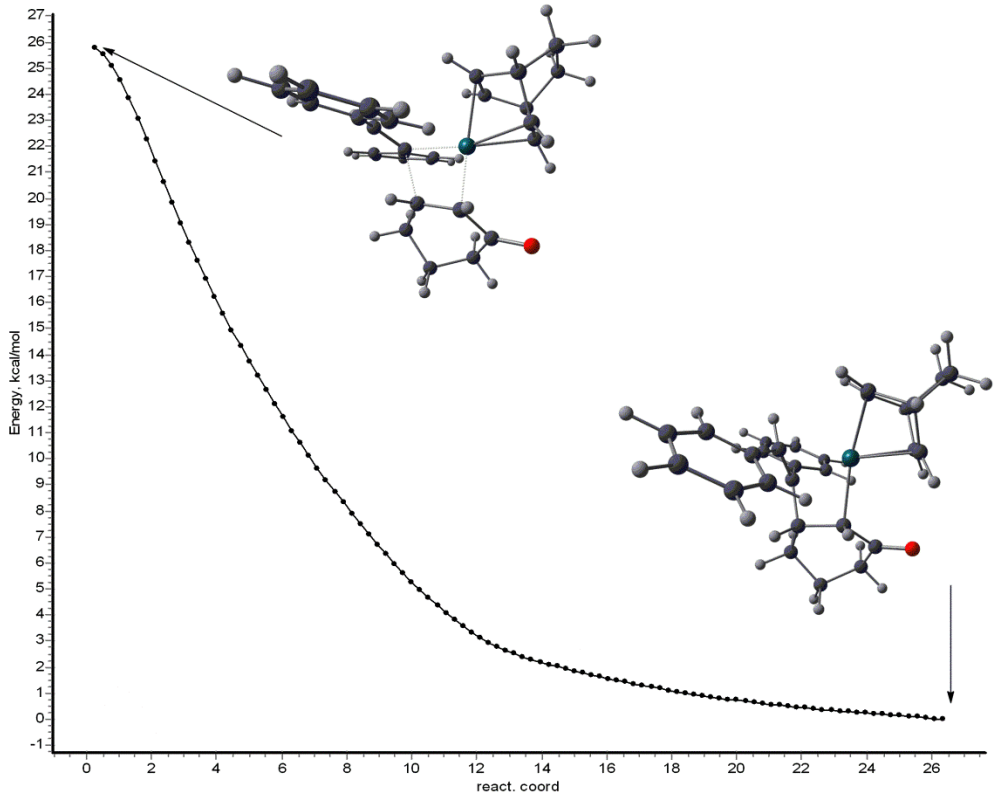


Non-rearranged lowest energy carborhodation (structure 12b)

Forward direction:

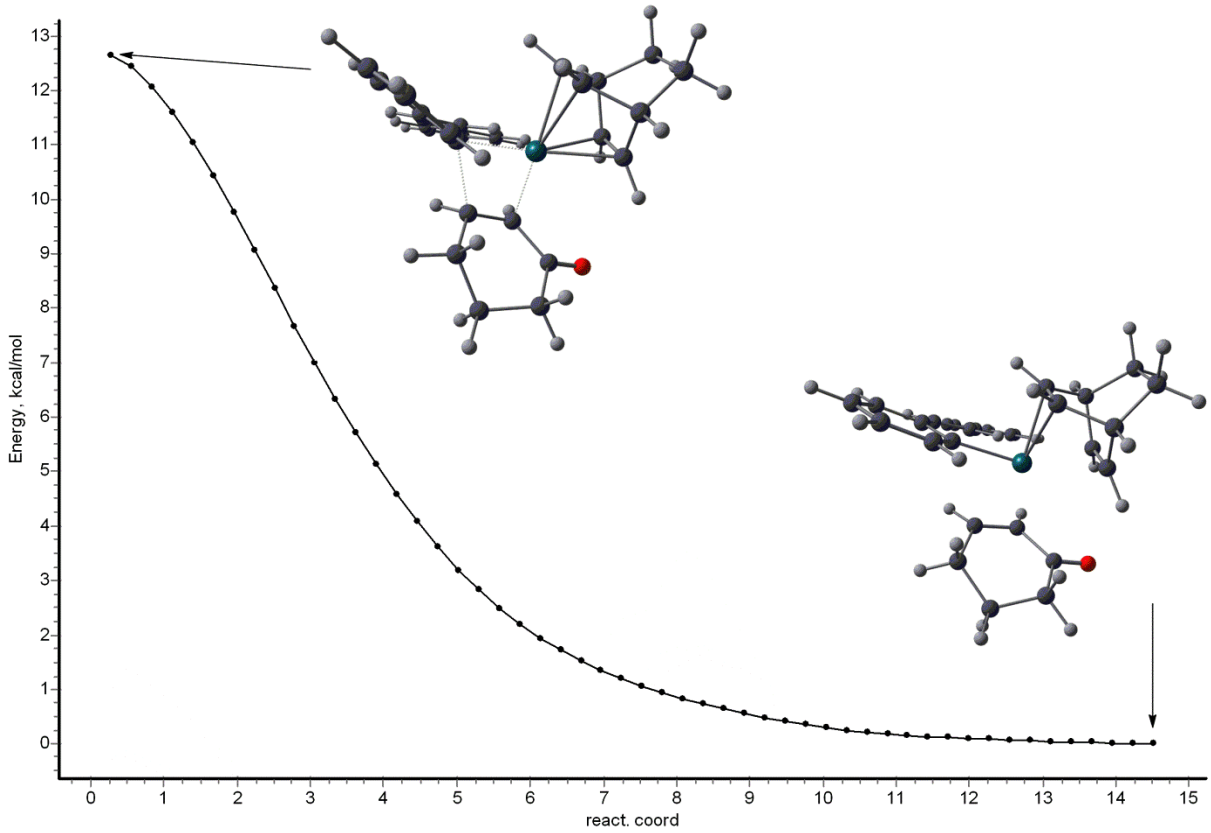


Reverse direction:

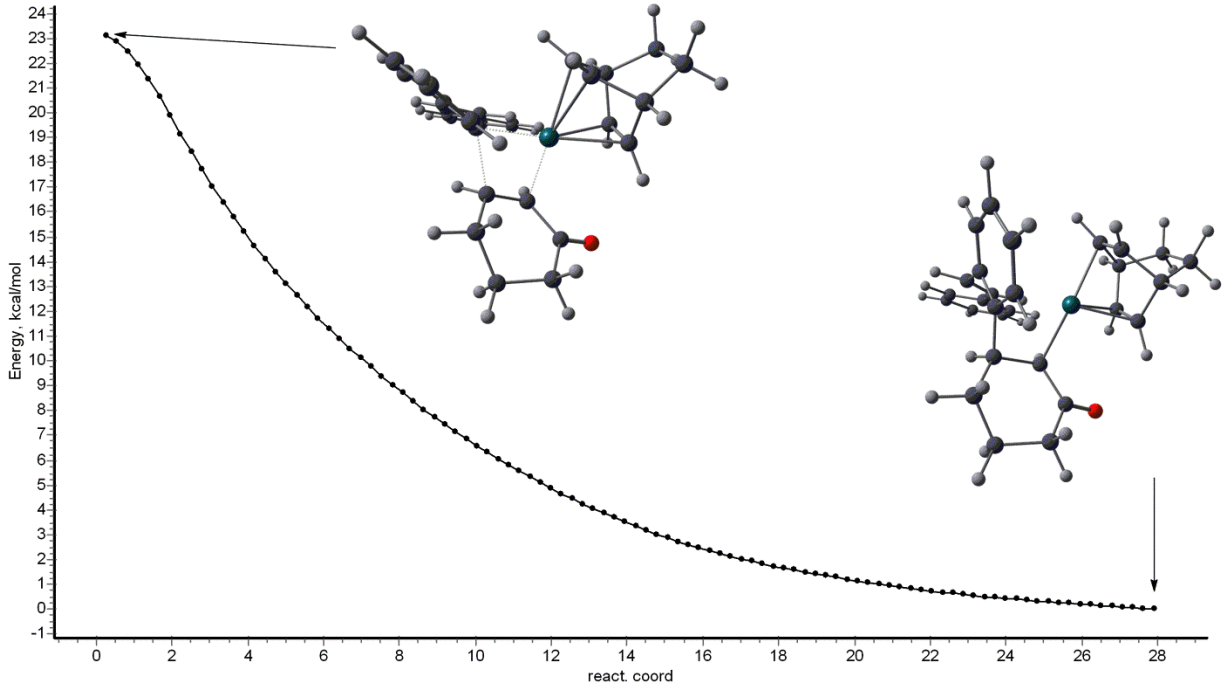


Rearranged lowest energy carborhodation (structure 15a)

Forward direction:



Reverse direction:



11. References:

1. Gaussian 09, Revision **A.02**, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.
2. (a) Biegler-König, F.; Schönbohm, J.; Bayles, D. *J. Comp. Chem.* **2001**, *22*, 545-549. (b) Biegler-König, F.; Schönbohm, J. *J. Comp. Chem.* **2002**, *23*, 1489-1494.
3. AIMAll (Version 11.10.16), Keith, T. A.; Gristmill software, Overland Park, KS, 2011.