Supporting Information

Mechanism and Stereochemistry of Rhodium-Catalyzed [5 + 2 + 1] Cycloaddition of Ene−Vinylcyclopropanes and Carbon Monoxide Revealed by Visual Kinetic Analysis and Quantum Chemical Calculations

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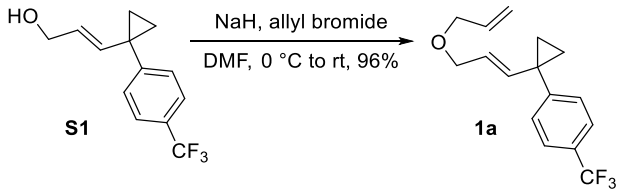
S1. General Information

All reactions were carried out in oven-dried glassware with magnetic stirring. All chemicals were used as received without further purification. Flash column chromatography was performed using silica gel (200−300 mesh). Analytical thin layer chromatography (TLC) was performed with 0.2−0.3 mm silica gel HSGF254 plates. Nuclear magnetic resonance (NMR) spectra were measured on Bruker AVANCE III 400 (^{1}H at 400 MHz, ^{13}C{^{1}H} at 101 MHz) and Bruker AVANCE III 500 (^{19}F at 471 MHz) NMR spectrometers. Data for ^{1}H NMR spectrum are reported as follows: chemical shift δ (ppm) referenced to tetramethylsilane (TMS, 0.00 ppm), multiplicity (d = doublet, t = triplet, dd = doublet of doublets, dt = doublet of triplets, dq = doublet of quartets, ddt = doublet of doublet of triplets, m = multiplet), coupling constant J (Hz), and integration. Data for ^{13}C{^{1}H} NMR spectrum are reported as follows: chemical shift δ (ppm) referenced to $CDCl_3$ (77.16 ppm), multiplicity (null = singlet, q = quartet), and coupling constant J (Hz). Distortionless enhancement by polarization transfer (DEPT) was used to distinguish carbon signals (CH_2, CH, or C). Data for ^{19}F NMR spectrum are reported in terms of chemical shift δ (ppm). High-resolution mass spectra (HRMS) were recorded on Bruker Solarix XR Fourier transform ion cyclotron resonance (FTICR) mass spectrometer (electrospray ionization, ESI).

S2. Synthesis of Substrate 1a and [5 + 2 + 1] Cycloadduct 2a



(*E*)-1-(1-(3-(Allyloxy)prop-1-en-1-yl)cyclopropyl)-4-(trifluoromethyl)benzene (1a)

To a stirred suspension of NaH (180 mg, 60 wt%, 4.50 mmol, 1.5 equiv) in DMF (5 mL) was added dropwise a solution of alcohol **S1**[1] (727 mg, 3.00 mmol, 1.0 equiv) in DMF (5 mL) at 0 °C under a nitrogen atmosphere. The reaction mixture was allowed to warm to room temperature and stirred for 1 h. Then, a solution of allyl bromide (0.40 mL, 4.6 mmol, 1.5 equiv) in DMF (5 mL) was added dropwise. The reaction mixture was stirred at room temperature for 16 h, quenched with saturated aqueous NH_4Cl solution (15 mL) and water (100 mL) at 0 °C, and extracted with Et_2O (50 mL × 2). The combined organic layers were washed with brine (50 mL), dried over anhydrous Na_2SO_4, filtered, and concentrated by rotary evaporation. Purification of the crude product by flash column chromatography (silica gel, 40:1 petroleum ether/EtOAc) afforded the title compound **1a** (814 mg, 2.88 mmol, 96%) as a light yellow oil.

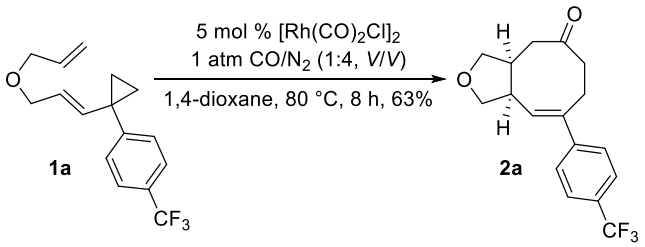
TLC (10:1 petroleum ether/EtOAc, R_f): 0.5.

^{1}H NMR (400 MHz, $CDCl_3$, δ): 7.55 (d, J = 8.1 Hz, 2H), 7.41 (d, J = 8.1 Hz, 2H), 5.89 (ddt, J = 17.1, 10.5, 5.7 Hz, 1H), 5.62 (dd, J = 15.5, 1.2 Hz, 1H), 5.25 (apparent dq, J = 17.1, 1.6 Hz, 1H), 5.19−5.10 (m, 2H), 3.94 (dt, J = 5.7, 1.2 Hz, 2H), 3.90 (dd, J = 6.1, 1.2 Hz, 2H), 1.13−1.08 (m, 2H), 1.07−1.02 (m, 2H).

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$, δ): 147.5 (C), 140.0 (CH), 134.8 (CH), 130.2 (2CH), 128.8 (q, J = 32 Hz, C), 125.3 (q, J = 4 Hz, 2CH), 125.2 (CH), 124.4 (q, J = 272 Hz, C), 117.3 (CH_2), 71.3 (CH_2), 70.6 (CH_2), 27.7 (C), 15.1 ($2CH_2$).

^{19}F NMR (471 MHz, $CDCl_3$, δ): −62.4.

HRMS (ESI−FTICR, m/z): $[M + H]^+$ calculated for $C_{16}H_{18}F_3O^+$: 283.1304; found: 283.1296.



***cis*-8-(4-(Trifluoromethyl)phenyl)-1,3a,4,6,7,9a-hexahydrocycloocta[*c*]furan-5(3*H*)-one (2a)**

A 25 mL eggplant-shaped flask equipped with an air condenser was charged with substrate **1a** (28.2 mg, 0.100 mmol), $[Rh(CO)_2Cl]_2$ (1.9 mg, 0.005 mmol, 5 mol %), and anhydrous 1,4-dioxane (2 mL). The reaction mixture was bubbled with balloon pressured (slightly higher than 1 atm) mix gas of CO and N_2 (1:4, *V*/*V*) at room temperature for 5 min and then stirred (1000 rpm) at 80 °C for 8 h under balloon pressured mix gas of CO and N_2 (1:4, *V*/*V*). After cooling, the reaction mixture was concentrated by rotary evaporation. Purification of the crude product by flash column chromatography (silica gel, 5:1 petroleum ether/EtOAc) afforded [5 + 2 + 1] cycloadduct **2a** as a light yellow oil. Run 1: **2a** (20.0 mg, 0.0645 mmol, 65%). Run 2: **2a** (18.8 mg, 0.0606 mmol, 61%). The average yield of two runs was 63%.

TLC (5:1 petroleum ether/EtOAc, R_f): 0.1.

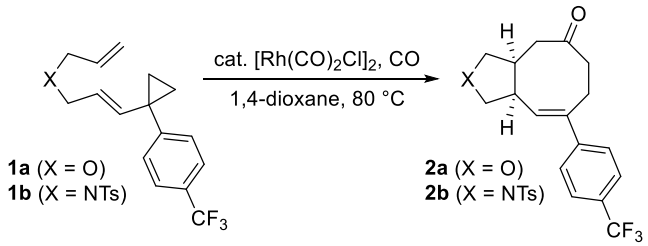
^{1}H NMR (400 MHz, $CDCl_3$, δ): 7.62 (d, *J* = 8.2 Hz, 2H), 7.55 (d, *J* = 8.2 Hz, 2H), 5.97 (d, *J* = 8.6 Hz, 1H), 4.04 (apparent t, *J* = 8.2 Hz, 1H), 4.00−3.95 (m, 2H), 3.35 (dd, *J* = 10.1, 8.3 Hz, 1H), 3.05−2.97 (m, 1H), 2.87−2.78 (m, 1H), 2.74−2.56 (m, 4H), 2.43 (apparent t, *J* = 11.4 Hz, 1H), 2.35 (dd, *J* = 11.4, 4.7 Hz, 1H).

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$, δ): 211.3 (C), 145.3 (C), 140.2 (C), 130.4 (CH), 129.6 (q, *J* = 32 Hz, C), 126.2 (2CH), 125.7 (q, *J* = 4 Hz, 2CH), 124.2 (q, *J* = 272 Hz, C), 74.2 (CH_2), 71.8 (CH_2), 46.3 (CH_2), 42.0 (CH), 41.1 (CH_2), 40.7 (CH), 27.2 (CH_2).

^{19}F NMR (471 MHz, $CDCl_3$, δ): −62.5.

HRMS (ESI−FTICR, *m*/*z*): $[M + H]^+$ calculated for $C_{17}H_{18}F_3O_2^+$: 311.1253; found: 311.1247.

S3. Visual Kinetic Analysis



Kinetic Measurements. In a nitrogen-regulated glovebox, a freshly prepared solution of substrate **1**,[1] 4-(trifluoromethoxy)anisole (internal standard), and $[Rh(CO)_2Cl]_2$ in anhydrous 1,4-dioxane was split into 1 mL aliquots and placed into 40 mL vials. The reaction mixture was vigorously stirred at 80 °C for indicated time under balloon pressured mix gas of CO and N_2 (Figure S1). After cooling, the reaction mixture was investigated by ^{19}F NMR spectroscopy (Tables S1 and S2). In some cases, $CDCl_3$ was added to facilitate locking and shimming.

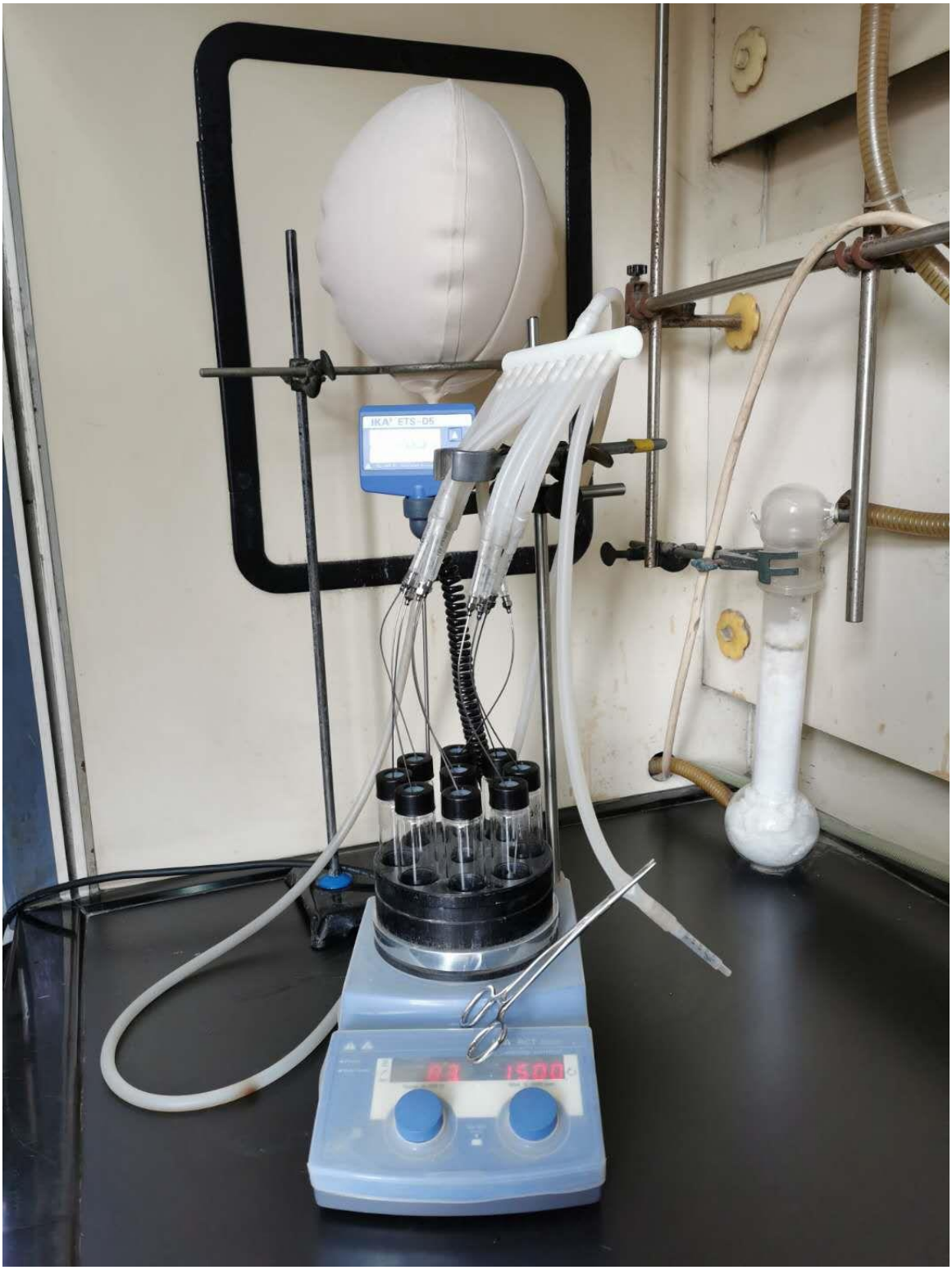


Figure S1. Parallel reactions for kinetic measurements.

Table S1. Kinetic Data for Substrate 1a

entry	$[catalyst]_T$ (mM)[a]	$[\mathbf{1a}]_0$ (M)	*p*(CO) (atm)	*t* (min)	[**1a**] (M)	[**2a**] (M)
A1	2.5	0.050	0.2	0	0.050	0
A2	2.5	0.050	0.2	20	0.040	0.006
A3	2.5	0.050	0.2	40	0.032	0.012
A4	2.5	0.050	0.2	60	0.026	0.017
A5	2.5	0.050	0.2	80	0.020	0.022
A6	2.5	0.050	0.2	100	0.015	0.027
A7	2.5	0.050	0.2	120	0.010	0.031
B1	1.25	0.050	0.2	0	0.050	0
B2	1.25	0.050	0.2	20	0.044	0.004
B3	1.25	0.050	0.2	40	0.038	0.008
B4	1.25	0.050	0.2	60	0.033	0.012
B5	1.25	0.050	0.2	80	0.028	0.015
B6	1.25	0.050	0.2	100	0.024	0.018
B7	1.25	0.050	0.2	120	0.020	0.021
C1	2.5	0.075	0.2	0	0.075	0
C2	2.5	0.075	0.2	30	0.059	0.012
C3	2.5	0.075	0.2	60	0.043	0.024
C4	2.5	0.075	0.2	90	0.031	0.034
C5	2.5	0.075	0.2	120	0.022	0.043
C6	2.5	0.075	0.2	150	0.013	0.051
D1	2.5	0.100	0.2	0	0.100	0
D2	2.5	0.100	0.2	30	0.078	0.014
D3	2.5	0.100	0.2	60	0.062	0.027
D4	2.5	0.100	0.2	90	0.049	0.039
D5	2.5	0.100	0.2	120	0.036	0.051
D6	2.5	0.100	0.2	150	0.024	0.060
E1	2.5	0.050	1	0	0.050	0
E2[b]	2.5	0.050	1	30	0.038	0.005
E3[b]	2.5	0.050	1	60	0.027	0.010
E4[b]	2.5	0.050	1	90	0.018	0.014

[a]$[catalyst]_T$ is the total concentration of catalyst added.

[b]The mass balance was poor due to the formation of side products.

Table S2. Kinetic Data for Substrate 1b

entry	[catalyst]$_T$ (mM)[a]	[**1b**]$_0$ (M)	*p*(CO) (atm)	*t* (min)	[**1b**] (M)	[**2b**] (M)
A1	2.5	0.050	0.2	0	0.050	0
A2	2.5	0.050	0.2	60	0.037	0.012
A3	2.5	0.050	0.2	120	0.027	0.021
A4	2.5	0.050	0.2	180	0.018	0.029
A5	2.5	0.050	0.2	240	0.012	0.035
A6	2.5	0.050	0.2	300	0.007	0.040
B1	1.25	0.050	0.2	0	0.050	0
B2	1.25	0.050	0.2	90	0.038	0.011
B3	1.25	0.050	0.2	180	0.027	0.021
B4	1.25	0.050	0.2	270	0.018	0.030
B5	1.25	0.050	0.2	360	0.012	0.036
C1	2.5	0.100	0.2	0	0.100	0
C2	2.5	0.100	0.2	30	0.089	0.009
C3	2.5	0.100	0.2	60	0.080	0.017
C4	2.5	0.100	0.2	90	0.072	0.025
C5	2.5	0.100	0.2	120	0.065	0.031
C6	2.5	0.100	0.2	180	0.052	0.043
C7	2.5	0.100	0.2	240	0.040	0.055
D1	2.5	0.050	1	0	0.050	0
D2	2.5	0.050	1	120	0.037	0.011
D3	2.5	0.050	1	240	0.026	0.021
D4	2.5	0.050	1	360	0.017	0.029
D5	2.5	0.050	1	480	0.009	0.036

[a][catalyst]$_T$ is the total concentration of catalyst added.

Time adjustment. To identify catalyst deactivation or product inhibition, we shifted the concentration profiles of oxygen-tethered substrate **1a** on the time scale (Figure S2).[2] The overlay of the curves indicates the absence of catalyst deactivation and product inhibition.

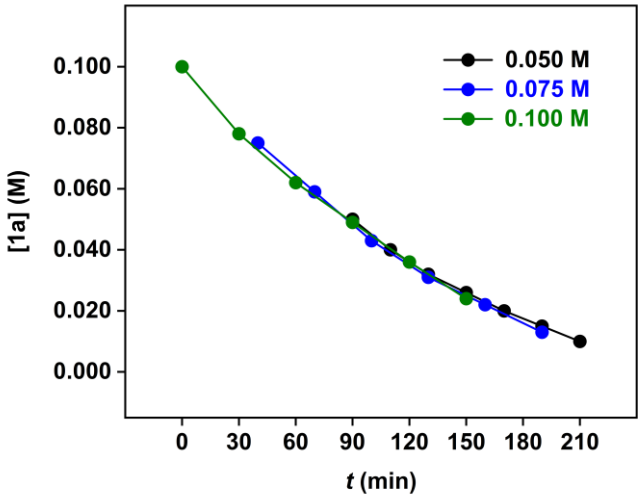


Figure S2. Concentration profiles of **1a** after time adjustment (+90 min for $[\mathbf{1a}]_0$ = 0.050 M; +40 min for $[\mathbf{1a}]_0$ = 0.075 M). Reaction conditions: **1a** (0.050, 0.075, 0.100 M), $[Rh(CO)_2Cl]_2$ (2.5 mM), CO (0.2 atm), 1,4-dioxane, 80 °C.

Order in catalyst. To determine the order in catalyst (*n*), we performed normalized time scale analysis[3] via plotting the concentration of **1** against $t[\text{catalyst}]_T^n$ ($[\text{catalyst}]_T$ is the total concentration of catalyst added). *n* was adjusted until the curves overlaid. For both **1a** (Figure 1b) and **1b** (Figure S3), *n* equals 0.5.

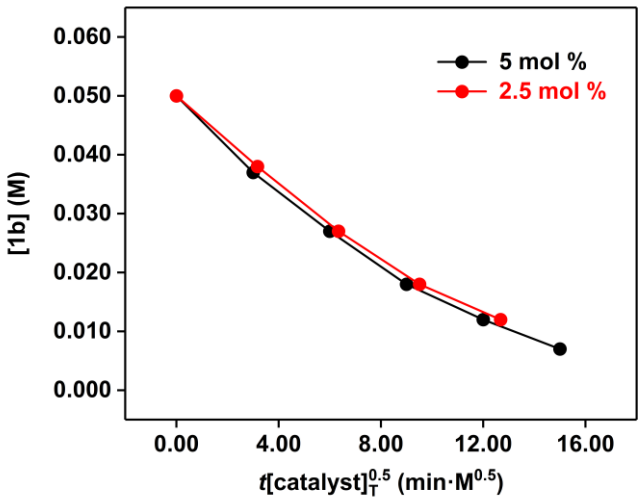


Figure S3. Normalized time scale analysis to determine the order in catalyst. Reaction conditions: **1b** (0.050 M), $[Rh(CO)_2Cl]_2$ (5, 2.5 mol %), CO (0.2 atm), 1,4-dioxane, 80 °C.

For substrate **1a**, when *n* equals 0, the curves did not overlay (Figure S4).

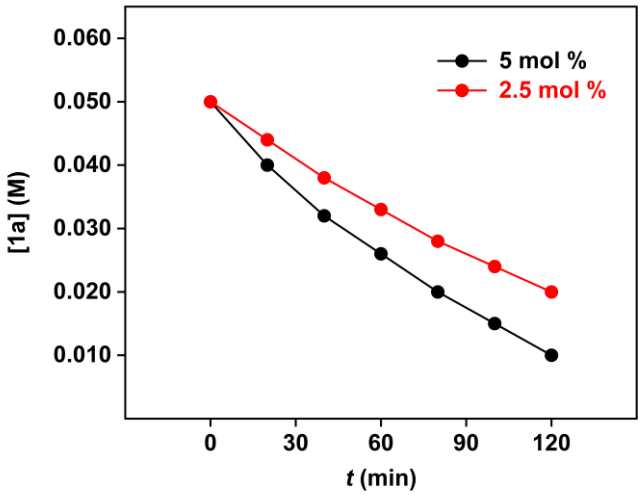


Figure S4. Kinetic profiles of substrate **1a**. Reaction conditions: **1a** (0.050 M), $[Rh(CO)_2Cl]_2$ (5, 2.5 mol %), CO (0.2 atm), 1,4-dioxane, 80 °C.

For substrate **1a**, when *n* equals 1, the curves did not overlay (Figure S5).

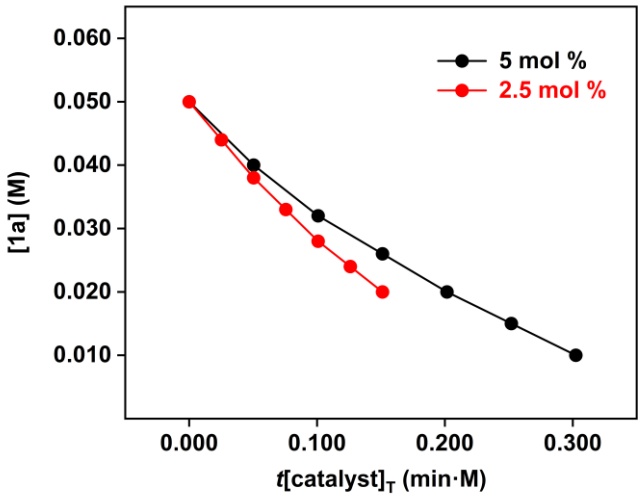


Figure S5. Normalized time scale analysis (*n* = 1). Reaction conditions: **1a** (0.050 M), $[Rh(CO)_2Cl]_2$ (5, 2.5 mol %), CO (0.2 atm), 1,4-dioxane, 80 °C.

Order in substrate. To determine the order in substrate (*a*), we performed variable time normalization analysis[4] via plotting the concentration of cycloadduct **2** against $\Sigma[\mathbf{1}]^{a}\Delta t$. *a* was adjusted until the curves overlaid and became straight lines. For both **1a** (Figure 1c) and **1b** (Figure S6), *a* equals 0.5.

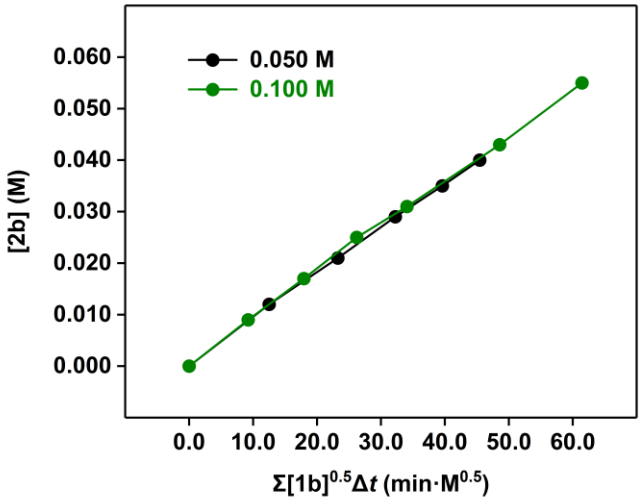


Figure S6. Variable time normalization analysis to determine the order in substrate **1b**. Reaction conditions: **1b** (0.050, 0.100 M), $[Rh(CO)_2Cl]_2$ (2.5 mM), CO (0.2 atm), 1,4-dioxane, 80 °C.

Order in CO. To determine the order in CO (*b*), we performed normalized time scale analysis[3] via plotting the concentration of cycloadduct **2** against $t[p(CO)]^{b}$. *b* was adjusted until the curves overlaid. For **1a**, *b* equals 0 (Figure 1d). For **1b**, *b* equals ca. −0.5 (Figure S7).

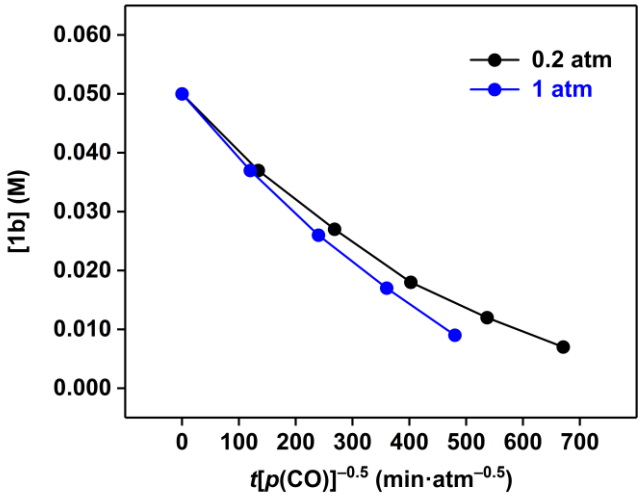
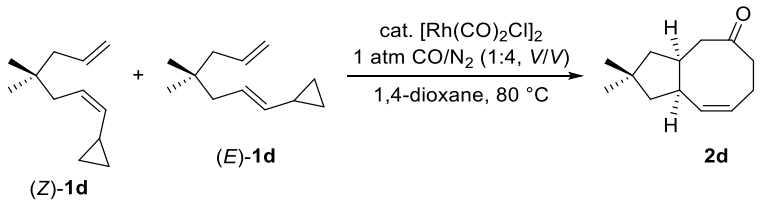


Figure S7. Normalized time scale analysis to determine the order in CO. Reaction conditions: **1b** (0.050 M), $[Rh(CO)_2Cl]_2$ (5 mol %), CO (0.2, 1 atm), 1,4-dioxane, 80 °C. When the order in CO was adjusted to −0.4, the best overlay was obtained.

S4. Influence of the Double-Bond Configuration on the Reactivity

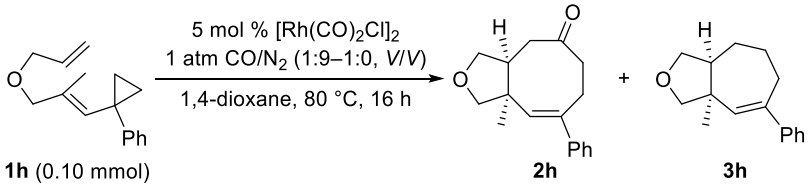


A reaction tube charged with $[Rh(CO)_2Cl]_2$ (7.0 mg, 0.018 mmol) was evacuated under vacuum and then back-filled with argon for three times. 1 mL of anhydrous 1,4-dioxane was added, and the resulting solution was bubbled with balloon pressured mix gas of CO and N_2 (1:4, *V*/*V*) for 5 min. A mixture of (*Z*)- and (*E*)-**1d**[5] (63.3 mg, 0.385 mmol, 1.3:1 *Z*:*E* as determined by ^{1}H NMR analysis) and *n*-tetradecane (internal standard, 49.1 mg, 0.247 mmol) was transferred to the reaction tube by 4 mL of anhydrous 1,4-dioxane. The solution was bubbled again with balloon pressured mix gas of CO and N_2 (1:4, *V*/*V*) for 5 min. The reaction tube was immersed in a preheated oil bath at 80 °C. Aliquots of the reaction mixture were extracted and analyzed (Table S3) by gas chromatography (GC) on an Agilent GC6820 instrument equipped with a Varian CP75 capillary column (25 m × 0.25 μm) and a flame ionization detector (FID). Nitrogen was used as the carrier gas. The following temperature program was used: 120 °C for 5 min, 5 °C/min to 145 °C, 15 °C/min to 225 °C, and 225 °C for 5 min.

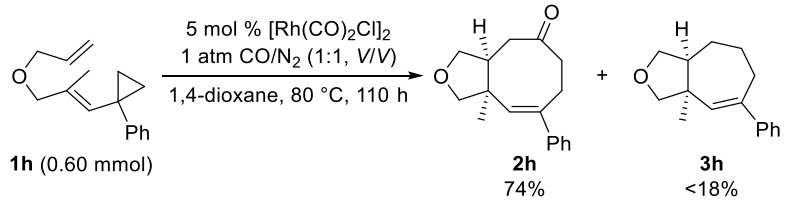
Table S3. Kinetic Data for Substrates (*Z*)- and (*E*)-1d

entry	*t* (h)	[(*Z*)-**1d**] (mM)	[(*E*)-**1d**] (mM)
1	0	43.6	33.5
2	1.16	45.3	29.4
3	2.58	43.3	24.4
4	3.5	41.5	20.8
5	7.67	39.8	8.8
6	9	39.6	6.7
7	23	35.6	2.4
8	24	36.3	2.3
9	26.83	33.2	2.2
10	29.5	34.1	2.3
11	46.5	30.5	2.3
12	56.5	26.9	2.2
13	71.5	23.7	2.3
14	95.17	20.5	2.2
15	101.67	19.6	2.0
16	143	13.6	1.8

S5. Influence of the Pressure of CO on the Chemoselectivity



Reaction performed on 0.10 mmol scale. A 25 mL reaction tube was charged with substrate **1h**[6] (22.8 mg, 0.100 mmol), $[Rh(CO)_2Cl]_2$ (1.9 mg, 0.005 mmol, 5 mol %), and anhydrous 1,4-dioxane (2 mL). The reaction mixture was stirred (500 rpm) at 80 °C for 16 h under balloon pressured mix gas of CO and N_2. After cooling, the reaction mixture was concentrated by rotary evaporation and the residue was analyzed by ^{1}H NMR spectroscopy. The **2h**/**3h** ratio was 1.7:1, 7.6:1, >20:1, and >20:1 when the pressure of CO was 0.1, 0.2, 0.5, and 1.0 atm, respectively.



Reaction performed on 0.60 mmol scale. A 50 mL eggplant-shaped flask equipped with an air condenser was charged with substrate **1h**[6] (137.2 mg, 0.601 mmol), $[Rh(CO)_2Cl]_2$ (11.7 mg, 0.030 mmol, 5 mol %), and anhydrous 1,4-dioxane (12 mL). The reaction mixture was bubbled with balloon pressured mix gas of CO and N_2 (1:1, *V*/*V*) at room temperature for 5 min and then stirred (1000 rpm) at 80 °C for 110 h under balloon pressured mix gas of CO and N_2 (1:1, *V*/*V*). After cooling, the reaction mixture was concentrated by rotary evaporation. Purification of the crude product by flash column chromatography (silica gel, 50:1−5:1 petroleum ether/EtOAc) afforded [5 + 2 + 1] cycloadduct **2h**[6] as a pale yellow solid and [5 + 2] cycloadduct **3h**[6] as a light yellow oil. Run 1: **2h** (111.0 mg, 0.433 mmol, 72%) and **3h** (with some inseparable impurities, <28.0 mg, <0.123 mmol, <20%). Run 2: **2h** (116.6 mg, 0.455 mmol, 76%) and **3h** (with some inseparable impurities, <22.4 mg, <0.098 mmol, <16%). The average yields of two runs were 74% and <18% for **2h** and **3h**, respectively.

S6. Benchmark Calculations

Figure S8 depicts several important elementary steps involved in $[Rh(CO)_2Cl]_2$-catalyzed cycloadditions, including dimer dissociation, complexation, oxidative addition, migratory insertion, reductive elimination, and oxidative cyclometalation. All these steps were studied using quantum chemical calculations with the Gaussian 09 software package.[7] For DFT calculations, pruned integration grids with 99 radial shells and 590 angular points per shell were used. Geometry optimizations of all the stationary points were carried out in the gas phase at the TPSS[8]/def2-TZVPP[9,10] level (density fitting approximation[11,12] using the W06 auxiliary basis set[13] was applied). Unscaled harmonic frequency calculations at the same level were performed to validate each structure as either a minimum or a transition state. For each transition state, we have considered the variation of the configuration of the rhodium center and only the most favored one is reported. On the basis of the optimized structures, single-point energy refinements were performed at the CCSD(T)[14]/def2-TZVPP level (frozen core approximation was applied). In total, 40 relative electronic energies (26 ΔE and 14 $\Delta E^{\ddagger}$, zero-point uncorrected) were obtained (Figure S8 and Table S4).

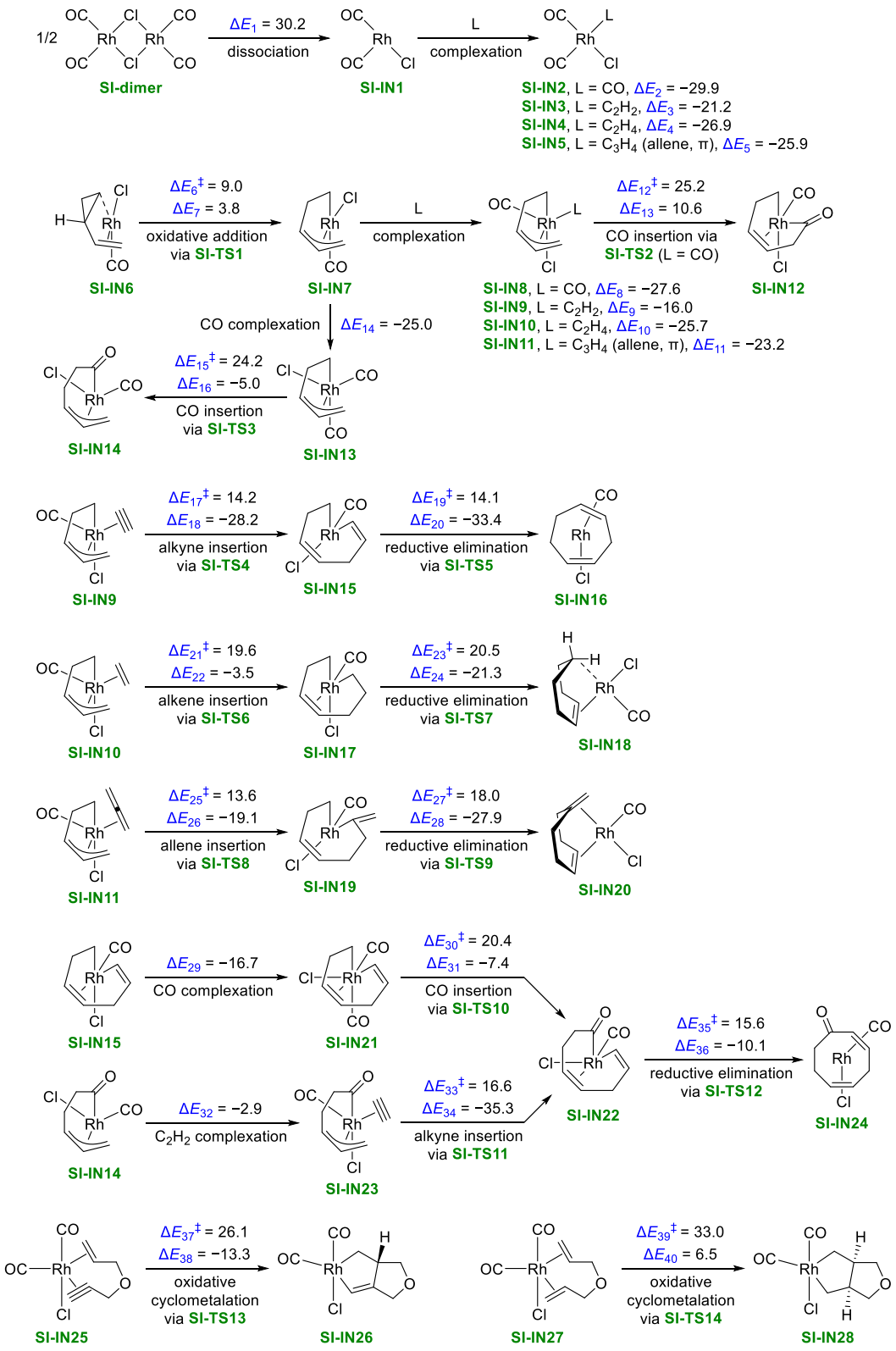


Figure S8. Elementary steps involved in $[Rh(CO)_2Cl]_2$-catalyzed cycloadditions. Relative electronic energies (zero-point uncorrected) are reported in kcal/mol, computed at the CCSD(T)/def2-TZVPP//TPSS/def2-TZVPP/W06 level.

Table S4. Assessment of Several Computational Methods for $[Rh(CO)_2Cl]_2$-Catalyzed Cycloadditions

	CCSD(T)	DLPNO-CCSD(T)	BP86	BP86-D3(BJ)	PBE	PBE-D3(BJ)	PBE0	PBE0-D3(BJ)	B3LYP	B3LYP-D3(BJ)	BMK	BMK-D3(BJ)	M06-L	M06-L-D3(0)	M06	M06-D3(0)	M06-2X	M06-2X-D3(0)	M11-L	M11	TPSS	TPSS-D3(BJ)	TPSSh	TPSSh-D3(BJ)	ωB97X	ωB97XD
RMSD	**0.0**	**1.3**	**4.2**	**4.2**	**4.2**	**4.3**	**3.3**	**3.4**	**4.6**	**2.3**	**2.2**	**2.8**	**3.1**	**3.0**	**3.5**	**3.4**	**5.5**	**5.5**	**2.9**	**3.1**	**2.9**	**3.3**	**2.2**	**2.7**	**3.1**	**2.4**
ΔE_1	30.2	30.3	24.4	29.2	25.1	27.4	27.4	29.7	24.1	28.6	29.3	34.3	27.8	27.9	29.7	30.0	29.1	29.2	28.0	28.7	26.2	29.4	26.9	30.0	29.3	28.2
ΔE_2	−29.9	−30.4	−31.2	−34.6	−32.2	−34.0	−31.9	−33.6	−28.1	−31.5	−29.5	−32.6	−31.0	−31.0	−32.5	−32.6	−24.8	−24.9	−31.3	−26.4	−32.1	−34.6	−31.9	−34.2	−31.4	−30.6
ΔE_3	−21.2	−21.5	−18.7	−24.1	−20.1	−23.1	−21.0	−23.8	−15.2	−20.7	−21.4	−26.2	−19.6	−19.7	−22.3	−22.6	−18.2	−18.2	−20.1	−19.3	−20.5	−24.4	−20.7	−24.4	−21.2	−20.6
ΔE_4	−26.9	−27.2	−22.0	−28.0	−23.5	−26.9	−25.0	−28.2	−19.0	−25.0	−26.1	−31.2	−24.1	−24.2	−27.5	−27.9	−22.9	−23.0	−24.6	−24.6	−24.1	−28.5	−24.5	−28.7	−25.6	−25.3
ΔE_5	−25.9	−26.1	−20.8	−28.1	−22.5	−26.4	−22.8	−26.6	−16.3	−23.4	−23.7	−30.1	−22.0	−22.2	−24.3	−24.9	−19.0	−19.1	−21.7	−21.2	−22.9	−28.2	−22.9	−27.9	−22.8	−23.0
$\Delta E_6^{‡}$	9.0	8.6	8.1	7.6	8.7	8.5	11.4	11.2	10.2	9.7	7.5	7.0	13.3	13.3	12.6	12.5	18.4	18.4	10.7	16.2	7.6	7.3	8.8	8.5	13.5	11.4
ΔE_7	3.8	2.2	4.2	3.6	5.3	5.0	8.6	8.3	6.1	5.5	2.6	2.0	10.7	10.7	11.4	11.4	16.7	16.7	5.8	14.2	3.1	2.7	4.6	4.3	11.0	8.7
ΔE_8	−27.6	−27.9	−30.8	−36.0	−32.7	−35.5	−31.1	−33.9	−25.7	−30.8	−26.2	−30.6	−29.4	−29.5	−26.6	−27.1	−22.0	−22.2	−27.2	−25.9	−31.0	−34.9	−30.5	−34.1	−27.4	−28.6
ΔE_9	−16.0	−16.1	−12.6	−20.6	−14.9	−19.4	−15.7	−20.0	−8.4	−16.3	−15.0	−21.6	−13.3	−13.6	−13.5	−14.2	−12.5	−12.7	−13.2	−16.0	−14.4	−20.4	−14.7	−20.4	−13.9	−15.4
ΔE_{10}	−25.7	−26.0	−18.4	−27.4	−21.2	−26.4	−23.3	−28.2	−14.6	−23.5	−22.6	−29.9	−21.1	−21.5	−22.3	−23.2	−21.2	−21.5	−20.2	−25.1	−20.8	−27.6	−21.6	−28.1	−21.9	−24.0
ΔE_{11}	−23.2	−23.2	−14.5	−25.1	−17.4	−23.4	−18.7	−24.4	−10.0	−20.3	−16.9	−25.6	−16.7	−17.1	−17.6	−18.8	−16.1	−16.4	−14.9	−19.8	−16.8	−24.7	−17.2	−24.8	−17.2	−19.7
$\Delta E_{12}^{‡}$	25.2	27.4	18.1	17.9	17.3	17.2	21.2	21.1	21.7	21.4	26.6	26.6	20.9	21.0	22.8	22.8	18.2	18.2	24.1	22.8	21.8	21.6	23.0	22.8	25.5	24.0
ΔE_{13}	10.6	13.0	4.2	4.2	2.9	2.8	4.5	4.5	6.3	6.2	10.6	10.8	6.2	6.2	7.2	7.2	1.7	1.7	8.2	7.0	8.2	8.1	8.4	8.4	8.1	7.3
ΔE_{14}	−25.0	−25.1	−27.7	−33.0	−29.4	−32.3	−27.7	−30.5	−22.6	−27.7	−22.1	−26.6	−26.3	−26.5	−24.3	−24.8	−19.3	−19.4	−24.5	−22.7	−27.9	−31.8	−27.3	−31.0	−24.2	−25.4
$\Delta E_{15}^{‡}$	24.2	26.3	15.5	15.6	15.1	15.0	19.4	19.4	18.5	18.5	25.7	25.9	18.5	18.5	20.6	20.5	16.8	16.8	22.6	21.4	19.8	19.8	21.2	21.2	23.4	21.9
ΔE_{16}	−5.0	−2.8	−10.5	−10.4	−11.8	−11.8	−11.0	−10.9	−9.1	−9.1	−5.3	−5.0	−9.9	−9.8	−8.6	−8.6	−12.1	−12.1	−9.1	−8.1	−7.1	−7.0	−7.1	−7.1	−8.1	−8.4
$\Delta E_{17}^{‡}$	14.2	14.5	10.9	10.9	10.5	10.5	11.4	11.4	13.6	13.5	11.4	11.4	14.7	14.7	15.5	15.6	12.3	12.3	14.7	13.3	12.6	12.6	12.8	12.8	14.1	13.4
ΔE_{18}	−28.2	−27.7	−30.7	−30.0	−31.1	−30.8	−32.8	−32.5	−31.4	−30.9	−30.4	−29.6	−27.7	−27.7	−27.3	−27.2	−33.9	−33.9	−27.9	−29.5	−27.1	−26.7	−28.1	−27.7	−31.6	−31.3
$\Delta E_{19}^{‡}$	14.1	16.4	13.1	13.5	12.5	12.7	11.8	12.0	14.4	14.7	17.0	17.3	12.0	12.0	7.7	7.7	11.7	11.7	10.3	13.6	14.0	14.3	13.6	13.9	12.3	12.4
ΔE_{20}	−33.4	−31.8	−30.8	−29.8	−31.9	−31.4	−36.7	−36.2	−32.2	−31.3	−32.0	−31.2	−35.0	−35.0	−38.7	−38.7	−36.4	−36.4	−36.0	−35.0	−30.3	−29.7	−32.4	−31.7	−38.5	−37.1
$\Delta E_{21}^{‡}$	19.6	20.2	17.3	17.4	17.0	17.0	17.4	17.4	19.0	19.0	17.5	17.7	19.7	19.7	20.1	20.1	14.1	14.1	19.8	17.2	20.2	20.3	20.2	20.2	18.8	18.7
ΔE_{22}	−3.5	−2.8	−5.4	−4.7	−5.7	−5.4	−6.9	−6.6	−6.9	−6.2	−5.8	−5.1	−3.9	−3.9	−4.8	−4.8	−10.9	−10.9	−4.7	−5.6	−1.0	−0.6	−1.9	−1.5	−7.1	−6.6
$\Delta E_{23}^{‡}$	20.5	22.3	19.3	19.1	18.9	18.7	20.0	19.9	22.7	22.3	25.9	25.9	19.2	19.2	16.4	16.4	22.7	22.7	19.1	21.9	19.3	19.1	19.8	19.6	21.1	20.9
ΔE_{24}	−21.3	−19.7	−19.5	−18.5	−20.1	−19.7	−24.0	−23.5	−21.7	−20.8	−17.2	−16.2	−24.5	−24.5	−25.8	−25.9	−28.6	−28.6	−23.2	−25.8	−17.2	−16.6	−19.0	−18.4	−27.5	−25.4
$\Delta E_{25}^{‡}$	13.6	14.1	12.4	12.3	12.2	12.1	12.3	12.2	13.7	13.7	11.9	11.9	15.3	15.2	15.6	15.6	10.2	10.2	15.7	13.0	14.3	14.2	14.2	14.1	13.7	13.3
ΔE_{26}	−19.1	−18.4	−18.1	−17.8	−18.2	−18.2	−20.6	−20.6	−20.2	−20.1	−20.3	−19.9	−16.6	−16.6	−18.8	−18.9	−26.2	−26.2	−17.7	−20.4	−14.2	−14.2	−15.5	−15.4	−22.1	−21.1
$\Delta E_{27}^{‡}$	18.0	19.9	17.4	17.6	16.8	16.9	15.9	16.0	18.6	18.7	20.0	20.3	16.6	16.6	12.2	12.3	16.5	16.6	13.9	17.4	17.8	17.9	17.3	17.5	16.2	16.3
ΔE_{28}	−27.9	−26.3	−24.8	−24.1	−26.1	−25.8	−31.4	−31.1	−25.6	−25.2	−26.1	−25.5	−27.4	−27.4	−33.0	−32.9	−30.3	−30.3	−30.6	−29.3	−24.8	−24.4	−27.0	−26.5	−32.5	−31.1
ΔE_{29}	−16.7	−16.9	−17.8	−23.4	−19.8	−22.9	−18.3	−21.3	−12.7	−18.0	−14.7	−19.3	−18.1	−18.3	−16.1	−16.7	−9.7	−9.9	−15.5	−14.1	−19.2	−23.3	−18.5	−22.5	−16.2	−16.7
$\Delta E_{30}^{‡}$	20.4	21.9	14.0	14.1	13.2	13.3	15.9	16.0	17.1	17.2	20.4	20.6	15.0	15.0	17.5	17.6	13.8	13.8	17.7	17.2	17.1	17.2	17.9	18.0	18.6	17.8
ΔE_{31}	−7.4	−5.4	−13.9	−13.0	−14.9	−14.5	−13.9	−13.4	−12.7	−11.9	−7.8	−6.9	−12.7	−12.7	−11.6	−11.5	−14.9	−14.9	−12.7	−10.5	−10.1	−9.5	−10.1	−9.5	−11.0	−11.0
ΔE_{32}	−2.9	−3.5	1.5	−6.1	−0.7	−5.0	−1.7	−5.8	4.5	−3.0	−2.5	−8.8	−0.9	−1.2	−1.8	−2.6	−1.1	−1.4	0.9	−3.7	−1.1	−6.8	−1.4	−6.8	−2.3	−2.5
$\Delta E_{33}^{‡}$	16.6	16.8	12.4	12.5	11.9	12.0	13.3	13.4	15.8	15.9	14.1	14.2	17.1	17.1	17.7	17.7	15.3	15.3	17.6	16.4	14.4	14.4	14.7	14.8	16.6	15.5
ΔE_{34}	−35.3	−34.8	−38.2	−37.5	−38.8	−38.5	−40.4	−40.0	−38.0	−37.3	−37.9	−37.2	−34.7	−34.7	−33.8	−33.7	−38.5	−38.5	−36.6	−35.5	−34.7	−34.3	−35.7	−35.2	−38.0	−38.1
$\Delta E_{35}^{‡}$	15.6	17.1	15.5	16.3	14.7	15.1	12.4	12.7	15.1	15.8	15.4	16.1	13.6	13.6	8.5	8.5	10.2	10.2	10.6	13.3	16.2	16.7	15.1	15.6	11.5	12.4
ΔE_{36}	−10.1	−10.0	−6.0	−4.9	−6.9	−6.4	−12.8	−12.3	−9.2	−8.2	−11.3	−10.2	−10.5	−10.5	−15.8	−15.8	−15.7	−15.7	−9.1	−13.1	−5.5	−4.8	−8.0	−7.3	−17.0	−15.4
$\Delta E_{37}^{‡}$	26.1	25.1	19.9	20.7	19.2	19.5	23.1	23.5	25.5	26.2	24.5	25.3	24.5	24.5	26.4	26.4	27.4	27.4	24.0	29.5	21.8	22.2	23.1	23.6	29.3	26.8
ΔE_{38}	−13.3	−15.0	−14.9	−12.8	−15.5	−14.6	−16.0	−15.0	−13.9	−12.1	−16.4	−14.2	−10.9	−10.9	−9.0	−8.9	−11.7	−11.7	−15.4	−8.9	−13.6	−12.3	−14.0	−12.7	−12.3	−12.8
$\Delta E_{39}^{‡}$	33.0	31.8	27.1	28.3	26.7	27.3	30.4	30.9	32.0	33.1	32.1	33.3	31.7	31.7	32.1	32.1	33.1	33.1	31.3	36.5	29.8	30.5	31.0	31.7	35.2	33.3
ΔE_{40}	6.5	4.7	7.0	8.4	6.6	7.1	5.9	6.5	7.0	8.2	4.3	5.9	8.5	8.6	8.5	8.6	6.4	6.5	4.6	9.0	8.9	9.7	8.4	9.2	6.9	7.0

Relative electronic energies (zero-point uncorrected) are reported in kcal/mol. The def2-TZVPP basis set was used.

Then, we used these results to assess the performance of several computational methods (Table S4), including DLPNO-CCSD(T)[15,16] (performed with ORCA 4.2.1[17,18] using the def2-TZVPP/C auxiliary basis set and tight thresholds), BP86,[19,20] PBE,[21] PBE0,[22] B3LYP,[23,24] BMK,[25] M06-L,[26] M06,[27] M06-2X,[27] M11-L,[28] M11,[29] TPSS,[8] TPSSh,[30] ωB97X,[31] and ωB97XD[32], by performing gas-phase single-point energy calculations (with the def2-TZVPP basis set) on the optimized geometries computed at the TPSS/def2-TZVPP/W06 level. For some density functionals, the influence of empirical dispersion was considered.[33,34] The smallest root-mean-square deviation (RMSD) was obtained with the DLPNO-CCSD(T) method (1.3 kcal/mol). Among the density functionals tested, B3LYP-D3(BJ), BMK, and TPSSh gave the best results: the RMSDs are ca. 2 kcal/mol. To make a choice among these three functionals, we further investigated the competition between [5 + 2] and [5 + 2 + 1] cycloadditions (Figure S9). The electronic energy difference between the reductive elimination transition state **SI-TS5** and the CO insertion transition state **SI-TS10** is 10.4 kcal/mol at the CCSD(T)/def2-TZVPP//TPSS/def2-TZVPP/W06 level. The smallest deviation (0.9 kcal/mol) was obtained when the BMK functional was utilized. Therefore, we finally decided to use the BMK functional and the DLPNO-CCSD(T) method for geometry optimizations and single-point energy refinements, respectively.

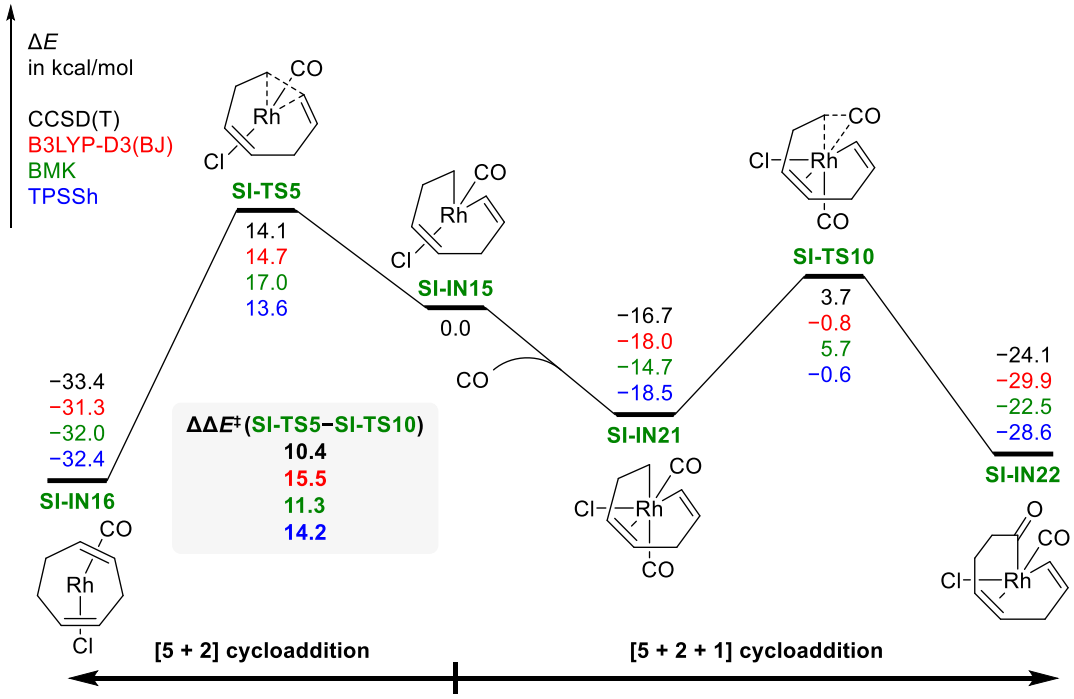
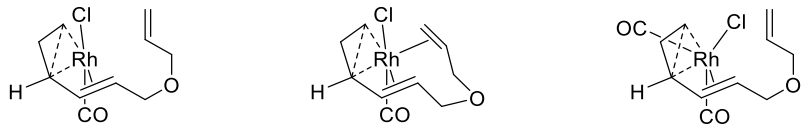


Figure S9. Competition between [5 + 2] and [5 + 2 + 1] cycloadditions. Relative electronic energies (zero-point uncorrected) are reported. The def2-TZVPP basis set was used.

S7. Additional Computational Results

Discussion of the Cyclopropane Cleavage Step. Compared with the 16-electron cyclopropane cleavage transition state **TS1**, 18-electron transition states **TS17** and **TS18** (with the complexation of the terminal alkene and an additional CO ligand, respectively) are disfavored (Figure S10).



TS1 (21.7) **TS17** (24.7) **TS18** (24.9)

Figure S10. Cyclopropane cleavage transition states. Relative Gibbs energies are reported in kcal/mol, computed at the DLPNO-CCSD(T)/def2-TZVPP:SMD(1,4-dioxane)//BMK/def2-SVP level.

Discussion of the CO Insertion Step. As depicted in Figure S11, **TS3** and **TS19** are the most favored CO insertion transition states with two CO ligands. **TS20** and **TS21** are the most favored CO insertion transition states with three CO ligands. Among them, **TS3** is the most favored one.

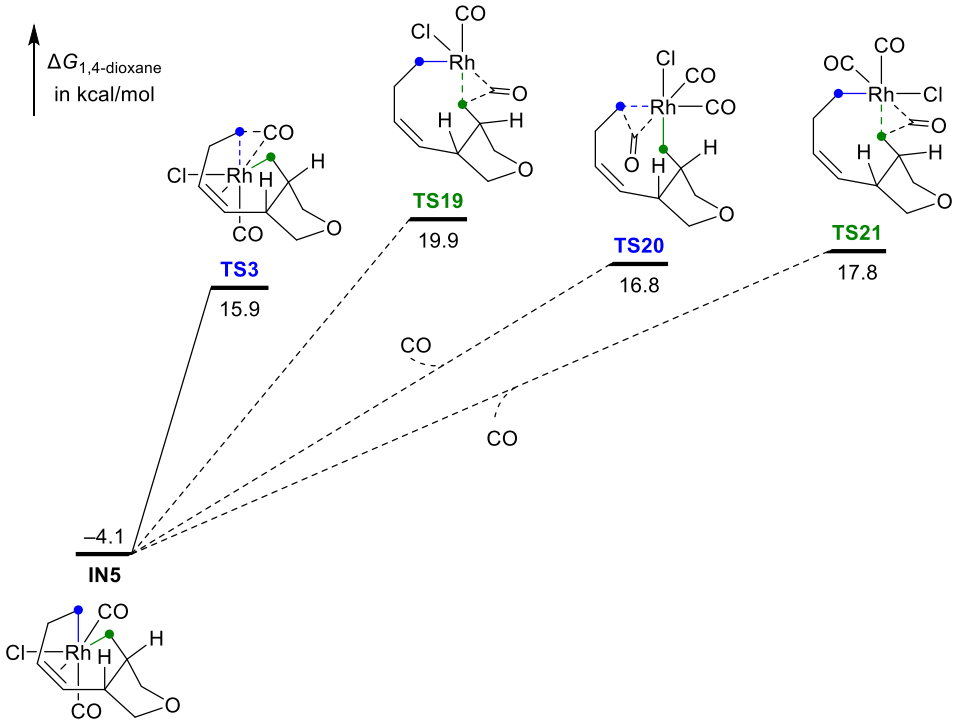


Figure S11. CO insertion transition states, computed at the DLPNO-CCSD(T)/def2-TZVPP:SMD(1,4-dioxane)//BMK/def2-SVP level.

Discussion of the Chemoselectivity. In the main text, we have discussed the competition between [5 + 2] and [5 + 2 + 1] cycloadditions. Herein, we will discuss the chemoselectivity in more detail (Figure S12).

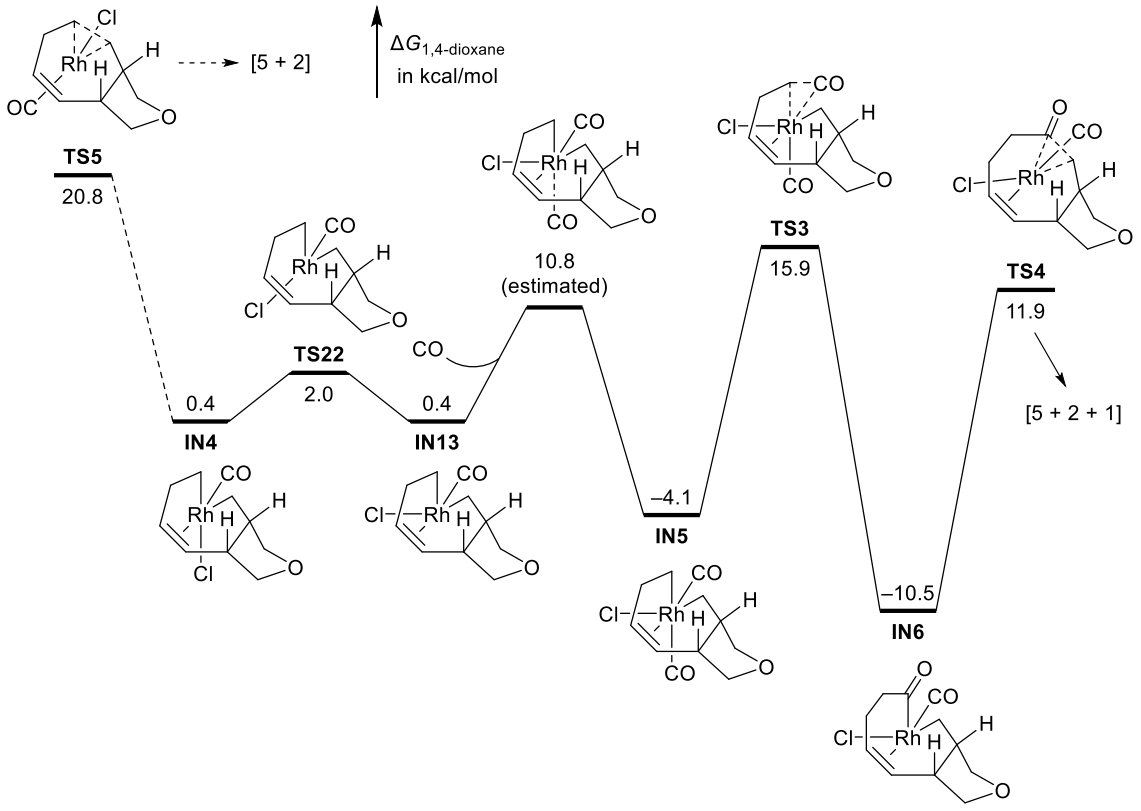


Figure S12. Competition between [5 + 2] and [5 + 2 + 1] cycloadditions, computed at the DLPNO-CCSD(T)/def2-TZVPP:SMD(1,4-dioxane)//BMK/def2-SVP level.

(i) We assume that the concentration of CO always reaches saturation (1.4 mM in 1,4-dioxane at 0.2 atm and 80 °C).[35] If the mass transfer of CO from the gas phase to the solution phase is inefficient, the concentration of CO in the solution will be even lower.

(ii) For rhodium intermediates with different configurations, such as **IN4** and **IN13**, the interconversion between the isomers is easy.[36,37] We assume that similar equilibria exist during the entire catalytic reaction (see **IN2** and **IN14** in Figure S13 for another example).

(iii) Unfortunately, we cannot locate the transition state for the CO complexation process (**IN13** + CO → **IN5**). The diffusion limit for the first-order rate constant of CO complexation is ca. 10^8 $M^{-1}{\cdot}s^{-1}$ (the typical second-order diffusion rate constant in water)[38] × 1.4 mM (the concentration of CO). The corresponding activation Gibbs energy is ca. 10.4 kcal/mol at 298 K.[39,40] We assume that there exists an equilibrium between **IN13** and **IN5**. We also assume that similar equilibria exist for the reactions discussed in Table 1.

(iv) Because the Gibbs energy of the C(sp^2)–C(sp^3) reductive elimination transition state **TS4** is lower than that of the CO insertion transition state **TS3**, the CO insertion step (**IN5** → **TS3** → **IN6**) is irreversible. Therefore, we can predict the chemoselectivity by applying the following equation:

$$[5+2] \xleftarrow{k_{[5+2]}} \mathbf{IN4} \underset{}{\overset{K_1}{\rightleftharpoons}} \mathbf{IN13} \overset{\overset{CO}{K_2}}{\rightleftharpoons} \mathbf{IN5} \xrightarrow{k_{[5+2+1]}} [5+2+1]$$

$$\frac{r_{[5+2+1]}}{r_{[5+2]}} = \frac{k_{[5+2+1]}[\mathbf{IN5}]}{k_{[5+2]}[\mathbf{IN4}]} = \frac{k_{[5+2+1]}K_1K_2[\mathrm{CO}][\mathbf{IN4}]}{k_{[5+2]}[\mathbf{IN4}]} = \frac{[\mathrm{CO}]}{c^\circ}\mathrm{e}^{-\frac{G(\mathbf{TS3})-G(\mathbf{TS5})-G(\mathrm{CO})}{RT}}$$

where c° is the standard state concentration of CO.

When computing the Gibbs energies, we used 1.4 mM (the CO concentration under our reaction conditions) as the standard state concentration of CO. Standard state concentration of 1.0 M was used for the other species.[41]

We suggest that the above discussion applies not only to this work, but also to other [*m* + *n*] versus [*m* + *n* + 1] cycloadditions if there is a CO complexation−dissociation equilibrium before the irreversible CO insertion.

Discussion of Pathway II. As was mentioned above, the diffusion limit for the activation Gibbs energy of CO complexation is ca. 10.4 kcal/mol. We assume that there exists an equilibrium between **IN2** and **IN7** in pathway II (Figure S13). Generation of **IN7** may also take place via a stepwise ligand transposition/CO complexation mechanism or through oxidative addition via **TS18** (Figure S10).

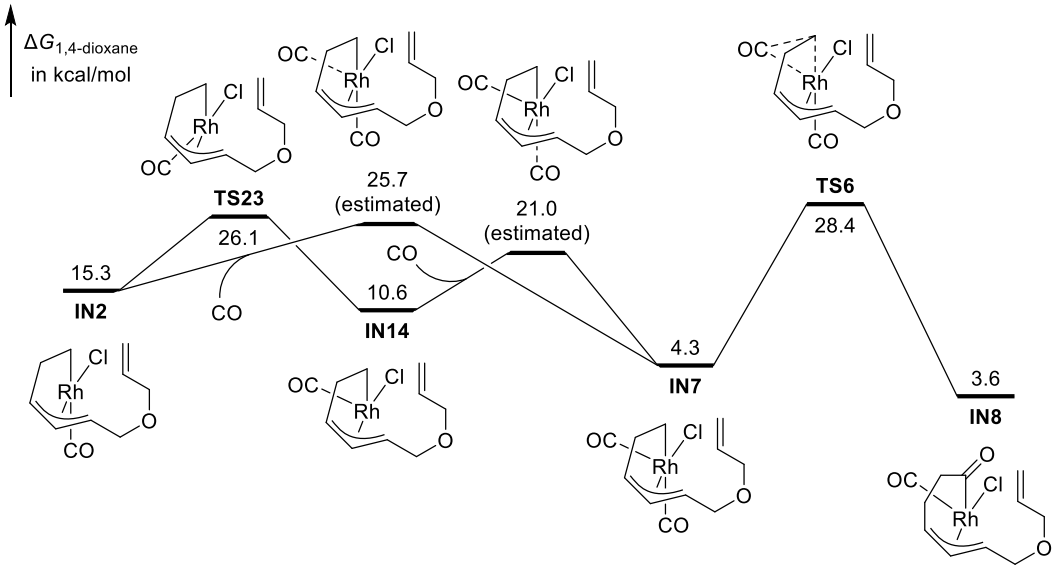


Figure S13. CO complexation and insertion in pathway II, computed at the DLPNO-CCSD(T)/def2-TZVPP:SMD(1,4-dioxane)//BMK/def2-SVP level.

S8. Computed Energies of the Stationary Points

Table S5. Thermal Corrections to Gibbs Energies (TCGs) and Single-Point Energies (SPEs)

	TCG[a,b] (a.u.)	SPE[a] (a.u.)	SPE[c] (a.u.)	SPE[d] (a.u.)
CO	−0.013860	−113.172745	−113.167803	−113.158173
$[Rh(CO)_2Cl]_2$	−0.005421	−1592.916752	−1592.917033	−1593.122136
1c	0.172762	−425.889224	−425.895549	−425.765417
2c	0.192174	−539.157244	−539.167450	−539.000051
(*Z*)-**4**	0.219957	−391.258220	−391.263628	−391.132127
(*E*)-**4**	0.219156	−391.259760	−391.265378	−391.132897
IN1	0.177761	−1109.132451	−1109.145911	−1109.131961
IN2	0.177970	−1109.134380	−1109.145186	−1109.133911
IN3	0.185353	−1109.171442	−1109.181199	−1109.173282
IN4	0.185451	−1109.169181	−1109.182266	−1109.162785
IN5	0.193309	−1222.369540	−1222.380299	−1222.350523
IN6	0.193623	−1222.383619	−1222.399967	−1222.355332
IN7	0.185069	−1222.344102	−1222.352656	−1222.331080
IN8	0.188140	−1222.352145	−1222.365704	−1222.330187
IN9	0.188466	−1222.356301	−1222.366015	−1222.340486
IN10	0.190905	−1222.345924	−1222.358045	−1222.330381
(*Z*)-**IN11**	0.225055	−1074.495257	−1074.507590	−1074.493883
(*E*)-**IN11**	0.224605	−1074.500999	−1074.513987	−1074.499578
IN12-Me	0.291075	−1379.147796	−1379.163645	−1379.034674
IN12-H	0.263754	−1339.894377	−1339.910536	−1339.790890
IN13	0.184761	−1109.168719	−1109.181822	−1109.162163
IN14	0.178476	−1109.141080	−1109.153247	−1109.140589
TS1	0.177760	−1109.123838	−1109.135111	−1109.122961
TS2	0.186587	−1109.141925	−1109.153111	−1109.139089
TS3	0.192025	−1222.337797	−1222.351676	−1222.314193
TS4	0.193625	−1222.354321	−1222.369049	−1222.321310
TS5	0.185442	−1109.132149	−1109.143780	−1109.131759
TS6	0.185677	−1222.311571	−1222.323242	−1222.290137
TS7	0.189270	−1222.305813	−1222.316360	−1222.292231
(*Z*)-**TS8**	0.224995	−1074.483013	−1074.493424	−1074.483231
(*E*)-**TS8**	0.224365	−1074.490215	−1074.501345	−1074.489850
cis-**TS9-H**	0.282974	−1868.170834	−1868.190011	−1867.888072
trans-**TS9-H**	0.281645	−1868.163673	−1868.183002	−1867.883637
cis-**TS9-Me**	0.311150	−1907.423986	−1907.442752	−1907.129561
trans-**TS9-Me**	0.309714	−1907.421332	−1907.439908	−1907.131769
cis-**TS10**	0.309815	−1907.420976	−1907.440425	−1907.126957
trans-**TS10**	0.308747	−1907.411865	−1907.430237	−1907.119318

cis-**TS11**	0.387679	−2138.142228	−2138.162668	−2137.749678
trans-**TS11**	0.387645	−2138.142575	−2138.163986	−2137.753618
TS12-Me	0.288405	−1379.109464	−1379.124181	−1379.002283
TS12-H	0.261976	−1339.855085	−1339.870056	−1339.757645
TS13-Me	0.295502	−1492.301980	−1492.319694	−1492.172537
TS13-H	0.268368	−1453.053615	−1453.070545	−1452.934752
TS14-Me	0.296504	−1492.304821	−1492.319561	−1492.177464
TS14-H	0.269088	−1453.058528	−1453.074487	−1452.936082
TS15-Me	0.301953	−1605.494635	−1605.508660	−1605.349083
TS15-H	0.274961	−1566.250825	−1566.265504	−1566.114861
TS16-Me	0.303137	−1605.502948	−1605.517337	−1605.358179
TS16-H	0.277119	−1566.251376	−1566.266231	−1566.116081
TS17	0.180736	−1109.122430	−1109.136536	−1109.118361
TS18	0.184225	−1222.313090	−1222.324661	−1222.294444
TS19	0.191668	−1222.329873	−1222.343114	−1222.308033
TS20	0.197105	−1335.528263	−1335.539614	−1335.490619
TS21	0.198538	−1335.527424	−1335.539373	−1335.489840
TS22	0.186032	−1109.167751	−1109.179288	−1109.162405
TS23	0.177087	−1109.119220	−1109.128607	−1109.117205

[a]Computed at the BMK/def2-SVP level.

[b]Computed at 1 atm and 298 K.

[c]Computed at the SMD(1,4-dioxane)/BMK/def2-SVP//BMK/def2-SVP level.

[d]Computed at the DLPNO-CCSD(T)/def2-TZVPP//BMK/def2-SVP level.

Table S6. Zero-Point Energies (ZPEs) and Selected Single-Point Energies in Benchmark Calculations

	ZPE[a] (a.u.)	TPSS[a] (a.u.)	BMK[b] (a.u.)	DLPNO-CCSD(T)[c] (a.u.)	CCSD(T)[d] (a.u.)
SI-CO	0.004875	−113.374477	−113.309117	−113.158297	−113.159057
SI-C_2H_2	0.026510	−77.374299	−77.299671	−77.188474	−77.189038
SI-C_2H_4	0.050360	−78.633957	−78.553122	−78.439787	−78.440102
SI-C_3H_4	0.054241	−116.725665	−116.609560	−116.434895	−116.435732
SI-dimer	0.036814	−1595.437285	−1593.834377	−1593.129136	−1592.556505
SI-IN1	0.017436	−797.676906	−796.870537	−796.516209	−796.230097
SI-IN2	0.025067	−911.102609	−910.226709	−909.722880	−909.436766
SI-IN3	0.045445	−875.083903	−874.204346	−873.738920	−873.452922
SI-IN4	0.070598	−876.349287	−875.465175	−874.999380	−874.713039
SI-IN5	0.073906	−914.439117	−913.517916	−912.992623	−912.707180
SI-IN6	0.124299	−879.697734	−878.783824	−878.291325	−878.004850
SI-IN7	0.123415	−879.692846	−878.779725	−878.287777	−877.998763

SI-IN8	0.132544	−993.116702	−992.130619	−991.490461	−991.201764
SI-IN9	0.152502	−957.090048	−956.103244	−955.501945	−955.213330
SI-IN10	0.178325	−958.359849	−957.368871	−956.769071	−956.479750
SI-IN11	0.181785	−996.445198	−995.416258	−994.759609	−994.471404
SI-IN12	0.133534	−993.103716	−992.113667	−991.469778	−991.184863
SI-IN13	0.132196	−993.111802	−992.124131	−991.486020	−991.197733
SI-IN14	0.134105	−993.123046	−992.132520	−991.490528	−991.205719
SI-IN15	0.157223	−957.133230	−956.151701	−955.546105	−955.258248
SI-IN16	0.160089	−957.181573	−956.202762	−955.596730	−955.311549
SI-IN17	0.180525	−958.361421	−957.378188	−956.773594	−956.485324
SI-IN18	0.183121	−958.388754	−957.405618	−956.804917	−956.519244
SI-IN19	0.185216	−996.467847	−995.448667	−994.788983	−994.501903
SI-IN20	0.187894	−996.507332	−995.490280	−994.830891	−994.546328
SI-IN21	0.165326	−1070.538233	−1069.484206	−1068.731393	−1068.443886
SI-IN22	0.167211	−1070.554381	−1069.496607	−1068.739987	−1068.455727
SI-IN23	0.162453	−1070.499060	−1069.436154	−1068.684523	−1068.399428
SI-IN24	0.169248	−1070.563119	−1069.514650	−1068.755978	−1068.471899
SI-IN25	0.140051	−1106.449048	−1105.381770	−1104.595537	−1104.311864
SI-IN26	0.142981	−1106.470822	−1105.407856	−1104.619517	−1104.333083
SI-IN27	0.164784	−1107.712850	−1106.641385	−1105.858178	−1105.574164
SI-IN28	0.166383	−1107.698705	−1106.634472	−1105.850712	−1105.563758
SI-TS1	0.122610	−879.685566	−878.771902	−878.277653	−877.990583
SI-TS2	0.131962	−993.082028	−992.088161	−991.446813	−991.161537
SI-TS3	0.131704	−993.080180	−992.083204	−991.444058	−991.159116
SI-TS4	0.153582	−957.069959	−956.085115	−955.478822	−955.190651
SI-TS5	0.156681	−957.110862	−956.124601	−955.519985	−955.235791
SI-TS6	0.179104	−958.327569	−957.340916	−956.736952	−956.448458
SI-TS7	0.179847	−958.330668	−957.336837	−956.738127	−956.452700
SI-TS8	0.182789	−996.422456	−995.397314	−994.737148	−994.449712
SI-TS9	0.184465	−996.439509	−995.416745	−994.757305	−994.473264
SI-TS10	0.165315	−1070.510925	−1069.451628	−1068.696513	−1068.411367
SI-TS11	0.163558	−1070.476187	−1069.413717	−1068.657792	−1068.372944
SI-TS12	0.166937	−1070.528651	−1069.472032	−1068.712720	−1068.430882
SI-TS13	0.140206	−1106.414410	−1105.342776	−1104.555525	−1104.270261
SI-TS14	0.165014	−1107.665451	−1106.590207	−1105.807549	−1105.521654

[a]Computed at the TPSS/def2-TZVPP/W06 level.

[b]Computed at the BMK/def2-TZVPP//TPSS/def2-TZVPP/W06 level.

[c]Computed at the DLPNO-CCSD(T)/def2-TZVPP//TPSS/def2-TZVPP/W06 level.

[d]Computed at the CCSD(T)/def2-TZVPP//TPSS/def2-TZVPP/W06 level.

S9. Cartesian Coordinates of the Stationary Points

CO

O	0.000000	0.000000	0.482549
C	0.000000	0.000000	-0.643398

$[Rh(CO)_2Cl]_2$

Rh	1.627119	0.000015	-0.097814
Rh	-1.627012	0.000024	-0.097844
Cl	0.000090	1.661827	-0.900430
Cl	-0.000122	-1.661664	-0.900317
O	3.464891	-2.196441	0.854893
O	3.465517	2.195998	0.855227
O	-3.465573	2.195950	0.855086
O	-3.465368	-2.195964	0.855013
C	2.788142	-1.357307	0.502231
C	2.788535	1.357155	0.502425
C	-2.788426	1.357179	0.502348
C	-2.788252	-1.357175	0.502257

1c

O	1.886898	-1.151520	-0.163680
C	-3.413782	1.422921	0.320635
C	-4.129914	0.102515	0.083436
C	-2.710824	0.309552	-0.476259
C	-1.573748	-0.417319	0.138340
C	-0.507544	-0.891229	-0.522536
C	0.617734	-1.666772	0.122620
C	2.157410	0.090834	0.419228
C	3.598578	0.445796	0.167732
C	4.017191	1.635637	-0.272467
H	-3.751105	2.306295	-0.230820
H	-3.038690	1.634958	1.327816
H	-4.958716	0.078699	-0.631206
H	-4.242081	-0.585001	0.928873
H	-2.632015	0.459800	-1.559055
H	-1.637217	-0.573686	1.226378
H	-0.422395	-0.739360	-1.607630
H	0.450616	-1.719702	1.220786
H	0.626076	-2.701047	-0.263557
H	1.490430	0.884381	0.025415
H	1.978408	0.035637	1.518011
H	4.320510	-0.350778	0.389569
H	5.081310	1.852522	-0.407884
H	3.309080	2.437827	-0.511632

2c

O	1.925783	-1.841981	0.920694
O	-2.971399	0.020138	-0.154229
C	1.704647	-1.091062	0.004169
C	2.638567	0.078865	-0.298279
C	2.085340	1.420112	0.264635
C	0.882613	1.970960	-0.475848
C	-0.388293	1.576003	-0.299276
C	-0.835549	0.496971	0.660238
C	-2.338215	0.586154	0.965632
C	-2.145081	-0.960370	-0.739446
C	-0.800920	-0.925363	0.023720
C	0.432712	-1.247949	-0.834224
H	2.793997	0.170362	-1.387631
H	3.601784	-0.146468	0.186248
H	2.901621	2.159572	0.225111
H	1.850282	1.269907	1.333421
H	1.083178	2.741059	-1.231336
H	-1.172519	2.027010	-0.921523
H	-0.225463	0.516978	1.578900
H	-2.576491	0.022821	1.891296
H	-2.699476	1.620390	1.086836
H	-2.621350	-1.956571	-0.677582
H	-2.005264	-0.718286	-1.810272
H	-0.823904	-1.652372	0.853849
H	0.381495	-2.301428	-1.160682
H	0.462126	-0.604154	-1.726274

(*Z*)-**4**

C	-3.171796	0.816450	0.678209
C	-3.613650	0.110141	-0.594012
C	-2.115316	0.186992	-0.249364
C	-1.414467	-1.044116	0.195631
C	-0.139449	-1.391484	-0.053103
C	0.877111	-0.610101	-0.851432
C	1.920385	0.183787	-0.008546

C	2.954565	0.792869	-0.974389
C	2.638439	-0.753873	0.980875
C	1.219487	1.314233	0.767561
H	-3.229715	1.908879	0.716184
H	-3.358071	0.319851	1.636715
H	-3.975642	0.717855	-1.429445
H	-4.100660	-0.866727	-0.501193
H	-1.521971	0.891430	-0.840657
H	-2.027386	-1.732585	0.794424
H	0.208283	-2.342880	0.368439
H	1.432556	-1.318438	-1.494804
H	0.373696	0.098177	-1.532191
H	3.495946	0.004487	-1.526190
H	3.699198	1.395336	-0.425438
H	2.466269	1.450607	-1.714833
H	1.937567	-1.160492	1.729162
H	3.432386	-0.211158	1.522956
H	3.109031	-1.603114	0.453799
H	0.744480	2.032364	0.075515
H	1.945340	1.872386	1.384658
H	0.436835	0.914637	1.434318

(*E*)-**4**

C	3.652125	0.972640	0.142050
C	4.005074	-0.421661	-0.355861
C	2.691449	-0.198218	0.413415
C	1.398572	-0.266247	-0.312608
C	0.251955	-0.746274	0.193164
C	-1.054203	-0.820334	-0.556451
C	-2.198825	0.083629	-0.011236
C	-3.459983	-0.182373	-0.855486
C	-1.805695	1.567208	-0.134038
C	-2.497622	-0.251644	1.462959
H	4.211215	1.381034	0.990037
H	3.337780	1.720478	-0.594175
H	4.806152	-0.969432	0.150743
H	3.930566	-0.621380	-1.430435
H	2.662399	-0.573523	1.443027
H	1.409213	0.108661	-1.347431
H	0.256196	-1.125192	1.224714
H	-0.879756	-0.561701	-1.617024
H	-1.417457	-1.866766	-0.541015
H	-3.275781	0.034172	-1.922418
H	-4.299093	0.452224	-0.521039
H	-3.778133	-1.236554	-0.773517
H	-0.894285	1.787533	0.446423
H	-2.616705	2.217930	0.237183
H	-1.609869	1.837617	-1.186924
H	-2.734377	-1.323471	1.587447
H	-3.364091	0.329384	1.824098
H	-1.641052	-0.011371	2.114861

IN1

Rh	-1.354297	-0.170661	-0.020898
Cl	-3.636731	-0.530719	-0.429590
O	-0.969403	-3.090305	0.530250
O	3.031179	-0.177417	-0.147488
C	-1.111883	-1.983442	0.314750
C	-1.637994	2.242101	-0.456724
C	-0.544562	3.189482	-0.015505
C	-0.726233	2.028284	0.915639
C	0.147418	0.825679	0.972297
C	0.716071	0.303256	-0.218541
C	1.770627	-0.777452	-0.165258
C	4.088244	-1.081556	-0.193716
C	5.414020	-0.369014	-0.156353
C	5.560091	0.955982	-0.078449
H	-2.684869	2.507761	-0.291267
H	-1.449775	1.689473	-1.392342
H	-0.856087	4.171879	0.351904
H	0.371070	3.205057	-0.615958
H	-1.307514	2.221374	1.822315
H	0.440994	0.455055	1.960439
H	0.809525	0.945937	-1.105633
H	1.624935	-1.410218	0.737655
H	1.672264	-1.442047	-1.050183
H	4.033771	-1.795059	0.660088
H	4.033104	-1.704470	-1.115491
H	6.292952	-1.024901	-0.198112
H	6.553460	1.413535	-0.054926
H	4.684964	1.610417	-0.035959

IN2

Rh	1.114661	0.266429	0.176263
Cl	1.523789	2.347573	-0.803008
O	-1.493610	1.715813	1.370774
O	-2.067410	-0.877753	-0.389649
C	-0.635768	1.114252	0.954467
C	2.918025	-0.468807	-0.468198
C	2.952541	-1.759102	0.371426
C	1.673931	-1.628735	1.201493
C	0.400499	-1.720970	0.627179
C	0.245584	-1.365631	-0.765865
C	-1.139114	-1.237660	-1.365207
C	-3.361551	-0.655681	-0.882595
C	-4.303484	-0.440763	0.270672
C	-5.140971	0.594696	0.373057
H	3.696020	0.254861	-0.177216
H	2.974743	-0.625463	-1.557409
H	3.829577	-1.821199	1.034547
H	2.929490	-2.686859	-0.227470
H	1.733727	-1.649361	2.296505
H	-0.489550	-1.751966	1.263877
H	0.976037	-1.745442	-1.491050
H	-1.108214	-0.489522	-2.184976
H	-1.426021	-2.209969	-1.826498
H	-3.378489	0.217178	-1.567458
H	-3.690252	-1.541652	-1.469839
H	-4.283088	-1.217689	1.045706
H	-5.829329	0.689320	1.218425
H	-5.168797	1.385623	-0.385398

IN3

Rh	0.456528	-0.043655	0.092366
Cl	-0.253001	-1.736657	-1.596324
O	3.074104	-1.655993	0.146744
O	-3.176688	0.353081	0.350373
C	2.120063	-1.048530	0.146939
C	1.187882	1.436993	1.352226
C	1.637049	2.411121	0.241506
C	1.240951	1.676701	-1.042715
C	-0.107760	1.444534	-1.386406
C	-1.132777	1.416852	-0.394414
C	-2.520067	0.917159	-0.750752
C	-2.573545	-0.810059	0.831924
C	-1.263188	-0.538265	1.541313
C	-0.238664	-1.463890	1.684393
H	2.028338	1.104177	1.981084
H	0.409793	1.850861	2.014258
H	2.725392	2.579662	0.249567
H	1.154162	3.403702	0.293900
H	1.984465	1.524244	-1.832929
H	-0.309664	0.971137	-2.354075
H	-1.099778	2.145886	0.424559
H	-3.152206	1.760206	-1.078283
H	-2.440391	0.186177	-1.578865
H	-3.270564	-1.225063	1.581763
H	-2.420235	-1.560089	0.033335
H	-1.286784	0.321150	2.222803
H	0.463498	-1.370197	2.517737
H	-0.307779	-2.436584	1.185160

IN4

Rh	0.987199	-0.079950	0.101882
Cl	1.089691	2.027550	1.304859
O	3.000515	0.870015	-1.963928
O	-3.369693	1.170422	-0.599375
C	2.258025	0.520413	-1.186818
C	1.074989	-2.069010	-0.512368
C	0.124873	-2.720944	0.518010
C	0.002431	-1.599799	1.536609
C	-0.896890	-0.566589	1.498927
C	-2.078890	-0.433645	0.562403
C	-2.759632	0.950477	0.648766
C	-3.005594	0.181552	-1.528351
C	-1.753633	-0.509974	-0.950394
C	-0.471672	0.260064	-1.280889
H	2.111445	-2.430831	-0.386679
H	0.771896	-2.253515	-1.555745
H	0.527902	-3.636047	0.982493
H	-0.857846	-2.971003	0.090921
H	0.732271	-1.590161	2.360099
H	-0.815182	0.188686	2.289976
H	-2.814423	-1.224189	0.805549

H	-3.519261	0.992093	1.449129
H	-2.001529	1.732998	0.850889
H	-3.826509	-0.552943	-1.658360
H	-2.812261	0.653031	-2.507548
H	-1.679537	-1.547760	-1.307816
H	-0.138726	0.020940	-2.303958
H	-0.637572	1.349324	-1.205181

IN5

Rh	-0.719665	0.021795	0.134236
Cl	-2.336093	0.516742	-1.684454
O	0.349301	2.847963	-0.870987
O	-2.825101	1.001668	2.097618
O	3.174616	1.063203	-0.363840
C	0.059422	1.839647	-0.461072
C	-2.026807	0.673880	1.368925
C	-1.507548	-1.894651	0.511922
C	-0.439194	-2.751574	-0.186239
C	-0.000447	-1.725073	-1.208261
C	1.092125	-0.895491	-1.119515
C	2.287320	-1.062442	-0.187232
C	3.475095	-0.252053	-0.740001
C	2.763436	1.011030	0.980087
C	2.095746	-0.382334	1.200924
C	0.637344	-0.339096	1.684676
H	-2.478907	-1.960535	-0.000771
H	-1.623304	-2.120513	1.582595
H	-0.818952	-3.675929	-0.653008
H	0.382864	-3.014091	0.498193
H	-0.672741	-1.580916	-2.062319
H	1.226736	-0.186666	-1.947155
H	2.519570	-2.134664	-0.078135
H	4.425677	-0.597028	-0.281240
H	3.580130	-0.292417	-1.835361
H	3.635933	1.129625	1.652662
H	2.079014	1.853564	1.172008
H	2.702413	-0.935742	1.940921
H	0.378099	-1.302783	2.153736
H	0.552505	0.418981	2.485348

IN6

Rh	0.724023	-0.260699	-0.294051
Cl	2.620048	0.531746	-1.595152
O	2.294486	-2.841133	0.182957
O	1.369134	-0.473213	2.443021
O	-3.984015	-0.852727	-0.525497
C	1.712346	-1.891618	0.011598
C	1.080377	0.288789	1.573879
C	1.080170	1.817347	1.764899
C	-0.044193	2.506165	0.977659
C	-0.023594	2.000211	-0.445219
C	-0.985094	1.216651	-1.026427
C	-2.292472	0.787661	-0.390219
C	-3.205757	-0.017663	-1.338231
C	-3.513511	-0.866658	0.804230
C	-2.116040	-0.219311	0.771332
C	-0.983185	-1.201380	0.431663
H	2.064428	2.145058	1.380851
H	1.041899	2.025882	2.846391
H	0.118500	3.597268	0.976722
H	-1.018478	2.316173	1.453269
H	0.804448	2.345246	-1.074701
H	-0.861919	1.012913	-2.101594
H	-2.834709	1.682814	-0.033578
H	-3.863620	0.630783	-1.943335
H	-2.592024	-0.620754	-2.039272
H	-4.205653	-0.296494	1.455388
H	-3.478110	-1.907271	1.170492
H	-1.898157	0.289063	1.725676
H	-0.773773	-1.841122	1.306211
H	-1.315811	-1.872377	-0.387460

IN7

Rh	1.021443	-0.133054	-0.082860
Cl	0.621789	-1.331937	1.987355
O	3.107500	-2.175901	-1.045110
O	-1.496417	-1.889291	-0.992283
O	-2.340018	0.920473	0.101445
C	2.316410	-1.432598	-0.727571
C	-0.655368	-1.184801	-0.735810
C	2.664931	0.936403	0.617913

C	2.669523	2.004336	-0.493418
C	1.451660	1.626747	-1.345198
C	0.136209	1.750244	-0.831554
C	-0.115700	1.640327	0.562121
C	-1.520697	1.467227	1.091668
C	-3.623603	0.574838	0.547483
C	-4.464239	0.161757	-0.630130
C	-5.169248	-0.971276	-0.689579
H	3.598695	0.356339	0.650189
H	2.465392	1.310360	1.632366
H	3.579310	1.947673	-1.111608
H	2.590319	3.043381	-0.124600
H	1.555868	1.559353	-2.433897
H	-0.710097	1.602205	-1.512002
H	0.571315	2.100427	1.278674
H	-1.472482	0.804140	1.980316
H	-1.926502	2.448356	1.425582
H	-3.573662	-0.240607	1.298043
H	-4.091659	1.452977	1.045010
H	-4.487859	0.875229	-1.464042
H	-5.791799	-1.210674	-1.557173
H	-5.149993	-1.700241	0.128818

IN8

Rh	0.702742	-0.281580	-0.180087
Cl	-0.503078	-1.761956	1.232364
O	2.128224	-2.625876	-1.594294
O	2.940427	-0.682505	1.429453
O	-2.487713	0.867531	0.091371
C	1.615192	-1.762296	-1.078495
C	2.398352	0.141895	0.769886
C	2.918328	1.573971	0.575007
C	2.600278	2.038197	-0.850403
C	1.272998	1.481375	-1.359557
C	-0.008583	1.666855	-0.748630
C	-0.272747	1.538256	0.633886
C	-1.695991	1.366696	1.122459
C	-3.636987	0.186907	0.524282
C	-4.381563	-0.336050	-0.673327
C	-5.682902	-0.135127	-0.899071
H	3.996062	1.577774	0.804540
H	2.424581	2.201915	1.335956
H	3.392720	1.676084	-1.526205
H	2.607560	3.141006	-0.918789
H	1.224797	1.402423	-2.452643
H	-0.883801	1.515539	-1.394811
H	0.416853	1.920725	1.391375
H	-1.674526	0.664002	1.978091
H	-2.094002	2.339070	1.489646
H	-3.328379	-0.661786	1.170453
H	-4.292899	0.855223	1.120387
H	-3.784661	-0.941368	-1.367465
H	-6.186330	-0.571630	-1.767261
H	-6.294798	0.468072	-0.218013

IN9

Rh	-0.189622	-0.562001	0.154049
Cl	-0.889645	-0.555445	-2.174653
O	1.406788	-2.988078	-0.921232
O	0.766218	-0.702010	3.026339
O	-2.374495	2.267608	0.133856
C	0.843416	-2.102523	-0.493887
C	0.419198	-0.658562	1.947485
C	3.661570	1.902880	-0.403713
C	3.640504	0.380250	-0.302894
C	2.493526	1.188826	0.302437
C	1.152477	1.196957	-0.359328
C	-0.001737	1.714770	0.247147
C	-1.133489	2.397305	-0.499053
C	-2.954306	0.996842	0.046873
C	-2.267825	-0.029736	0.927741
C	-2.203292	-1.403305	0.651848
H	4.371206	2.459421	0.216780
H	3.457657	2.355574	-1.379926
H	4.347078	-0.106050	0.377281
H	3.422283	-0.187706	-1.214449
H	2.472385	1.275628	1.396141
H	1.167572	1.142576	-1.456199
H	0.072419	2.018767	1.301283
H	-0.921148	3.481190	-0.512886
H	-1.170474	2.035406	-1.542732
H	-3.990835	1.117098	0.408674

H	-2.986743	0.636547	-0.997522
H	-2.166820	0.293948	1.972721
H	-2.125985	-2.125594	1.470026
H	-2.579974	-1.786591	-0.301942

IN10

Rh	0.542266	-0.859226	0.328858
Cl	-0.722872	-2.068711	-1.247545
O	2.804750	-1.303623	-1.898133
O	2.050902	0.253218	2.716080
O	-3.638346	0.884747	-0.545724
C	2.058606	-1.096466	-1.079910
C	1.510175	-0.130626	1.797115
C	1.228431	3.299292	-0.936419
C	2.350262	2.290265	-0.698850
C	1.015253	2.118709	0.028638
C	0.043968	1.031383	-0.356331
C	-1.415558	1.344542	0.048191
C	-2.419469	1.230951	-1.132429
C	-3.328171	-0.103244	0.397883
C	-2.042061	0.391344	1.116502
C	-1.106755	-0.747174	1.585698
H	1.326861	4.301545	-0.507575
H	0.708369	3.265008	-1.899851
H	3.223606	2.608485	-0.120294
H	2.579362	1.598429	-1.517404
H	1.003914	2.394635	1.090988
H	0.104078	0.868905	-1.447536
H	-1.445308	2.379730	0.427963
H	-2.546718	2.172387	-1.690108
H	-2.079918	0.437960	-1.830619
H	-4.185659	-0.224279	1.078104
H	-3.120795	-1.069481	-0.102650
H	-2.343845	0.999275	1.985165
H	-0.843030	-0.617579	2.648534
H	-1.600601	-1.730363	1.496623

(*Z*)-**IN11**

Rh	1.272416	-0.122689	-0.057442
Cl	3.292013	0.304358	1.061383
O	2.086913	-2.949284	-0.607489
C	1.782192	-1.875089	-0.392305
C	0.607719	2.238919	0.352618
C	-0.573106	2.820299	-0.395967
C	0.171197	1.779523	-1.180567
C	-0.184227	0.357081	-1.440510
C	-0.793558	-0.524356	-0.504775
C	-1.732973	-0.239242	0.657074
C	-3.251895	-0.401379	0.337564
C	-4.027022	-0.185162	1.652267
C	-3.552956	-1.816710	-0.193900
C	-3.705898	0.643973	-0.697997
H	1.533704	2.813692	0.430761
H	0.373044	1.636949	1.243284
H	-0.474867	3.851948	-0.747520
H	-1.572767	2.568402	-0.033682
H	0.871219	2.181718	-1.919868
H	0.011732	0.006204	-2.459310
H	-0.943436	-1.532546	-0.911382
H	-1.484175	-0.948903	1.467873
H	-1.578728	0.767107	1.076251
H	-3.751686	-0.943688	2.405383
H	-5.115156	-0.255468	1.481730
H	-3.815407	0.810313	2.080554
H	-3.113317	-1.984899	-1.191064
H	-4.642439	-1.966561	-0.285415
H	-3.162523	-2.591158	0.489872
H	-3.599702	1.669708	-0.302580
H	-4.769848	0.499281	-0.953840
H	-3.120720	0.571946	-1.630784

(*E*)-**IN11**

Rh	-1.238201	-0.208422	-0.002180
Cl	-3.497026	-0.635851	-0.477416
O	-0.749999	-3.110345	0.547682
C	-0.936008	-2.009504	0.332490
C	-1.590954	2.200819	-0.434549
C	-0.526143	3.180332	0.008915
C	-0.675206	2.007609	0.932999
C	0.238499	0.832663	0.992769
C	0.838475	0.323305	-0.185806
C	1.925002	-0.733630	-0.140524

C	3.387783	-0.201105	-0.169138
C	4.328006	-1.421862	-0.127756
C	3.663213	0.693330	1.053919
C	3.653745	0.593874	-1.462462
H	-2.645276	2.435422	-0.269563
H	-1.388436	1.655984	-1.371490
H	-0.865558	4.152549	0.378806
H	0.387128	3.224144	-0.594006
H	-1.261703	2.181194	1.840243
H	0.530861	0.470348	1.984386
H	0.861654	0.958708	-1.082824
H	1.797591	-1.344745	0.772097
H	1.794685	-1.417057	-0.999686
H	4.163723	-2.019123	0.785998
H	5.384774	-1.103845	-0.139536
H	4.162051	-2.080651	-0.997809
H	3.023152	1.591811	1.052453
H	4.714673	1.029257	1.058917
H	3.480719	0.145503	1.995563
H	3.420386	-0.010381	-2.356856
H	4.715720	0.888465	-1.522230
H	3.053866	1.518632	-1.506879

IN12-Me

Rh	-0.007746	1.013080	0.078417
Cl	-0.229061	1.065060	-2.355144
O	0.051419	4.051903	0.186058
O	3.954195	-1.174100	-0.989807
C	0.013145	2.922916	0.144772
C	-0.104647	0.781423	2.145863
C	-0.298780	-0.748468	2.220382
C	-0.615432	-1.096492	0.761588
C	0.373376	-1.294457	-0.184422
C	1.862938	-1.509363	0.037342
C	2.623684	-1.488787	-1.311407
C	4.033440	-0.520158	0.254596
C	2.577100	-0.316572	0.733554
C	2.022847	1.030198	0.245265
C	-2.056622	-1.093563	0.338546
C	-3.019447	-0.355361	1.062281
C	-4.359064	-0.327679	0.657306
C	-4.769280	-1.048074	-0.468994
C	-3.829315	-1.800147	-1.186950
C	-2.491214	-1.821518	-0.790403
C	2.131420	-2.851598	0.753119
H	-0.966652	1.334608	2.557122
H	0.796506	1.120529	2.681116
H	-1.110434	-1.076400	2.889448
H	0.615491	-1.261867	2.545007
H	0.039915	-1.449795	-1.216622
H	2.600704	-2.469900	-1.817385
H	2.178897	-0.736530	-1.993094
H	4.608637	-1.142103	0.967586
H	4.564490	0.442987	0.145118
H	2.509046	-0.383760	1.830879
H	2.373976	1.840306	0.905308
H	2.359798	1.245827	-0.783144
H	-2.726347	0.213544	1.946879
H	-5.082867	0.260170	1.228953
H	-5.816528	-1.029862	-0.784095
H	-4.141222	-2.377741	-2.061708
H	-1.780496	-2.429491	-1.353930
H	1.631398	-3.677019	0.219331
H	1.765819	-2.848146	1.792469
H	3.212678	-3.066203	0.764807

IN12-H

Rh	-0.147453	0.886900	0.005550
Cl	0.063860	0.663379	2.429152
O	-0.416244	3.905739	0.232920
O	-3.965083	-1.776836	0.623008
C	-0.299640	2.784283	0.150935
C	-0.034164	0.888463	-2.077677
C	0.280903	-0.605724	-2.323626
C	0.629634	-1.077354	-0.910792
C	-0.358489	-1.455580	-0.022450
C	-1.816169	-1.720193	-0.340627
C	-2.628526	-2.082122	0.919516
C	-4.061222	-0.916996	-0.486888
C	-2.619264	-0.497516	-0.853414
C	-2.179273	0.782885	-0.133766
C	2.059697	-1.002064	-0.464363

C	2.974359	-0.148392	-1.120306
C	4.304408	-0.055273	-0.694362
C	4.752415	-0.821350	0.386442
C	3.860529	-1.684552	1.038091
C	2.532087	-1.773256	0.620213
H	0.786364	1.544838	-2.415687
H	-0.956140	1.219056	-2.581733
H	1.108935	-0.791539	-3.025939
H	-0.592461	-1.160543	-2.697011
H	-0.050469	-1.697842	1.000095
H	-1.894035	-2.539106	-1.080832
H	-2.549264	-3.150720	1.183635
H	-2.263269	-1.485733	1.780929
H	-4.543232	-1.448817	-1.330444
H	-4.689729	-0.044006	-0.233639
H	-2.521922	-0.370615	-1.941595
H	-2.606231	1.665641	-0.637733
H	-2.508064	0.782919	0.919943
H	2.650213	0.459397	-1.967516
H	4.990859	0.619495	-1.213648
H	5.792403	-0.751825	0.718032
H	4.203104	-2.296081	1.877541
H	1.859616	-2.465261	1.131272

IN13

Rh	-0.777678	-0.113706	0.004163
Cl	-1.954119	0.551970	2.012370
O	-2.952754	-2.125111	-0.642689
O	3.280508	-0.852273	1.134278
C	-2.132612	-1.393013	-0.381121
C	-1.373567	1.095886	-1.531561
C	-0.246051	2.137323	-1.474251
C	0.207217	1.992690	-0.031946
C	1.245890	1.214474	0.400398
C	2.331027	0.576474	-0.450844
C	3.583336	0.309015	0.400036
C	2.276693	-1.602695	0.488699
C	1.958170	-0.876134	-0.835778
C	0.519574	-1.030949	-1.339001
H	-2.346392	1.513078	-1.223653
H	-1.470257	0.589227	-2.503239
H	-0.589172	3.163442	-1.692432
H	0.565838	1.881786	-2.172752
H	-0.401869	2.491006	0.731459
H	1.385888	1.137583	1.488134
H	2.543469	1.193344	-1.338921
H	4.462759	0.152523	-0.256295
H	3.821443	1.123016	1.104976
H	2.620512	-2.639364	0.324055
H	1.378028	-1.652104	1.142080
H	2.677592	-1.221669	-1.603438
H	0.437915	-0.608777	-2.356573
H	0.289695	-2.109163	-1.441513

IN14

Rh	1.329735	-0.071618	-0.169195
Cl	1.200663	-2.298633	0.581551
O	4.353540	-0.306300	-0.673829
O	-3.120860	-0.068623	-0.067531
C	3.239983	-0.210813	-0.500870
C	1.688107	1.105285	1.456978
C	1.258328	2.437245	0.830247
C	0.901227	2.028864	-0.606233
C	-0.263643	1.265663	-0.871551
C	-0.800330	0.390855	0.109946
C	-1.852321	-0.629884	-0.247976
C	-4.164337	-0.971691	-0.239731
C	-5.498376	-0.300803	-0.046415
C	-5.658937	0.992437	0.245337
H	2.744161	1.076667	1.760654
H	1.062298	0.730090	2.280290
H	2.076783	3.173269	0.820741
H	0.394287	2.899317	1.340489
H	1.353738	2.572871	-1.442097
H	-0.545892	1.106455	-1.921971
H	-0.841728	0.723861	1.154421
H	-1.717456	-0.966795	-1.299750
H	-1.716601	-1.523578	0.394520
H	-4.129692	-1.426409	-1.256486
H	-4.073101	-1.820574	0.475336
H	-6.369475	-0.958402	-0.162159
H	-6.656336	1.422809	0.374957

H	-4.789977	1.646433	0.360963

TS1

Rh	1.030820	0.255103	-0.038138
Cl	2.204742	2.297894	-0.222543
O	-1.451715	2.098632	0.277131
O	-2.220804	-0.897165	-0.153969
C	-0.597404	1.371785	0.135496
C	2.898462	-0.776698	-0.282944
C	2.836857	-2.136865	0.401963
C	1.714414	-1.533553	1.181984
C	0.335949	-1.529515	0.783363
C	0.036453	-1.526661	-0.615985
C	-1.397021	-1.501191	-1.100435
C	-3.547615	-0.725158	-0.572092
C	-4.365661	-0.188349	0.570673
C	-5.151797	0.888275	0.488652
H	3.679847	-0.106104	0.090144
H	2.844109	-0.798969	-1.385238
H	3.714749	-2.416555	0.998666
H	2.530423	-2.969539	-0.245541
H	1.934876	-1.174858	2.194830
H	-0.451541	-1.383574	1.526880
H	0.702755	-2.053808	-1.311719
H	-1.443863	-0.961697	-2.071141
H	-1.739509	-2.542460	-1.298104
H	-3.600720	-0.038295	-1.442629
H	-3.963224	-1.703969	-0.899746
H	-4.296600	-0.756763	1.506946
H	-5.751067	1.222999	1.340818
H	-5.223442	1.475623	-0.434078

TS2

Rh	0.772782	-0.077112	-0.014304
Cl	-0.031241	-1.924697	-1.422304
O	3.417339	-1.361967	0.476330
O	-3.545284	-0.211505	0.413699
C	2.411739	-0.869165	0.288494
C	1.338263	1.667376	0.993508
C	0.891892	2.799384	0.032182
C	0.432221	2.115438	-1.246712
C	-0.607529	1.229039	-1.270643
C	-1.524947	0.942214	-0.085150
C	-2.865579	0.389481	-0.637937
C	-2.594933	-0.998180	1.062852
C	-1.361959	-0.105147	1.290368
C	-0.097967	-0.871148	1.601405
H	2.423249	1.720118	1.172248
H	0.839348	1.731053	1.976113
H	1.706857	3.505536	-0.189994
H	0.060403	3.397059	0.449680
H	0.959799	2.308639	-2.188849
H	-0.853016	0.720585	-2.208432
H	-1.675526	1.899998	0.432460
H	-3.486869	1.196483	-1.056582
H	-2.629297	-0.348051	-1.431048
H	-3.013035	-1.350571	2.018287
H	-2.295906	-1.866217	0.442041
H	-1.562603	0.625189	2.086131
H	0.371494	-0.599236	2.555893
H	-0.192633	-1.958676	1.474449

TS3

Rh	-0.731402	0.192250	0.043346
Cl	-2.251635	0.346030	-1.876342
O	-0.549265	3.215843	-0.124388
O	-2.903037	-0.080354	2.035616
O	3.706482	0.806587	-0.468415
C	-0.560220	2.085691	-0.075595
C	-2.068845	-0.216029	1.245221
C	-1.660022	-1.865579	0.586328
C	-0.368551	-2.525569	-0.010622
C	0.236363	-1.722794	-1.154269
C	1.410381	-1.040251	-1.097988
C	2.410093	-1.065632	0.042748
C	3.793852	-0.594294	-0.433242
C	2.739788	1.267184	0.449257
C	2.128615	0.015646	1.120888
C	0.672731	0.121224	1.601410
H	-2.522137	-2.002555	-0.083488
H	-1.854594	-2.335442	1.561034
H	-0.652017	-3.534400	-0.361514

H	0.369403	-2.654181	0.794546
H	-0.351219	-1.671477	-2.077751
H	1.701337	-0.465298	-1.987810
H	2.450573	-2.071114	0.492764
H	4.575462	-0.934156	0.276248
H	4.062013	-0.957166	-1.439202
H	3.203861	1.940883	1.192237
H	1.981536	1.852790	-0.103475
H	2.765223	-0.230994	1.993028
H	0.447432	-0.758687	2.231328
H	0.575488	0.993856	2.271975

TS4

Rh	-0.789961	-0.211513	0.036418
Cl	-2.439724	-1.155325	1.400901
O	-2.625392	-1.189956	-2.319274
O	-1.084411	1.841210	-1.840404
O	3.062707	-1.646780	-0.810055
C	-1.946408	-0.831346	-1.495658
C	-0.398230	1.589743	-0.872659
C	-0.058190	2.707781	0.132301
C	0.484680	2.242006	1.494524
C	0.021532	0.834685	1.843591
C	0.762734	-0.311492	1.608116
C	2.131875	-0.333074	0.953327
C	2.572270	-1.761308	0.503078
C	3.377136	-0.306602	-1.059873
C	2.255522	0.486763	-0.357493
C	0.971962	0.443958	-1.202967
H	-1.017980	3.237604	0.250059
H	0.627633	3.414811	-0.369075
H	0.127444	2.927278	2.279613
H	1.583550	2.290483	1.521107
H	-0.845592	0.739906	2.506074
H	0.456036	-1.224440	2.134417
H	2.864826	0.055616	1.685473
H	3.351516	-2.163146	1.178286
H	1.726419	-2.470348	0.497955
H	4.365716	-0.033113	-0.633491
H	3.413348	-0.149794	-2.149705
H	2.567462	1.526027	-0.177265
H	1.118095	1.000821	-2.139194
H	0.812544	-0.595571	-1.558229

TS5

Rh	0.875692	0.015793	-0.023762
Cl	2.311932	-1.799619	-0.554984
O	3.097362	1.716917	-1.375660
O	-3.777163	-0.070487	-1.184064
C	2.265418	1.123593	-0.892122
C	0.299950	-0.725465	1.931753
C	-0.112255	0.662631	2.444013
C	0.140294	1.556729	1.239209
C	-0.704650	1.517528	0.114070
C	-2.087691	0.880886	0.093934
C	-2.748894	0.865933	-1.297676
C	-3.304496	-1.159862	-0.434129
C	-2.138689	-0.626114	0.462027
C	-0.803021	-1.277166	0.117895
H	1.348291	-0.992725	2.133467
H	-0.338728	-1.544980	2.276607
H	0.511458	0.960595	3.302693
H	-1.166113	0.698968	2.766412
H	0.856795	2.379546	1.338662
H	-0.567303	2.315744	-0.628214
H	-2.751317	1.448504	0.773378
H	-3.184088	1.834985	-1.589199
H	-2.004195	0.571259	-2.070114
H	-4.142751	-1.563168	0.156496
H	-2.937590	-1.966021	-1.101029
H	-2.382473	-0.776794	1.524462
H	-0.703268	-2.329386	0.411509
H	-0.645095	-1.237285	-0.987178

TS6

Rh	1.027560	-0.187600	-0.093929
Cl	0.632804	-1.473291	1.914039
O	3.869828	-1.044637	-0.538390
O	-0.408528	-2.263123	-1.779603
O	-2.637858	0.625814	0.205230
C	2.880294	-0.503037	-0.256337
C	0.122594	-1.474408	-1.166544

C	2.821990	1.107679	0.523115
C	2.311841	2.156443	-0.509264
C	1.119247	1.557662	-1.281918
C	-0.231076	1.593624	-0.751028
C	-0.485678	1.545307	0.611074
C	-1.830534	1.189221	1.188154
C	-3.891645	0.209882	0.673537
C	-4.639815	-0.469876	-0.441016
C	-5.889650	-0.165644	-0.801389
H	3.910342	1.136672	0.660567
H	2.388844	1.187918	1.534964
H	3.117563	2.384101	-1.224001
H	2.044505	3.101379	-0.004506
H	1.201321	1.546494	-2.373877
H	-1.057438	1.347233	-1.426963
H	0.230220	1.963412	1.328963
H	-1.659355	0.476118	2.023739
H	-2.308337	2.098151	1.619587
H	-3.756003	-0.500748	1.517934
H	-4.475717	1.072240	1.058875
H	-4.096032	-1.276276	-0.949245
H	-6.403565	-0.714421	-1.596567
H	-6.447189	0.640136	-0.309539

TS7

Rh	0.187766	-0.833221	0.109200
Cl	-0.920706	-1.132131	-2.026552
O	2.598217	-1.666192	-1.528484
O	1.514247	-1.159113	2.836594
O	-3.180289	1.725488	0.005299
C	1.723642	-1.288104	-0.912178
C	1.009835	-1.040785	1.827333
C	2.179353	3.180676	-0.194485
C	2.995628	1.897034	-0.337191
C	1.656876	1.856179	0.394783
C	0.470371	1.193278	-0.246053
C	-0.865807	1.402363	0.379833
C	-1.933168	2.010723	-0.543603
C	-3.169638	0.362331	0.286900
C	-1.877497	0.017945	1.050120
C	-1.576364	-1.466116	1.066847
H	2.531566	3.950159	0.499888
H	1.677563	3.567756	-1.087800
H	3.913782	1.796189	0.250281
H	3.039029	1.433035	-1.329433
H	1.698671	1.774957	1.488661
H	0.463676	1.301935	-1.341012
H	-0.770531	1.979530	1.309621
H	-1.818080	3.104400	-0.607735
H	-1.827092	1.568352	-1.553809
H	-4.044963	0.121675	0.910660
H	-3.198376	-0.241249	-0.640346
H	-1.907377	0.395866	2.079594
H	-1.541789	-1.904175	2.069596
H	-2.150342	-2.061859	0.348109

(*Z*)-**TS8**

Rh	-1.222164	0.013354	-0.056347
Cl	-3.212540	-0.339200	1.169388
O	-2.376576	2.843083	-0.580946
C	-1.919793	1.827692	-0.378213
C	-0.693284	-2.018156	0.394244
C	0.304158	-2.522037	-0.643908
C	-0.166236	-1.390206	-1.501630
C	0.292066	-0.036528	-1.505287
C	0.795725	0.624139	-0.329184
C	1.784105	0.146393	0.723041
C	3.289538	0.333310	0.357930
C	4.115376	-0.010679	1.613311
C	3.585805	1.788027	-0.055435
C	3.687741	-0.618512	-0.785547
H	-1.635380	-2.576229	0.428554
H	-0.284370	-1.831584	1.400500
H	0.090424	-3.514022	-1.063981
H	1.360362	-2.453863	-0.356963
H	-0.878343	-1.640723	-2.298479
H	0.033097	0.565076	-2.382665
H	0.886028	1.707532	-0.482665
H	1.582145	0.733305	1.638301
H	1.628579	-0.906605	0.996680
H	3.887336	0.682915	2.441155
H	5.196556	0.056367	1.401839

H	3.901258	-1.036299	1.961434
H	3.113036	2.046722	-1.017685
H	4.672866	1.938873	-0.171801
H	3.227073	2.501356	0.707879
H	3.566197	-1.674181	-0.484236
H	4.746707	-0.472683	-1.061017
H	3.078409	-0.445817	-1.689182

(*E*)-**TS8**

Rh	-1.205837	-0.085129	-0.002397
Cl	-3.363534	-0.746070	-0.700454
O	-0.855243	-3.052317	0.818827
C	-0.936662	-1.971980	0.490305
C	-1.686268	1.914157	-0.609977
C	-0.872534	2.905063	0.212792
C	-0.724379	1.779593	1.186094
C	0.309726	0.785382	1.142672
C	0.866344	0.424027	-0.122787
C	1.920987	-0.657679	-0.241725
C	3.400349	-0.171514	-0.233226
C	4.299876	-1.416609	-0.361459
C	3.722605	0.554334	1.086396
C	3.673190	0.769535	-1.422960
H	-2.772691	2.017945	-0.517832
H	-1.357534	1.782361	-1.655666
H	-1.419851	3.775555	0.597377
H	0.074814	3.219519	-0.245677
H	-1.368165	1.785118	2.073998
H	0.548878	0.224721	2.052302
H	0.913462	1.192519	-0.905320
H	1.792295	-1.383219	0.583206
H	1.750024	-1.215239	-1.181348
H	4.131834	-2.116641	0.475479
H	5.366185	-1.132146	-0.356288
H	4.097506	-1.957543	-1.302194
H	3.112895	1.465637	1.208232
H	4.784434	0.854511	1.114017
H	3.536256	-0.101001	1.955931
H	3.407227	0.288179	-2.380540
H	4.743540	1.035418	-1.465197
H	3.104185	1.710972	-1.342266

cis-**TS9-H**

Rh	2.494515	0.357111	-0.025731
Cl	0.880028	2.138343	0.483929
S	-3.098893	-1.518036	-0.447945
O	4.565027	2.254919	-1.025152
O	-3.439064	-2.442558	0.611947
O	-3.443908	-1.757278	-1.832091
N	-1.457404	-1.367546	-0.408544
C	3.780232	1.530019	-0.641407
C	-3.749767	0.102219	0.009389
C	-3.964535	1.057891	-0.991698
C	-4.420691	2.329203	-0.624587
C	-4.661405	2.627737	0.723448
C	-4.456625	1.655822	1.712098
C	-3.999929	0.380548	1.359012
C	3.782687	-1.280727	-0.226350
C	3.649159	-2.019161	1.130227
C	2.801263	-1.122174	2.018274
C	1.521470	-0.768445	1.697364
C	0.730967	-1.338755	0.519428
C	-0.767514	-1.181843	0.850807
C	-0.756228	-0.570396	-1.396547
C	0.718408	-0.940125	-1.197479
C	1.674727	0.049460	-1.821488
H	-3.794517	0.794214	-2.039103
H	-4.594239	3.086823	-1.393976
H	-5.017129	3.623143	1.004790
H	-4.658854	1.888885	2.761362
H	-3.857027	-0.402245	2.108891
H	4.827116	-0.979224	-0.399575
H	3.478585	-1.913537	-1.078227
H	4.625469	-2.204222	1.604037
H	3.157742	-3.004021	1.023640
H	3.224995	-0.711923	2.943173
H	0.982860	-0.071695	2.346922
H	1.000589	-2.400802	0.441241
H	-1.093347	-1.932474	1.585965
H	-0.933987	-0.160866	1.252459
H	-1.092951	-0.830043	-2.410927
H	-0.888036	0.516430	-1.216266
H	0.907275	-1.947647	-1.590706

H	2.354767	-0.387375	-2.564309
H	1.191402	0.967854	-2.181903

trans-**TS9-H**

Rh	-2.392851	0.214347	-0.106081
Cl	-3.396405	-1.866316	0.766481
S	3.159422	-1.576425	0.006983
O	-5.085263	0.999427	-1.190572
O	3.551370	-2.190116	-1.242399
O	3.573433	-2.073275	1.299926
N	1.515702	-1.579065	0.010555
C	-4.071000	0.716247	-0.770431
C	3.646294	0.163725	-0.079425
C	3.859035	0.875804	1.108759
C	4.189819	2.234364	1.034259
C	4.312827	2.861559	-0.213465
C	4.118906	2.131697	-1.394341
C	3.788258	0.772349	-1.334136
C	-1.571324	2.058457	-0.615135
C	-1.375717	2.659039	0.799588
C	-1.764407	1.565223	1.795334
C	-1.201876	0.306205	1.787335
C	-0.241039	-0.150279	0.742386
C	0.765633	-1.200470	1.203291
C	0.785982	-1.298492	-1.220955
C	-0.677115	-1.222189	-0.819915
C	-1.692081	-0.736345	-1.772713
H	3.797768	0.357850	2.069923
H	4.366554	2.801009	1.953051
H	4.576512	3.921933	-0.266126
H	4.238591	2.618457	-2.366529
H	3.670292	0.174140	-2.241905
H	-2.229231	2.689646	-1.231754
H	-0.623837	1.938634	-1.168523
H	-2.032057	3.528598	0.958598
H	-0.343571	3.005170	0.998154
H	-2.461899	1.796873	2.608838
H	-1.520022	-0.429625	2.534184
H	0.299927	0.689837	0.286938
H	1.436297	-0.767165	1.962559
H	0.260939	-2.070423	1.659692
H	1.117401	-0.358712	-1.708584
H	0.915930	-2.123149	-1.939507
H	-1.010130	-2.140747	-0.319272
H	-2.410524	-1.502235	-2.087674
H	-1.341918	-0.081727	-2.582436

cis-**TS9-Me**

Rh	2.473751	0.378595	-0.120304
Cl	0.890160	2.161707	0.510661
S	-3.127497	-1.522252	-0.500994
O	4.435059	2.426181	-1.038983
O	-3.445326	-2.437417	0.573908
O	-3.481174	-1.785013	-1.878752
N	-1.488064	-1.347904	-0.479571
C	3.694354	1.642185	-0.685635
C	-3.800236	0.093895	-0.060285
C	-4.042307	1.030666	-1.072989
C	-4.518306	2.298767	-0.720011
C	-4.751557	2.612688	0.625854
C	-4.519228	1.659363	1.626504
C	-4.042528	0.387623	1.287470
C	3.806382	-1.165206	-0.583965
C	3.566206	-2.190971	0.541797
C	2.897755	-1.412538	1.658437
C	1.609230	-0.945445	1.601655
C	0.696350	-1.328992	0.411540
C	-0.787448	-1.126793	0.769131
C	-0.813911	-0.540649	-1.475982
C	0.676995	-0.862050	-1.297295
C	1.569128	0.205977	-1.888463
C	1.005242	-0.272841	2.820979
H	-3.878358	0.754197	-2.118081
H	-4.713772	3.041451	-1.498678
H	-5.123354	3.605276	0.896159
H	-4.715887	1.904061	2.674175
H	-3.878279	-0.381491	2.047049
H	4.848207	-0.808154	-0.550086
H	3.630255	-1.583763	-1.589591
H	4.493743	-2.665138	0.900957
H	2.899106	-3.006623	0.209185
H	3.470363	-1.199571	2.569660

H	0.869622	-2.401132	0.250049
H	-1.117516	-1.854338	1.524916
H	-0.949271	-0.095430	1.136874
H	-1.155115	-0.804815	-2.487636
H	-0.971078	0.542642	-1.291787
H	0.914227	-1.837446	-1.741099
H	2.219482	-0.149073	-2.698165
H	1.042267	1.133655	-2.148721
H	1.788862	-0.100206	3.574148
H	0.240149	-0.926533	3.273988
H	0.546023	0.693925	2.570192

trans-**TS9-Me**

Rh	-2.187083	0.238883	-0.225605
Cl	-3.483628	-1.784409	0.376430
S	3.265057	-1.487397	-0.189770
O	-4.756447	1.354333	-1.315950
O	3.734518	-1.901708	-1.492715
O	3.776707	-2.031838	1.047458
N	1.637078	-1.762498	-0.192040
C	-3.787115	0.945964	-0.892546
C	3.436876	0.312012	-0.098530
C	3.477052	0.933125	1.157455
C	3.516296	2.331284	1.221480
C	3.524752	3.090004	0.042036
C	3.511293	2.455034	-1.207397
C	3.471213	1.057060	-1.285159
C	-1.169964	2.003589	-0.633025
C	-0.926787	2.497073	0.810679
C	-1.455216	1.411909	1.750331
C	-1.021838	0.097319	1.739382
C	-0.098595	-0.366612	0.648813
C	0.862597	-1.497517	1.016247
C	0.878059	-1.425934	-1.396072
C	-0.578376	-1.298111	-0.978186
C	-1.539143	-0.689951	-1.921104
C	-1.418343	-0.876173	2.825517
H	3.508620	0.322441	2.064082
H	3.555904	2.829159	2.194646
H	3.558988	4.181961	0.097449
H	3.543175	3.048930	-2.125304
H	3.494204	0.539150	-2.247946
H	-1.751279	2.731828	-1.219303
H	-0.234372	1.811286	-1.187364
H	-1.474227	3.430690	1.013289
H	0.138921	2.701916	1.032776
H	-2.120921	1.703407	2.571916
H	0.496540	0.466526	0.253030
H	1.528548	-1.186173	1.836287
H	0.330430	-2.403904	1.349189
H	1.227073	-0.483960	-1.862892
H	0.964130	-2.228061	-2.146348
H	-0.976870	-2.224988	-0.545180
H	-2.311309	-1.378987	-2.281946
H	-1.120516	-0.030781	-2.693752
H	-2.191807	-0.437339	3.473268
H	-0.537451	-1.112112	3.449075
H	-1.822647	-1.806697	2.398683

cis-**TS10**

Rh	-2.400720	0.458246	-0.112692
Cl	-4.033138	-1.272725	-0.709340
S	3.190093	-1.536742	-0.347790
O	-4.233323	2.583686	-1.109928
O	3.569298	-1.950628	-1.680059
O	3.500534	-2.312120	0.832751
N	1.549858	-1.370980	-0.368004
C	-3.535775	1.776783	-0.722430
C	3.837731	0.130653	-0.089763
C	4.040159	0.589315	1.218495
C	4.500923	1.897144	1.412933
C	4.757583	2.723524	0.310148
C	4.564770	2.245556	-0.993324
C	4.104882	0.939532	-1.201840
C	-0.984337	1.844374	0.522270
C	-0.917657	1.565225	2.036037
C	-1.649672	0.259418	2.322389
C	-1.594523	-0.922299	1.629979
C	-0.644365	-1.263492	0.452748
C	0.827694	-1.051046	0.848157
C	0.893314	-0.695874	-1.470980
C	-0.620335	-0.884461	-1.241370

C	-1.451848	0.226084	-1.852662
C	-2.378630	-2.119163	2.131815
H	3.863341	-0.084324	2.061625
H	4.671197	2.267702	2.427864
H	5.121072	3.743254	0.467374
H	4.783484	2.887549	-1.851414
H	3.976383	0.534597	-2.209492
H	-1.240640	2.896045	0.320339
H	-0.021120	1.652043	0.019423
H	-1.440313	2.359200	2.593100
H	0.109691	1.537002	2.449122
H	-2.307393	0.249479	3.201233
H	-0.783796	-2.343973	0.333543
H	1.014475	-0.009534	1.174996
H	1.117786	-1.737541	1.657064
H	1.136777	0.387537	-1.480108
H	1.204345	-1.134343	-2.430575
H	-0.962012	-1.843032	-1.650149
H	-2.141089	-0.126917	-2.629739
H	-0.876124	1.106228	-2.172661
H	-3.037822	-1.841856	2.967926
H	-1.677651	-2.897949	2.482446
H	-2.996917	-2.536302	1.320934

trans-**TS10**

Rh	2.391757	0.135149	-0.168522
Cl	1.527417	2.401799	-0.694813
S	-3.106910	-1.550153	-0.381686
O	5.082740	1.196854	-1.076355
O	-3.478287	-2.357699	0.759813
O	-3.455811	-1.900013	-1.741489
N	-1.468803	-1.436460	-0.352807
C	4.088239	0.796056	-0.711272
C	-3.717589	0.122461	-0.078261
C	-3.826823	1.014371	-1.153941
C	-4.247344	2.325741	-0.904496
C	-4.563363	2.727084	0.401028
C	-4.471321	1.817616	1.463184
C	-4.048613	0.503350	1.228560
C	3.231981	-1.712719	0.318945
C	2.598916	-2.017396	1.687064
C	2.241273	-0.664411	2.280883
C	1.210140	0.129956	1.845080
C	0.330495	-0.242411	0.675305
C	-0.749942	-1.294724	0.909215
C	-0.739527	-0.922739	-1.504284
C	0.725244	-1.108202	-1.178241
C	1.771692	-0.522424	-2.004771
C	0.878043	1.438288	2.534043
H	-3.607865	0.671795	-2.169045
H	-4.336277	3.033720	-1.733278
H	-4.893535	3.752738	0.589557
H	-4.739063	2.128856	2.477013
H	-4.000441	-0.233536	2.034983
H	4.325485	-1.627420	0.425730
H	3.034610	-2.497728	-0.431948
H	3.266016	-2.573321	2.366739
H	1.684502	-2.622873	1.573031
H	2.840502	-0.285831	3.118666
H	-0.161518	0.674659	0.322128
H	-0.357738	-2.264115	1.260479
H	-1.425039	-0.915391	1.696137
H	-0.981157	-1.528292	-2.392356
H	-0.960007	0.140083	-1.731033
H	0.927492	-2.134804	-0.847942
H	2.491211	-1.226709	-2.438281
H	1.480888	0.306631	-2.661488
H	1.619730	1.672882	3.313404
H	-0.114470	1.359615	3.012584
H	0.845545	2.261899	1.802854

cis-**TS11**

Rh	-1.700491	-1.287098	0.425355
Cl	-0.226270	-0.315506	2.187254
S	3.220696	0.366986	-1.532167
O	-3.762942	-1.387628	2.618043
O	2.497867	1.466803	-2.142031
O	4.341938	-0.229757	-2.235808
N	2.065505	-0.778038	-1.167250
C	-2.993360	-1.340421	1.787088
C	3.804327	0.833980	0.108227
C	5.182293	1.017812	0.273019

C	5.657591	1.451147	1.516641	H	-1.971878	4.305123	1.680416
C	4.761985	1.680295	2.570212	H	-3.693838	5.544131	0.355647
C	3.386655	1.477702	2.388115	H	-4.771106	4.439919	-1.611016
C	2.894023	1.059340	1.146975	H	-4.132669	2.133042	-2.250224
C	-3.124856	-1.782803	-1.000060				
C	-3.286784	-0.420075	-1.713671			*trans*-**TS11**	
C	-2.259429	0.535450	-1.083564	Rh	1.473834	-1.292316	0.546927
C	-0.917410	0.179407	-1.042198	Cl	2.285262	-2.417441	-1.502924
C	-0.380151	-1.136069	-1.502534	S	-3.844333	0.340692	-1.379944
C	1.010177	-0.980197	-2.136585	O	3.994237	-2.034522	2.009351
C	2.513647	-2.029491	-0.578162	O	-5.140980	-0.291357	-1.269885
C	1.383853	-2.628549	0.261066	O	-3.510502	1.247801	-2.456420
C	0.003072	-2.761265	-0.389974	N	-2.732897	-0.878550	-1.420961
C	-1.043388	-3.208354	0.559208	C	3.047258	-1.741820	1.457864
C	-2.670753	1.905293	-0.658749	C	-3.562576	1.243426	0.165081
C	-2.069567	2.535386	0.450473	C	-2.759510	2.389693	0.152367
C	-2.438878	3.834720	0.810290	C	-2.511292	3.055565	1.360066
C	-3.407741	4.527294	0.071317	C	-3.061881	2.574980	2.555927
C	-4.014377	3.907317	-1.027609	C	-3.878754	1.435089	2.549695
C	-3.656126	2.602414	-1.384716	C	-4.140581	0.765508	1.348648
H	5.858049	0.813124	-0.561513	C	0.800761	-0.136623	2.137255
H	6.730841	1.602000	1.663772	C	0.979149	1.282330	1.546254
H	5.139742	2.009948	3.542669	C	1.498360	1.088682	0.113978
H	2.685202	1.633143	3.212580	C	0.778776	0.312376	-0.784875
H	1.824428	0.868387	1.017606	C	-0.462560	-0.461219	-0.463005
H	-4.078180	-2.119156	-0.564639	C	-1.348797	-0.574407	-1.725329
H	-2.773930	-2.587857	-1.667713	C	-2.987618	-2.136178	-0.733815
H	-4.295545	-0.015361	-1.546748	C	-2.067914	-2.349189	0.474808
H	-3.139819	-0.468549	-2.809166	C	-0.586392	-2.359021	0.085325
H	-0.178405	0.899029	-0.672168	C	0.367335	-2.905749	1.075195
H	-1.041091	-1.606986	-2.238190	C	2.701380	1.830672	-0.365907
H	1.226306	-1.879227	-2.747336	C	3.583340	1.257341	-1.306719
H	0.970343	-0.115056	-2.815034	C	4.683574	1.981625	-1.774608
H	2.846645	-2.724255	-1.376341	C	4.922504	3.285030	-1.316733
H	3.380075	-1.841062	0.075197	C	4.057263	3.858497	-0.377479
H	1.680193	-3.651353	0.556914	C	2.960023	3.133445	0.101676
H	1.269320	-2.034565	1.181824	H	-2.357087	2.760029	-0.794448
H	0.000218	-3.315933	-1.339046	H	-1.895954	3.959984	1.363554
H	-1.766347	-3.941642	0.181618	H	-2.866069	3.099224	3.495811
H	-0.675854	-3.433195	1.568558	H	-4.325986	1.075508	3.480870
H	-1.337411	1.986511	1.052963	H	-4.805094	-0.102709	1.317643

H	1.380571	-0.260878	3.064242
H	-0.251325	-0.373825	2.373058
H	1.718878	1.858110	2.121448
H	0.043419	1.872323	1.534190
H	1.139560	0.233234	-1.815853
H	-1.022480	-0.002535	0.360873
H	-1.326623	0.380289	-2.270980
H	-0.938860	-1.340298	-2.408621
H	-4.048383	-2.174099	-0.449251
H	-2.820531	-2.957518	-1.456005
H	-2.264443	-1.609080	1.271443
H	-2.296415	-3.341300	0.901898
H	-0.404392	-2.793313	-0.906614
H	0.875110	-3.821360	0.748828
H	0.022504	-2.929508	2.118241
H	3.422546	0.226457	-1.644609
H	5.364805	1.518966	-2.494642
H	5.785333	3.847799	-1.684780
H	4.236573	4.874287	-0.013114
H	2.288820	3.594041	0.832278

TS12-Me

Rh	-0.177886	1.048612	0.057209
Cl	-0.420953	3.416234	-0.009137
O	1.727705	1.631748	2.458377
O	-3.914726	-1.543751	1.112830
C	1.060022	1.388197	1.581140
C	-0.585415	0.745644	-2.034865
C	0.145248	-0.601946	-2.063945
C	0.620384	-0.805879	-0.619478
C	-0.337566	-1.077733	0.390124
C	-1.760896	-1.595705	0.188087
C	-2.573389	-1.498198	1.502500
C	-4.071579	-0.924250	-0.141324
C	-2.644253	-0.697084	-0.720388
C	-2.205962	0.757872	-0.582892
C	2.088036	-0.986174	-0.364892
C	3.032072	-0.147194	-0.993210
C	4.400541	-0.307131	-0.762067
C	4.857341	-1.316105	0.098550
C	3.932972	-2.161981	0.720609
C	2.560498	-1.999867	0.489065
C	-1.748820	-3.062458	-0.288522
H	0.051183	1.615018	-2.267324
H	-1.466769	0.789713	-2.682033
H	0.998438	-0.574910	-2.760197
H	-0.510988	-1.425568	-2.385264
H	0.077194	-1.366110	1.366301
H	-2.376801	-2.340720	2.187040
H	-2.331777	-0.555841	2.037567
H	-4.676423	-1.584428	-0.787828
H	-4.614446	0.035264	-0.039018
H	-2.608876	-1.019243	-1.772720
H	-2.723060	1.458728	-1.249121
H	-2.389978	1.114246	0.452937
H	2.685610	0.658405	-1.648924
H	5.114323	0.362605	-1.250562
H	5.928682	-1.441828	0.279635
H	4.278822	-2.959198	1.385262
H	1.848467	-2.681495	0.962649
H	-1.158214	-3.688369	0.401873
H	-1.307950	-3.159433	-1.294196
H	-2.775593	-3.464381	-0.315783

TS12-H

Rh	-0.303407	0.912042	0.098059
Cl	-0.637605	3.269805	0.111596
O	1.643984	1.515530	2.463748
O	-3.876533	-2.212438	0.859916
C	0.961385	1.263707	1.600613
C	-0.713299	0.661200	-2.002216
C	0.087513	-0.645416	-2.085566
C	0.591585	-0.864736	-0.654791
C	-0.358641	-1.235758	0.329354
C	-1.738640	-1.813666	0.039601
C	-2.563296	-2.082181	1.312825
C	-4.099750	-1.231673	-0.119260
C	-2.708181	-0.893726	-0.750599
C	-2.316203	0.564579	-0.534229
C	2.066967	-0.974071	-0.409793
C	2.962231	-0.076360	-1.028368
C	4.338417	-0.167361	-0.806071

C	4.852351	-1.163920	0.036530
C	3.977050	-2.067119	0.648888
C	2.596694	-1.975091	0.425497
H	-0.125315	1.568809	-2.213545
H	-1.605679	0.680960	-2.635525
H	0.923930	-0.552435	-2.796423
H	-0.529441	-1.497412	-2.415774
H	0.047955	-1.544950	1.301606
H	-1.624574	-2.774668	-0.496668
H	-2.276751	-3.007173	1.837916
H	-2.454125	-1.230303	2.020565
H	-4.814120	-1.633165	-0.855652
H	-4.547336	-0.322282	0.330807
H	-2.714190	-1.139729	-1.822933
H	-2.866230	1.292442	-1.143331
H	-2.485810	0.842676	0.529975
H	2.570267	0.720554	-1.668759
H	5.013181	0.546710	-1.287153
H	5.929727	-1.235523	0.211170
H	4.367956	-2.855225	1.299280
H	1.926446	-2.703066	0.890822

TS13-Me

Rh	-1.718645	-0.659367	-0.178997
Cl	-2.720751	-1.956915	1.599445
O	-0.972804	-2.422742	-2.419099
O	-4.502497	0.413942	-0.863166
O	0.734572	3.997539	-0.302589
C	-1.100095	-1.793594	-1.463762
C	-3.466811	0.070560	-0.572439
C	0.153606	-1.915677	-0.032966
C	0.724953	-1.088031	1.166744
C	1.652764	0.038419	0.742409
C	1.332252	1.347605	0.660660
C	0.017970	2.090437	0.866075
C	0.359755	3.598027	0.982641
C	-0.039641	3.297927	-1.248104
C	-0.766899	2.147060	-0.493249
C	-0.847886	0.856117	-1.319437
C	3.029597	-0.390965	0.319234
C	3.784306	-1.302732	1.085340
C	5.071901	-1.683999	0.691736
C	5.632112	-1.171543	-0.485150
C	4.893110	-0.271527	-1.262265
C	3.607405	0.112090	-0.864257
C	-0.852557	1.653984	2.057370
H	0.951625	-2.006667	-0.785996
H	-0.149672	-2.914867	0.312279
H	1.308361	-1.827026	1.742371
H	-0.060282	-0.760605	1.858034
H	2.133651	2.009384	0.307921
H	-0.533941	4.155050	1.335735
H	1.193537	3.802746	1.674243
H	-0.767063	3.973661	-1.736780
H	0.633501	2.903319	-2.030677
H	-1.790556	2.488364	-0.246062
H	-1.417385	1.053891	-2.244586
H	0.166146	0.553075	-1.629237
H	3.376123	-1.701777	2.018644
H	5.641727	-2.382469	1.311809
H	6.636160	-1.474612	-0.795786
H	5.314570	0.129268	-2.188955
H	3.032649	0.803663	-1.487280
H	-0.244190	1.521489	2.968014
H	-1.409081	0.712101	1.912834
H	-1.613300	2.426237	2.263115

TS13-H

Rh	-1.720709	-0.679127	-0.133695
Cl	-2.657728	-1.783342	1.778978
O	-0.718009	-2.271407	-2.400526
O	-4.548568	0.180485	-0.915081
O	0.200844	4.167958	0.105205
C	-0.938459	-1.701058	-1.423596
C	-3.499547	-0.086442	-0.593014
C	0.214648	-1.848922	0.095295
C	0.756758	-0.941318	1.244965
C	1.676983	0.165703	0.763930
C	1.296161	1.457780	0.687612
C	-0.069591	2.024113	0.990607
C	0.019941	3.520104	1.338746
C	-0.397323	3.428105	-0.932222

C	-0.953807	2.126031	-0.295786
C	-0.949453	0.919247	-1.235877
C	3.047866	-0.241700	0.316865
C	3.805813	-1.188040	1.036597
C	5.094338	-1.545421	0.623959
C	5.652388	-0.973734	-0.525997
C	4.909061	-0.040206	-1.258786
C	3.622231	0.318387	-0.843037
H	1.035579	-2.000616	-0.621648
H	-0.112264	-2.822300	0.489165
H	1.325328	-1.630694	1.893575
H	-0.048869	-0.559419	1.889668
H	2.030290	2.190450	0.327902
H	-0.581205	1.454890	1.783803
H	-0.911819	3.855576	1.838563
H	0.872248	3.764386	1.993027
H	-1.199615	4.014700	-1.416353
H	0.364706	3.196747	-1.700899
H	-1.987785	2.328730	0.042512
H	-1.549833	1.133591	-2.136303
H	0.078520	0.706132	-1.572217
H	3.400849	-1.635302	1.948702
H	5.666258	-2.272297	1.208381
H	6.657376	-1.257486	-0.851431
H	5.328121	0.405501	-2.165824
H	3.043222	1.032884	-1.435340

TS14-Me

Rh	0.110438	1.744072	0.052801
Cl	1.019173	1.480403	2.250376
O	2.196276	3.921047	-0.499890
O	-2.263349	2.191781	-1.702360
O	-4.179962	-1.924543	1.002603
C	1.454587	3.093658	-0.301179
C	-1.423772	1.954797	-0.950378
C	0.818918	0.777409	-1.636564
C	0.170995	-0.597383	-1.825830
C	0.383211	-1.517557	-0.635977
C	-0.624198	-2.009224	0.112712
C	-2.119585	-1.842264	-0.087900
C	-2.886500	-2.428729	1.124641
C	-4.039541	-0.561534	0.724166
C	-2.711147	-0.380793	-0.098725
C	-1.850003	0.713946	0.554859
C	1.803348	-1.848796	-0.295604
C	2.712291	-2.244746	-1.298134
C	4.030919	-2.586289	-0.978275
C	4.472081	-2.525260	0.350097
C	3.584394	-2.116525	1.352692
C	2.263835	-1.778441	1.033833
C	-2.592927	-2.601640	-1.350832
H	1.896087	0.667329	-1.421513
H	0.702734	1.391183	-2.544113
H	0.626282	-1.053619	-2.727199
H	-0.899095	-0.486833	-2.051399
H	-0.338456	-2.675823	0.937959
H	-2.926457	-3.530058	1.120759
H	-2.410544	-2.094978	2.073677
H	-4.932275	-0.217776	0.177803
H	-3.970546	0.013787	1.670124
H	-2.972736	-0.095613	-1.130406
H	-2.494440	1.485461	1.010222
H	-1.250925	0.294281	1.383016
H	2.381311	-2.312205	-2.338966
H	4.715437	-2.904899	-1.770227
H	5.504460	-2.786794	0.600119
H	3.922765	-2.044894	2.390569
H	1.589389	-1.416041	1.814862
H	-2.261042	-3.652463	-1.313296
H	-2.188881	-2.152897	-2.271852
H	-3.693838	-2.587253	-1.406980

TS14-H

Rh	0.642323	-0.874156	-0.127075
Cl	0.675662	-0.778716	2.330544
O	3.008921	-2.641866	-0.193370
O	-1.292331	-3.187809	0.049412
O	1.925776	3.224190	0.998051
C	2.306971	-1.710185	-0.190175
C	-0.581622	-2.312142	-0.030118
C	0.410372	-0.747265	-2.199677
C	-0.800018	0.209707	-2.329059

C	-1.061884	0.765159	-0.919138
C	-0.055565	1.408717	-0.238502
C	1.238270	1.955189	-0.842511
C	1.421371	3.392463	-0.299205
C	2.618482	1.995737	1.113779
C	2.565523	1.365096	-0.294672
C	2.967026	-0.144825	-0.398880
C	-2.419781	0.612042	-0.307768
C	-3.561397	0.711006	-1.127177
C	-4.846114	0.636480	-0.576352
C	-5.010501	0.442242	0.799860
C	-3.880793	0.327130	1.621565
C	-2.595561	0.414063	1.077961
H	0.236530	-1.706309	-2.709765
H	1.329994	-0.308983	-2.622549
H	-1.687727	-0.345159	-2.665417
H	-0.636847	1.026190	-3.056579
H	-0.265440	1.768143	0.776015
H	1.199733	1.929679	-1.941965
H	2.125105	3.957009	-0.944743
H	0.475942	3.956261	-0.245139
H	3.662813	2.175811	1.427249
H	2.126299	1.358551	1.868712
H	3.357424	1.861277	-0.885559
H	3.351656	-0.319756	-1.417033
H	3.809511	-0.280005	0.300188
H	-3.449493	0.870437	-2.203452
H	-5.720169	0.728412	-1.227745
H	-6.013877	0.373536	1.230083
H	-3.997691	0.159099	2.696116
H	-1.722154	0.291201	1.728396

TS15-Me

Rh	-1.575194	-0.813448	-0.058001
Cl	-2.417443	-2.941661	0.853345
O	-0.629337	-2.653530	-2.490213
O	-4.433242	-0.273846	-1.041926
O	-1.667225	0.582791	2.605905
O	-0.257934	4.532391	-0.946630
C	-0.948297	-1.967982	-1.656731
C	-3.369782	-0.476284	-0.725424
C	-1.501076	-0.007967	1.632184
C	0.140352	-1.021475	1.464273
C	1.217995	-0.004153	1.876256
C	2.010014	0.519002	0.693709
C	1.739933	1.664236	0.033513
C	0.644585	2.701018	0.226325
C	0.970428	3.937019	-0.669329
C	-1.082049	3.472966	-1.330335
C	-0.783818	2.294467	-0.353157
C	-0.914030	0.935679	-1.071427
C	3.111035	-0.370282	0.195298
C	4.022769	-0.976713	1.083813
C	5.059685	-1.788907	0.612207
C	5.203266	-2.026917	-0.760647
C	4.300886	-1.441604	-1.656729
C	3.267564	-0.624913	-1.182819
C	0.482131	3.235738	1.668948
H	0.557867	-1.714690	0.715274
H	-0.188132	-1.663156	2.296645
H	1.898994	-0.535824	2.561461
H	0.782513	0.813089	2.463617
H	2.406365	1.876618	-0.813240
H	1.625242	4.669908	-0.171068
H	1.460838	3.607219	-1.610981
H	-2.131622	3.805949	-1.303626
H	-0.840965	3.157174	-2.369193
H	-1.505732	2.360012	0.476295
H	-1.624363	1.070266	-1.906757
H	0.050196	0.679098	-1.540126
H	3.941180	-0.791968	2.158814
H	5.761636	-2.235726	1.322601
H	6.009980	-2.667580	-1.128271
H	4.395152	-1.627398	-2.730852
H	2.559017	-0.184275	-1.890712
H	1.463152	3.448113	2.125989
H	-0.073739	2.551563	2.325600
H	-0.094956	4.174998	1.625059

TS15-H

Rh	-1.758145	-0.515972	-0.105406
Cl	-2.974209	-2.465458	0.785501

O	-1.360469	-2.434374	-2.629127
O	-4.449189	0.699311	-0.936894
O	-1.525133	0.620323	2.670763
O	1.031784	4.237549	-0.667880
C	-1.476430	-1.717444	-1.769711
C	-3.450581	0.244553	-0.675340
C	-1.473176	0.132678	1.630358
C	-0.019405	-1.136564	1.295228
C	1.204079	-0.386492	1.859549
C	2.082907	0.277969	0.808797
C	1.835472	1.521869	0.348690
C	0.663657	2.391177	0.721674
C	1.034670	3.884825	0.690280
C	0.091376	3.457006	-1.363478
C	-0.448110	2.380708	-0.377897
C	-0.742704	1.055626	-1.089114
C	3.226628	-0.514391	0.255405
C	4.048280	-1.304245	1.086077
C	5.131641	-2.018655	0.562896
C	5.415003	-1.970809	-0.807735
C	4.604894	-1.198349	-1.648986
C	3.524378	-0.481607	-1.123175
H	0.301768	-1.737309	0.427886
H	-0.443867	-1.848994	2.019040
H	1.793795	-1.147014	2.396012
H	0.890258	0.339317	2.626501
H	2.515536	1.948668	-0.400442
H	0.255802	2.113274	1.702753
H	0.288603	4.475122	1.262382
H	2.033611	4.093965	1.105990
H	-0.729319	4.088512	-1.754075
H	0.591488	2.983265	-2.229853
H	-1.370486	2.769072	0.091660
H	-1.326724	1.287863	-1.998412
H	0.209284	0.620317	-1.437152
H	3.860359	-1.342521	2.162808
H	5.760554	-2.612797	1.232627
H	6.258423	-2.534162	-1.217265
H	4.808781	-1.159130	-2.723252
H	2.888805	0.104458	-1.793436

TS16-Me

Rh	0.807487	-1.473026	-0.116542
Cl	2.141712	-2.381704	1.752155
O	-1.508084	-1.871073	2.046565
O	0.695733	-4.330725	-1.223140
O	3.087049	-0.316621	-1.710595
O	2.353921	4.029921	0.956237
C	-0.751742	-1.686377	1.234279
C	0.691972	-3.281863	-0.808332
C	2.242040	-0.649317	-1.004109
C	-0.455799	-0.865727	-1.691799
C	-0.689244	0.648949	-1.802378
C	-1.345452	1.286337	-0.590558
C	-0.745363	2.256222	0.132726
C	0.608233	2.900293	-0.098661
C	0.993348	3.781055	1.117392
C	2.937740	2.798052	0.641488
C	1.876434	1.965557	-0.170341
C	1.758555	0.562523	0.456842
C	-2.719828	0.815163	-0.223935
C	-3.623325	0.365008	-1.209802
C	-4.920734	-0.039579	-0.874358
C	-5.347138	-0.016984	0.458637
C	-4.458715	0.410769	1.453598
C	-3.163961	0.816145	1.115952
C	0.570376	3.819696	-1.343767
H	-1.420273	-1.384102	-1.556549
H	-0.034751	-1.224068	-2.646590
H	-1.329392	0.839576	-2.686497
H	0.261986	1.151105	-2.021910
H	-1.326313	2.703737	0.949938
H	0.451407	4.740339	1.147029
H	0.792733	3.232159	2.065164
H	3.863677	2.978858	0.073176
H	3.203760	2.256190	1.571498
H	2.217437	1.893720	-1.214682
H	2.679206	0.271725	0.985080
H	0.968620	0.564017	1.225662
H	-3.321147	0.346832	-2.259844
H	-5.602351	-0.372468	-1.662822
H	-6.359386	-0.337339	0.721419

H	-4.770700	0.418913	2.502225
H	-2.476254	1.119604	1.910440
H	-0.261460	4.539193	-1.264201
H	0.430910	3.243113	-2.271494
H	1.512929	4.386498	-1.419078

TS16-H

Rh	0.853634	-1.316945	-0.090995
Cl	2.126065	-2.147710	1.854896
O	-1.543184	-1.714463	1.983927
O	0.849639	-4.210601	-1.104272
O	3.190443	-0.183809	-1.614613
O	2.282149	4.363861	0.441401
C	-0.759473	-1.525000	1.199351
C	0.805535	-3.148932	-0.726126
C	2.313659	-0.500117	-0.940423
C	-0.363515	-0.802945	-1.738419
C	-0.673499	0.692490	-1.918853
C	-1.342448	1.357516	-0.728911
C	-0.748429	2.382900	-0.080777
C	0.586964	2.991522	-0.437330
C	0.890976	4.274940	0.378025
C	2.725539	3.070789	0.716069
C	1.886675	2.128647	-0.198622
C	1.750782	0.752723	0.463700
C	-2.687078	0.855465	-0.305894
C	-3.564628	0.255298	-1.233675
C	-4.838282	-0.182271	-0.850381
C	-5.265881	-0.041870	0.474523
C	-4.402613	0.537920	1.413737
C	-3.132538	0.975527	1.028631
H	-1.305564	-1.365568	-1.623185
H	0.112400	-1.171797	-2.663018
H	-1.326800	0.806777	-2.806502
H	0.253823	1.228701	-2.169021
H	-1.288333	2.856167	0.748689
H	0.575725	3.267189	-1.504456
H	0.494128	5.192291	-0.083119
H	0.458647	4.180956	1.398722
H	3.807066	3.009208	0.519849
H	2.545937	2.812477	1.782568
H	2.421900	2.043296	-1.156919
H	2.650917	0.497644	1.045541
H	0.921277	0.770043	1.188501
H	-3.261560	0.142511	-2.277426
H	-5.499697	-0.634226	-1.595582
H	-6.258904	-0.387761	0.775459
H	-4.715363	0.640564	2.457099
H	-2.465072	1.397635	1.785053

TS17

Rh	0.384533	-0.194046	-0.056923
Cl	2.262220	-1.729561	0.197002
O	-0.694249	-2.386703	-1.857761
O	-3.127864	0.728557	0.149965
C	-0.340341	-1.553186	-1.172760
C	1.638729	1.518907	1.011859
C	1.687238	2.876485	0.332633
C	1.507858	1.830957	-0.704980
C	0.256323	1.389898	-1.347551
C	-0.925720	1.422887	-0.526269
C	-2.337283	1.084899	-0.955473
C	-2.757517	-0.415181	0.861313
C	-1.490410	-0.271923	1.687627
C	-0.634317	-1.283095	1.997187
H	2.585523	1.049192	1.290860
H	0.828519	1.403496	1.740880
H	2.650767	3.396227	0.337174
H	0.837828	3.539946	0.528547
H	2.422777	1.500218	-1.207293
H	0.266650	1.177322	-2.420576
H	-0.932563	2.152259	0.296268
H	-2.843389	1.962419	-1.393796
H	-2.336150	0.280971	-1.721348
H	-3.593183	-0.602541	1.559150
H	-2.678879	-1.303733	0.200509
H	-1.393617	0.691408	2.205527
H	0.148999	-1.154466	2.749093
H	-0.775487	-2.296820	1.608350

TS18

Rh	0.826067	-0.193420	-0.089439

Cl	1.661226	-1.252392	1.996273
O	-1.549080	-2.111791	0.169763
O	2.407249	-2.181495	-1.898249
O	-2.447150	0.733058	0.265707
C	-0.724461	-1.351423	0.026311
C	1.788662	-1.473436	-1.267404
C	2.687971	1.157191	-0.020859
C	2.414717	2.605007	-0.394276
C	1.371816	1.879466	-1.156535
C	0.013098	1.609502	-0.736843
C	-0.222692	1.481335	0.684760
C	-1.635073	1.355637	1.215916
C	-3.715456	0.388080	0.724503
C	-4.550636	-0.201943	-0.379873
C	-4.148929	-0.353043	-1.644372
H	3.495888	0.683855	-0.586755
H	2.690872	0.921929	1.051641
H	3.180722	3.107146	-0.996003
H	2.055527	3.232430	0.429294
H	1.605412	1.664394	-2.205675
H	-0.784557	1.543528	-1.479752
H	0.430166	2.022881	1.381172
H	-1.618875	0.778327	2.164119
H	-2.040110	2.364269	1.455377
H	-3.640809	-0.344821	1.559233
H	-4.236816	1.279418	1.139987
H	-5.556687	-0.518704	-0.077066
H	-4.809319	-0.793622	-2.396906
H	-3.147551	-0.042874	-1.956289

TS19

Rh	-1.344461	-0.259673	-0.106906
Cl	-1.908937	-0.972168	2.098702
O	0.187303	-0.363611	-2.685166
O	-4.321967	-0.010225	-0.748862
O	4.476402	-0.883794	-0.107977
C	-0.291242	-0.372427	-1.635966
C	-3.223073	-0.077635	-0.498408
C	-1.284531	1.796372	-0.296417
C	0.121444	2.399445	-0.214187
C	0.846439	2.052688	1.062309
C	1.975001	1.333658	1.150118
C	2.734364	0.746144	-0.018471
C	4.219828	0.419156	0.338062
C	3.287583	-1.598047	0.037175
C	2.204165	-0.647282	-0.519472
C	0.791919	-1.068371	-0.116436
H	-1.896921	2.119055	0.564260
H	-1.780938	2.119724	-1.225409
H	-0.006443	3.500109	-0.268768
H	0.710198	2.110999	-1.099898
H	0.376819	2.402564	1.991023
H	2.371674	1.126400	2.152728
H	2.704597	1.452356	-0.861792
H	4.940701	1.099140	-0.141086
H	4.361971	0.485078	1.436734
H	3.368920	-2.544004	-0.521083
H	3.081069	-1.834084	1.105044
H	2.303481	-0.668332	-1.617136
H	0.640030	-2.137560	-0.353312
H	0.661359	-0.956875	0.974815

TS20

Rh	-1.122303	-0.161493	0.007649
Cl	-3.361372	0.695545	-0.564719
O	-2.532274	-0.772299	2.807994
O	-1.839359	-2.797272	-1.388433
O	0.063587	1.333680	-2.318074
O	4.299784	-1.301777	0.125366
C	-1.989885	-0.582621	1.840402
C	-1.578782	-1.849449	-0.835086
C	-0.343372	0.878315	-1.343601
C	-0.480181	2.058897	0.220688
C	0.886792	2.773231	0.204053
C	1.932122	2.206795	1.143741
C	2.731933	1.162157	0.881729
C	2.703864	0.333962	-0.377528
C	4.100226	-0.209092	-0.732143
C	3.066464	-1.907199	0.426792
C	1.945431	-1.017341	-0.181210
C	0.685632	-1.017987	0.690896
H	-0.799128	1.917778	1.266462

H	-1.269450	2.654160	-0.263696
H	0.685782	3.819253	0.494713
H	1.273577	2.819829	-0.828357
H	2.032897	2.700885	2.118382
H	3.446284	0.839028	1.651025
H	2.282501	0.910013	-1.213665
H	4.129517	-0.520583	-1.797253
H	4.907341	0.522533	-0.564340
H	3.026074	-2.935554	0.019769
H	2.961592	-1.976955	1.526443
H	1.704802	-1.401182	-1.189662
H	0.457486	-2.069586	0.943922
H	0.912299	-0.513360	1.645068

TS21

Rh	-1.232428	-0.046477	-0.083855
Cl	-1.911025	-1.833547	1.475801
O	-1.581083	1.817850	2.488627
O	-4.145996	-0.027999	-1.035651
O	0.065574	-1.755079	-2.195606
O	4.531347	-1.040817	0.239609
C	-1.455259	1.199132	1.556513
C	-3.079169	0.007269	-0.671150
C	-0.311686	-1.147054	-1.293420
C	-0.862824	1.596336	-1.363635
C	0.595075	2.083574	-1.432991
C	1.170513	2.423461	-0.082048
C	2.206670	1.792274	0.490771
C	3.001863	0.684546	-0.164459
C	4.243480	0.259600	0.654411
C	3.303485	-1.701269	0.202522
C	2.281889	-0.695556	-0.418324
C	0.900571	-0.920589	0.206655
H	-1.504704	2.424918	-1.013866
H	-1.205403	1.347884	-2.382526
H	0.626162	2.988084	-2.073207
H	1.218646	1.327342	-1.937025
H	0.677700	3.237354	0.468425
H	2.524065	2.110241	1.493137
H	3.358004	1.042204	-1.144562
H	5.124721	0.895812	0.479768
H	4.003395	0.283477	1.741043
H	3.408159	-2.625841	-0.385761
H	2.977713	-1.973591	1.229681
H	2.243649	-0.879312	-1.503530
H	0.738987	-1.979468	0.464948
H	0.829220	-0.379350	1.163449

TS22

Rh	-0.890244	0.069355	-0.001840
Cl	-2.245428	-1.265985	-1.474630
O	-2.661213	2.523431	-0.342363
O	3.545148	0.501106	-1.230764
C	-2.010608	1.605285	-0.240420
C	-0.759846	0.315989	2.041728
C	-0.027897	-0.990929	2.416633
C	-0.068934	-1.758302	1.104156
C	0.820044	-1.595547	0.072810
C	2.125734	-0.828091	0.117717
C	2.784836	-0.678212	-1.272098
C	3.323251	1.212299	-0.036123
C	2.017439	0.650938	0.558006
C	0.760234	1.293833	-0.043902
H	-1.798772	0.326811	2.413231
H	-0.246921	1.223945	2.393784
H	-0.540380	-1.554922	3.212494
H	1.009449	-0.816938	2.740058
H	-0.887070	-2.472076	0.948223
H	0.638378	-2.206152	-0.822084
H	2.820619	-1.360132	0.795546
H	3.433855	-1.536588	-1.521046
H	2.008057	-0.603599	-2.059724
H	4.170194	1.063571	0.664152
H	3.252584	2.290165	-0.262511
H	2.015485	0.758612	1.652995
H	0.599636	2.288639	0.405219
H	0.901151	1.439582	-1.134878

TS23

Rh	-0.745172	0.322391	-0.013791
Cl	0.055349	1.338328	1.940983
O	1.424135	2.811550	-1.273447

O	1.568214	-1.568418	0.026177
C	0.778891	1.923225	-1.032358
C	-2.681517	0.258967	0.561738
C	-3.265760	-0.426026	-0.683815
C	-2.029316	-0.623801	-1.567490
C	-0.974489	-1.453404	-1.167358
C	-0.792954	-1.705601	0.255017
C	0.549792	-2.232522	0.728273
C	2.640781	-1.113519	0.797130
C	3.608111	-0.335182	-0.051113
C	3.502814	-0.159696	-1.372385
H	-2.987722	1.314040	0.665877
H	-2.855918	-0.261222	1.515732
H	-4.003214	0.204738	-1.204413
H	-3.754275	-1.393910	-0.469640
H	-2.046213	-0.284480	-2.609596
H	-0.150925	-1.654209	-1.862087
H	-1.647866	-2.055668	0.848379
H	0.629113	-2.043620	1.814859
H	0.632203	-3.328798	0.570487
H	2.271897	-0.457733	1.614935
H	3.178163	-1.964514	1.270989
H	4.448503	0.107643	0.498507
H	4.244892	0.424621	-1.924615
H	2.676258	-0.605764	-1.933233

SI-CO

O	0.000000	0.000000	0.486234
C	0.000000	0.000000	-0.648312

SI-C_2H_2

C	0.000000	0.000000	0.601497
C	0.000000	0.000000	-0.601497
H	0.000000	0.000000	1.666980
H	0.000000	0.000000	-1.666980

SI-C_2H_4

C	0.000000	0.000000	0.665371
C	0.000000	0.000000	-0.665371
H	0.000000	0.923905	1.237257
H	0.000000	-0.923905	1.237257

SI-C_3H_4

C	0.000000	0.000000	1.306303
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	-1.306303
H	0.000000	0.928417	1.872194
H	0.000000	-0.928417	1.872194
H	-0.928417	0.000000	-1.872194
H	0.928417	0.000000	-1.872194

SI-dimer

Rh	0.000000	1.541472	-0.123066
Rh	0.000000	-1.541472	-0.123066
Cl	-1.600456	0.000000	-1.011325
Cl	1.600456	0.000000	-1.011325
O	2.128475	3.330956	0.997427
O	-2.128475	3.330956	0.997427
O	-2.128475	-3.330956	0.997427
O	2.128475	-3.330956	0.997427
C	1.311261	2.648189	0.564305
C	-1.311261	2.648189	0.564305
C	-1.311261	-2.648189	0.564305
C	1.311261	-2.648189	0.564305

SI-IN1

Rh	0.000000	0.277414	0.000000
Cl	-2.182777	0.781365	0.000000
O	3.012730	0.353564	0.000000
O	0.150177	-2.667897	0.000000
C	1.861965	0.308381	0.000000
C	0.105361	-1.517080	0.000000

SI-IN2

Rh	0.000000	0.000000	0.085457
Cl	0.000000	0.000000	-2.238681
O	0.000000	3.073110	-0.127073
O	0.000000	0.000000	3.102794
O	0.000000	-3.073110	-0.127073
C	0.000000	1.938279	-0.024082

C	0.000000	0.000000	1.951965	H	-1.521158	-0.508643	2.553320
C	0.000000	-1.938279	-0.024082	H	-2.916604	-1.616179	2.015839

SI-IN3

Rh	-0.075122	-0.053842	-0.005197	Rh	-0.315327	-0.041769	-0.062099
Cl	2.252196	-0.229570	-0.054941	Cl	-1.277992	2.054342	0.016581
O	-3.054908	0.299080	-0.221960	O	-2.850863	-1.547255	0.171900
O	0.381680	2.938175	0.148632	C	-1.872155	-0.938941	0.071905
C	-1.914490	0.159847	-0.120052	C	1.925457	1.022628	-0.286052
C	0.194454	1.811223	0.074433	C	3.178137	0.208544	-0.126847
C	0.130143	-2.269745	-0.353006	C	2.041923	-0.163542	0.779647
C	-0.588391	-2.152908	0.636583	C	1.168527	-1.344717	0.591414
H	0.797939	-2.557156	-1.136722	C	0.787042	-1.766720	-0.701840
H	-1.249269	-2.305829	1.463456	H	1.875808	2.024730	0.118280
				H	1.390855	0.889839	-1.232419

SI-IN4

				H	4.027786	0.697871	0.335724
Rh	-0.064809	0.002989	-0.049654	H	3.426862	-0.484184	-0.923425
Cl	2.245115	-0.238497	-0.070000	H	2.112372	0.198131	1.799088
O	-3.059662	0.284803	-0.075094	H	0.935078	-1.936156	1.471198
O	0.359079	3.013968	0.162647	H	1.342486	-1.464879	-1.587950
C	-1.910013	0.180951	-0.063279	H	0.237664	-2.695018	-0.812457
C	0.194217	1.886253	0.067484				
C	-0.208952	-2.221516	-0.518710				
C	-0.211813	-2.087873	0.850380				
H	-1.130761	-2.378494	-1.070042				
H	0.721865	-2.377785	-1.053853				
H	-1.133458	-2.129856	1.421534				
H	0.715862	-2.130975	1.411125				

SI-IN5

Rh	0.093419	0.111336	-0.239290				
Cl	1.348556	-1.841496	-0.253790				
O	-1.516572	2.652168	-0.393106				
O	2.566848	1.510167	0.916918				
C	-0.900141	1.680396	-0.327551				
C	1.652491	1.007828	0.448168				
C	-1.632068	-1.119735	-0.856295				
C	-1.675073	-0.940355	0.498662				
C	-2.048577	-1.013202	1.752271				
H	-2.292218	-0.547153	-1.503899				
H	-1.181342	-2.020973	-1.264825				

SI-IN6

SI-IN7

SI-IN8

Rh	-0.044576	-0.044095	0.098286
Cl	-1.765024	1.118116	-1.251078
O	-0.847329	-2.634940	-1.350825
O	-1.949363	-0.194951	2.479877
C	-0.530187	-1.680236	-0.804970
C	-1.244510	-0.148183	1.578276
C	1.630521	-0.931436	1.059295
C	2.680414	-0.496792	0.030804
C	1.912188	0.348519	-0.983733
C	1.279272	1.552389	-0.636667
C	0.911500	1.839479	0.707657
H	1.508217	-2.011632	1.127220
H	1.763994	-0.511925	2.057062
H	3.118955	-1.360297	-0.476458
H	3.507854	0.076972	0.467798
H	2.015246	0.126419	-2.042347
H	0.806801	2.122941	-1.431209
H	1.571602	1.582510	1.530434
H	0.256999	2.687994	0.876572

SI-IN9

Rh	0.036647	0.053681	0.134204
Cl	2.067457	-0.876587	-0.962882
O	0.862510	2.766329	-0.962933
C	0.533569	1.755717	-0.526265
C	-1.805748	0.715869	0.931670
C	-2.664219	0.335523	-0.280180
C	-1.645118	-0.266809	-1.245928
C	-1.013725	-1.506779	-0.987969
C	-0.895335	-1.986610	0.332405
C	1.170414	-0.623131	1.974095
C	0.998682	0.591484	2.093223
H	-1.791921	1.786828	1.133581
H	-2.022158	0.165381	1.849366
H	-3.135037	1.210506	-0.736448
H	-3.461436	-0.381487	-0.048024
H	-1.575285	0.127698	-2.255925
H	-0.378728	-1.933689	-1.758446
H	-1.682684	-1.830511	1.062945
H	-0.242235	-2.834934	0.507010
H	1.489288	-1.638301	2.066120
H	1.033119	1.592648	2.466816

SI-IN10

Rh	0.026472	0.032333	0.102945
Cl	2.000943	-0.916730	-1.064662
O	0.823598	2.788662	-0.937640
C	0.515624	1.760287	-0.530437
C	-1.746493	0.719315	1.020893
C	-2.680335	0.429693	-0.161683
C	-1.745490	-0.165735	-1.213476
C	-1.123997	-1.421043	-1.045626
C	-0.948724	-1.963409	0.250581
C	0.959109	-0.717940	2.007810
C	1.391599	0.584767	1.813640
H	-1.684770	1.778103	1.273768
H	-1.954376	0.135653	1.921126
H	-3.138556	1.342907	-0.551111
H	-3.494226	-0.265493	0.079655
H	-1.715974	0.276338	-2.205778
H	-0.538865	-1.823195	-1.867279
H	-1.716313	-1.847288	1.009491
H	-0.304474	-2.829498	0.354793
H	0.153625	-0.932468	2.702289
H	1.582344	-1.546962	1.692670
H	0.931636	1.405882	2.353958
H	2.356117	0.770532	1.354037

SI-IN11

Rh	0.057088	0.016730	0.042385
Cl	-0.858206	2.213283	-0.675470
O	-1.371490	-1.175017	-2.373174
C	-0.823120	-0.750973	-1.459069
C	1.025728	-1.767235	0.621962
C	2.326520	-1.528592	-0.155629
C	2.108630	-0.174038	-0.828104
C	2.008136	1.024030	-0.094502
C	1.641384	0.997136	1.272324
C	-1.080153	0.342630	1.927794
C	-1.753260	-0.546294	1.132738
C	-2.738332	-1.377572	0.861254

H	0.470806	-2.642470	0.286091
H	1.138576	-1.796589	1.708252
H	2.487995	-2.294860	-0.918735
H	3.221130	-1.508802	0.479578
H	2.238446	-0.090867	-1.903917
H	1.927616	1.959562	-0.639835
H	2.001509	0.210647	1.928452
H	1.389084	1.937750	1.749440
H	-0.485441	-0.018787	2.762605
H	-1.337701	1.398553	1.910004
H	-2.805222	-1.954452	-0.053362
H	-3.547514	-1.492763	1.579869

SI-IN12

Rh	0.257495	0.002890	-0.285798
Cl	1.509848	-2.014668	-0.130710
O	2.627400	1.845224	-0.207948
O	-0.057777	1.240590	2.305463
C	1.726224	1.134660	-0.242697
C	-0.421229	0.447196	1.490624
C	-1.010553	1.516321	-1.072097
C	-2.364099	0.806340	-1.012423
C	-1.973980	-0.660510	-0.921703
C	-1.606823	-1.290294	0.234034
C	-1.549607	-0.593373	1.580715
H	-0.656980	1.657688	-2.097192
H	-0.968975	2.457565	-0.524493
H	-3.001299	0.995268	-1.882815
H	-2.926266	1.104320	-0.120993
H	-1.957692	-1.244194	-1.840311
H	-1.325162	-2.337315	0.199745
H	-2.475663	-0.069633	1.847483
H	-1.299221	-1.292932	2.382739

SI-IN13

Rh	-0.089162	0.028124	0.157098
Cl	-0.717206	-0.900752	-1.991407
O	-2.394986	2.090769	-0.422626
O	-1.724266	-1.869593	1.876321
C	-1.525597	1.395654	-0.164973
C	-1.139474	-1.137336	1.214062
C	1.490594	-1.374253	0.183187
C	2.527442	-0.495196	-0.520886
C	1.872758	0.875213	-0.670058
C	1.426333	1.633512	0.415407
C	1.123812	1.032830	1.677060
H	1.166914	-2.223784	-0.414759
H	1.764907	-1.686428	1.192440
H	2.743775	-0.884784	-1.517743
H	3.481189	-0.413099	0.017212
H	1.883850	1.352799	-1.645410
H	1.065798	2.640560	0.214910
H	1.774706	0.266225	2.084373
H	0.622466	1.643747	2.421143

SI-IN14

Rh	0.304024	-0.121968	-0.375551
Cl	0.682291	2.186776	-0.645852
O	3.124292	-0.938221	0.470657
O	0.297021	-0.241980	2.464719
C	2.072517	-0.599012	0.161565
C	-0.340326	0.061561	1.502127
C	-1.723964	0.708182	1.490739
C	-2.604642	0.038433	0.428185
C	-1.895742	-0.017701	-0.914262
C	-1.266002	-1.174990	-1.409943
C	-0.627049	-2.110507	-0.548835
H	-1.548388	1.759133	1.231567
H	-2.141712	0.643485	2.500970
H	-3.543777	0.591369	0.329497
H	-2.861547	-0.975253	0.755601
H	-2.145436	0.756190	-1.634039
H	-1.010393	-1.197186	-2.469632
H	-1.048554	-2.353715	0.422315
H	-0.039490	-2.904832	-0.997455

SI-IN15

Rh	-0.377331	-0.052842	0.064602
Cl	-1.658331	1.920309	0.395247
O	-2.757206	-1.886290	0.046124
C	-1.862724	-1.165284	0.073491
C	0.358650	-0.821830	-1.747061

C	1.596192	0.064572	-1.886829
C	1.294215	1.181385	-0.905177
C	1.659457	1.145231	0.415499
C	2.644914	0.162578	1.020431
C	2.042566	-1.206268	1.212375
C	0.806419	-1.506701	0.794858
H	-0.443672	-0.572098	-2.445058
H	0.560795	-1.891554	-1.743151
H	1.731545	0.444958	-2.905603
H	2.497435	-0.478968	-1.591304
H	0.715815	2.032243	-1.257635
H	1.340316	1.976240	1.040972
H	3.545474	0.096274	0.391072
H	2.982246	0.556825	1.987081
H	2.644740	-1.947123	1.743144
H	0.416343	-2.515935	0.919677

SI-IN16

Rh	-0.445217	0.027727	-0.029627
Cl	-1.836647	-1.812383	0.214561
O	-2.679148	2.038669	0.137495
C	-1.843439	1.247304	0.093174
C	2.018890	0.801758	1.430046
C	2.466634	-0.619560	1.023011
C	1.431024	-1.368212	0.204297
C	1.206430	-1.068259	-1.118353
C	1.774006	0.210052	-1.712791
C	1.018638	1.296883	-0.954027
C	1.076082	1.466712	0.449370
H	1.502424	0.752576	2.395016
H	2.899993	1.442692	1.588181
H	2.707134	-1.193990	1.921033
H	3.389077	-0.556964	0.431356
H	1.013201	-2.287243	0.605861
H	0.644550	-1.753577	-1.746185
H	2.865994	0.281664	-1.601754
H	1.543165	0.273196	-2.777573
H	0.580804	2.096838	-1.544171
H	0.655029	2.398160	0.825615

SI-IN17

Rh	0.392279	0.144214	-0.184515
Cl	1.135687	-2.029683	-0.874991
O	3.034471	1.153522	0.786234
C	2.028436	0.739072	0.408482
C	-0.389730	2.099195	-0.251784
C	-1.780289	1.804019	-0.828663
C	-1.618898	0.378236	-1.322448
C	-1.832969	-0.744256	-0.569429
C	-2.406485	-0.794618	0.820005
C	-1.278768	-1.077759	1.834543
C	-0.227048	0.017160	1.792828
H	0.248818	2.649988	-0.949274
H	-0.408781	2.615704	0.710509
H	-2.067774	2.477774	-1.643409
H	-2.555252	1.863580	-0.059462
H	-1.271976	0.236502	-2.346851
H	-1.612465	-1.704325	-1.030409
H	-2.903144	0.146276	1.079119
H	-3.156506	-1.592255	0.867164
H	-1.698384	-1.132822	2.851844
H	-0.820348	-2.045605	1.611642
H	-0.612386	0.987736	2.117421
H	0.657713	-0.242044	2.378643

SI-IN18

Rh	-0.590429	0.010022	-0.032541
Cl	-1.900219	1.902327	-0.148038
O	-2.807247	-1.924530	0.120944
C	-1.946796	-1.153208	0.067718
C	1.910127	0.907909	1.369079
C	1.863402	-0.614742	1.612273
C	0.836856	-1.361000	0.774297
C	0.853361	-1.443575	-0.641715
C	1.859475	-0.809659	-1.583754
C	2.634727	0.415890	-1.056325
C	1.809887	1.307520	-0.114462
H	1.111166	1.400818	1.932871
H	2.856965	1.296174	1.763732
H	1.655649	-0.793590	2.671323
H	2.854062	-1.049868	1.416243

H	0.328612	-2.168631	1.296460
H	0.345955	-2.299931	-1.083130
H	2.569783	-1.587540	-1.903241
H	1.317388	-0.518545	-2.492689
H	3.536852	0.094451	-0.523077
H	2.977968	1.000198	-1.915585
H	2.099018	2.360334	-0.211698
H	0.751337	1.377025	-0.500413

SI-IN19

Rh	-0.419823	0.068097	-0.054538
Cl	-1.725857	1.884899	0.733384
O	-2.685834	-1.897305	-0.107821
C	-1.827686	-1.133819	-0.064488
C	0.322068	-0.533819	-1.919409
C	1.494152	0.441563	-2.035726
C	1.166676	1.477284	-0.975805
C	1.570419	1.410349	0.330942
C	2.547396	0.426067	0.917885
C	1.777952	-0.714671	1.624033
C	0.826796	-1.367708	0.647841
C	0.817799	-2.683113	0.408774
H	-0.510292	-0.299645	-2.588583
H	0.599954	-1.584567	-1.986155
H	1.569976	0.899415	-3.028802
H	2.439761	-0.060253	-1.814706
H	0.530216	2.311539	-1.264697
H	1.201526	2.186580	0.999087
H	3.189930	-0.001177	0.142266
H	3.188770	0.945987	1.637662
H	2.472813	-1.462922	2.030182
H	1.220724	-0.292880	2.470184
H	0.140511	-3.159050	-0.293511
H	1.500943	-3.345054	0.942052

SI-IN20

Rh	-0.508509	0.029588	-0.216523
Cl	-2.075319	-1.685890	-0.045232
O	-2.827539	1.879829	0.439283
C	-1.957508	1.197253	0.117961
C	1.897466	1.226310	1.115762
C	1.780754	-0.122838	1.876755
C	0.812577	-1.062712	1.188557
C	1.068876	-1.564938	-0.093602
C	2.345601	-1.198794	-0.831714
C	2.280671	0.275564	-1.278524
C	1.428976	1.096289	-0.321325
C	0.441677	1.934947	-0.831736
H	1.275877	1.974042	1.615928
H	2.933332	1.592732	1.138113
H	1.462006	0.061811	2.905352
H	2.763138	-0.614702	1.932371
H	0.078964	-1.573972	1.805248
H	0.518962	-2.447749	-0.409348
H	3.211084	-1.364205	-0.173596
H	2.484942	-1.847769	-1.700238
H	3.284260	0.720355	-1.346007
H	1.834911	0.334234	-2.276693
H	0.057766	2.760436	-0.240025
H	0.283836	2.008350	-1.905709

SI-IN21

Rh	0.257924	-0.056893	0.124470
Cl	1.922484	0.772715	-1.509673
O	0.816351	-2.953241	-0.941347
O	2.449367	0.055721	2.197421
C	0.586765	-1.898834	-0.568760
C	1.622818	-0.009686	1.407618
C	-0.237596	1.944792	0.760558
C	-1.514875	2.155444	-0.050120
C	-1.249582	1.162144	-1.159282
C	-1.726362	-0.127986	-1.209396
C	-2.842046	-0.682870	-0.337057
C	-2.418247	-0.878114	1.093644
C	-1.156653	-0.680525	1.482741
H	0.590703	2.567976	0.425261
H	-0.377244	1.984375	1.839688
H	-1.638396	3.174520	-0.431261
H	-2.401710	1.880707	0.525451
H	-0.576019	1.486908	-1.948652
H	-1.453890	-0.707881	-2.089037
H	-3.708056	-0.005376	-0.389896

H	-3.184482	-1.636030	-0.760834
H	-3.180717	-1.207382	1.803085
H	-0.870074	-0.839794	2.521239

SI-IN22

Rh	-0.347096	0.132532	-0.282628
Cl	-1.542445	-1.739074	-1.197329
O	-2.981916	1.596051	0.027515
O	-0.885450	0.424381	2.502071
C	-1.988046	1.039069	-0.076045
C	-0.199611	-0.140448	1.699089
C	0.808785	-1.241716	2.065043
C	2.012845	-1.262252	1.119439
C	1.491165	-1.306673	-0.290477
C	1.716954	-0.348483	-1.246061
C	2.647179	0.839866	-1.099580
C	1.937805	1.996291	-0.450463
C	0.687710	1.864270	0.018759
H	0.245625	-2.180343	1.984730
H	1.087947	-1.096238	3.113168
H	2.626723	-2.147326	1.324742
H	2.628943	-0.374066	1.283957
H	0.946167	-2.202421	-0.580772
H	1.319510	-0.542173	-2.242970
H	3.541918	0.560334	-0.524961
H	3.007660	1.125708	-2.096794
H	2.472988	2.946191	-0.383605
H	0.213632	2.707650	0.520448

SI-IN23

Rh	0.216239	0.063339	0.074036
Cl	2.553679	-0.789459	-0.387565
O	0.650940	1.531866	-2.554690
O	-1.964429	1.739010	1.103328
C	0.465563	1.012971	-1.547840
C	-1.678617	0.852053	0.336543
C	-2.705731	0.189794	-0.584416
C	-2.434152	-1.319019	-0.590990
C	-0.947051	-1.620149	-0.730206
C	-0.153085	-2.064230	0.371016
C	-0.324851	-1.505459	1.645464
C	1.486523	1.019333	1.779498
C	0.885124	1.951443	1.259740
H	-2.536878	0.604653	-1.586854
H	-3.721725	0.449470	-0.267962
H	-2.978569	-1.800820	-1.409045
H	-2.808082	-1.751868	0.343320
H	-0.612663	-1.947592	-1.711440
H	0.766360	-2.601601	0.161981
H	-1.289087	-1.153650	1.998124
H	0.406494	-1.728552	2.414832
H	2.130926	0.346973	2.300865
H	0.445471	2.886125	0.991192

SI-IN24

Rh	0.701159	0.073886	0.079702
Cl	2.383641	-1.316791	-0.703620
O	2.426605	2.511467	-0.255176
O	-3.184736	1.631202	-0.747643
C	1.770825	1.571920	-0.149763
C	-2.224889	0.879682	-0.677103
C	-2.154283	-0.395898	-1.491312
C	-2.022332	-1.676190	-0.634784
C	-0.695630	-1.880826	0.065190
C	-0.411730	-1.475992	1.344678
C	-1.248268	-0.445728	2.077219
C	-0.722589	0.856222	1.480325
C	-1.056647	1.315464	0.181161
H	-1.281807	-0.320705	-2.154813
H	-3.060475	-0.447180	-2.100867
H	-2.176381	-2.530554	-1.300970
H	-2.837818	-1.696248	0.098299
H	-0.001409	-2.574817	-0.401821
H	0.458491	-1.886459	1.850415
H	-2.324249	-0.576093	1.912299
H	-1.063186	-0.479266	3.152018
H	-0.277738	1.568978	2.168432
H	-0.851186	2.369639	0.000862

SI-IN25

Rh	0.526753	0.101723	-0.061848
Cl	0.098423	-2.254485	-0.120159

O	1.150309	3.044720	-0.029763
O	3.468795	-0.809681	0.067072
O	-3.105536	0.398867	0.087634
C	0.908449	1.919510	-0.038535
C	2.385322	-0.437709	0.017862
C	-0.159307	0.275140	-2.156488
C	-1.203580	0.231239	-1.472015
C	-2.629795	-0.043629	-1.177827
C	-2.426426	-0.208520	1.199840
C	-1.153009	0.516796	1.534289
C	-0.041400	-0.036772	2.156455
H	0.446001	0.324440	-3.039383
H	-3.256511	0.462861	-1.917910
H	-2.770979	-1.131057	-1.274507
H	-3.127452	-0.096456	2.035960
H	-2.245132	-1.275996	1.023567
H	-1.266204	1.599468	1.552307
H	0.649318	0.598466	2.700348
H	0.003791	-1.100614	2.364467

SI-IN26

Rh	0.933825	0.065316	-0.284027
Cl	1.423464	-2.217382	-0.320579
O	0.387777	2.946811	-0.982572
O	3.511090	0.421793	1.477481
O	-4.014246	-0.116967	0.456767
C	0.581963	1.854359	-0.678988
C	2.583617	0.322541	0.818928
C	-0.801094	-0.399536	-1.278026
C	-1.911053	-0.133913	-0.581688
C	-3.360383	-0.535963	-0.761424
C	-3.018969	-0.079011	1.488031
C	-1.777873	0.513821	0.776012
C	-0.415371	0.171046	1.336211
H	-0.781542	-0.948168	-2.218744
H	-3.860950	-0.027046	-1.591482
H	-3.464978	-1.622234	-0.897635
H	-3.412735	0.536895	2.298930
H	-2.800275	-1.090544	1.864799
H	-1.911646	1.602160	0.703524
H	-0.011981	0.874274	2.064495
H	-0.338915	-0.862201	1.679409

SI-IN27

Rh	0.123755	0.476812	0.000000
Cl	2.487633	0.205224	0.000000
O	0.850123	3.473274	0.000000
O	-2.830309	1.052104	0.000000
O	-1.093291	-2.979424	0.000000
C	0.544450	2.367967	0.000000
C	-1.705264	0.801706	0.000000
C	0.064153	-0.157715	2.169694
C	0.064153	-1.328482	1.408341
C	-1.140923	-2.210214	1.204562
C	-1.140923	-2.210214	-1.204562
C	0.064153	-1.328482	-1.408341
C	0.064153	-0.157715	-2.169694
H	0.994651	0.211404	2.585524
H	-0.850641	0.204718	2.630567
H	1.023200	-1.807478	1.225861
H	-1.170646	-2.968913	1.995525
H	-2.073866	-1.626779	1.260243
H	-1.170646	-2.968913	-1.995525
H	-2.073866	-1.626779	-1.260243
H	1.023200	-1.807478	-1.225861
H	0.994651	0.211404	-2.585524
H	-0.850641	0.204718	-2.630567

SI-IN28

Rh	0.889826	0.188895	-0.296805
Cl	1.554614	-2.040891	-0.551781
O	3.289911	0.461268	1.722546
O	0.071239	3.088368	-0.375053
O	-3.478989	0.333448	0.822157
C	2.428406	0.378837	0.977907
C	0.364182	1.975564	-0.330882
C	-0.508107	-0.270429	1.208188
C	-1.616064	-1.107870	0.584986
C	-2.940884	-0.895811	1.333369
C	-2.900188	0.608176	-0.473013
C	-1.967796	-0.565760	-0.813573
C	-0.714704	-0.213043	-1.622049

H	0.085898	-0.811796	1.945404
H	-0.863460	0.676856	1.614311
H	-1.312773	-2.156184	0.542469
H	-3.628190	-1.731669	1.132673
H	-2.832465	-0.785315	2.417779
H	-3.706303	0.723415	-1.206393
H	-2.357601	1.561094	-0.408699
H	-2.549380	-1.328186	-1.348292
H	-0.338258	-1.079668	-2.170691
H	-0.894436	0.603682	-2.328838

SI-TS1

Rh	-0.183822	-0.034622	-0.091064
Cl	-1.345192	1.978942	0.050910
O	-2.784519	-1.596325	0.245556
C	-1.817129	-0.995548	0.083264
C	1.611853	1.187205	-0.401644
C	2.823379	0.449155	0.126209
C	1.830361	-0.319294	0.935033
C	1.169034	-1.518631	0.504003
C	0.926329	-1.705675	-0.880457
H	1.390627	2.142574	0.060707
H	1.461095	1.154991	-1.483968
H	3.522673	1.042988	0.713141
H	3.355452	-0.151121	-0.611370
H	1.690904	-0.018543	1.969650
H	0.768462	-2.195197	1.251489
H	1.598213	-1.295164	-1.630022
H	0.366005	-2.577249	-1.200090

SI-TS2

Rh	-0.249481	-0.103363	-0.103883
Cl	-1.603665	1.821425	-0.558615
O	-2.540240	-1.999254	-0.477196
O	0.018278	-0.244188	2.851046
C	-1.651497	-1.273969	-0.376974
C	0.097794	-0.012484	1.711360
C	1.153794	-1.698237	-0.352556
C	2.504714	-1.020648	-0.627444
C	2.208317	0.328168	-1.237650
C	1.612750	1.317341	-0.512074
C	1.351663	1.214431	0.947136
H	0.795555	-2.210955	-1.247180
H	1.167818	-2.389607	0.490685
H	3.129526	-1.630248	-1.288794
H	3.066211	-0.890804	0.307014
H	2.406747	0.499806	-2.292346
H	1.297916	2.235558	-0.996895
H	2.168574	0.763570	1.509448
H	0.967078	2.129699	1.387681

SI-TS3

Rh	0.348605	-0.029417	-0.019783
Cl	1.284538	2.130661	0.284607
O	3.027538	-1.271660	-0.639570
O	-0.557455	-1.654953	2.291084
C	2.008593	-0.772954	-0.451289
C	-0.363445	-0.893410	1.429219
C	-1.623813	0.639994	1.097452
C	-2.733028	0.350419	0.090325
C	-2.250641	0.533971	-1.331465
C	-1.343779	-0.295469	-1.909199
C	-0.753059	-1.430282	-1.200758
H	-1.192978	1.638239	1.000275
H	-1.918822	0.480508	2.133955
H	-3.574353	1.023758	0.295618
H	-3.115953	-0.669485	0.230520
H	-2.612365	1.394175	-1.888177
H	-0.978231	-0.058551	-2.905998
H	-1.435521	-2.014177	-0.584647
H	-0.101788	-2.072647	-1.787439

SI-TS4

Rh	0.120445	0.126153	0.114934
Cl	2.062181	-0.949928	-0.956828
O	1.520674	2.767813	0.016845
C	0.973739	1.754478	0.055983
C	-1.689243	0.955085	0.841825
C	-2.545396	0.852056	-0.428243
C	-1.658320	0.166503	-1.458106
C	-1.073598	-1.072721	-1.257831
C	-1.123341	-1.815335	0.021339

C	-0.015995	-1.612626	1.677929
C	0.634855	-0.545731	1.953193
H	-1.561331	1.980960	1.185105
H	-2.029406	0.331824	1.672583
H	-2.824107	1.841449	-0.800470
H	-3.480900	0.293124	-0.285255
H	-1.541868	0.616473	-2.441225
H	-0.456880	-1.500238	-2.041507
H	-2.060636	-1.744179	0.568629
H	-0.757093	-2.829478	-0.101514
H	-0.195633	-2.613840	2.027777
H	1.249162	-0.136956	2.738631

SI-TS5

Rh	0.407717	-0.051315	0.027456
Cl	1.821032	1.788014	-0.103492
O	2.813690	-1.853747	-0.205097
C	1.892451	-1.169116	-0.125014
C	-1.049467	-1.363173	1.136385
C	-1.919892	-0.205673	1.636628
C	-1.279822	1.048047	1.068862
C	-1.425289	1.366769	-0.260021
C	-2.380776	0.646057	-1.196228
C	-1.955925	-0.779335	-1.444855
C	-0.973042	-1.389901	-0.738760
H	-0.183701	-1.546442	1.783147
H	-1.583739	-2.310398	1.058069
H	-1.940143	-0.185428	2.730337
H	-2.950570	-0.311169	1.280368
H	-0.736257	1.721783	1.725288
H	-0.960037	2.279650	-0.621582
H	-3.410228	0.695426	-0.804649
H	-2.401835	1.179794	-2.153881
H	-2.409266	-1.298793	-2.288883
H	-0.688001	-2.403547	-1.005599

SI-TS6

Rh	0.148849	0.185496	0.042434
Cl	1.931375	-1.094456	-1.034438
O	1.704459	2.715153	-0.002979
C	1.096422	1.732961	0.015945
C	-1.562986	1.155937	0.815052
C	-2.543424	0.977024	-0.357302
C	-1.821387	0.134720	-1.400710
C	-1.263730	-1.090008	-1.129224
C	-1.292630	-1.728073	0.228937
C	0.019794	-1.736117	1.491395
C	0.728987	-0.491898	1.880194
H	-1.378756	2.204926	1.045994
H	-1.870361	0.642197	1.731814
H	-2.803352	1.942428	-0.799371
H	-3.490730	0.501462	-0.065297
H	-1.780961	0.489783	-2.428075
H	-0.763016	-1.637772	-1.920557
H	-2.167472	-1.420489	0.798909
H	-1.269004	-2.808924	0.103858
H	-0.637130	-2.123603	2.271142
H	0.700629	-2.484368	1.095092
H	0.313634	0.077216	2.710074
H	1.813001	-0.572932	1.890436

SI-TS7

Rh	0.401310	0.034875	-0.086308
Cl	1.996193	-1.692158	-0.069170
O	2.637421	2.090151	-0.256904
C	1.795032	1.308105	-0.213767
C	-0.837673	-0.862314	1.542610
C	-1.535120	0.464896	1.836045
C	-0.959077	1.424682	0.811257
C	-1.265740	1.370400	-0.563135
C	-2.398828	0.595508	-1.219753
C	-2.520150	-0.865621	-0.754517
C	-1.129785	-1.437984	-0.567920
H	0.089953	-1.032052	2.088253
H	-1.470682	-1.742265	1.607295
H	-1.292333	0.794976	2.852306
H	-2.625833	0.394542	1.772121
H	-0.440152	2.303866	1.183235
H	-0.927993	2.222376	-1.151317
H	-3.343973	1.136436	-1.064579
H	-2.215981	0.605607	-2.300003
H	-3.108646	-0.949297	0.164764

H	-3.061637	-1.449150	-1.512111
H	-1.056807	-2.475894	-0.255229
H	-0.531446	-1.319082	-1.494672

SI-TS8

Rh	0.043158	0.131912	-0.093498
Cl	1.321867	-1.236838	-1.674203
O	1.327530	2.656311	-1.041455
C	0.817308	1.687116	-0.683289
C	-1.307593	1.181791	1.157606
C	-2.616796	0.984956	0.374790
C	-2.293439	0.078873	-0.804285
C	-1.682213	-1.147114	-0.675617
C	-1.218723	-1.707470	0.623369
C	0.540290	-1.554091	1.442613
C	1.247498	-0.285819	1.419175
C	2.222942	0.282268	2.115522
H	-1.034403	2.230844	1.264545
H	-1.299834	0.714561	2.145899
H	-2.991069	1.939430	-0.004885
H	-3.424508	0.552026	0.982513
H	-2.610169	0.377653	-1.800863
H	-1.476341	-1.734307	-1.564237
H	-1.832844	-1.411667	1.470178
H	-1.097548	-2.784236	0.555088
H	0.120749	-1.836887	2.406745
H	1.050778	-2.354704	0.911807
H	2.596211	1.273479	1.882735
H	2.709273	-0.249538	2.931679

SI-TS9

Rh	-0.436559	-0.035132	0.066332
Cl	-2.079046	-1.584467	-0.484231
O	-2.688375	1.998639	0.181156
C	-1.809873	1.259857	0.122854
C	1.090139	0.870598	1.467038
C	1.650923	-0.519268	1.827249
C	0.942325	-1.532619	0.947136
C	1.106945	-1.637548	-0.421063
C	2.106027	-0.935763	-1.314947
C	2.402000	0.517471	-0.912497
C	1.157868	1.240387	-0.418835
C	0.871059	2.492281	-0.844401
H	0.254136	1.184849	2.094390
H	1.850203	1.645352	1.537316
H	1.448136	-0.732960	2.881148
H	2.736969	-0.561090	1.693009
H	0.305472	-2.269094	1.429588
H	0.560109	-2.448932	-0.896440
H	3.034983	-1.524902	-1.354298
H	1.694376	-0.946101	-2.329316
H	3.172269	0.547100	-0.131948
H	2.812282	1.065571	-1.767919
H	0.053077	3.081417	-0.445305
H	1.469427	2.954182	-1.627663

SI-TS10

Rh	-0.290654	0.191187	0.038186
Cl	-1.900215	-0.505470	-1.646707
O	-1.327719	3.010887	-0.107691
O	-1.825338	-0.900543	2.336675
C	-0.906345	1.942758	-0.074343
C	-1.126699	-0.714074	1.418845
C	-0.106113	-2.070028	0.681346
C	1.274177	-2.039710	-0.041150
C	1.258408	-1.114762	-1.245741
C	1.973636	0.034935	-1.362559
C	3.007054	0.546208	-0.379987
C	2.462080	0.917707	0.975703
C	1.173100	0.857077	1.325539
H	-0.874378	-2.569548	0.091633
H	0.018839	-2.530678	1.660820
H	1.503686	-3.069629	-0.348635
H	2.039422	-1.720927	0.669362
H	0.620910	-1.413894	-2.073724
H	1.861400	0.590837	-2.291362
H	3.797197	-0.211904	-0.258994
H	3.510204	1.418762	-0.815289
H	3.198350	1.272364	1.701966
H	0.876105	1.180771	2.322096

SI-TS11

Rh	0.262155	0.122696	0.026245
Cl	2.631315	-0.389198	-0.580422
O	0.843956	2.864786	-1.051078
O	-1.925706	1.291636	1.604906
C	0.594801	1.825530	-0.624976
C	-1.652534	0.747454	0.565358
C	-2.709811	0.462066	-0.508565
C	-2.496301	-0.966452	-1.026611
C	-1.085874	-1.178817	-1.523453
C	-0.073564	-1.839423	-0.844556
C	-0.071751	-2.106270	0.611133
C	0.545280	-0.953393	2.103492
C	0.785484	0.295835	1.979840
H	-2.543362	1.180588	-1.321568
H	-3.712039	0.624271	-0.096279
H	-3.193009	-1.172071	-1.846416
H	-2.726152	-1.674259	-0.222280
H	-0.910579	-0.989665	-2.580520
H	0.837414	-2.095942	-1.374638
H	-1.038046	-2.324679	1.058432
H	0.703343	-2.821311	0.869066
H	0.595911	-1.751978	2.822750
H	1.096809	1.149550	2.557009

SI-TS12

Rh	0.497996	-0.109314	0.100066
Cl	1.963307	-1.764016	-0.598150
O	2.875706	1.689844	0.659451
O	-0.243701	2.522162	-1.022366
C	1.977734	1.016786	0.426494
C	-0.778806	1.461967	-0.685445
C	-1.759378	0.809778	-1.672088
C	-2.321218	-0.545156	-1.244792
C	-1.238974	-1.426950	-0.668740
C	-1.088654	-1.613152	0.685550
C	-1.974513	-0.914184	1.698160
C	-1.658690	0.551267	1.803262
C	-0.935091	1.320337	0.942309
H	-1.187630	0.715267	-2.601142
H	-2.559726	1.534957	-1.863944
H	-2.769878	-1.043593	-2.110768
H	-3.121041	-0.400276	-0.511177
H	-0.668845	-2.055232	-1.348073
H	-0.433417	-2.399640	1.049077
H	-3.045365	-1.070526	1.493012
H	-1.801745	-1.348725	2.689679
H	-1.942982	1.015530	2.750569
H	-0.645942	2.299456	1.313422

SI-TS13

Rh	-0.729043	-0.076708	-0.135900
Cl	-0.344582	2.237059	-0.556357
O	-1.481866	-3.013880	-0.192612
O	-3.474449	0.839127	0.662036
O	3.629124	-0.172205	0.322310
C	-1.176126	-1.906350	-0.164075
C	-2.413186	0.474249	0.400823
C	0.588375	-0.575225	-1.731983
C	1.526781	-0.428536	-0.859380
C	2.981611	-0.001326	-0.923293
C	2.708519	0.271750	1.311769
C	1.408379	-0.495810	1.127728
C	0.227325	0.014602	1.785138
H	0.522937	-0.598217	-2.809244
H	3.510217	-0.603297	-1.666417
H	2.999354	1.057894	-1.221097
H	3.155210	0.040959	2.282461
H	2.525802	1.353985	1.237268
H	1.541636	-1.575459	1.199698
H	-0.324256	-0.654469	2.438523
H	0.241387	1.056018	2.098160

SI-TS14

Rh	0.725122	0.139905	-0.167010
Cl	1.216789	-2.179244	-0.491243
O	3.505287	0.287720	0.995866
O	0.434855	3.141863	-0.482782
O	-3.648955	-0.152434	0.423075
C	2.413662	0.228767	0.638229
C	0.519123	1.998822	-0.371515
C	-0.186576	-0.147112	1.719779

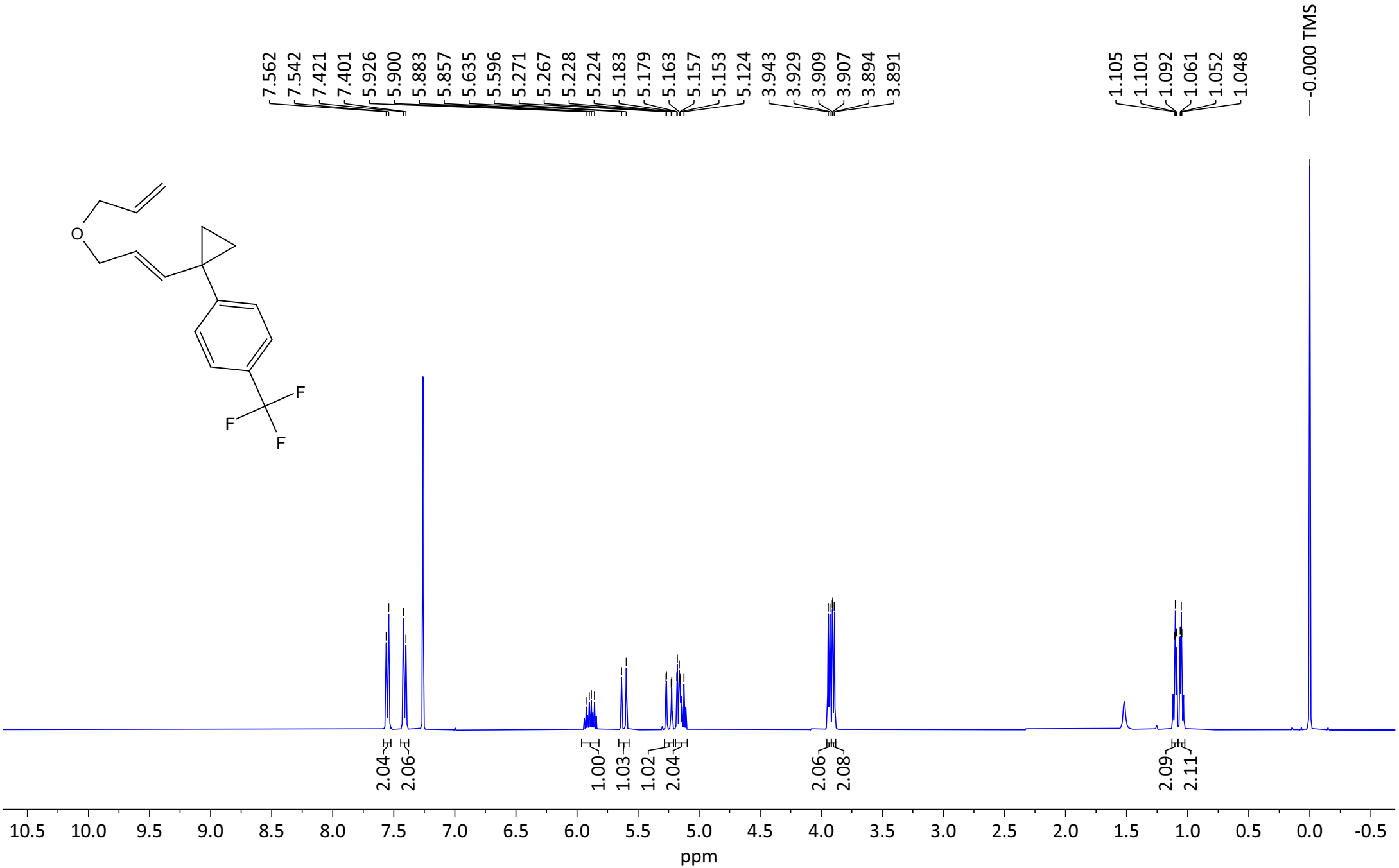
C	-1.403893	-0.655832	1.090098
C	-2.698676	0.063876	1.459980
C	-2.956899	0.141482	-0.781771
C	-1.613907	-0.581390	-0.803410
C	-0.651000	-0.041180	-1.798822
H	0.420029	-0.879554	2.245183
H	-0.248448	0.815513	2.224258
H	-1.470172	-1.739265	1.167487
H	-3.132461	-0.330567	2.382667
H	-2.503816	1.142284	1.586092
H	-3.582847	-0.202212	-1.610331
H	-2.795861	1.227916	-0.880858
H	-1.692729	-1.661779	-0.897974
H	-0.220500	-0.771151	-2.476547
H	-0.949602	0.888447	-2.278090

S10. Copies of NMR Spectra

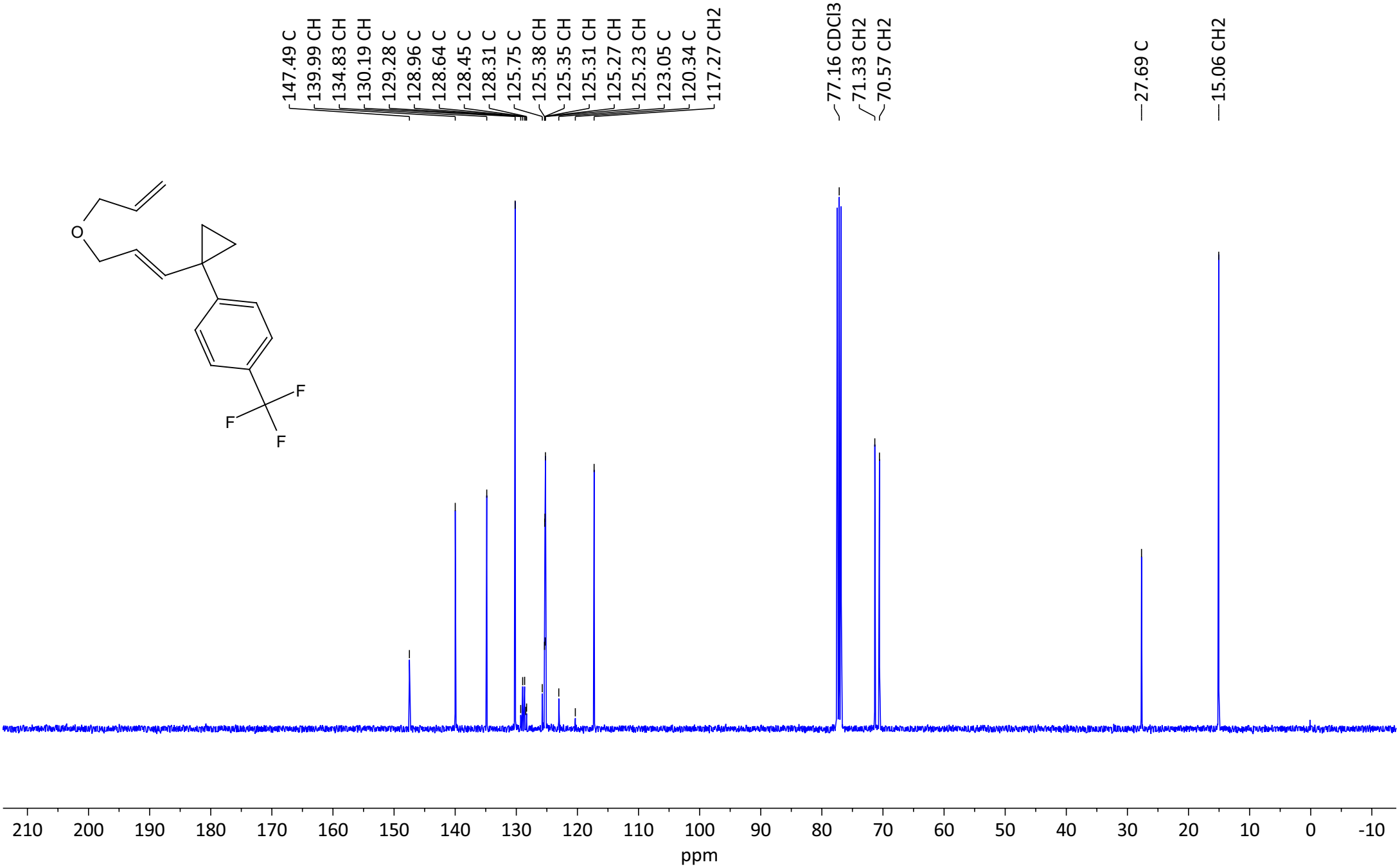
Table S7. Summary of NMR Spectra

compound	NMR	page
1a	^{1}H NMR, 400 MHz, $CDCl_3$	S58
1a	$^{13}C\{^{1}H\}$ NMR, 101 MHz, $CDCl_3$	S59
1a	^{19}F NMR, 471 MHz, $CDCl_3$	S60
2a	^{1}H NMR, 400 MHz, $CDCl_3$	S61
2a	$^{13}C\{^{1}H\}$ NMR, 101 MHz, $CDCl_3$	S62
2a	^{19}F NMR, 471 MHz, $CDCl_3$	S63

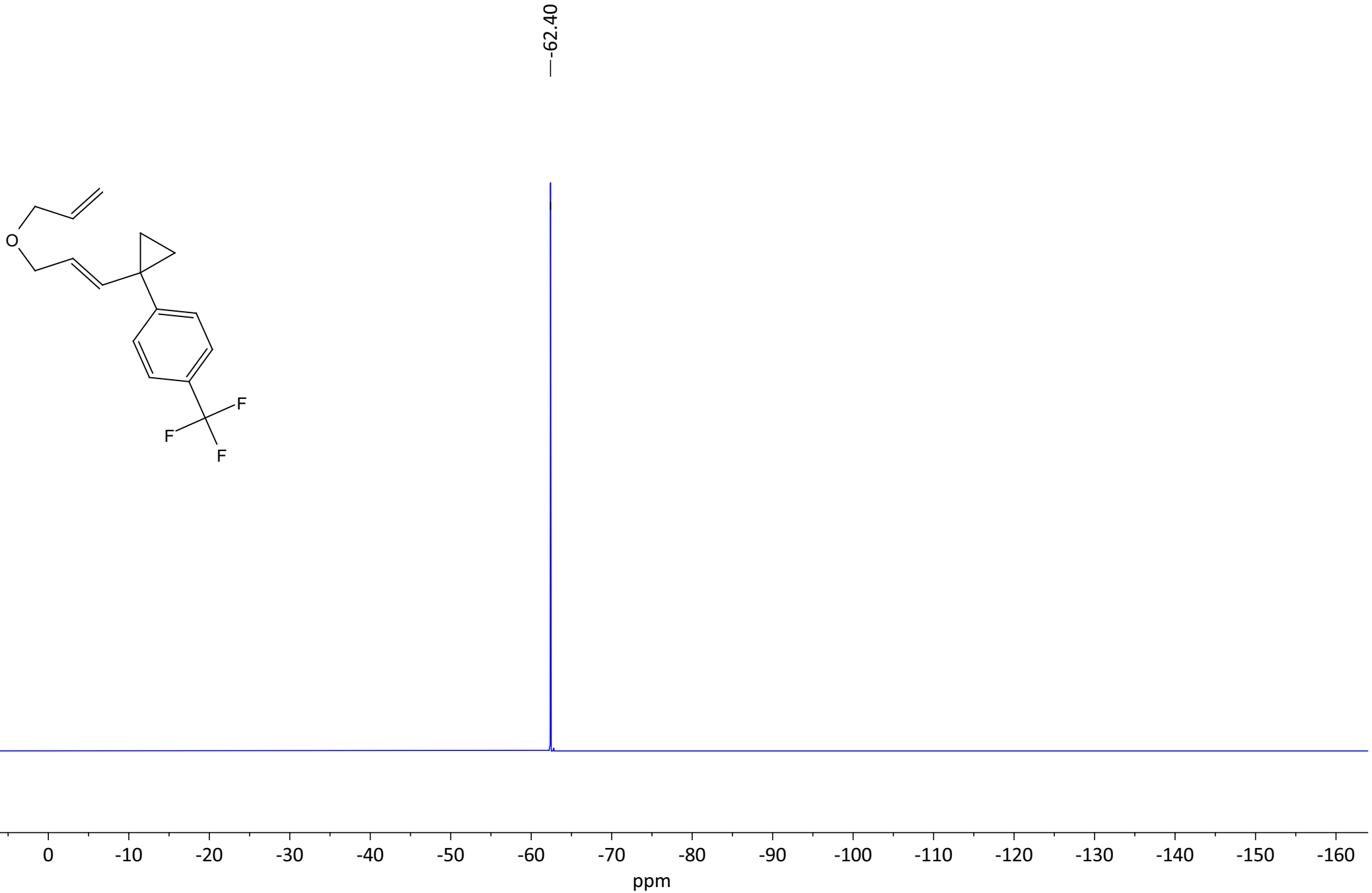
Compound **1a**: ^{1}H NMR (400 MHz, $CDCl_3$)



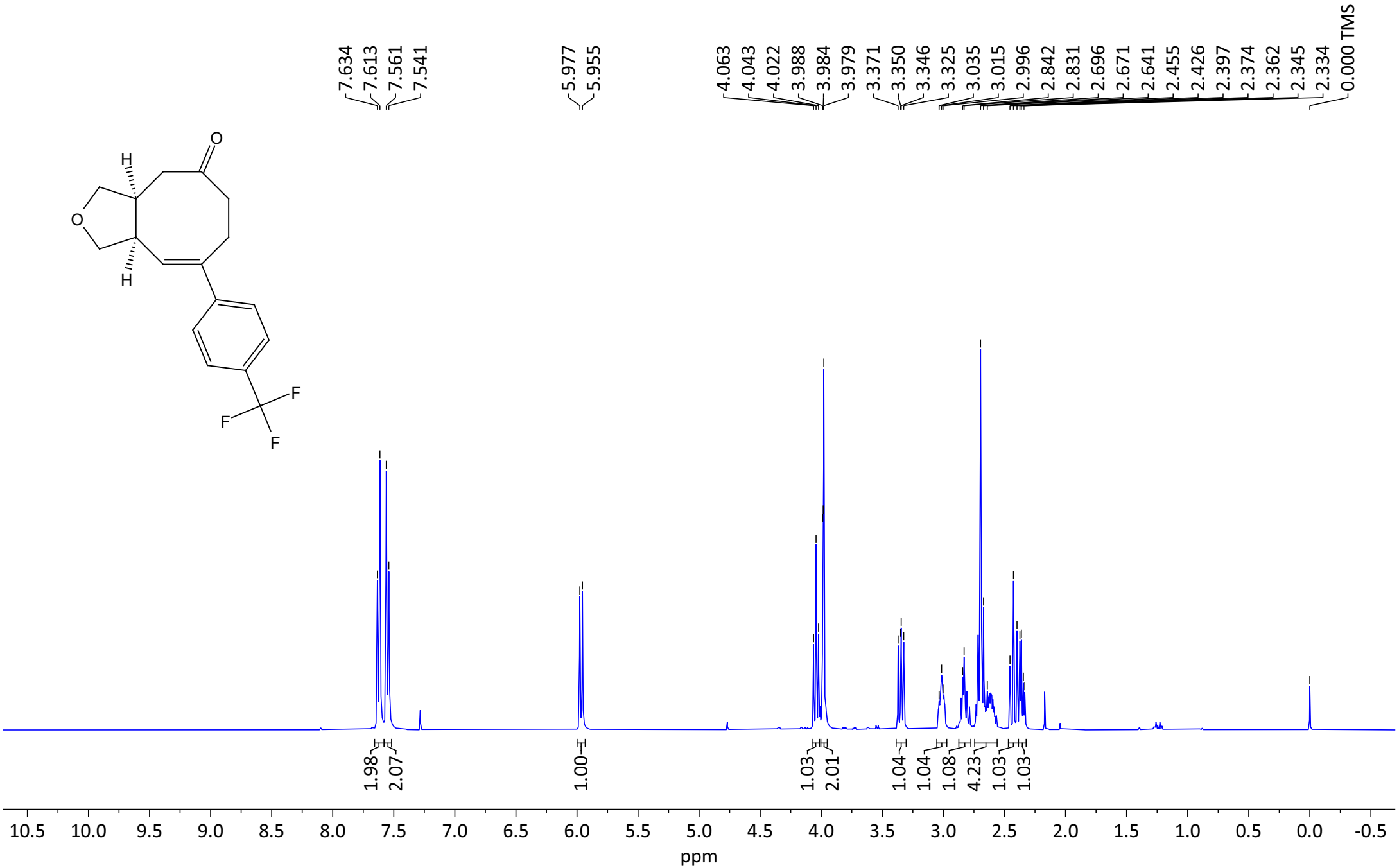
Compound **1a**: $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$)



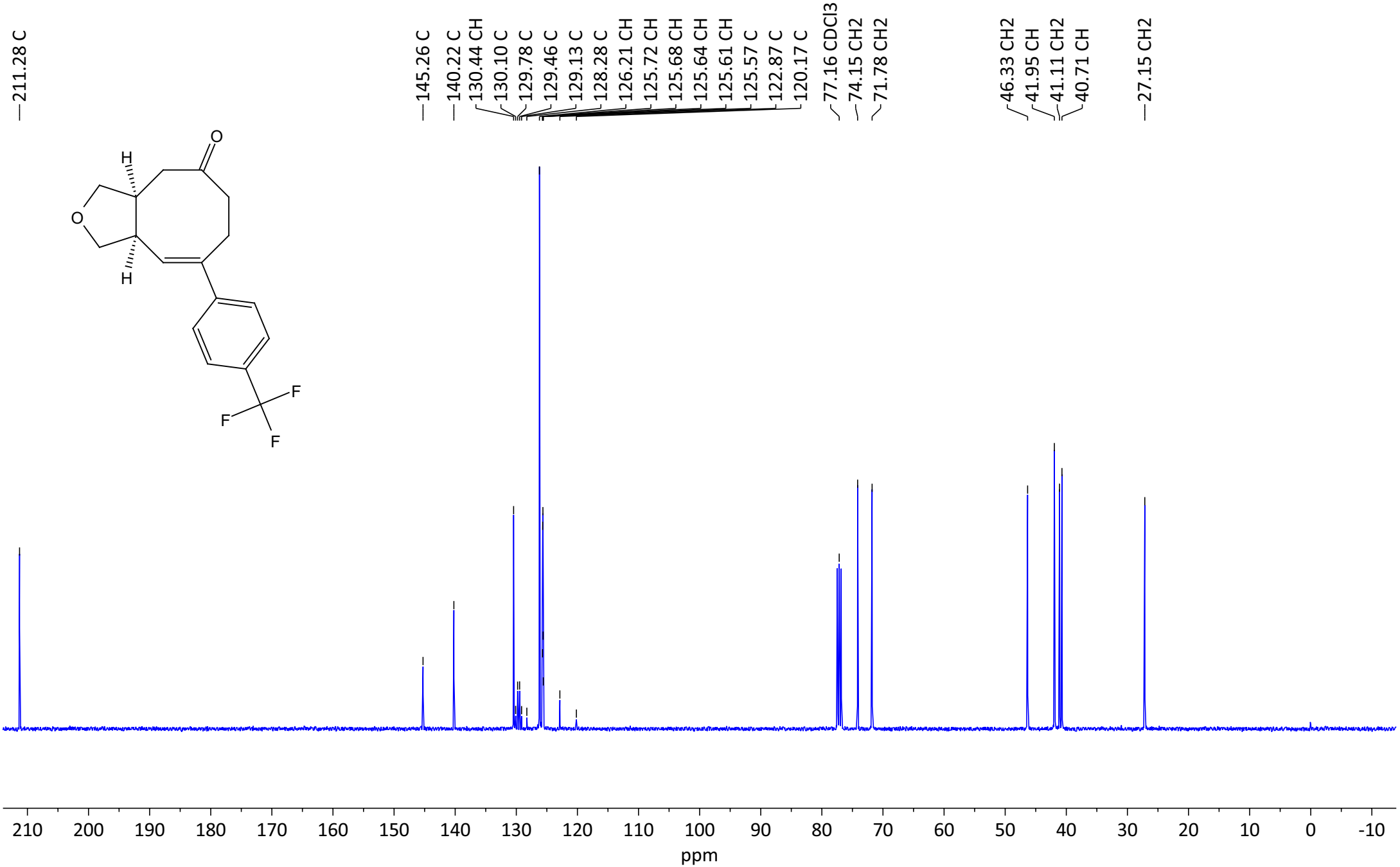
Compound **1a**: ^{19}F NMR (471 MHz, $CDCl_3$)



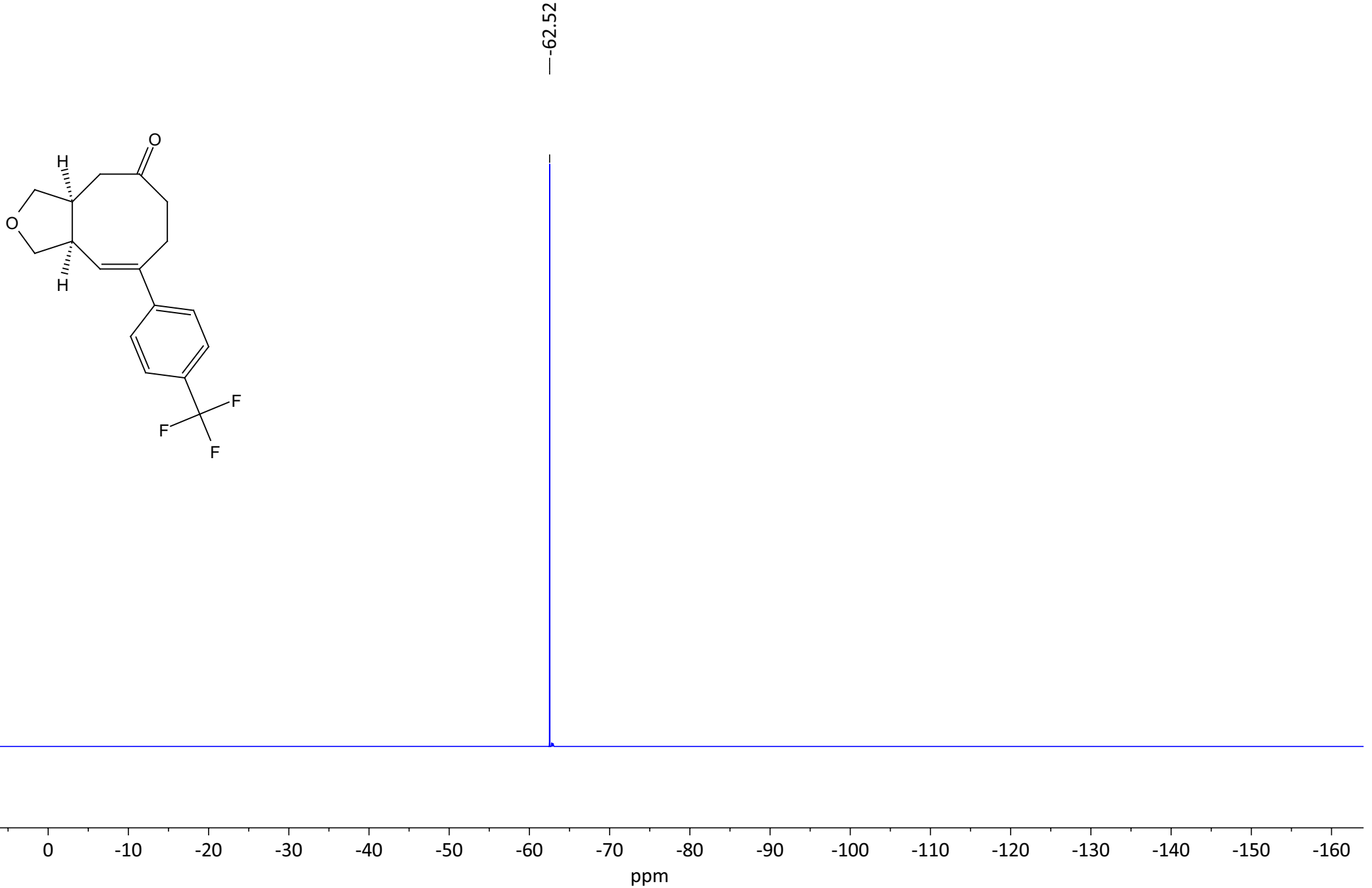
Compound **2a**: ^{1}H NMR (400 MHz, $CDCl_3$)



Compound **2a**: $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$)



Compound **2a**: ^{19}F NMR (471 MHz, $CDCl_3$)



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