Electronic Supplementary Material (ESI) for Green Chemistry.


# Supporting Information

## Dehydrogenative ester synthesis from enol ethers and water with a ruthenium complex catalyzing two reactions in synergy

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## 1. General Information

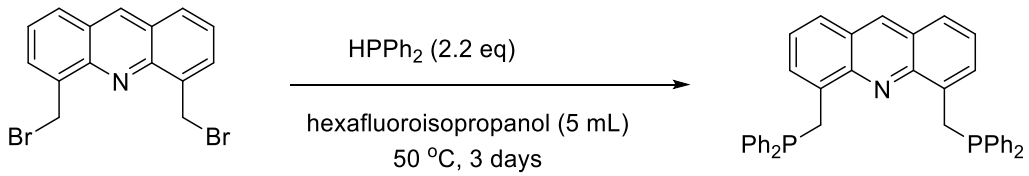
All experiments were carried out under an inert atmosphere (with $N_2$ or Ar) using standard Schlenk techniques. Complexes RuH(CO)Acr*PNP(*i*-Pr) (**1**),[1] RuHCl(CO)AcrPNP(i-Pr) (**2**),[2] RuH(CO)PNN$_{BPy}$*(*t*-Bu)(**3**),[3] RuH(CO)P$^{tBu}$NNH*(*t*-Bu) (**4**),[4,5], RuH(CO)$_2$Acr*PNP(*i*-Pr) (**5**)[6] were prepared according to the previously reported procedures. All catalysts were weighed inside a nitrogen filled glove box. The enol ethers were purchased from standard commercial sources (some of the substrates contained KOH or amine in 100 ppm amount as stabilizers). All solvents were purified according to standard procedures under an argon atmosphere, bubbled with argon, and stored over 4 Å molecular sieves. 1,3,5-trimethylbenzene (mesitylene) was purchased from commercial sources and used as received. Deionized water was used for the reactions which was degassed by bubbling argon for 30 minutes prior to its use.

NMR spectra were recorded at room temperature on a Bruker AMX-300, AMX-400 or AMX-500 spectrometers. Chemical shifts of the NMR spectra are reported relative to residual signals of $CDCl_3$ ($^1$H NMR: δ = 7.26 ppm, $^{13}$C NMR: δ = 77.16 ppm), benzene-$d_6$ ($^1$H NMR: δ = 7.16 ppm, $^{13}$C NMR: δ = 128.06 ppm), dicholoromethane-$d_2$ ($^1$H NMR: δ = 5.32 ppm, $^{13}$C NMR: δ = 54.00 ppm) or the internal standard mesitylene. $^{31}$P{$^1$H} NMR chemical shifts are reported in ppm downfield from $H_3PO_4$ and referenced to an external 85% solution of phosphoric acid in $D_2O$. GC–MS was carried out on HP 6890 (flame ionization detector and thermal conductivity detector) and HP 5973 (MS detector) instruments equipped with a 30 m column (Restek 5MS, 0.32 mm internal diameter) with a 5% phenylmethylsilicone coating (0.25 mm) and helium as carrier gas. GC was carried out on HP 6890 or Agilent 7890B Series GC System with $N_2$ or Helium as carrier gas. IR spectra were recorded on a Nicolet FTIR spectrophotometer (KBr, thin Film).

**Caution:** Reactions are associated with $H_2$ gas. They should be carefully handled inside proper fume hoods without any flame, spark or static electricity sources nearby.

## 2. Syntheses and characterization of complex RuH(CO)Acr*PNP(Ph) (**6**)

*Synthesis of the ligand*




**Procedure:** Inside a $N_2$ glove box, 1 mmol (365 mg) of acridine dimethylenebromide was dissolved in 5 mL of hexafluoroisopropanol, to which 2.2 mmol (410 mg) of diphenylphosphine was added dropwise. The solution was transferred to a pressure tube and was heated at 50 °C for 3 days. Afterwards, it was cooled down to room temperature, and 20 mL dichloromethane (DCM) was added. The solution was quickly washed with 30 mL of 10% aqueous NaOH. The organic layer was collected, and the aqueous layer was washed once more with 20 mL DCM. The combined DCM solutions were dried with $MgSO_4$, and DCM was removed in vacuo, affording a crude yellow solid.

The solid was then taken inside a glove box and dissolved using small amounts of THF. The solution was filtered through a small Celite pad. The THF was then removed, and the resulting yellow solid was washed with pentane, sparing amounts of ether, and methanol to obtain the pure acridinePNP(Ph) ligand in ~70% (400 mg) yield.

$^{31}$P NMR (162 MHz, $CDCl_3$) δ -9.69.

$^{1}$H NMR (400 MHz, Chloroform-*d*) δ 8.76 (s, 1H), 7.89 (d, *J* = 8.2 Hz, 2H), 7.52 (t, 8H), 7.43 – 7.23 (m, 16H), 4.42 (d, *J* = 1.7 Hz, 4H).

$^{13}$C{$^{1}$H} NMR (101 MHz, Chloroform-*d*) δ 146.60, 139.34 (d, *J* = 16.7 Hz), 136.68 (d, *J* = 6.2 Hz), 136.14, 133.06 (d, *J* = 18.7 Hz), 129.72 (d, *J* = 9.3 Hz), 128.37, 128.24 (d, *J* = 6.4 Hz), 126.63, 126.23, 125.26, 31.20 (d, *J* = 15.2 Hz).

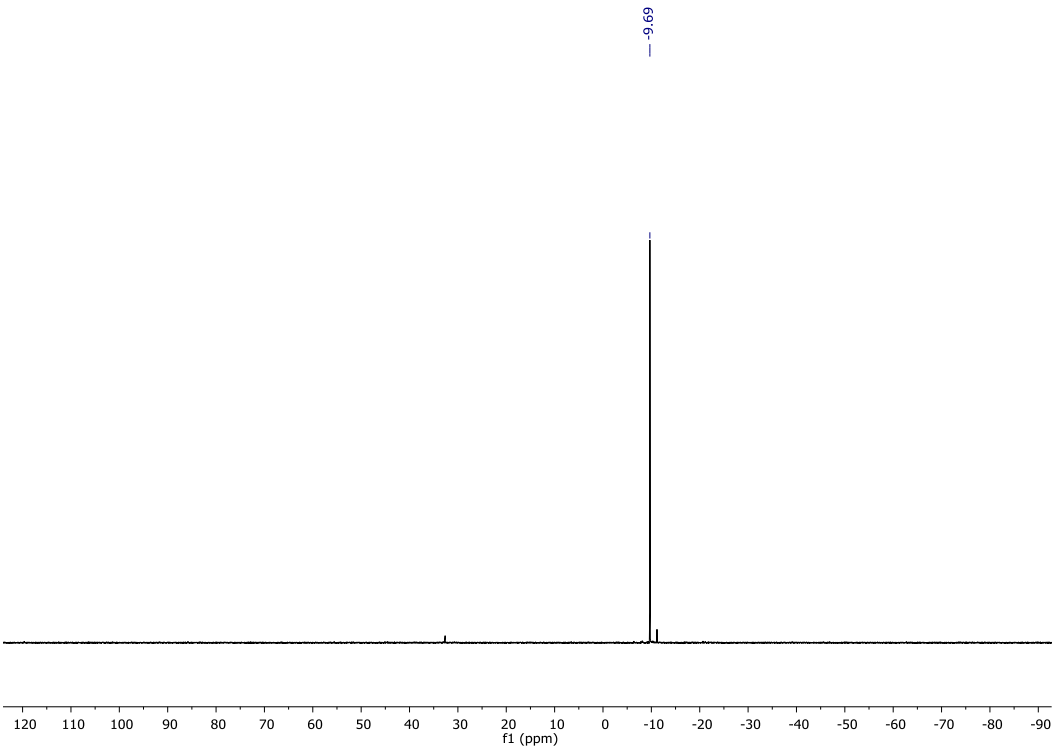



**Figure S1.** $^{31}P\{^{1}H\}$ NMR spectrum (162 MHz) of acridine PNP(Ph) ligand in $CDCl_3$.

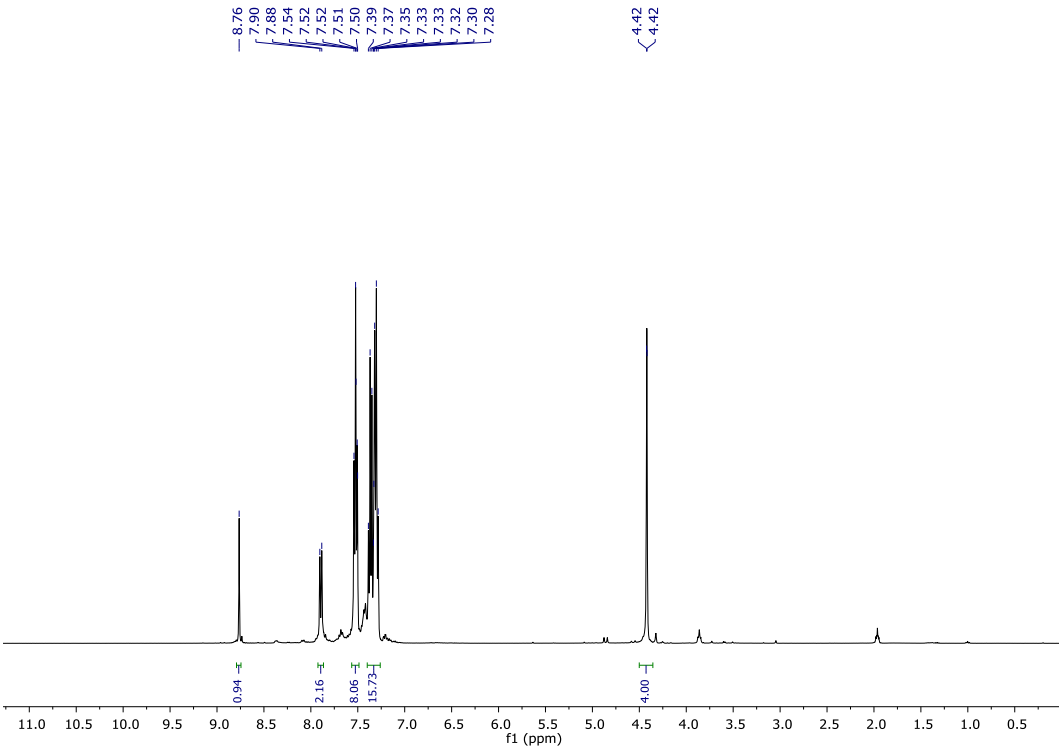



**Figure S2.** $^{1}H$ NMR spectrum (400 MHz) of acridine PNP(Ph) ligand in $CDCl_3$.

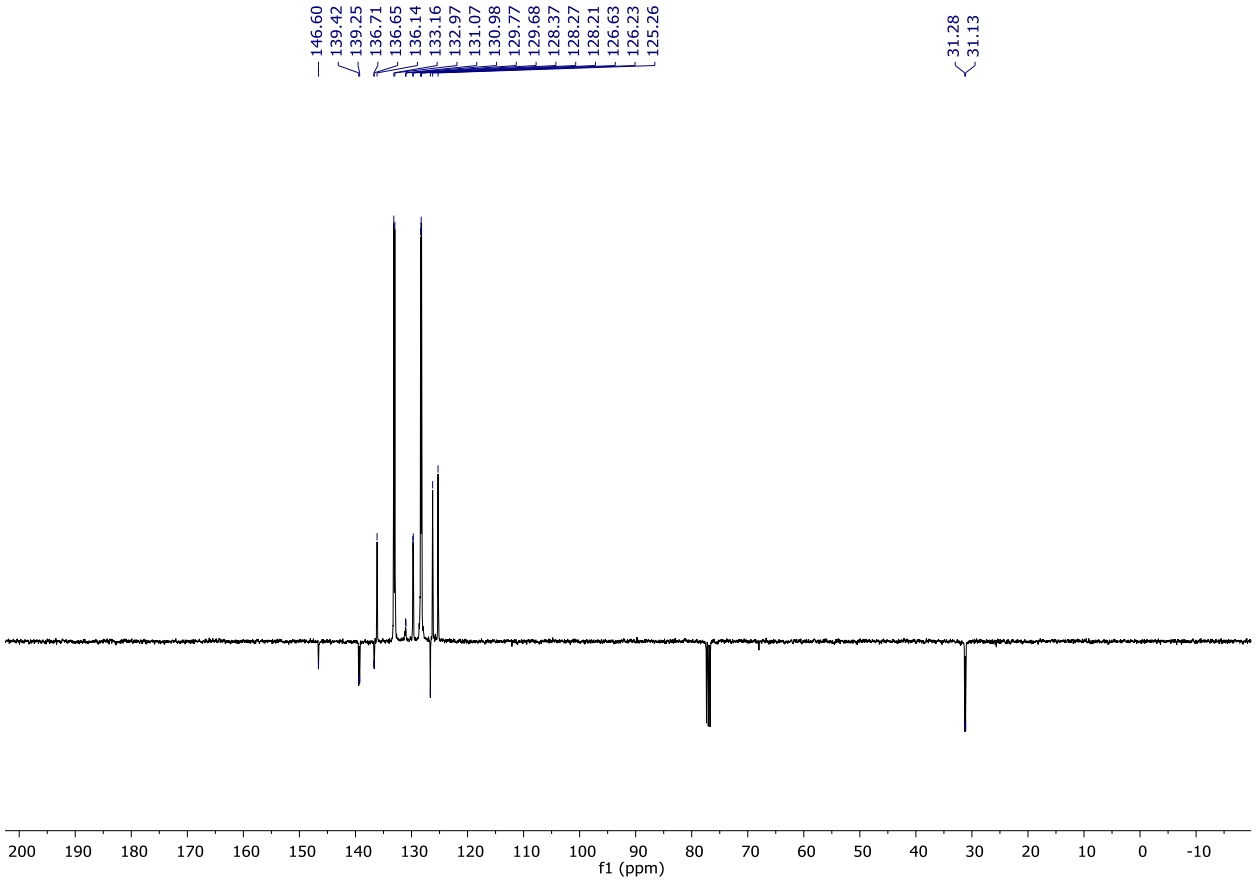
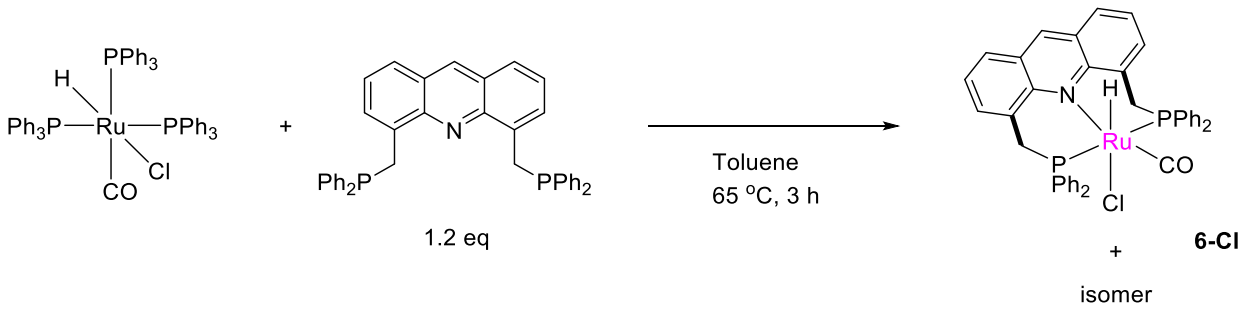



**Figure S3.** DEPT 135 NMR spectrum (101 MHz) of acridine PNP(Ph) ligand in $CDCl_3$.

*Synthesis of the aromatic acridine complex*




**Procedure:** Inside a $N_2$ glove box, 0.1 mmol of $RuHCl(CO)(PPh_3)_3$ (95.2 mg) and 0.12 mmol of the PNP(Ph) acridine ligand (69 mg) were suspended in 5 mL toluene. The solution was transferred to a pressure tube and was heated at 65 °C for 3 hours. Formation of yellow precipitates was observed during the reaction. After 3 hours, the reaction mixture was cooled to room temperature and the toluene was evaporated *in vacuo*. The resulting yellow solid was then washed with diethyl ether and THF for multiple times, affording the acridine complex as a yellow powder in 89% yield.

The complex is not soluble in less polar solvents such as benzene, toluene, or THF. NMR analysis of a $CD_2Cl_2$ solution showed the presence of two major isomers, along with one minor isomer, which can be directly used for the next step synthesis. The possibility of different isomers possible with the ruthenium acridine $PNP^{iPr}$ framework has been discussed before in the context of computational studies.[7] It is thus likely that while for the acridine $PNP^{iPr}$ complex only one isomer is thermodynamically favorable, for the $PNP^{Ph}$ complex, their energies are much more similar, leading to their co-observations. As mentioned before, both isomers lead to the generation of the same dearomatized complex upon the addition of super-hydride (next step).

$^{31}P$ NMR (162 MHz, $CD_2Cl_2$) δ 53.26 (minor, 0.44 P), 45.4 (major, 0.56 P).
$^{1}H$ NMR (500 MHz, $CD_2Cl_2$ ) δ 9.15 (s, 0.55H), 9.04 (s, 0.45H), 8.09 (d, J = 8.1 Hz, 1H), 7.98 (s, 3.1H), 7.88 (d, J = 5.5 Hz, 1.6H), 7.64 (d, J = 4.2 Hz, 1.7H), 7.53 (d, J = 6.8 Hz, 2.25H), 7.43 (M, 4.9), 7.34 (t, J = 7.0 Hz, 1.71), 7.31 – 7.24 (m, 1.6H), 7.24 – 7.08 (m, 5.6H), 6.91 (m, 1.6H), 5.37 (d, *J* = 7.9 Hz, 1.53H), 4.57 (d, *J* = 11.4 Hz, 1.1H), 4.05 (dd, J = 11.0, 3.9 Hz, 6H), -13.97 (t, J = 26.6 Hz, 1H), -16.71 (t, J = 19.9 Hz, 1H).
$^{13}C$ NMR (101 MHz, $CD_2Cl_2$) δ 153.37 151.93, 144.21, 142.83, 136.58, 135.51, 134.46, 133.71, 133.65, 133.59, 133.35, 132.89, 130.76, 130.32, 130.09, 129.71, 129.45, 129.07, 128.87, 128.46, 128.08, 127.84, 127.50, 127.45, 127.11, 124.97, 124.45, 35.53 (t, J = 10.4 Hz), 34.91 (J = 8.0 Hz).
IR (thin film, KBr) = 1953 $cm^{-1}$ (minor), 1931 $cm^{-1}$ (major) (CO).
HR-ESI-MS m/z calcd. for $C_{40}H_{32}NONaP_2ClRu$ [**6-Cl**-Na]$^+$: 764.0589, found: 764.1075.

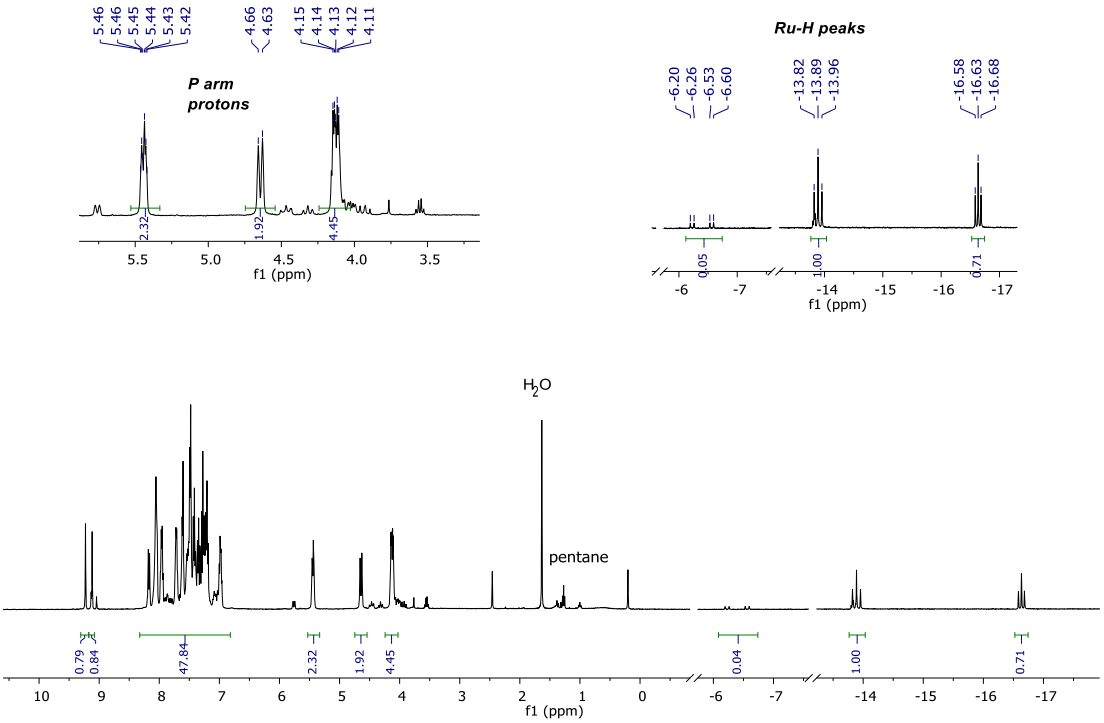



**Figure S4.** $^{1}H$ NMR spectrum (400 MHz) of Ru-Acr(Ph)HCl(CO) complex (**6-Cl**) in $CD_2Cl_2$. Two distinct hydride peaks of two different isomers are shown in inset.

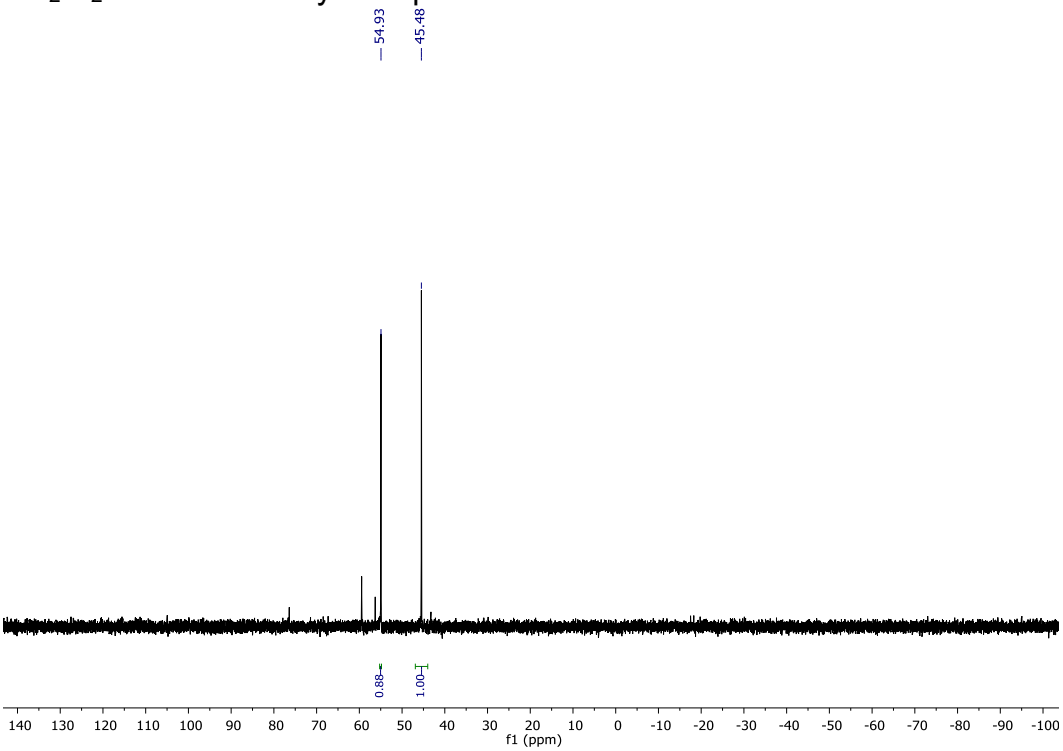



**Figure S5.** $^{31}P\{^{1}H\}$ NMR spectrum (162 MHz) of Ru-Acr(Ph)HCl(CO) (**6-Cl**) complex in $CD_2Cl_2$. Two distinct major isomers are seen, along with some minor complexes.

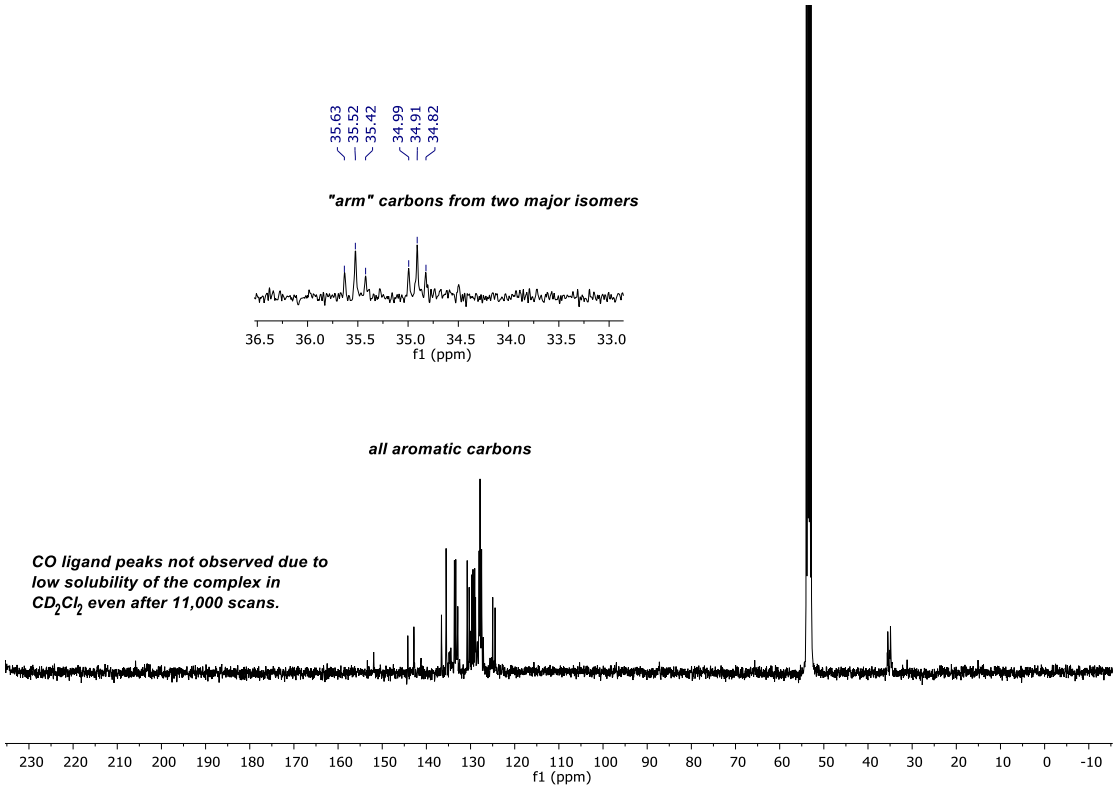



**Figure S6.** $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz) of Ru-Acr(Ph)HCl(CO) (**6-Cl**) complex in $C_6D_6$.

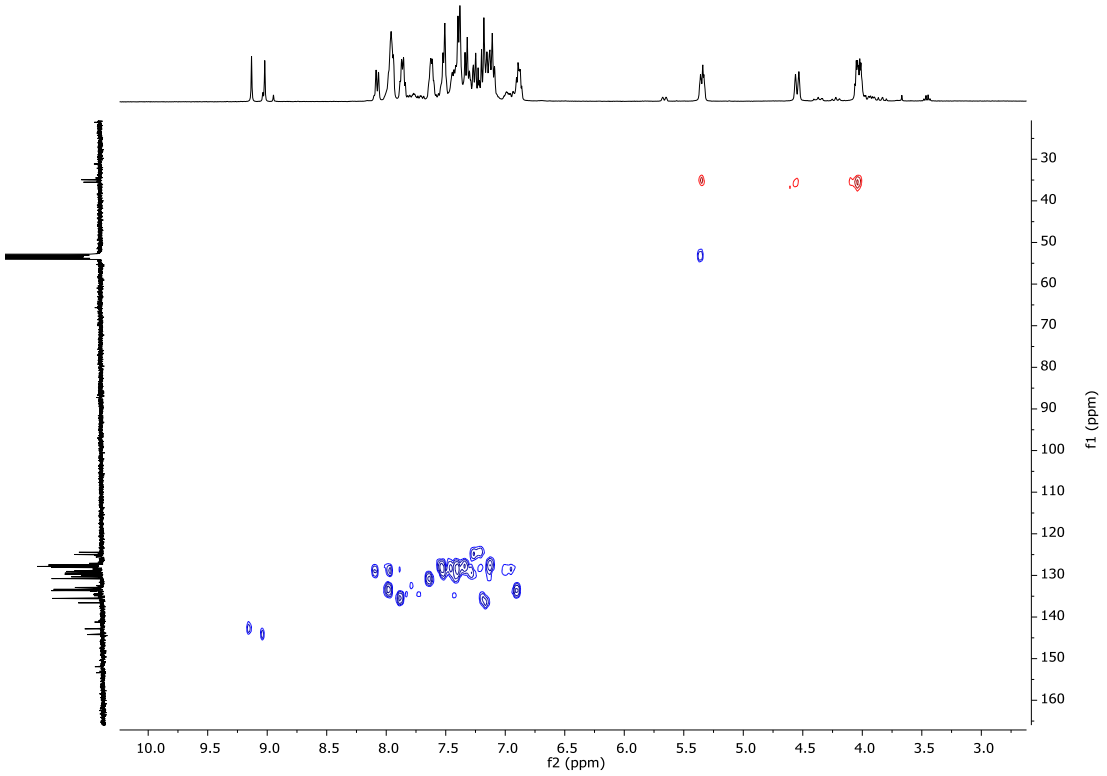
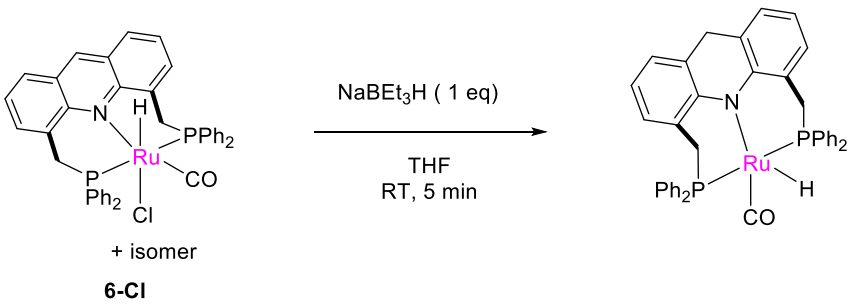



**Figure S7.** $^{1}H$-$^{13}C$ HSQC NMR spectrum of Ru-Acr(Ph)HCl(CO) (**6-Cl**) complex in $C_6D_6$.

*Synthesis of the acridine complex* **6**




**Procedure:** Inside a $N_2$ glove box, 25 mg of RuHCl(CO)Acr(Ph) complex (obtained in the previous step) was suspended in 5 mL THF. 1 eq of $NaBEt_3H$ (pre-dissolved in 3 mL THF) was then added to the solution dropwise over 5 minutes. The solution was allowed to stir for 5 mins at which the reaction solution turned from yellow to dark red. The stirring was then turned off, and the THF was removed *in vacuo*. The resulting solid was washed with diethyl ether (0.5 mLx3). Subsequently, the red solid was dissolved in 5 mL benzene and filtered through a short Celite® plug. The resulting filtrate was then frozen, and benzene was removed afterwards *in vacuo* to obtain complex **6** as red powder in 73% yield.

$^{31}$P NMR (162 MHz, Benzene-$d_6$) δ 53.70.

$^{1}$H NMR (400 MHz, Benzene-$d_6$) δ 7.70 – 7.48 (m, 3H), 7.47 – 7.30 (m, 3H), 7.06 (d, $J$ = 6.8 Hz, 2H), 7.02 – 6.90 (m, 13H), 6.77 – 6.43 (m, 5H), 3.97 (d, $J$ = 11.9 Hz, 2H), 3.79 (d, $J$ = 14.7 Hz, 1H), 3.71 (d, $J$ = 14.6 Hz, 1H), 3.42 (dt, $J$ = 12.1, 4.4 Hz, 2H), -21.35 (t, $J$ = 25.1 Hz, 1H).

$^{13}$C NMR (101 MHz, Benzene-$d_6$) δ 207.84, 152.89, 139.15 (t, $J$ = 24.1 Hz), 134.05 (t, $J$ = 7.6 Hz), 132.58 (t, $J$ = 18.1 Hz), 130.80, 130.18, 129.06, 128.74, 128.38 – 127.76 (m), 126.09, 120.15, 119.31, 36.12, 32.22 (t, $J$ = 11.7 Hz).

IR (thin film, KBr) = 1922 cm$^{-1}$ (carbonyl)

HR-ESI-MS m/z calcd. for $C_{40}H_{32}NOP_2Ru$ [**6-H**]$^+$: 706.1003 , found: 706.1011.

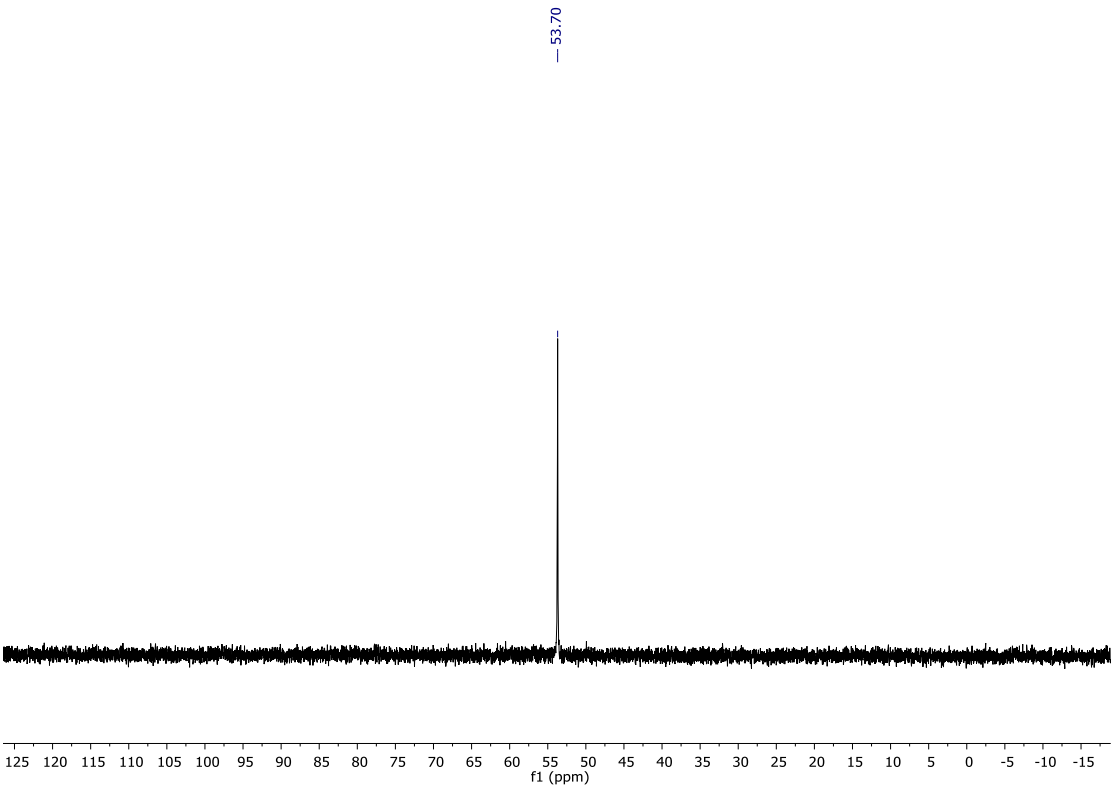



**Figure S8.** $^{31}P\{^{1}H\}$ NMR spectrum (162 MHz) of Ru-Acr*(Ph)H(CO) (**6**) complex in $C_6D_6$.

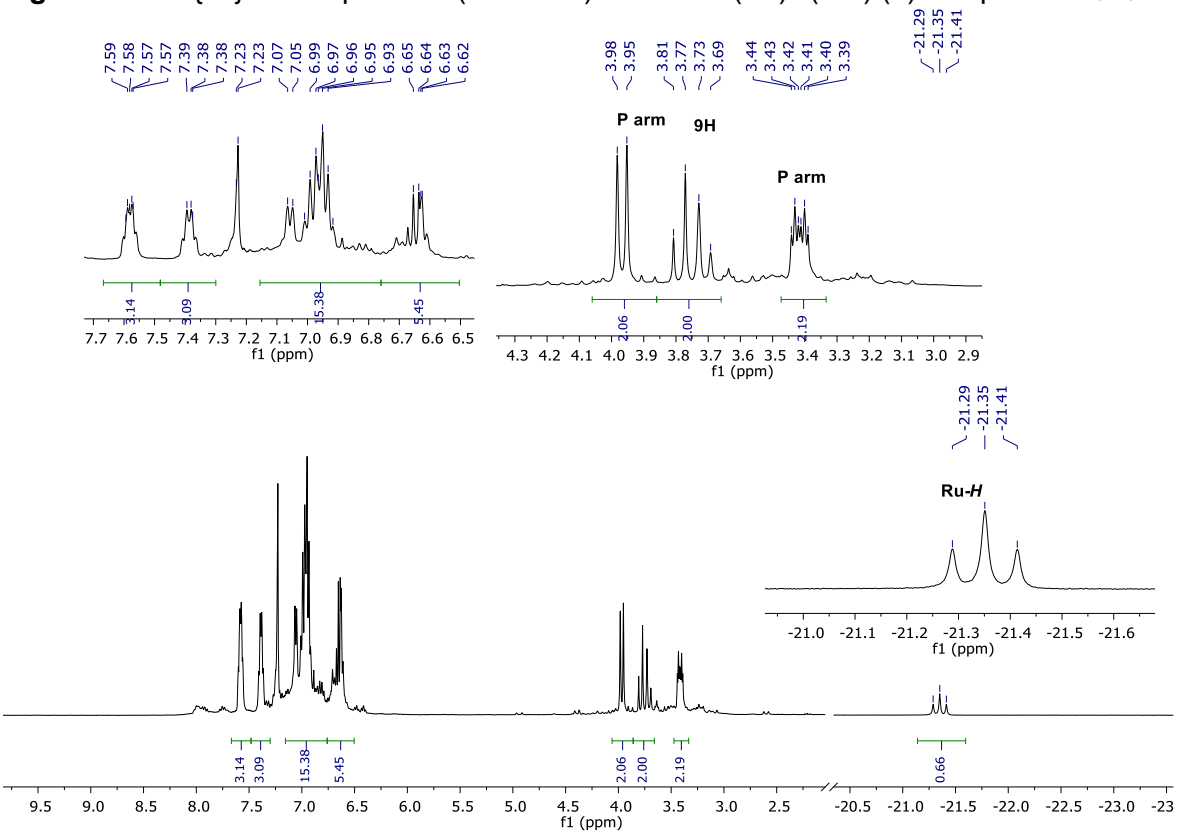



**Figure S9.** $^{1}H$ NMR spectrum (400 MHz) of Ru-Acr*(Ph)H(CO) (**6**) complex in $C_6D_6$.

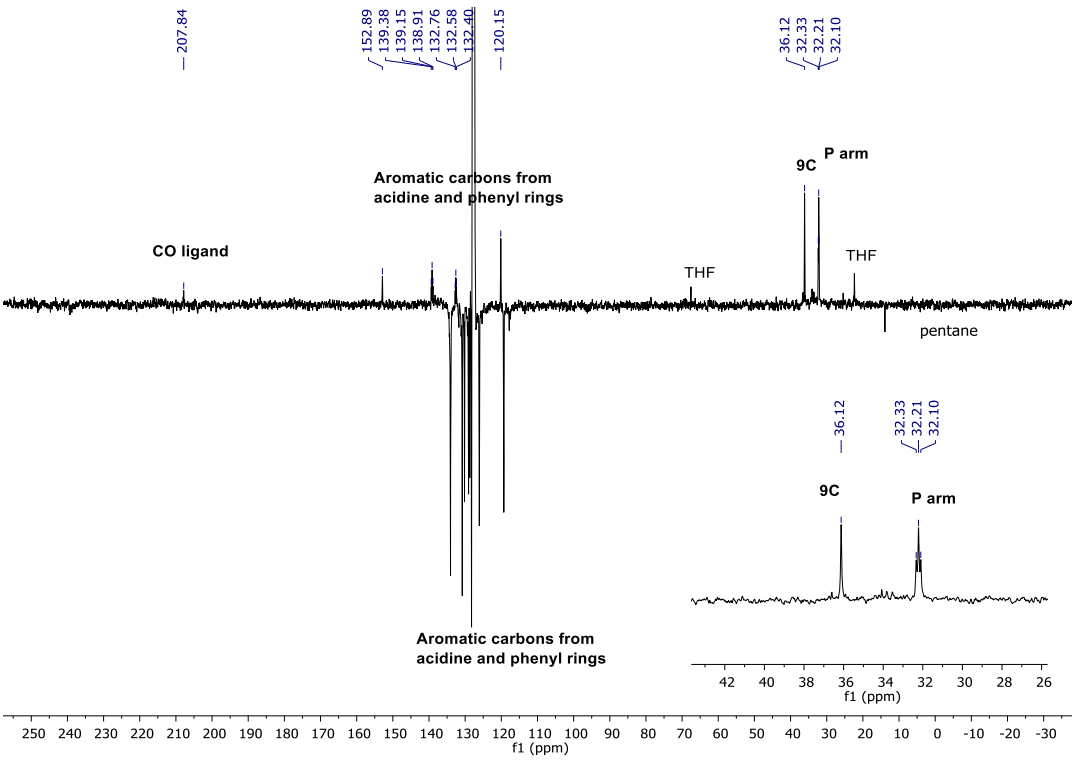



**Figure S10.** $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz) of Ru-Acr*(Ph)H(CO) (**6**) complex in $C_6D_6$.

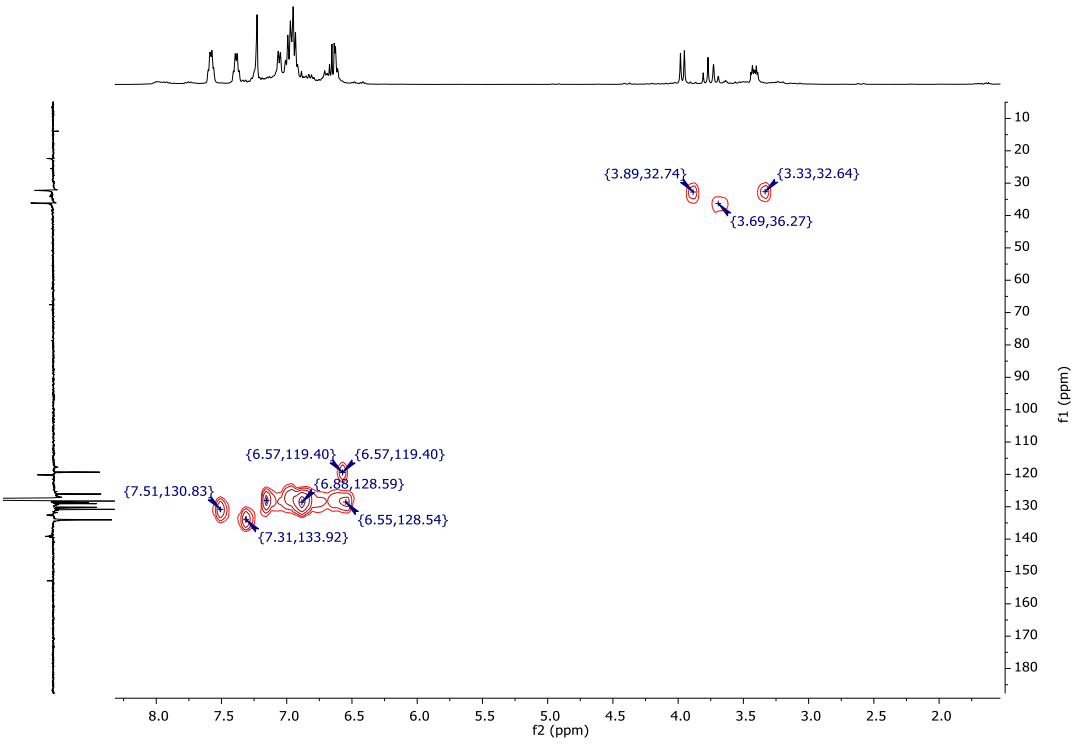
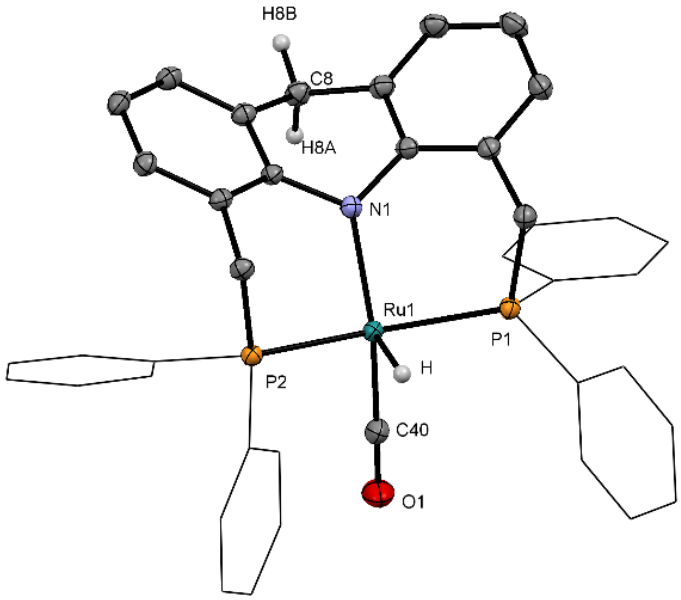
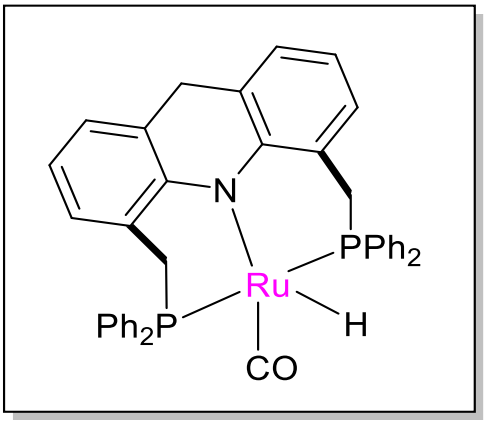



**Figure S11.** $^{1}H$-$^{13}C$ HSQC NMR spectrum of Ru-Acr*(Ph)H(CO) (**6**) complex in $C_6D_6$.

## 2.2. X-ray crystallography of complex 6 + $C_6H_6$



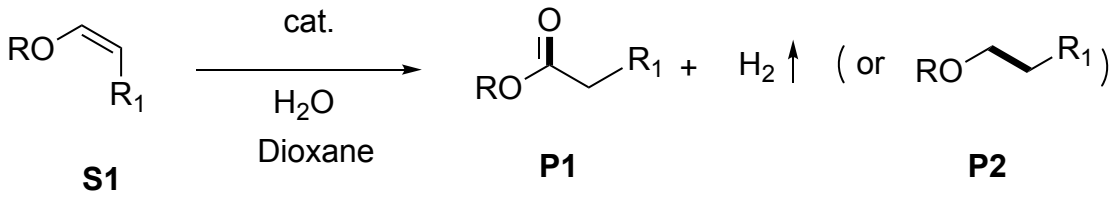

**Selected bond lengths (Å) and angles (º):** Ru(1)-H 1.47(2), Ru(1)-P(1) 2.3137(4), Ru(1)-P(2) 2.3087(4), Ru(1)-N(1) 2.0903(11), Ru(1)-C(40) 1.8288(15), P(1)-Ru(1)-H 80.5(9), P(2)-Ru(1)-H 80.1(9), P(2)-Ru(1)-P(1) 157.966(13), N(1)-Ru(1)-H 120.5(9), N(1)-Ru(1)-P(1) 90.48(3), N(1)-Ru(1)-P(2) 90.35(3), C(40)-Ru(1)-H 83.5(9), C(40)-Ru(1)-P(1) 94.47(5), C(40)-Ru(1)-P(2) 93.71(5), C(40)-Ru(1)-N(1) 155.92(6).

Data were collected on a Rigaku Synergy-S diffractometer dual source equipped with Dectris Pilatus R CdTe 300K detector and microfocus, with MoK$\alpha$ ($\lambda$=0.71073 Å). The data were processed with CrysAlis$^{PRO}$. Structure was solved by direct methods with SHELXT.[8] Data were refined as Full-matrix least-squares refinement based on $F^2$ with SHELXL[9] and OLEX2[10]. All non-hydrogen atoms were further refined with anisotropic displacement coefficients. Hydrogen atoms were assigned isotropic displacement coefficients, and their coordinates were allowed to ride on their respective carbons. Hydride was located in the electron density map. Crystallographic data and refinement parameters are summarized in Supplementary Table S1.

**Table S1.** Crystal data and structure refinement for complex **6** + $C_6H_6$

| | |
|---|---|
| Complex **6** + $C_6H_6$ | |
| Identification code | CCDC-2079903 |
| Empirical formula | $C_{46}$ $H_{39}$ N O $P_2$ Ru |
| Formula weight | 784.79 |
| Temperature | 100.00(10) K |
| Wavelength | 0.71073 A |
| Crystal system, space group | Monoclinic, P 1 21/n 1 |
| Unit cell dimensions | a = 12.7847(2) A alpha = 90 deg. |
| | b = 19.6339(3) A beta = 91.1120(10) deg. |
| | c = 14.6880(2) A gamma = 90 deg. |
| Volume | 3686.19(9) A^3 |
| Z, Calculated density | 4, 1.414 Mg/m^3 |
| Absorption coefficient | 0.550 mm^-1 |
| F(000) | 1616 |
| Crystal size | 0.181 x 0.131 x 0.055 mm |
| Theta range for data collection | 1.732 to 33.141 deg. |
| Limiting indices | -19<=h<=19, -30<=k<=30, -22<=l<=22 |
| Reflections collected / unique | 143025 / 14072 [R(int) = 0.0729] |
| Completeness to theta = 25.242 | 100.0 % |
| Absorption correction | Gaussian |
| Max. and min. transmission | 1.000 and 0.644 |
| Refinement method | Full-matrix least-squares on F^2 |
| Data / restraints / parameters | 14072 / 0 / 464 |
| Goodness-of-fit on F^2 | 1.053 |
| Final R indices [I>2sigma(I)] | R1 = 0.0322, wR2 = 0.0742 |
| R indices (all data) | R1 = 0.0414, wR2 = 0.0775 |
| Extinction coefficient | n/a |
| Largest diff. peak and hole | 0.539 and -0.490 e.A^-3 |

### 3. General procedure for the reactions




**S1** **P1** **P2**

In a $N_2$ glove box, the ruthenium catalyst (2.25 or 4.5 μmol) was dissolved in 2 mL of dry 1,4-dioxane. 0.3 mmol of enol ether was then added to the solution. The solution was transferred to a 25 mL Schlenk flask with a side arm and taken out of the box. The desired amount of water was then added to the solution under argon flow using Schlenk techniques. The flask was dipped into an oil bath preheated to the desired temperature. After suitable reaction time, the flask was cooled down to room temperature, opened, and a known amount of mesitylene was added to the solution as internal standard. Part of the reaction solution was then dried using $MgSO_4$ and analyzed via GC-MS, GC and $^1$H NMR. The yields were calculated based on the peak integration ratios in the GC or $^1$H NMR spectrum. For selected reactions, the accumulated gas volume in the headspace was measured and analyzed by GC.

All the ester products synthesized in this study have been reported previously in the literature. All products were identified by comparison of the $^1$H NMR spectra from literature or by GC-MS spectra with those of the commercially available compounds. The GC-MS retention times and observed m/z values are provided in Table S2.

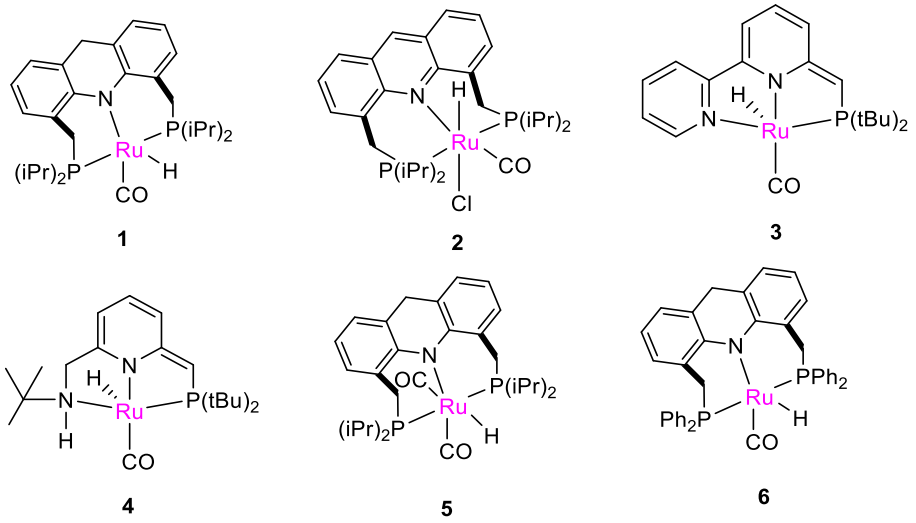
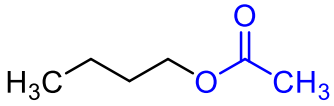
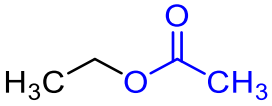
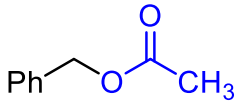
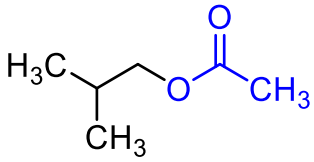
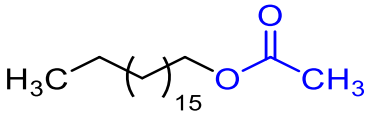
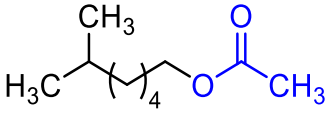
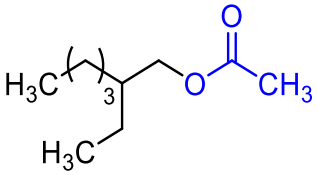
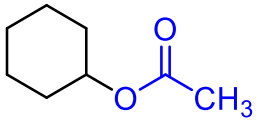
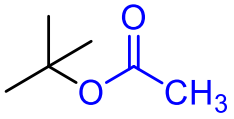
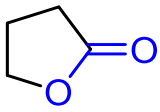
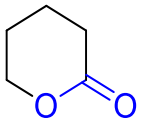
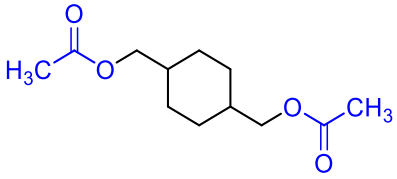
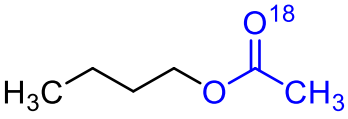



**Figure S12.** Complexes screened for oxidative dehydrogenative ester synthesis in this study.

**Table S2.** GC-MS data for esters using HP 6890 equipped with flame ionization and thermal conductivity detectors and HP 5973 (MS detector) instruments, equipped with a 30 m column (Restek 5MS, 0.32 mm internal diameter) with a 5% phenylmethylsilicone coating (0.25 mm) and helium as carrier gas with a flow-rate of 1 ml/min). The parameters are shown in Figure S13.

| | | |
|---|---|---|
|  <br>$t_r$ = 5.8 min<br>m/z = 101.0 (M-$CH_3$) |  <br>$t_r$ = 2.1 min<br>m/z = 88.1 |  <br>$t_r$ = 11.5 min<br>m/z = 150.1 |
|  <br>$t_r$ = 4.5 min<br>m/z = 115.0 (M-H) |  <br>$t_r$ = 19.8 min<br>m/z = 312.3 |  <br>$t_r$ = 11.5 min<br>m/z = 129.1 (M-$C_3H_8$) |
|  <br>$t_r$ = 11.4 min<br>m/z = 129.1 (M-$C_3H_8$) |  <br>$t_r$ = 10.0 min<br>m/z = 127.1 (M-$CH_3$) |  <br>$t_r$ = 2.9 min<br>m/z = 101.1 (M-$CH_3$) |
|  <br>$t_r$ = 8.0 min<br>m/z = 86.0 |  <br>$t_r$ = 11.7 min<br>m/z = 100.0 |  <br>$t_r$ = 15.8 min (30%), 15.85 min (70%)<br>m/z = 168.0 (minor), 168.1 (major) |
|  <br>$t_r$ = 5.8 min<br>m/z = 103.0 (M-$CH_3$) | | |

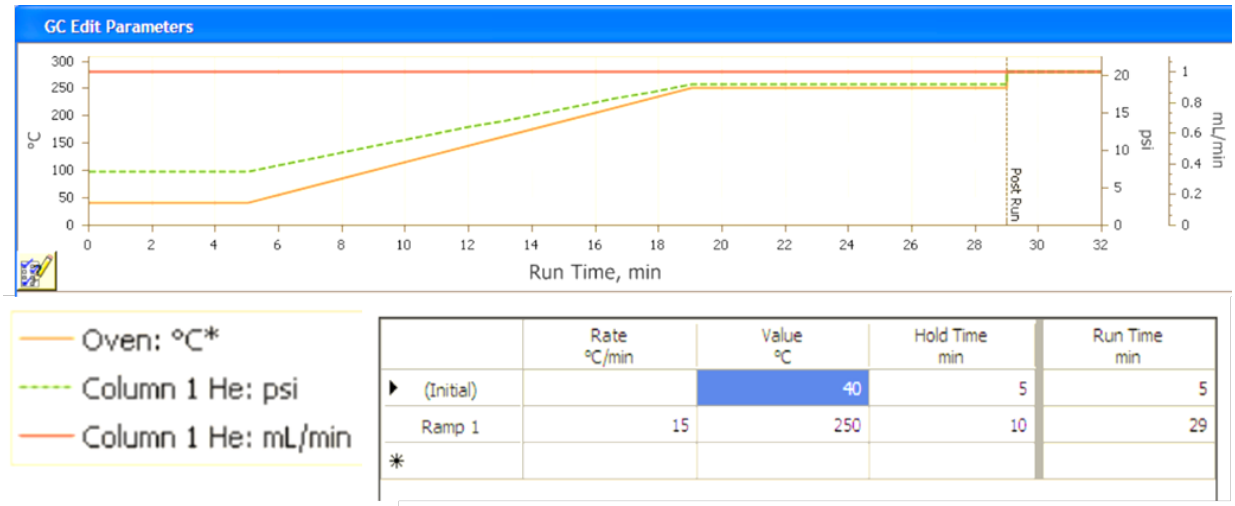



**Figure S13.** Method parameters for the GC-MS.

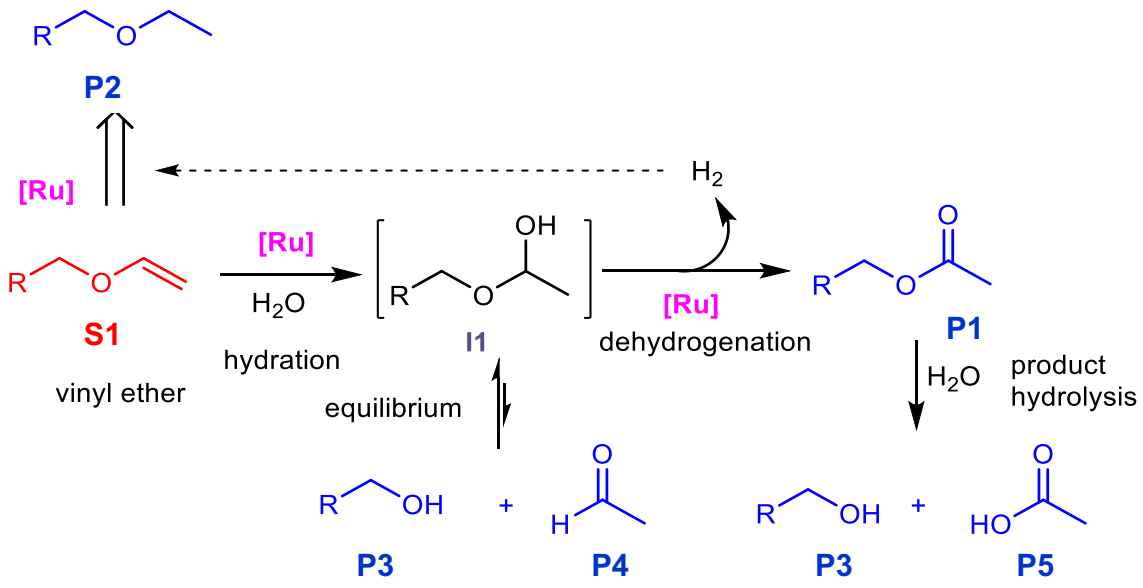



**Figure S14.** Simplified possible reaction sequences of enol ethers in presence of [Ru] and water.

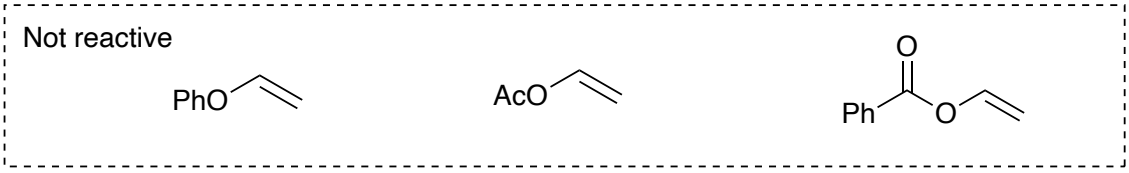



**Figure S15.** Unreactive vinyl ethers under the reaction condition of Table 2.

***GC analysis of the headspace gas mixture***

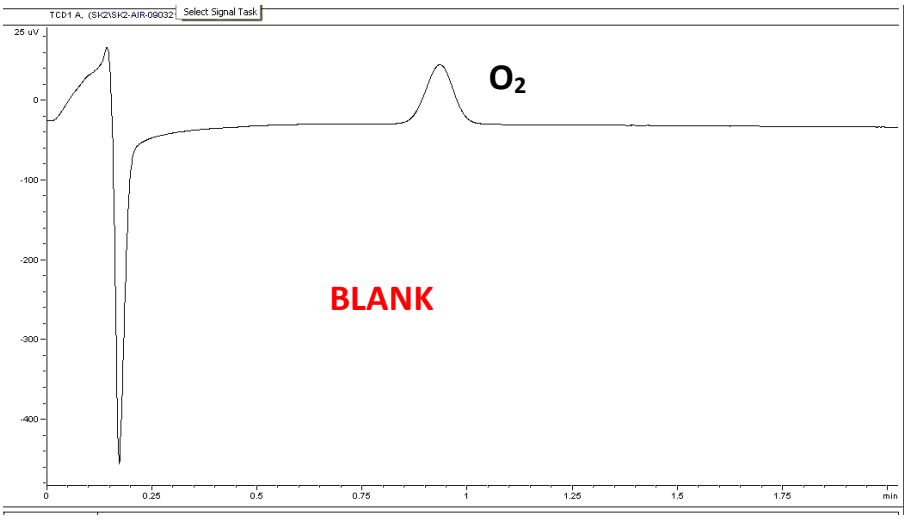



**Figure S16a.** GC of a blank air sample. The peak around 1 min is due to the presence of $O_2$ gas. $N_2$ was used as the carrier gas.

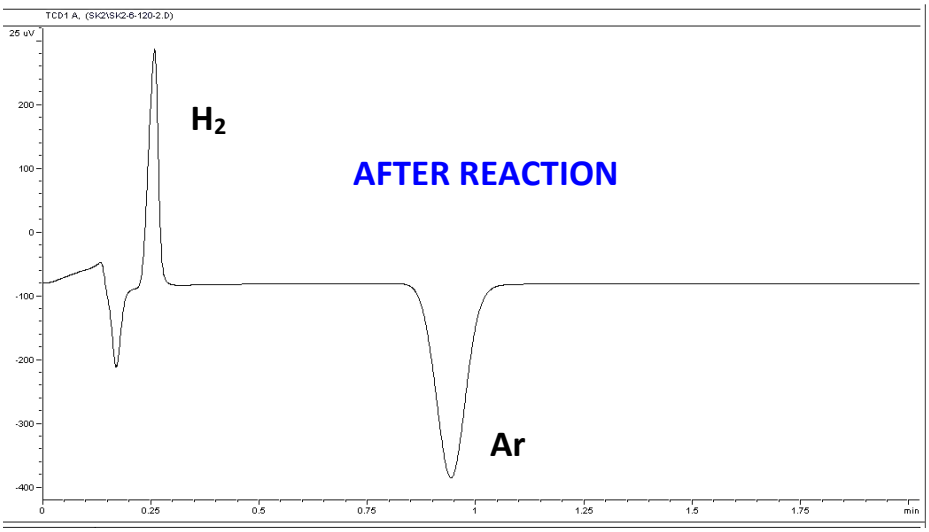
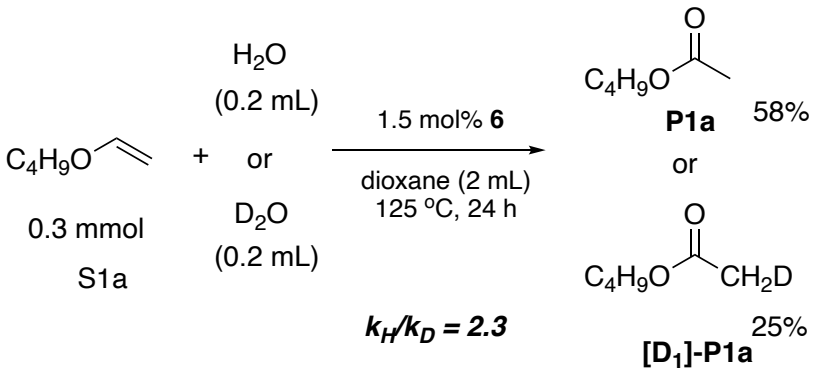



**Figure S16b.** Typical GC of the headspace gas after reaction. The peak at 0.25 min is due to the presence of $H_2$ gas. The negative peak at 0.9 min is for the Ar gas. $N_2$ was used as the carrier gas.

### 3.1. Procedure for the kinetic isotope effect experiment




**Procedure:** In a $N_2$ glove box, the ruthenium catalyst **6** (4.5 μmol) was dissolved in 2 mL of dry 1,4-dioxane. 0.3 mmol of butyl vinyl ether was then added to the solution. The solution was transferred to a 25 mL Schlenk flask with a side arm and taken out of the box. 0.25 mL of $H_2O$ or $D_2O$ was then added to the solution under argon flow using Schlenk techniques. The flask was dipped into an oil bath preheated to 125 °C. After 24 h, the flask was cooled down to room temperature, opened, and a known amount of mesitylene was added to the solution as internal standard. Part of the reaction solution was then dried using $MgSO_4$ and analyzed via GC-MS, and $^1H$ NMR. Yields were calculated from the $^1H$ NMR spectra. 58% of ester yield was observed when $H_2O$ was used (conversion 67%), whereas 25% of deuterated ester was observed when $D_2O$ was used (conversion 34%).

## 4. Representative GC and NMR spectra after reaction

### 4.1. Copies of $^1$H NMR spectra of selected crude reaction mixtures

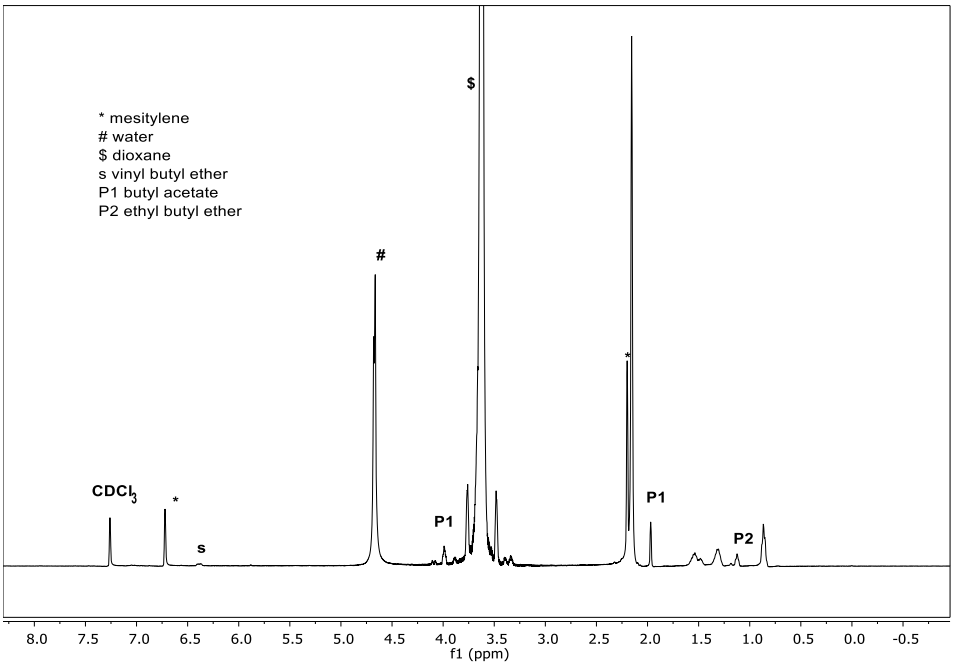



**Figure S17.** $^1$H NMR of the reaction mixture from table 1, entry 5 in $CDCl_3$. Reaction conditions: butyl vinyl ether (0.3 mmol), $H_2O$ (0.2 mL), **1** (1.5 mol%), 1,4-Dioxane (2 mL), 125 $^o$C, 24 h.

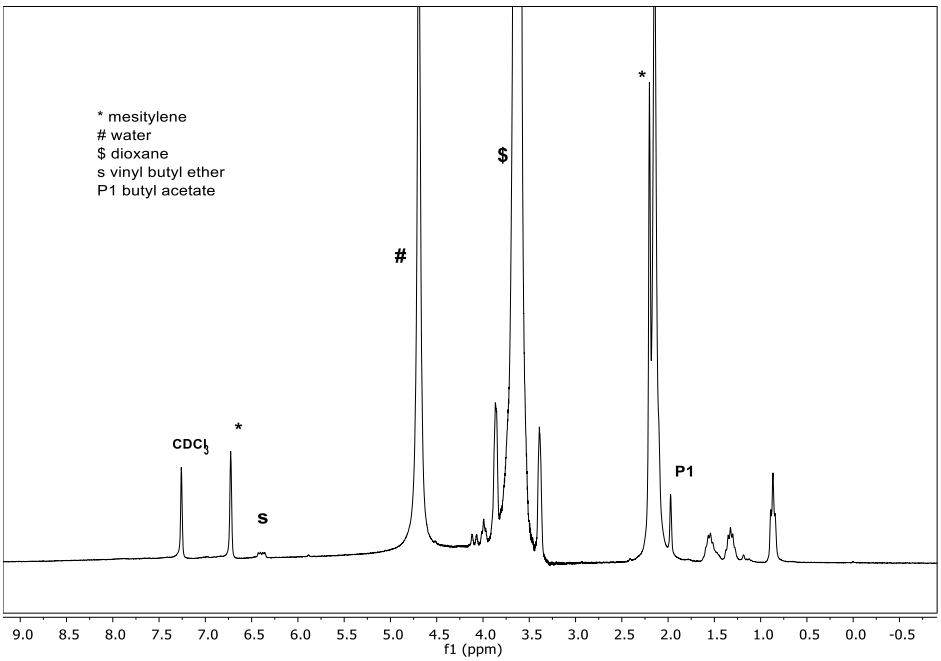



**Figure S18.** $^1$H NMR of the reaction mixture from table 1, entry 13. Reaction conditions: butyl vinyl ether (0.3 mmol), $H_2O$ (0.2 mL), **6** (1.5 mol%), 1,4-Dioxane (2 mL), 125 $^o$C, 24 h.

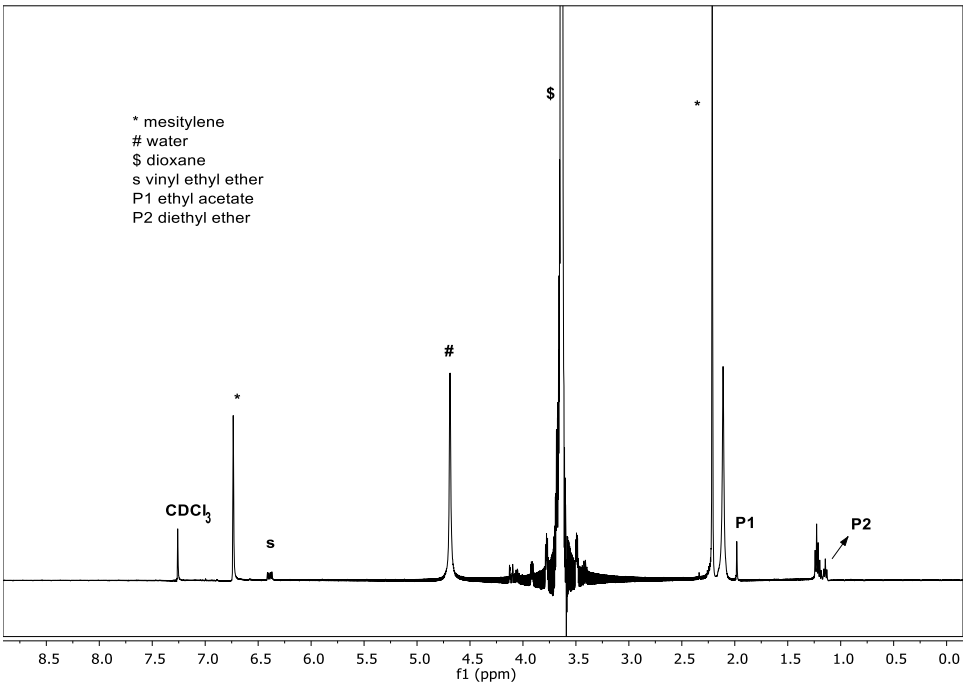



**Figure S19.** $^1$H NMR of the reaction mixture from table 1, entry 3. Reaction conditions: ethyl vinyl ether (0.3 mmol), $H_2O$ (0.2 mL), **1** (1.5 mol%), 1,4-Dioxane (2 mL), 125 $^oC$, 24 h.

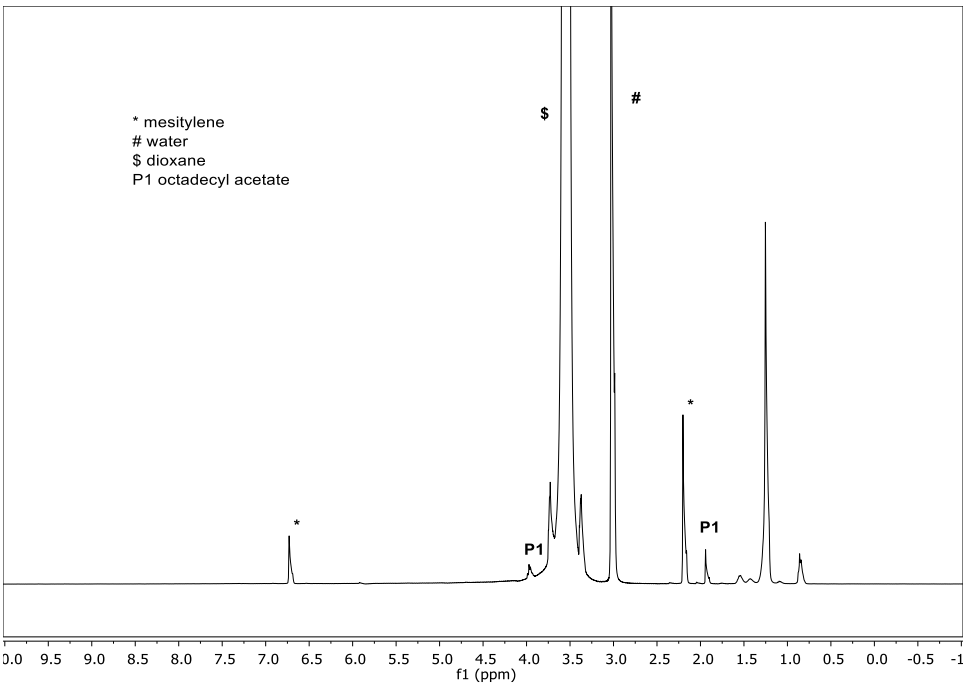



**Figure S20.** $^1$H NMR of the reaction mixture for the synthesis of **P1e**. Reaction conditions: vinyl octadecyl ether (0.3 mmol), $H_2O$ (0.25 mL), **6** (1.5 mol%), 1,4-Dioxane (2 mL), 125 $^oC$, 36 h.

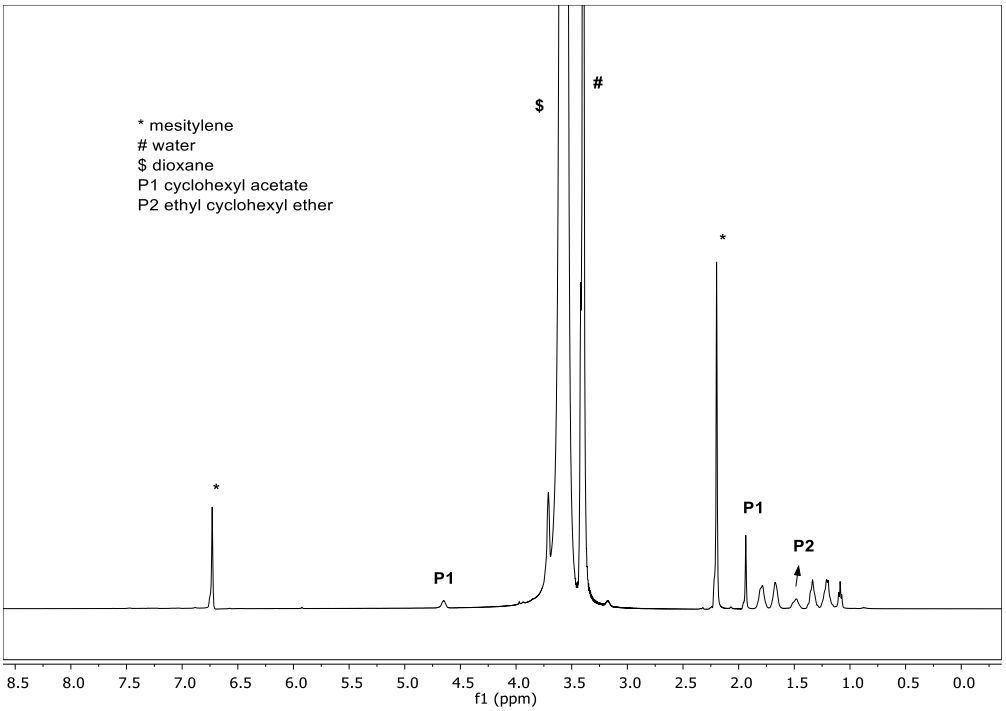



**Figure S21.** $^1$H NMR of the reaction mixture for the synthesis of **P1h**. Reaction conditions: vinyl cyclohexyl ether (0.3 mmol), $H_2O$ (0.25 mL), **6** (1.5 mol%), 1,4-Dioxane (2 mL), 125 $^o$C, 36 h.

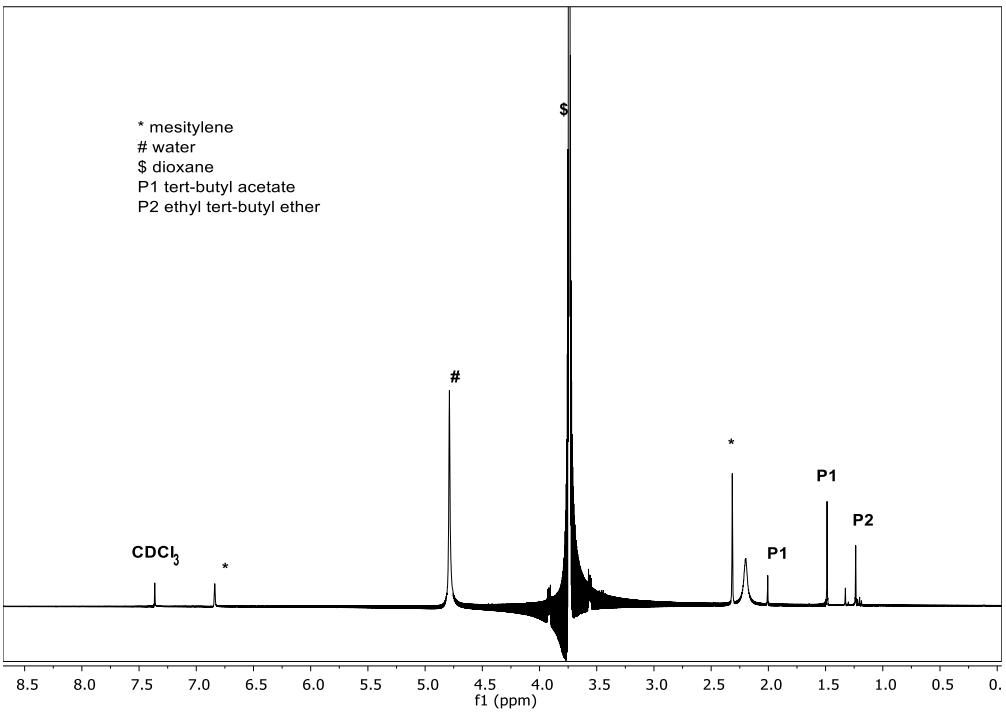



**Figure S22.** $^1$H NMR of the reaction mixture for the synthesis of **P1i**. Reaction conditions: vinyl *tert*-butyl ether (0.3 mmol), $H_2O$ (0.25 mL), **6** (1.5 mol%), 1,4-Dioxane (2 mL), 125 $^o$C, 36 h.

### 4.2. Copies of GC-MS chromatogram of selected crude reaction mixtures

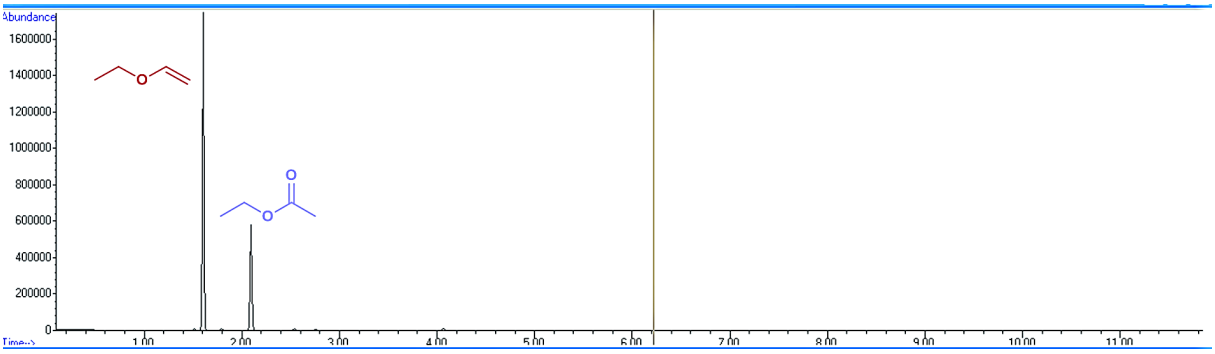



**Figure S23.** GC-MS chromatogram of the crude reaction mixture from Table 1, entry 2, showing the generation of ethyl acetate after the reaction (peak at 2.1 min). Detector off during 1,4-dioxane (3-4 min).

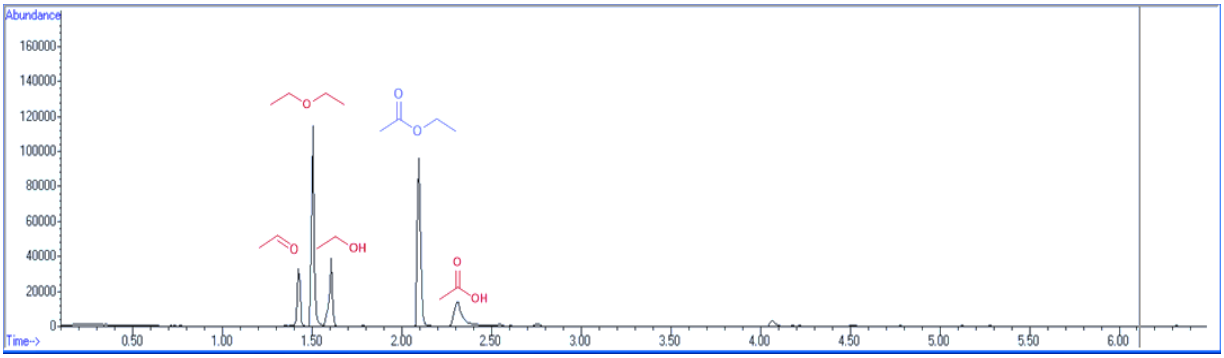



**Figure S24.** GC-MS chromatogram of the crude reaction mixture from Table 1, entry 4, showing the generation of other side products at higher water amount. Detector off during dioxane (3-4 min).

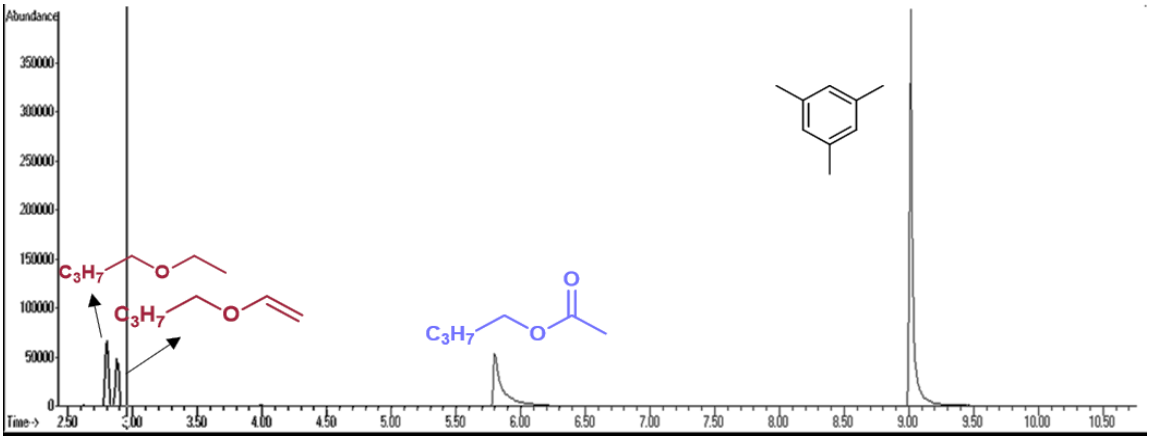



**Figure S25.** GC-MS chromatogram of the crude reaction mixture from Table 1, entry 5, showing the generation of ester and also hydrogenation side product when **1** is used as catalyst. Detector off during 1,4-dioxane (3-4 min).

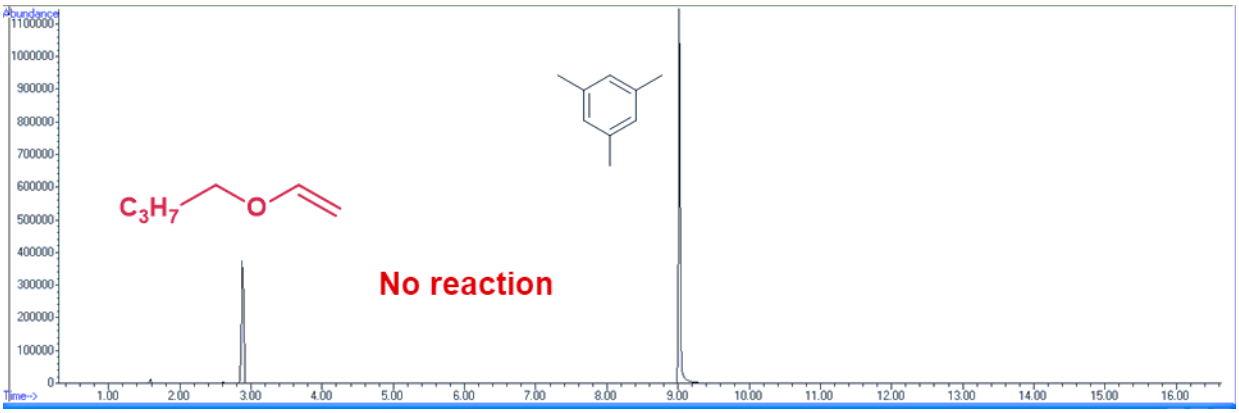



**Figure S26.** GC-MS chromatogram of the crude reaction mixture from Table 1, entry 7, showing thar complex **2** is not active in catalyzing the reaction. Detector off during 1,4-dioxane (3-4 min).

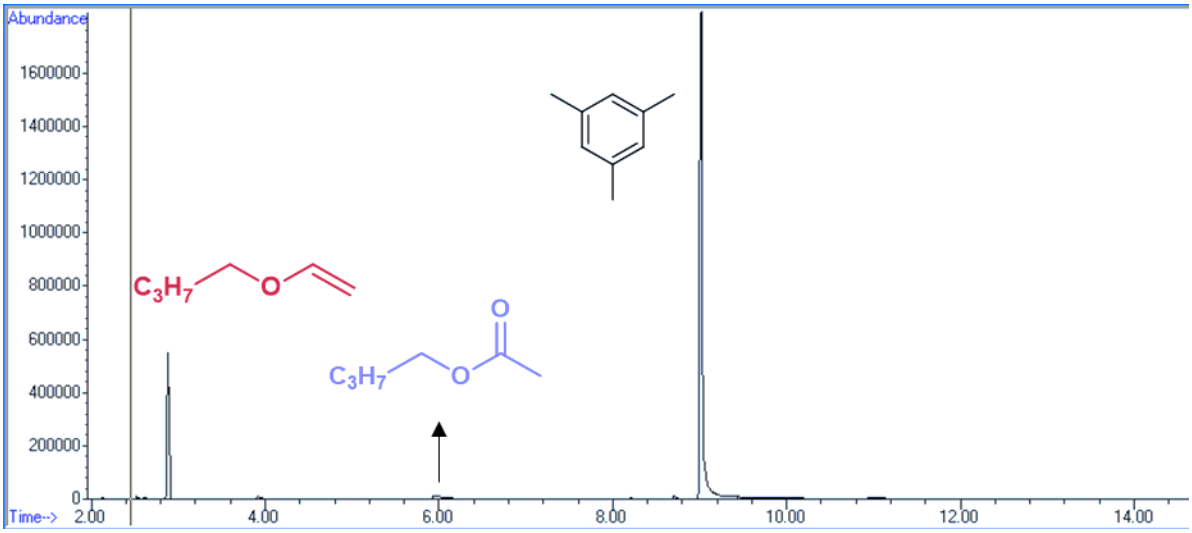



**Figure S27.** GC-MS chromatogram of the crude reaction mixture from Table 1, entry 9, showing that the coordinatively saturated dicarbonyl complex **5** is not a very effective catalyst for the transformation. Detector off during 1,4-dioxane (3-4 min).

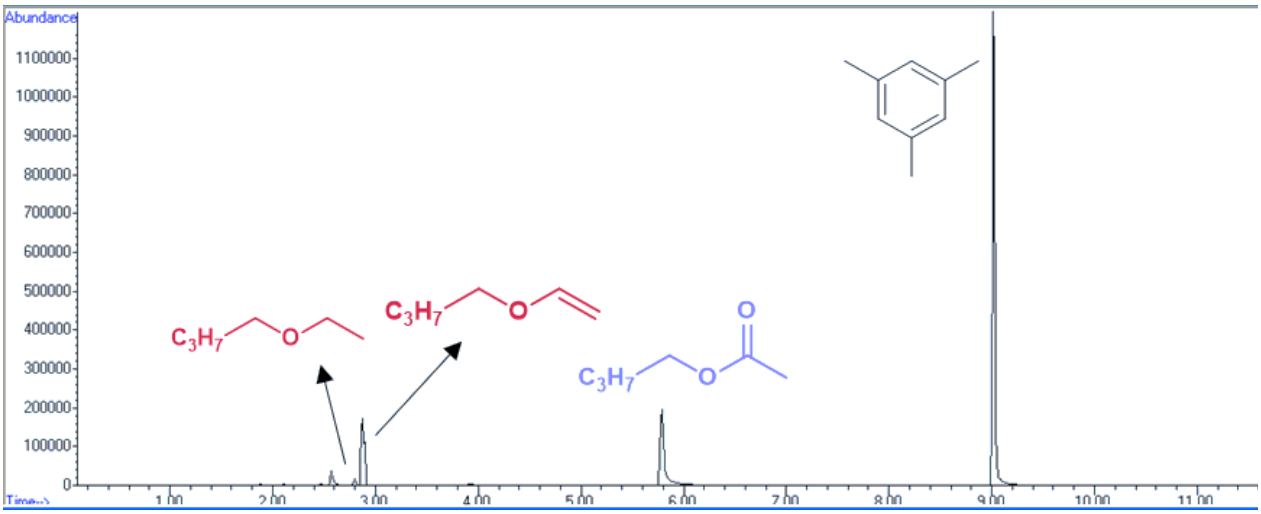



**Figure S28.** GC-MS chromatogram of the crude reaction mixture from Table 1, entry 10, showing the abatement in the hydrogenation side reaction when **6** is used as catalyst. Detector off during 1,4-dioxane (3-4 min)

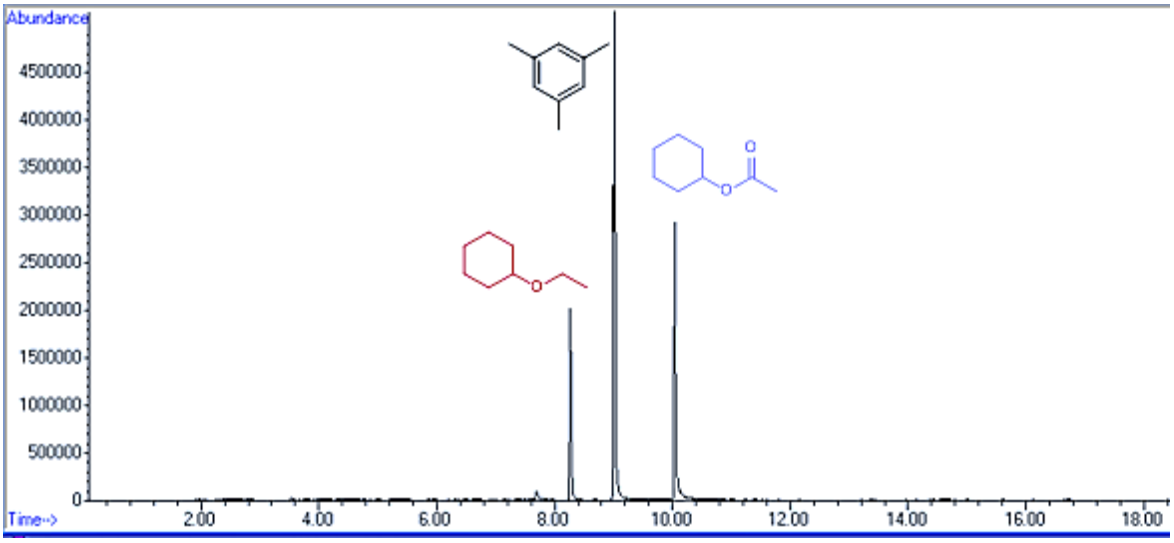



**Figure S29.** GC-MS chromatogram of the crude reaction mixture for the synthesis of **P1h**, showing the generation of the ester as major product along with hydrogenation side product. Detector off during 1,4-dioxane (3-4 min).

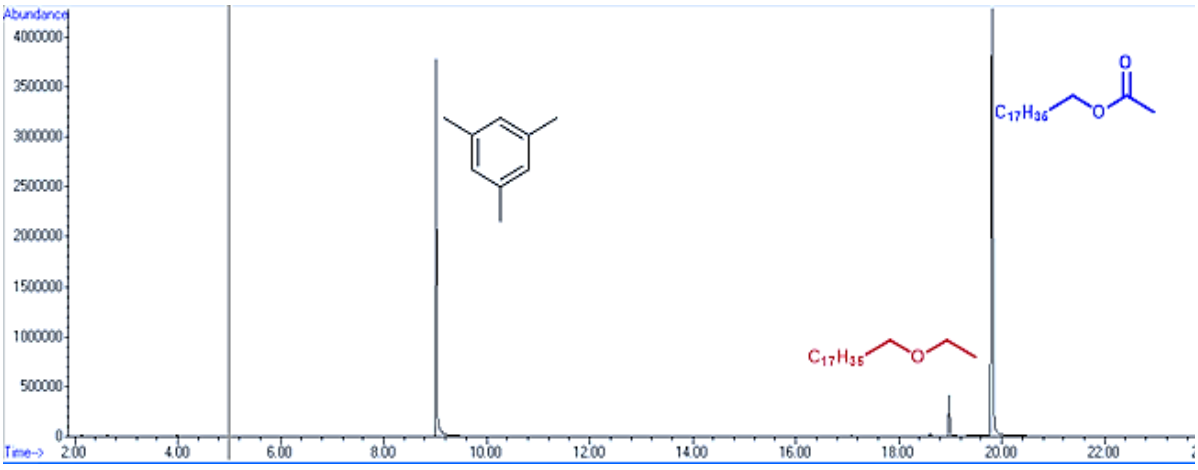



**Figure S30.** GC-MS chromatogram of the crude reaction mixture for the synthesis of **P1e**, showing the generation of the ester in high yield along with minimal hydrogenation side product. Detector off during 1,4-dioxane (3-4 min).

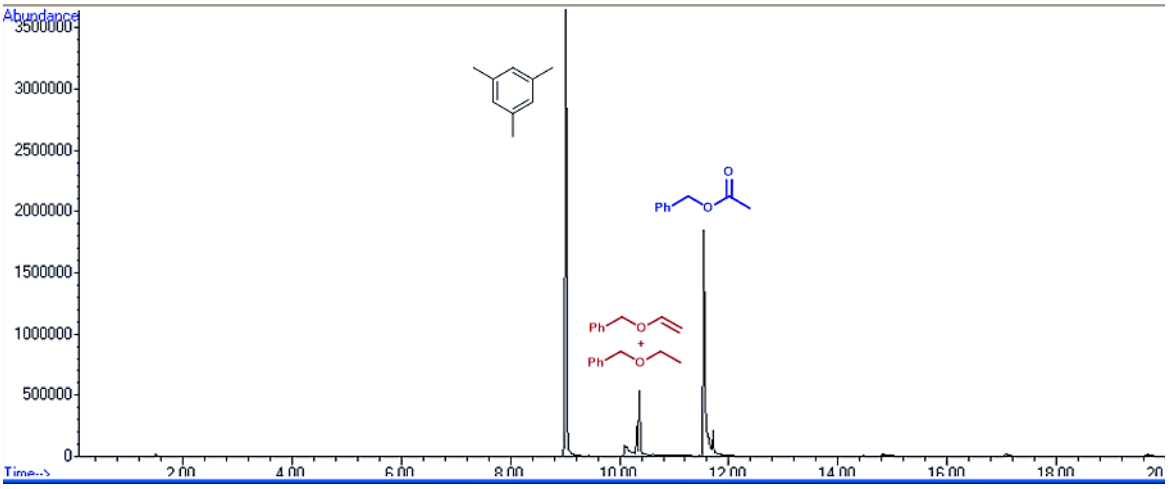



**Figure S31.** GC-MS chromatogram of the crude reaction mixture for the synthesis of **P1c**, showing the formation of benzyl acetate from vinyl benzyl ether via this method. Detector off during 1,4-dioxane (3-4 min).

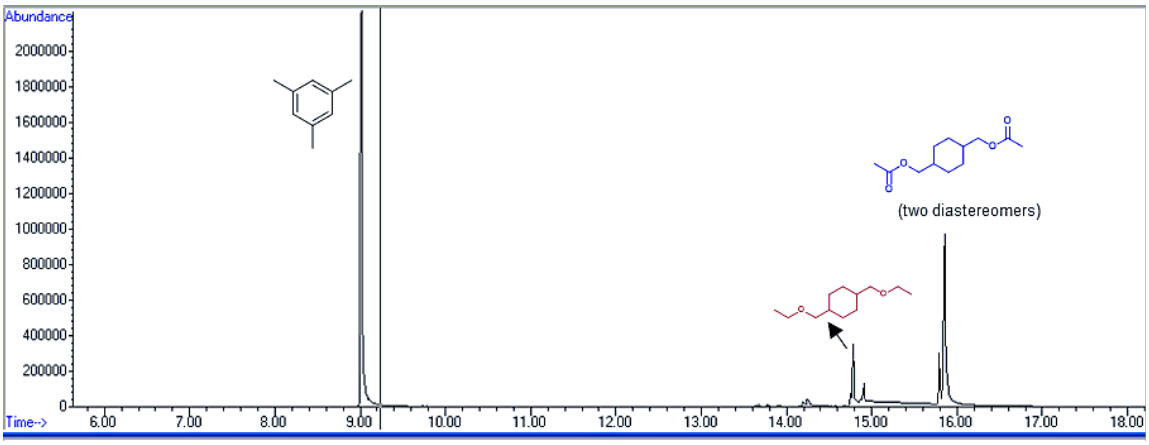



**Figure S32.** GC-MS chromatogram of the crude reaction mixture showing the formation of diester **P2j** via this method. Detector off during 1,4-dioxane (3-4 min).

### 4.3. MS of the labelled ester

For the synthesis of $^{18}O$ labelled ester, a standard reaction was set up with vinyl ether but instead of 0.25 mL of $H_2O$, 0.1 mL of $H_2{}^{18}O$ was used as reactant. After 36 h of reaction at a bath temperature of 125 $^oC$, the reaction mixture was worked up via the standard procedure and the GC and GC-MS specta were taken. 56% yield of the ester was observed and the MS spectra showed the presence of $^{18}O$ atom in the product in the fragmentation pattern.

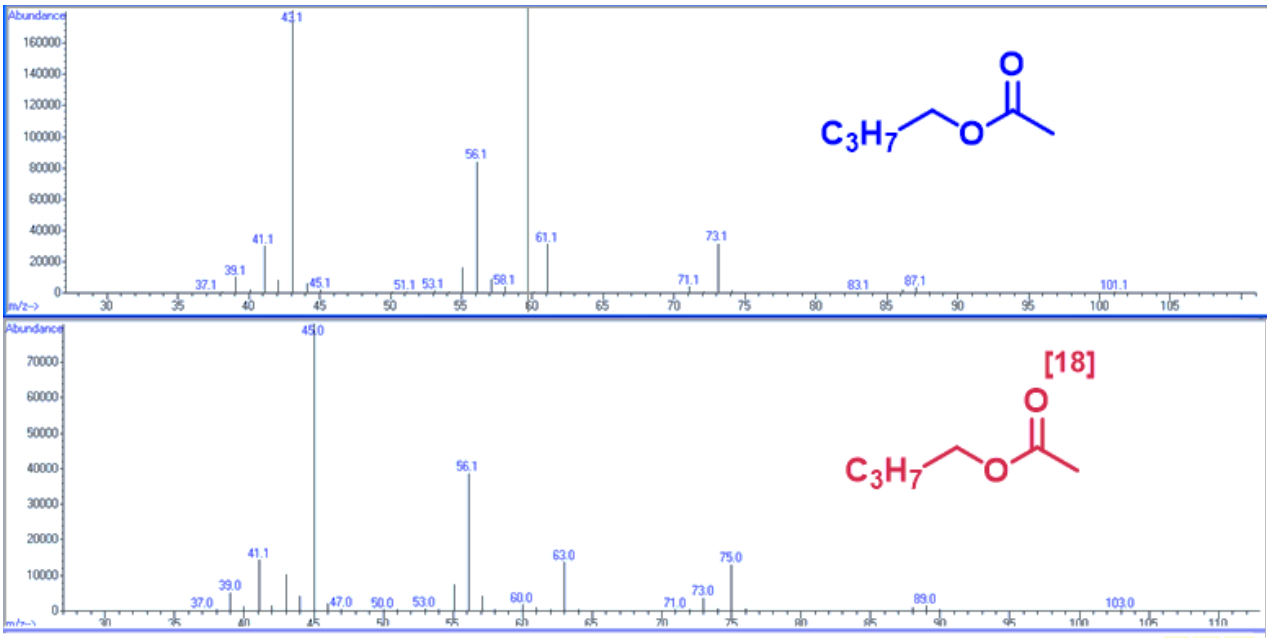



**Figure S33.** Comparison of the MS spectra of obtained unlabeled butyl acetate and $^{18}O$ labelled butyl acetate via this method. The fragmentation pattern clearly indicates the incorporation of an $^{18}O$ atom in the molecule.

## 5. Mechanistic studies

### 5.1. Reaction of complex 1 with vinyl butyl ether and water as observed in NMR

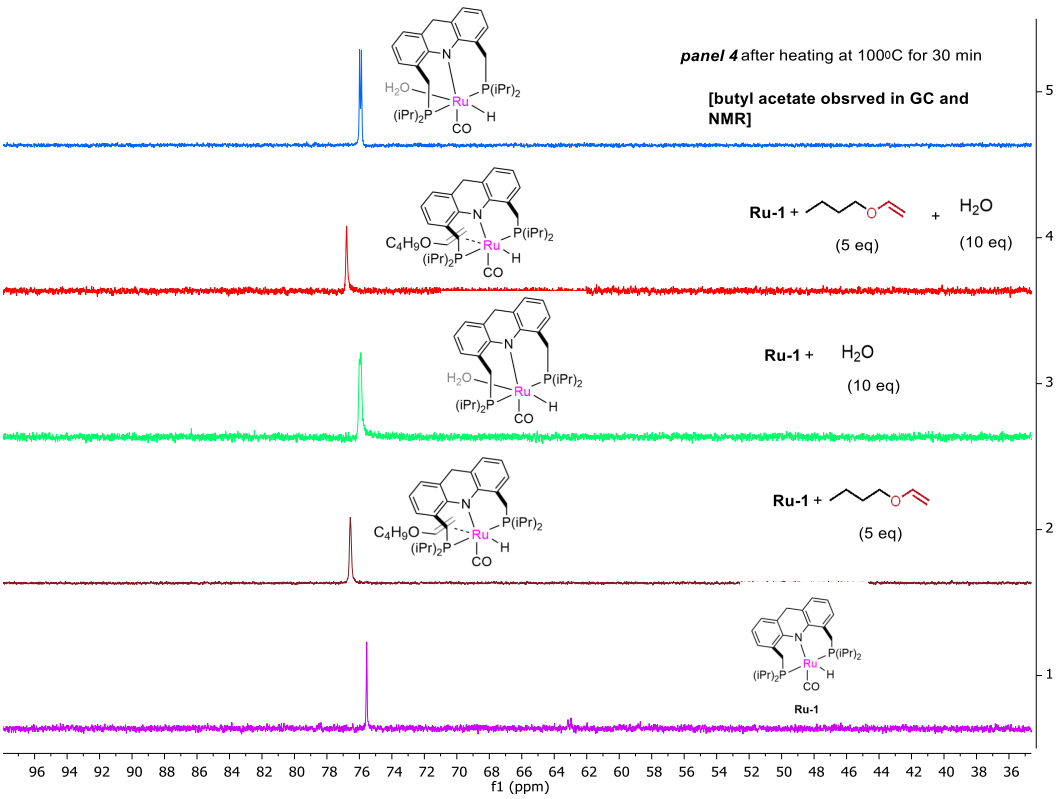



**Figure S34.** Reaction of complex **1** with vinyl butyl ether and water. [***panel 1***] $^{31}P\{^{1}H\}$ NMR spectrum of complex **1** (5 μmol) in 1,4-dioxane [***panel 2***] with 5 eq of vinyl butyl ether added, [***panel 3***] 10 eq of water added to complex **1** [***panel 4***] complex **1** with added vinyl butyl ether (5 eq) and water (10 eq) [***panel 5***] after heating panel 4 at 100 °C for half an hour. Water adduct is observed after consumption of all the vinyl ether. The proton NMR and GC-MS displayed the presence of butyl acetate and ethyl butyl ether in the solution of panel 5.

## 5.3. Reaction between complex 1 and various substrates

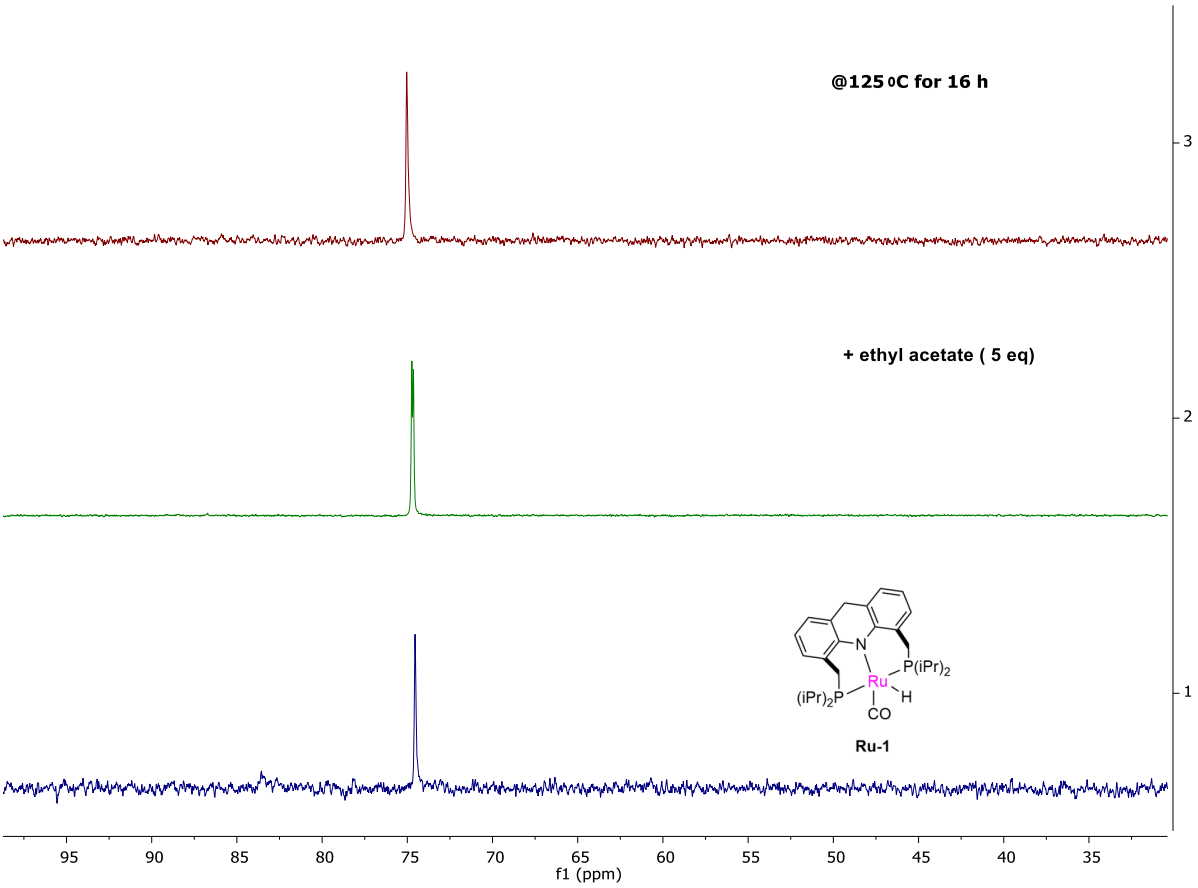



**Figure S35.** Reaction of complex **1** with ester as seen by $^{31}P\{^{1}H\}$ NMR. [***panel 1***] complex **1** in 1,4-dioxane, [***panel 2***] after adding 5 eq ethyl acetate, [***panel 3***] after heating the solution of panel 2 at 125 $^{o}$C overnight. $^{31}P\{^{1}H\}$ NMR spectra show no reaction between complex **1** and ethyl acetate.

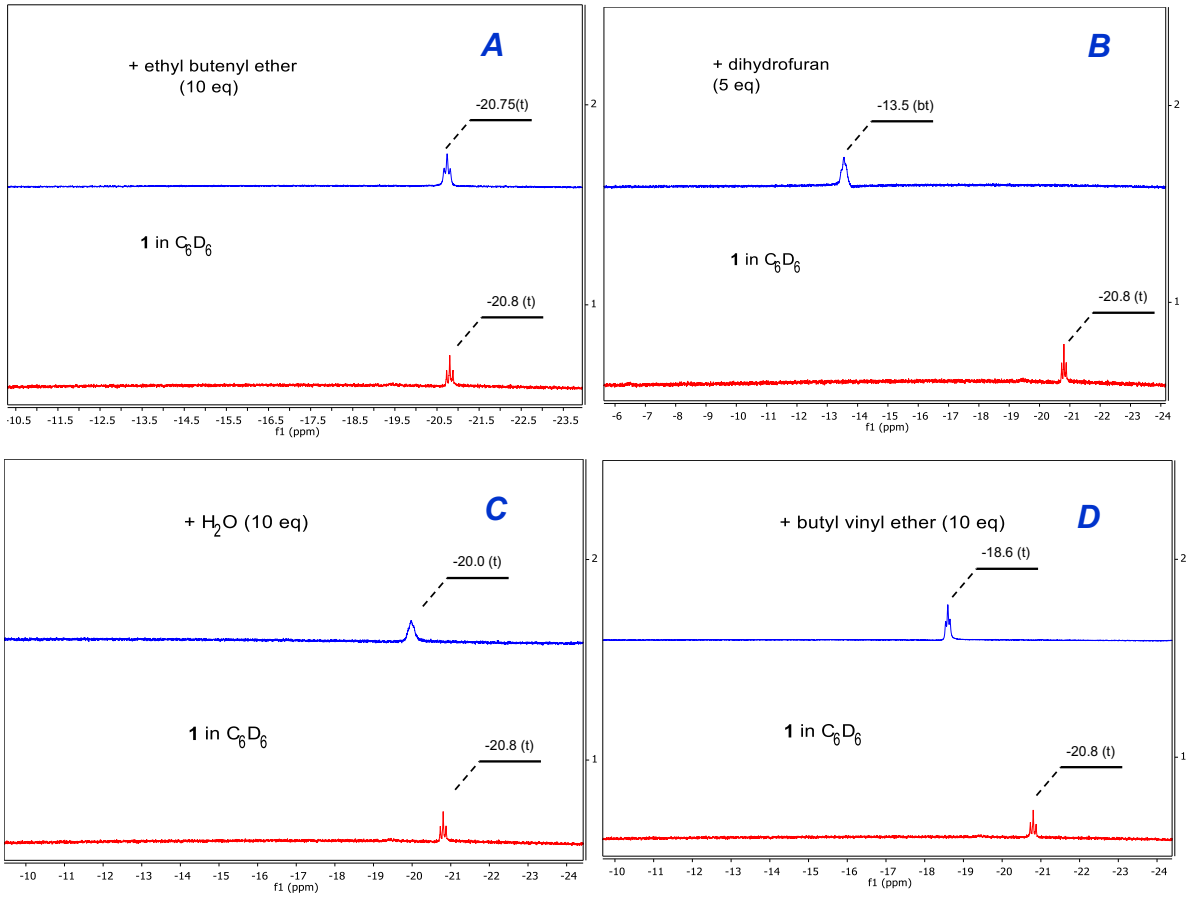



**Figure S36.** $^{1}$H NMR spectra of the hydride region of complex **1** in the presence of (A) ethyl butenyl ether, (B) dihydrofuran, (C) water and (D) butyl vinyl ether, showing the interaction between complex **1** and substrates. $C_6D_6$ was used as solvent.

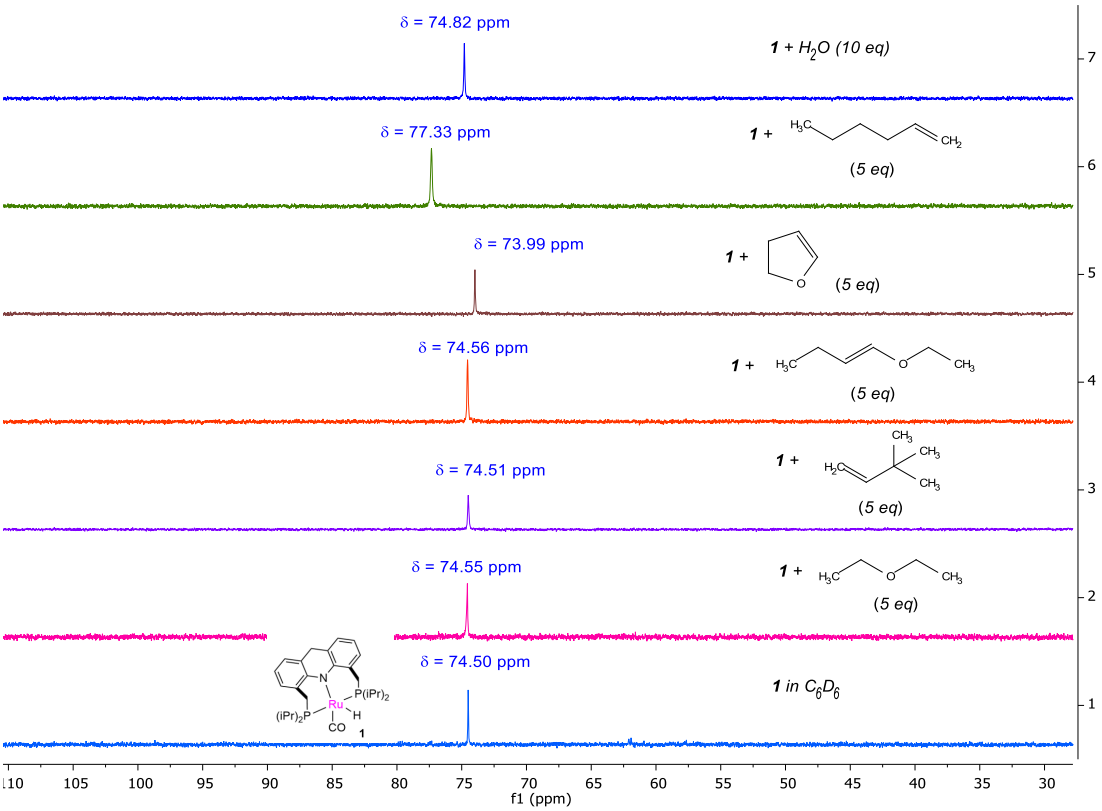



**Figure S37.** Stacked $^{31}P\{^{1}H\}$ NMR spectra showing interaction of different substrates with **1**.

## 6. Computational Studies

All geometries were optimized using Truhlar's M06-L functional,[11] the triple-ξ def2-TZVP basis set[12] and W06 density fitting to increase computational efficiency[13] as well as Grimme's D3(0) empirical dispersion correction.[14] To take the influence of the solvent into account optimizations were performed with the integral equation formalism variant (IEFPCM) with the SMD variation of Truhlar and co-workers, with 1,4-dioxane, except otherwise stated. Frequency calculations at this level of theory at 398.15 K were run in order to confirm stationary points and transition states, as well as to compute thermodynamic properties. Single point energies of the optimized structures were computed using the range-separated meta-GGA hybrid functional ωB97M-V of the Head-Gordon group[15] including dispersion correction,[16] together with the triple-ξ def2-TZVPP basis set[12] and the corresponding auxiliary basis sets, def2/J[13] and def2-TZVPP/C, [17] for RIJCOSX density fitting. The single point calculations include the same solvation (SMD) approach as described above in the optimizations. Gibbs free energies were computed by adding the free energy correction terms from the frequency calculations to the single point energies according to:

$$G^{\omega B97M\text{-}V}_{SMD} = E^{\omega B97M\text{-}V}_{el/SMD} + Gcorr^{M06\text{-}L}_{freq/SMD} \quad (1)$$

Free energy values ($G^o$) were then corrected to account for changes in standard states ($G^o \rightarrow G^{o\prime}$ *via* $\Delta G^{o\prime} = \Delta G^o + RT * \ln (Q^{o\prime}/Q^o)$.[18] Specifically, all species were corrected for the condensed phase (1 atm to 1M at 398.15 K), with the exception of $H_2$ (maintained at 1 atm standard state) and water (1 atm to 6.17 M at 398.15 K).[19] Optimizations and frequency calculations were done using the Gaussian 16 software suite in the C.01 revision.[20] Single point calculations were performed using ORCA Software in the 4.2.1 release.[21]

For the structures of **TS3** and **1a**-*mer*, and, structures were optimized, and frequency corrections were obtained in the gas phase at 398.15 K due to encountered optimization difficulty in dioxane continuum. Single point energies were calculated with the solvation model (dioxane). The resulting obtained values of free energies are likely to be within ±3 kcal/mol of the previously stated method in eq 1, verified with other selected structures.

### 6.1. Alternate hydration mechanism without the involvement of ruthenium complex

We considered the possibility of a reaction pathway where the initial hydration happens spontaneously without the involvement of ruthenium complex to generate a hemiacetal, from which dehydrogenation happens catalyzed by the ruthenium complex. This pathway is unlikely as our experimental results (Table 1) show that in the absence of acridine catalyst, no significant hydration products are observed under the reaction conditions. The computational analysis reveals that the uncatalyzed water assisted hydration pathway has a high activation barrier of around ~51.8 kcal/mol (with 2 water molecules involved in the transition state) under our reaction conditions, corroborating the experimental observations.

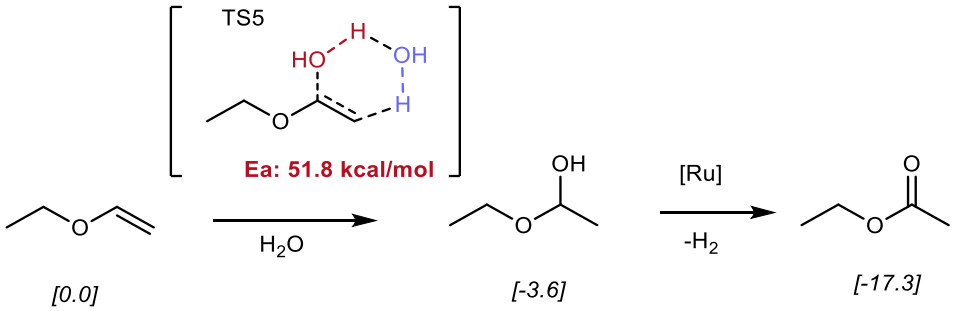



**Figure S38.** Uncatalyzed hydration pathway leading to the formation of a hemiacetal. The relevant transition state was found quite high in energy. Free energies (kcal/mol) were calculated at 398.15 K relative to ethyl vinyl ether+2*water and are calculated in a 1,4-dioxane continuum (all solutes are 1 M except for $H_2O$, which is at 6.17 M).

### 6.2. Discussion about the possibility of outer sphere pathway involving 6-*mer*

Another stepwise reaction mechanism involving a first step vinyl ether hydration catalyzed by [Ru], followed by subsequent [Ru] catalyzed dehydrogenation of the generated acetal was also considered. However, during our DFT calculations (with both complex **1** and **6**), we were unable to find the relevant zwitter ionic species resulting from initial nucleophilic water attack onto [Ru] bound vinyl ether. All optimization attempts from more than a dozen starting points resulted in spontaneous loss of water from the structure. This hints at the fact that such a zwitter ionic structure minima most likely does not exist in the potential energy surface, or if it does, is relatively very high in energy with facile loss of water being favorable from the structure. Furthermore, the experimental fact that both $P^iPr_2$ complex and the $PPh_2$ complex display similar catalytic activities for ester formation suggest the absence of such a stepwise mechanism where the Lewis acidity of the metal center in expected to play a big role in the reaction rate.

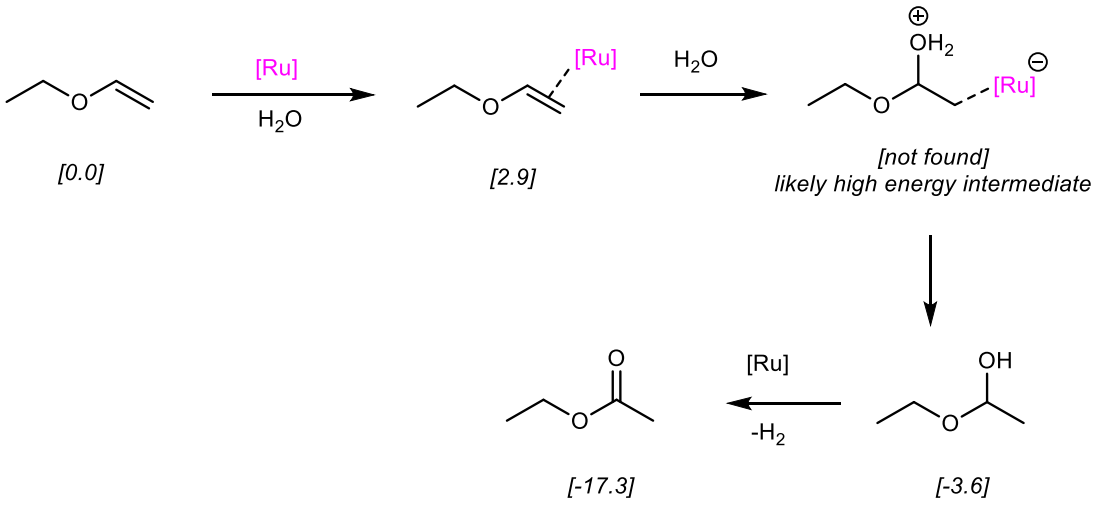



**Figure S39.** Stepwise Ru-catalyzed hydration-dehydrogenation pathway with complex **1/6**.

### 6.3. Reaction energy profile for ethyl vinyl ether oxidation by water catalyzed by 1

The energy profiles for both inner-sphere and outer-sphere reaction pathways were calculated also for complex **1** and compared to the energy profile associated with complex **6**. While a similar energy profile is observed, there are several differences worth mentioning. First, the *fac* isomer of complex **1** was energetically uphill by 12.0 kcal/mol with respect to the *mer* isomer, in contrast to the *Ph* complex **6** whose *fac* isomer is 5.6 kcal/mol uphill compared to the *mer* isomer. Second, the inner sphere $H_2$ evolution was found less facile with complex **1** (28.6 kcal/mol) as compared to complex **6** (22.4 kcal/mol). Similar trend is also observed for the hydroxide insertion onto bound vinyl ether transition state (28.6 kcal/mol for complex **1**, as compared to 17.2 kcal/mol for complex **1**, with respect to their *mer* isomers). Thus, in case of complex **1**, the initial $H_2$ evolution is also the most energetically demanding step under the reaction conditions, along with the hydroxide insertion step. An overall activation barrier of 28.6 kcal/mol was calculated for the Ru-Acr(iPr) system, as compared to the 26.0 kcal/mol for the Acr(Ph) system. These values are close and are also in agreement with the fact that similar reactivities are observed with complex **1** and **6** for the dehydrogenative oxidative ester synthesis from enol ethers.

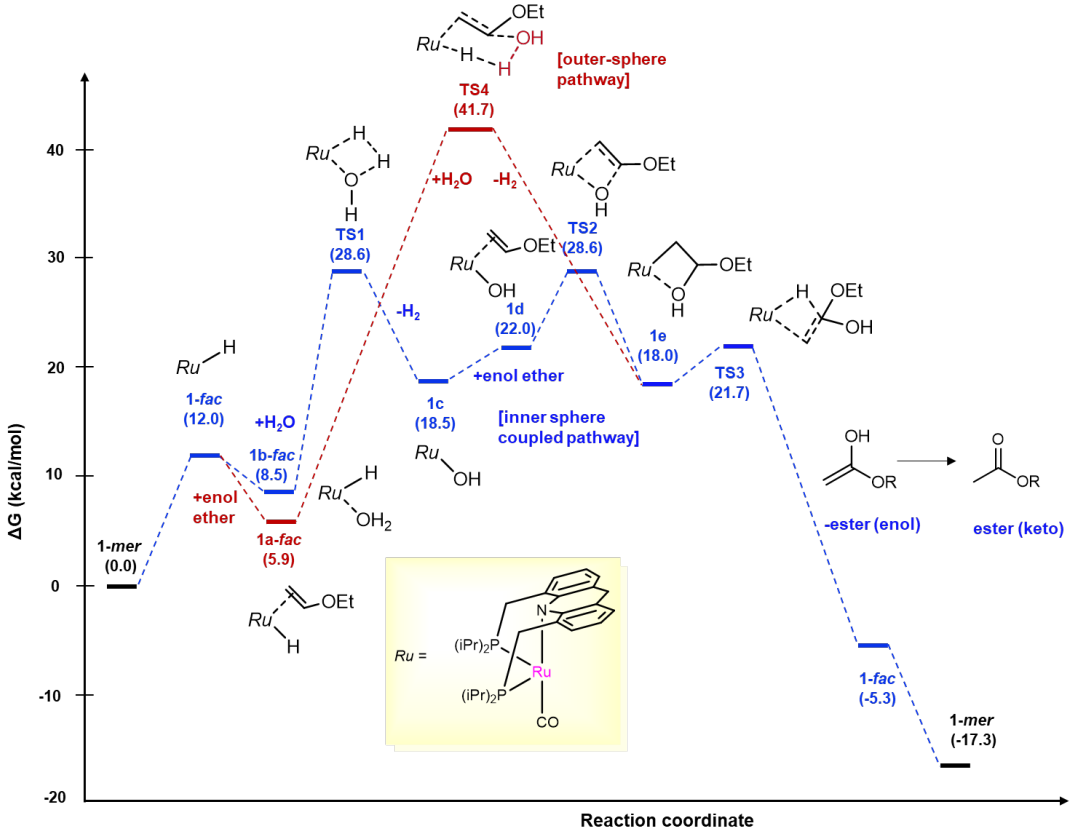


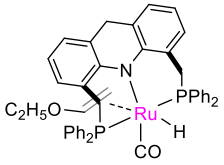
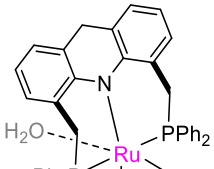
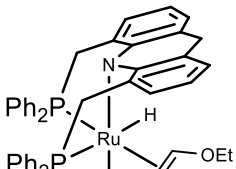
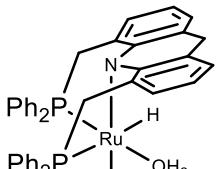
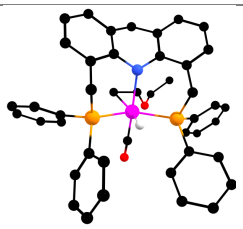
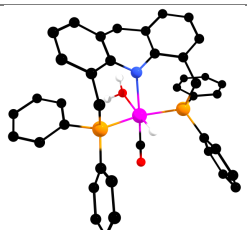
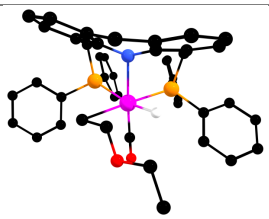
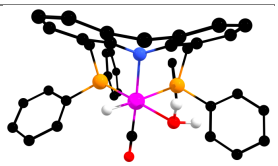

**Figure S40.** Energy profile of the inner sphere coupled catalytic pathway from enol ether to ester formation catalyzed by **1**. Free energies (kcal/mol) were calculated at 398.15 K relative to **1**-*mer*+water+ethyl vinyl ether and are calculated in a 1,4-dioxane continuum

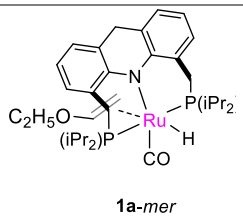
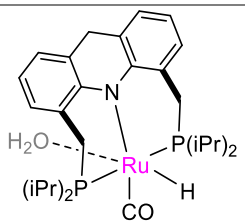
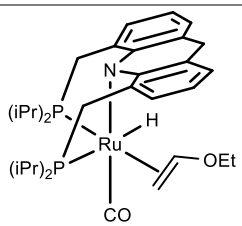
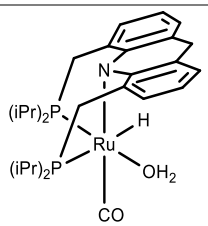
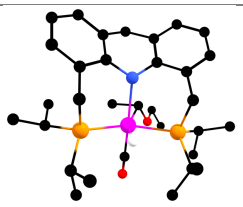
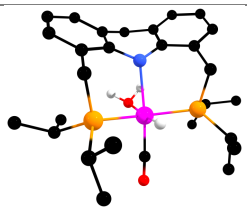
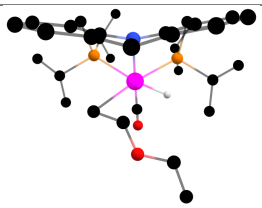
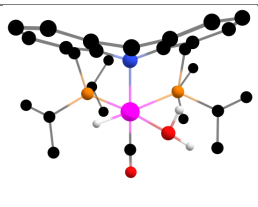
(all solutes are 1 M except for $H_2$ and $H_2O$, which are at 1 atm and 6.17 M, respectively). Mass balance is ensured throughout. The CO and acridine based ligands are omitted for clarity.

### 6.4. Energies of water and vinyl ether coordinated intermediates

The energies of the complexes, generating from the coordination of the vinyl ether or water to the metal center, with both complex **1** ($^i$Pr system) and **6** (Ph system), are shown in the following table.

**Table S3.**

| **Complex** |  **6a**-*mer* |  **6b**-*mer* |  **6a**-*fac* |  **6b**-*fac* |
|---|---|---|---|---|
| **Optimized Structure** |  |  |  |  |
| **$dG_{dioxane}^{398K}$** | +1.4 | +1.2 | -3.6 | -1.0 |

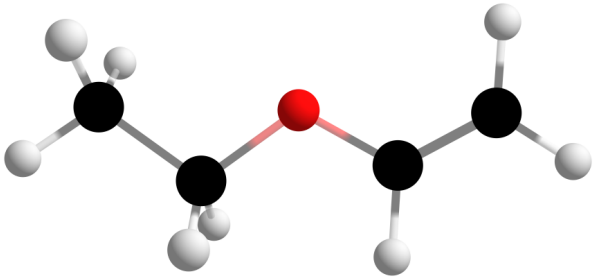
| **Complex** |  **1a**-*mer* |  **1b**-*mer* |  ***1a-fac*** |  ***1b-fac*** |
|---|---|---|---|---|
| **Optimized Structure** |  |  |  |  |
| **$dG_{dioxane}^{398K}$** | +3.4 | +2.18 | +5.9 | +8.5 |

## 6.5. Computed Structures, First Three Frequencies, Coordinates

*Note:* Only relevant hydrogen atoms shown for clarity.

*Color Scheme:* ruthenium (magenta), phosphorus (orange), nitrogen (blue), carbon (black), hydrogen (grey), oxygen (red).

### Ethyl vinyl ether



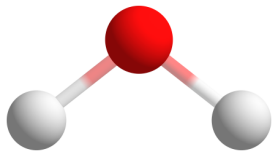
First three frequencies

| | 1 | 2 | 3 |
|---|---|---|---|
| | A | A | A |
| Frequencies -- | 49.3003 | 95.9505 | 209.9987 |
| Red. masses -- | 1.6505 | 4.2766 | 2.6950 |
| Frc consts -- | 0.0024 | 0.0232 | 0.0700 |
| IR Inten -- | 0.4389 | 2.3154 | 0.1639 |

Coordinates

| | | | |
|---|---|---|---|
| 6 | -2.798823000 | 0.195541000 | -0.009297000 |
| 6 | -1.677599000 | 0.904555000 | 0.015508000 |
| 1 | -2.792964000 | -0.884549000 | -0.061477000 |
| 1 | -3.751066000 | 0.700973000 | 0.023127000 |
| 8 | -0.452379000 | 0.341611000 | -0.022052000 |
| 1 | -1.691173000 | 1.991771000 | 0.068259000 |
| 6 | 0.639500000 | 1.262857000 | 0.014867000 |
| 6 | 1.918348000 | 0.482870000 | -0.032135000 |
| 1 | 0.575572000 | 1.864520000 | 0.928523000 |
| 1 | 0.562968000 | 1.950146000 | -0.835222000 |
| 1 | 1.997162000 | -0.193561000 | 0.817730000 |
| 1 | 2.771530000 | 1.158699000 | -0.006535000 |
| 1 | 1.983481000 | -0.109648000 | -0.943575000 |

### Water



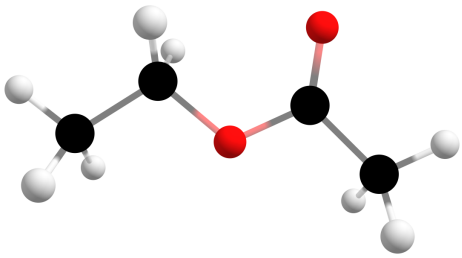
First three frequencies

| | 1 | 2 | 3 |
|---|---|---|---|
| | A | A | A |
| Frequencies -- | 1643.5791 | 3792.4424 | 3903.6700 |
| Red. masses -- | 1.0824 | 1.0454 | 1.0812 |
| Frc consts -- | 1.7227 | 8.8589 | 9.7077 |
| IR Inten -- | 76.0039 | 6.6593 | 54.3264 |

Coordinates

| | | | |
|---|---|---|---|
| 8 | -4.486777000 | 1.956755000 | -0.005133000 |
| 1 | -3.526897000 | 1.911854000 | 0.008495000 |
| 1 | -4.762492000 | 1.075811000 | 0.262233000 |

## Ethyl acetate



First three frequencies

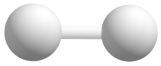
| | 1 | 2 | 3 |
|---|---|---|---|
| | ***A*** | A | A |
| Frequencies -- | ***46.4758*** | 71.6940 | 155.9772 |
| Red. masses -- | ***1.0609*** | 2.9443 | 1.8660 |
| Frc consts -- | ***0.0014*** | 0.0089 | 0.0267 |
| IR Inten -- | ***0.7146*** | 0.4160 | 4.5999 |

Coordinates

| | | | |
|---|---|---|---|
| 6 | -4.324713000 | -0.921502000 | -0.193250000 |
| 8 | -3.141328000 | -0.106406000 | -0.302443000 |
| 6 | -1.990721000 | -0.704870000 | 0.053006000 |
| 6 | -0.838596000 | 0.233072000 | -0.095353000 |
| 1 | -0.784273000 | 0.612724000 | -1.114401000 |
| 1 | 0.089375000 | -0.269510000 | 0.155652000 |
| 1 | -0.969977000 | 1.095163000 | 0.557333000 |
| 8 | -1.925201000 | -1.844965000 | 0.439144000 |
| 6 | -5.495448000 | -0.094630000 | -0.630039000 |
| 1 | -4.422339000 | -1.261554000 | 0.839656000 |
| 1 | -5.386071000 | 0.234963000 | -1.662340000 |
| 1 | -5.613735000 | 0.788296000 | -0.003388000 |

| | | | |
|---|---|---|---|
| 1 | -6.410444000 | -0.680700000 | -0.560228000 |
| 1 | -4.194979000 | -1.812214000 | -0.811179000 |

**$H_2$**



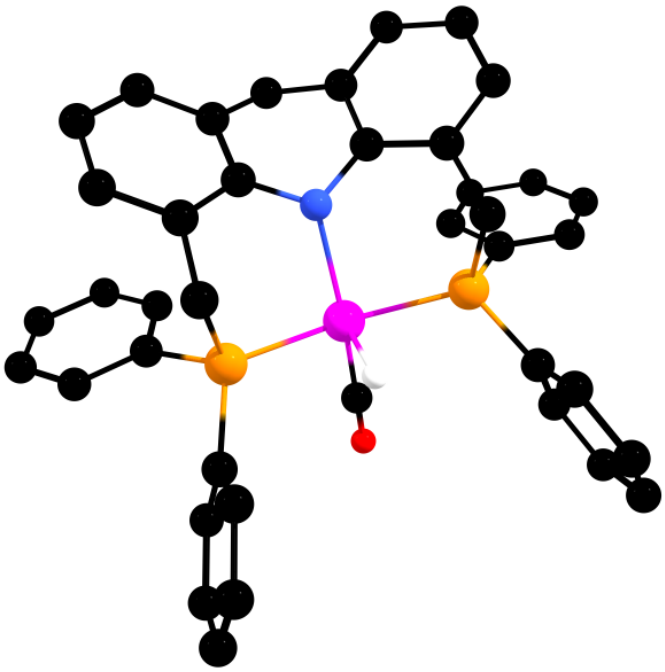
First frequency

| | 1 |
|---|---|
| | ***A*** |
| Frequencies -- | ***4338.4404*** |
| Red. masses -- | ***1.0078*** |
| Frc consts -- | ***11.1764*** |
| IR Inten -- | ***0.0000*** |

Coordinates

| | | | |
|---|---|---|---|
| 1 | -2.503763000 | 1.564580000 | 0.000000000 |
| 1 | -1.760653000 | 1.606642000 | 0.000000000 |

**6-*mer***



First three frequencies

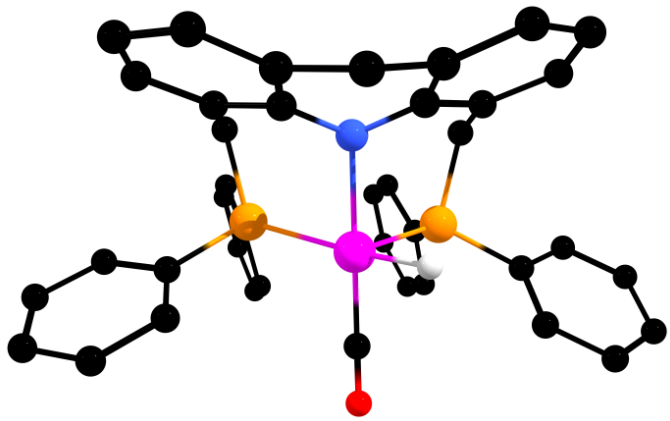
| | 1 | 2 | 3 |
|---|---|---|---|
| | ***A*** | A | A |
| Frequencies -- | ***16.8751*** | 19.9776 | 30.3156 |

| | | | |
|---|---|---|---|
| Red. masses -- | ***6.2059*** | 5.7436 | 5.6023 |
| Frc consts -- | ***0.0010*** | 0.0014 | 0.0030 |
| IR Inten -- | ***0.2628*** | 0.0510 | 0.4704 |

Coordinates

| | | | |
|---|---|---|---|
| 44 | 8.232659000 | 7.701367000 | 3.283387000 |
| 1 | 7.042300000 | 8.243090000 | 4.156724000 |
| 15 | 9.375237000 | 9.271257000 | 4.546515000 |
| 15 | 6.462067000 | 6.666987000 | 2.207288000 |
| 8 | 8.486700000 | 5.566393000 | 5.353813000 |
| 7 | 8.583211000 | 8.907255000 | 1.499914000 |
| 6 | 11.860759000 | 10.181954000 | 5.523633000 |
| 6 | 7.739401000 | 10.298700000 | 6.572235000 |
| 6 | 8.174441000 | 4.092286000 | -0.436541000 |
| 6 | 7.267479000 | 10.377839000 | 7.873063000 |
| 6 | 6.742874000 | 8.185179000 | 0.021731000 |
| 6 | 5.814437000 | 3.641842000 | -0.491285000 |
| 6 | 11.189565000 | 9.312636000 | 4.664279000 |
| 6 | 9.388457000 | 8.698106000 | 7.271960000 |
| 6 | 11.926895000 | 8.513129000 | 3.794763000 |
| 6 | 4.123904000 | 4.421988000 | 4.682953000 |
| 6 | 8.491683000 | 8.176397000 | -2.143947000 |
| 6 | 13.969307000 | 9.454474000 | 4.630358000 |
| 6 | 8.960986000 | 8.485195000 | -0.878621000 |
| 6 | 7.854122000 | 9.619751000 | 8.874517000 |
| 6 | 6.305923000 | 7.855406000 | -1.257465000 |
| 6 | 7.157196000 | 7.865740000 | -2.347707000 |
| 6 | 10.528905000 | 9.860808000 | 0.366583000 |
| 6 | 11.513043000 | 10.828207000 | 0.255135000 |
| 6 | 7.097756000 | 3.392457000 | -0.958350000 |
| 6 | 8.096391000 | 8.529014000 | 0.232952000 |
| 6 | 5.116940000 | 4.830684000 | 3.808801000 |
| 6 | 5.793047000 | 8.023535000 | 1.161104000 |
| 6 | 13.310937000 | 8.585601000 | 3.774470000 |
| 6 | 6.683036000 | 5.305190000 | 1.021511000 |
| 6 | 5.606198000 | 4.595342000 | 0.491437000 |
| 6 | 5.102349000 | 6.118768000 | 3.273239000 |
| 6 | 4.079507000 | 6.991009000 | 3.641039000 |
| 6 | 9.775929000 | 10.858935000 | 2.429644000 |
| 6 | 8.914685000 | 8.778684000 | 8.570649000 |
| 6 | 7.967464000 | 5.040511000 | 0.552776000 |
| 6 | 13.243732000 | 10.250424000 | 5.506604000 |
| 6 | 8.971291000 | 10.844518000 | 3.686148000 |
| 6 | 3.105450000 | 5.294800000 | 5.037265000 |
| 6 | 8.365854000 | 6.409613000 | 4.561471000 |
| 6 | 3.086347000 | 6.579184000 | 4.515949000 |
| 6 | 9.615724000 | 9.864943000 | 1.439307000 |
| 6 | 11.649737000 | 11.813520000 | 1.219286000 |
| 6 | 8.809379000 | 9.462300000 | 6.258638000 |
| 6 | 10.790259000 | 11.802955000 | 2.303147000 |
| 6 | 10.403888000 | 8.732837000 | -0.599390000 |

**6-*fac***



First three frequencies

| | 1 | 2 | 3 |
|---|---|---|---|
| | ***A*** | A | A |
| Frequencies -- | ***19.7479*** | 29.8199 | 34.7170 |
| Red. masses -- | ***5.4445*** | 5.5893 | 4.9142 |
| Frc consts -- | ***0.0013*** | 0.0029 | 0.0035 |
| IR Inten -- | ***0.0275*** | 0.3760 | 0.2620 |

Coordinates

| | | | |
|---|---|---|---|
| 15 | -2.307939000 | 7.574606000 | 3.019844000 |
| 15 | 0.498488000 | 6.172452000 | 5.022373000 |
| 8 | -2.323507000 | 7.613028000 | 7.087173000 |
| 7 | 0.673459000 | 8.523627000 | 2.996151000 |
| 6 | -1.572155000 | 7.868624000 | 1.361393000 |
| 6 | -0.913428000 | 9.207915000 | 1.293812000 |
| 6 | -1.385592000 | 10.182686000 | 0.422632000 |
| 6 | -0.729092000 | 11.394050000 | 0.275961000 |
| 6 | 0.419335000 | 11.635806000 | 1.017567000 |
| 6 | 0.889805000 | 10.705861000 | 1.930081000 |
| 6 | 0.215915000 | 9.480829000 | 2.095215000 |
| 6 | 2.077467000 | 10.965679000 | 2.807108000 |
| 6 | 2.807427000 | 9.699716000 | 3.138471000 |
| 6 | 4.165742000 | 9.658905000 | 3.412382000 |
| 6 | 4.771324000 | 8.489212000 | 3.850342000 |
| 6 | 4.007040000 | 7.340817000 | 3.996422000 |
| 6 | 2.652795000 | 7.340875000 | 3.690979000 |
| 6 | 2.035126000 | 8.536273000 | 3.270772000 |
| 6 | 1.837322000 | 6.092495000 | 3.764116000 |
| 6 | -1.661987000 | 7.762294000 | 6.142451000 |
| 44 | -0.603135000 | 8.032822000 | 4.665068000 |
| 6 | -3.609386000 | 8.852586000 | 3.081029000 |
| 6 | -4.723740000 | 8.820720000 | 2.243327000 |

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| 6 | -5.639887000 | 9.858645000 | 2.256200000 |
| 6 | -4.352626000 | 10.982307000 | 3.945241000 |
| 6 | -5.452989000 | 10.942243000 | 3.104157000 |
| 6 | 1.357738000 | 5.905076000 | 6.608373000 |
| 6 | 1.342516000 | 6.836543000 | 7.640173000 |
| 6 | 2.074689000 | 4.717579000 | 6.779536000 |
| 6 | 2.032098000 | 6.589449000 | 8.818802000 |
| 6 | 2.769191000 | 4.476981000 | 7.951397000 |
| 6 | 2.747723000 | 5.414363000 | 8.975278000 |
| 6 | -0.434237000 | 4.622446000 | 4.835500000 |
| 6 | -0.579833000 | 3.997433000 | 3.597547000 |
| 6 | -1.087392000 | 4.079053000 | 5.944226000 |
| 6 | -1.334991000 | 2.841076000 | 3.477696000 |
| 6 | -1.844639000 | 2.927015000 | 5.821023000 |
| 6 | -1.964870000 | 2.301436000 | 4.588268000 |
| 6 | -3.257609000 | 6.032414000 | 2.869398000 |
| 6 | -3.396077000 | 5.333454000 | 1.671273000 |
| 6 | -3.893222000 | 5.543428000 | 4.012827000 |
| 6 | -4.168930000 | 4.182217000 | 1.614622000 |
| 6 | -4.669432000 | 4.399695000 | 3.951374000 |
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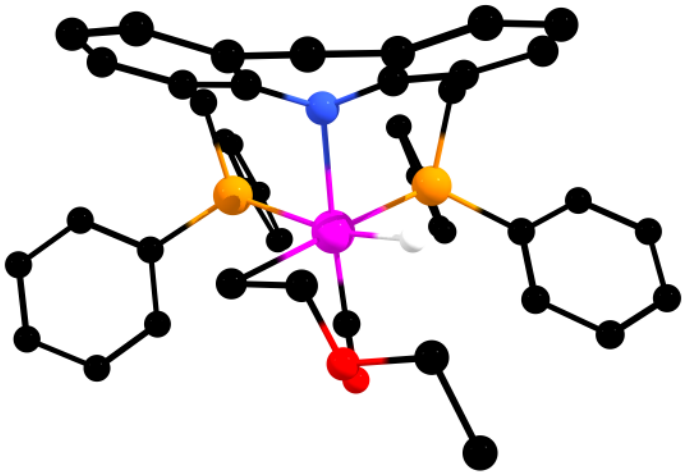
**6a-*fac***



First three frequencies

| | 1 | 2 | 3 |
|---|---|---|---|
| | ***A*** | A | A |
| Frequencies -- | ***22.5971*** | 25.8336 | 32.2733 |
| Red. masses -- | ***4.4374*** | 5.2156 | 4.5908 |
| Frc consts -- | ***0.0013*** | 0.0021 | 0.0028 |
| IR Inten -- | ***0.2870*** | 0.0982 | 0.0378 |

Coordinates

| | | | |
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| 15 | -2.438838000 | 7.610620000 | 2.956108000 |
| 15 | 0.311629000 | 6.098893000 | 4.934142000 |
| 8 | -2.489935000 | 7.624764000 | 7.062790000 |
| 7 | 0.621867000 | 8.481627000 | 2.912674000 |
| 6 | -1.624511000 | 7.891754000 | 1.333477000 |
| 1 | -0.899722000 | 7.072233000 | 1.269789000 |
| 1 | -2.335515000 | 7.766519000 | 0.516417000 |
| 6 | -0.916532000 | 9.201515000 | 1.210822000 |
| 6 | -1.339933000 | 10.153972000 | 0.293828000 |
| 1 | -2.218214000 | 9.948292000 | -0.308354000 |
| 6 | -0.637960000 | 11.334898000 | 0.106580000 |
| 1 | -0.974935000 | 12.063529000 | -0.618676000 |
| 6 | 0.513718000 | 11.555295000 | 0.846027000 |
| 1 | 1.082146000 | 12.468332000 | 0.701415000 |
| 6 | 0.956897000 | 10.635653000 | 1.785028000 |
| 6 | 0.235141000 | 9.443986000 | 1.996033000 |
| 6 | 2.182413000 | 10.905452000 | 2.609417000 |
| 1 | 2.932247000 | 11.429532000 | 2.009707000 |
| 1 | 1.940583000 | 11.615192000 | 3.414065000 |
| 6 | 2.767231000 | 9.651459000 | 3.190351000 |
| 6 | 4.079763000 | 9.609398000 | 3.641942000 |
| 1 | 4.689011000 | 10.503655000 | 3.558112000 |
| 6 | 4.614501000 | 8.460220000 | 4.203725000 |
| 1 | 5.634314000 | 8.448596000 | 4.565098000 |
| 6 | 3.833728000 | 7.314766000 | 4.266352000 |
| 1 | 4.248913000 | 6.392995000 | 4.659835000 |
| 6 | 2.530140000 | 7.316256000 | 3.793108000 |
| 6 | 1.956015000 | 8.509487000 | 3.299287000 |
| 6 | 1.718109000 | 6.068016000 | 3.752304000 |
| 1 | 2.328074000 | 5.182885000 | 3.936704000 |
| 1 | 1.256325000 | 5.970427000 | 2.765896000 |
| 6 | -1.847366000 | 7.800164000 | 6.109573000 |
| 44 | -0.797314000 | 8.094766000 | 4.644120000 |
| 6 | -1.631005000 | 10.232863000 | 4.458673000 |
| 6 | -0.439477000 | 10.372336000 | 5.143737000 |
| 1 | -1.661826000 | 10.492586000 | 3.409676000 |
| 1 | -2.558985000 | 10.343460000 | 5.004106000 |
| 8 | -0.427034000 | 10.653360000 | 6.461054000 |
| 1 | 0.486778000 | 10.567259000 | 4.610866000 |
| 6 | 0.866142000 | 10.596995000 | 7.068635000 |
| 6 | 0.700556000 | 10.722793000 | 8.552487000 |
| 1 | 1.489836000 | 11.399186000 | 6.657546000 |
| 1 | 1.342396000 | 9.646247000 | 6.794190000 |
| 1 | 0.240410000 | 11.671872000 | 8.824258000 |
| 1 | 1.670883000 | 10.664522000 | 9.043268000 |
| 1 | 0.073353000 | 9.921589000 | 8.943922000 |
| 6 | 1.134796000 | 5.844662000 | 6.550699000 |
| 6 | 0.978526000 | 6.720074000 | 7.620813000 |
| 6 | 1.968414000 | 4.735300000 | 6.713207000 |
| 6 | 1.645437000 | 6.502249000 | 8.818221000 |
| 6 | 2.642365000 | 4.523055000 | 7.903027000 |

| | | | |
|---|---|---|---|
| 6 | 2.482965000 | 5.408812000 | 8.959928000 |
| 1 | 0.334237000 | 7.582502000 | 7.516327000 |
| 1 | 2.088646000 | 4.026509000 | 5.901299000 |
| 1 | 1.507687000 | 7.192756000 | 9.640850000 |
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| 6 | -4.478878000 | 9.188304000 | 1.762006000 |
| 6 | -4.649051000 | 8.822356000 | 4.124324000 |
| 6 | -5.652340000 | 9.928118000 | 1.795811000 |
| 6 | -5.827550000 | 9.547397000 | 4.155855000 |
| 6 | -6.330126000 | 10.107918000 | 2.990193000 |
| 1 | -3.973802000 | 9.049932000 | 0.815509000 |
| 1 | -4.254790000 | 8.403569000 | 5.043291000 |
| 1 | -6.036409000 | 10.363042000 | 0.881728000 |
| 1 | -6.349446000 | 9.682394000 | 5.094666000 |
| 1 | -7.245859000 | 10.684608000 | 3.014615000 |
| 6 | -3.204696000 | 5.959787000 | 2.795934000 |
| 6 | -3.393344000 | 5.321650000 | 1.571467000 |
| 6 | -3.696742000 | 5.352114000 | 3.951985000 |
| 6 | -4.071094000 | 4.113026000 | 1.504529000 |
| 6 | -4.386267000 | 4.154184000 | 3.881744000 |
| 6 | -4.577170000 | 3.532019000 | 2.656068000 |
| 1 | -3.019642000 | 5.765500000 | 0.657777000 |
| 1 | -3.535809000 | 5.825039000 | 4.915005000 |
| 1 | -4.209536000 | 3.629582000 | 0.545525000 |
| 1 | -4.764156000 | 3.698745000 | 4.788381000 |
| 1 | -5.112012000 | 2.592211000 | 2.601442000 |
| 6 | -0.492943000 | 4.478245000 | 4.713063000 |
| 6 | -0.555919000 | 3.854785000 | 3.467269000 |
| 6 | -1.108455000 | 3.860629000 | 5.803650000 |
| 6 | -1.185815000 | 2.628198000 | 3.324472000 |
| 6 | -1.737491000 | 2.635575000 | 5.659061000 |
| 6 | -1.769826000 | 2.011764000 | 4.420423000 |
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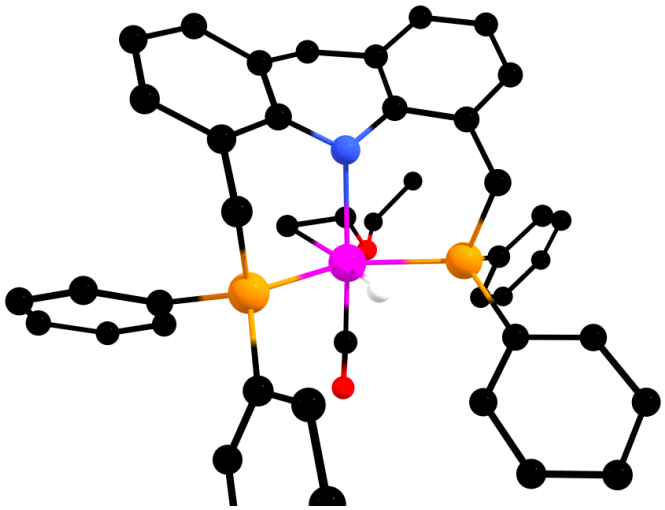
| 1 | -1.083609000 | 4.339333000 | 6.776485000 |
| 1 | -1.219915000 | 2.154208000 | 2.351586000 |
| 1 | -2.201566000 | 2.166102000 | 6.517331000 |
| 1 | -2.257853000 | 1.051982000 | 4.306914000 |
| 1 | 0.542843000 | 8.373157000 | 5.535132000 |

**6a-*mer***



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| Frequencies -- | ***21.5176*** | 25.0413 | 31.5158 |
| Red. masses -- | ***5.3981*** | 4.9867 | 3.1488 |
| Frc consts -- | ***0.0015*** | 0.0018 | 0.0018 |
| IR Inten -- | ***0.0486*** | 0.4067 | 0.5293 |

| | | | |
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| 15 | 1.596410000 | 5.267760000 | 2.888221000 |
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| 6 | -1.415948000 | 5.546997000 | 3.213800000 |
| 6 | 0.207264000 | 6.453212000 | -1.326151000 |
| 6 | 1.914849000 | 5.125061000 | -0.405634000 |
| 6 | -0.468804000 | 8.561333000 | -0.126976000 |
| 6 | -0.430577000 | 7.715119000 | -1.352747000 |
| 6 | -1.033655000 | 8.171148000 | -2.519544000 |
| 6 | -1.017843000 | 7.425884000 | -3.685345000 |
| 6 | -0.406491000 | 6.182207000 | -3.667254000 |
| 6 | 0.178980000 | 5.689719000 | -2.513099000 |
| 6 | 0.768567000 | 4.319841000 | -2.451521000 |
| 6 | 1.971977000 | 4.321824000 | -1.567979000 |
| 6 | 3.078302000 | 3.537667000 | -1.845291000 |
| 6 | 4.153120000 | 3.483747000 | -0.971683000 |
| 6 | 4.084239000 | 4.215036000 | 0.200269000 |
| 6 | 2.990693000 | 5.018997000 | 0.507032000 |
| 6 | 2.980770000 | 5.772862000 | 1.794191000 |
| 1 | 0.523636000 | 8.631963000 | 0.324673000 |
| 1 | -0.818415000 | 9.571429000 | -0.344090000 |
| 1 | -1.501040000 | 9.149455000 | -2.510535000 |
| 1 | -1.477106000 | 7.805483000 | -4.588327000 |
| 1 | -0.395376000 | 5.566375000 | -4.560262000 |
| 1 | 0.021251000 | 3.622602000 | -2.040320000 |
| 1 | 1.006163000 | 3.942522000 | -3.447375000 |
| 1 | 3.084681000 | 2.950132000 | -2.757259000 |

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| 1 | 4.915510000 | 4.189974000 | 0.897015000 |
| 1 | 3.934550000 | 5.672884000 | 2.315651000 |
| 1 | 2.800940000 | 6.840035000 | 1.632474000 |
| 1 | 0.395562000 | 7.123502000 | 2.299070000 |
| 6 | -1.653867000 | 4.462453000 | 0.486683000 |
| 1 | -2.652412000 | 4.304001000 | 0.872461000 |
| 1 | -1.594598000 | 4.858473000 | -0.518513000 |
| 6 | -0.623748000 | 3.681651000 | 1.009548000 |
| 1 | 0.267110000 | 3.467879000 | 0.426628000 |
| 8 | -0.893114000 | 2.770291000 | 2.012281000 |
| 6 | -0.794317000 | 1.412454000 | 1.579378000 |
| 1 | -1.498898000 | 1.245817000 | 0.753790000 |
| 1 | -1.149486000 | 0.828426000 | 2.429874000 |
| 6 | 0.597550000 | 0.980865000 | 1.189067000 |
| 1 | 1.308385000 | 1.164093000 | 1.993838000 |
| 1 | 0.962717000 | 1.487282000 | 0.295061000 |
| 1 | 0.600998000 | -0.087915000 | 0.975044000 |
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| 6 | -3.653481000 | 8.769265000 | -0.376110000 |
| 6 | -4.108897000 | 6.792431000 | 0.906737000 |
| 6 | -4.962520000 | 8.775214000 | -0.828272000 |
| 6 | -5.423023000 | 6.807468000 | 0.466201000 |
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| 1 | -6.871341000 | 7.799776000 | -0.764890000 |
| 6 | -1.621774000 | 8.957623000 | 2.515302000 |
| 6 | -2.769336000 | 9.051312000 | 3.300427000 |
| 6 | -0.513637000 | 9.737036000 | 2.850522000 |
| 6 | -2.806412000 | 9.901907000 | 4.395052000 |
| 6 | -0.558821000 | 10.598508000 | 3.933799000 |
| 6 | -1.704487000 | 10.680482000 | 4.712130000 |
| 1 | -3.641420000 | 8.455105000 | 3.059168000 |
| 1 | 0.399324000 | 9.662029000 | 2.271466000 |
| 1 | -3.703460000 | 9.956811000 | 4.998448000 |
| 1 | 0.308354000 | 11.200169000 | 4.175448000 |
| 1 | -1.736980000 | 11.348546000 | 5.563302000 |
| 6 | 1.970536000 | 3.592903000 | 3.493386000 |
| 6 | 1.011880000 | 2.972264000 | 4.297264000 |
| 6 | 3.174784000 | 2.935502000 | 3.255478000 |
| 6 | 1.256483000 | 1.728749000 | 4.852985000 |
| 6 | 3.415129000 | 1.683872000 | 3.805714000 |
| 6 | 2.458761000 | 1.079406000 | 4.605779000 |
| 1 | 0.068923000 | 3.469765000 | 4.488622000 |
| 1 | 3.935000000 | 3.397449000 | 2.641760000 |
| 1 | 0.504980000 | 1.263806000 | 5.478495000 |
| 1 | 4.355785000 | 1.185037000 | 3.609625000 |
| 1 | 2.647975000 | 0.104336000 | 5.036497000 |

| | | | |
|---|---|---|---|
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| 6 | 1.003356000 | 7.159819000 | 4.927928000 |
| 6 | 3.096003000 | 6.003935000 | 5.114025000 |
| 6 | 1.293925000 | 7.861894000 | 6.089575000 |
| 6 | 3.390455000 | 6.712893000 | 6.264893000 |
| 6 | 2.486675000 | 7.643867000 | 6.757901000 |
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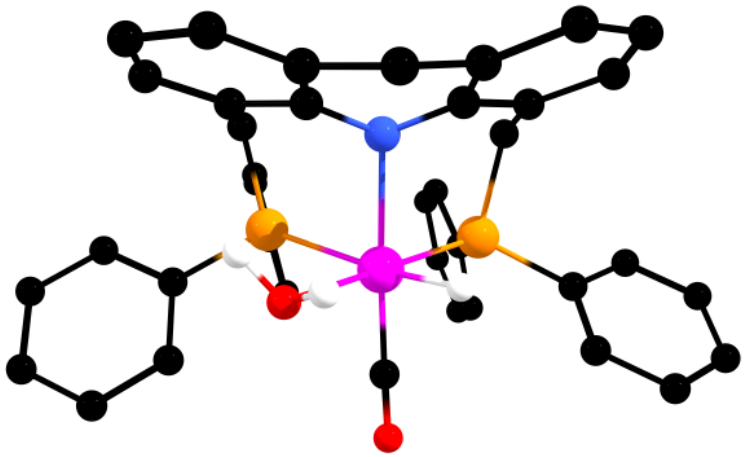
**6b-*fac***



| | 1 | 2 | 3 |
|---|---|---|---|
| | ***A*** | A | A |
| Frequencies -- | ***17.2825*** | 30.0457 | 37.6271 |
| Red. masses -- | ***5.2967*** | 4.9011 | 4.9864 |
| Frc consts -- | ***0.0009*** | 0.0026 | 0.0042 |
| IR Inten -- | ***0.0111*** | 0.3230 | 0.3332 |

| | | | |
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| 15 | 0.386366000 | 6.227777000 | 5.011486000 |
| 8 | -2.295868000 | 7.748198000 | 7.172414000 |
| 7 | 0.706976000 | 8.539430000 | 2.975866000 |
| 6 | -1.577559000 | 8.059304000 | 1.423051000 |
| 1 | -0.845154000 | 7.257316000 | 1.280547000 |
| 1 | -2.318260000 | 7.988790000 | 0.626201000 |
| 6 | -0.882921000 | 9.380979000 | 1.380680000 |
| 6 | -1.345838000 | 10.416829000 | 0.577405000 |
| 1 | -2.264434000 | 10.275919000 | 0.018026000 |
| 6 | -0.629181000 | 11.597645000 | 0.447679000 |
| 1 | -0.993398000 | 12.389836000 | -0.192730000 |
| 6 | 0.571117000 | 11.741258000 | 1.131525000 |

| | | | |
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| 6 | 1.040800000 | 10.746376000 | 1.975523000 |
| 6 | 0.305228000 | 9.554122000 | 2.129637000 |
| 6 | 2.284961000 | 10.910913000 | 2.799079000 |
| 1 | 2.998449000 | 11.570399000 | 2.299859000 |
| 1 | 2.030247000 | 11.432717000 | 3.735932000 |
| 6 | 2.911185000 | 9.592288000 | 3.143423000 |
| 6 | 4.261914000 | 9.459453000 | 3.428122000 |
| 1 | 4.907707000 | 10.326104000 | 3.331320000 |
| 6 | 4.786748000 | 8.250357000 | 3.862970000 |
| 1 | 5.839643000 | 8.163499000 | 4.096774000 |
| 6 | 3.948545000 | 7.152152000 | 3.992147000 |
| 1 | 4.347869000 | 6.198343000 | 4.319889000 |
| 6 | 2.600714000 | 7.245114000 | 3.675890000 |
| 6 | 2.062672000 | 8.481404000 | 3.265825000 |
| 6 | 1.694897000 | 6.062077000 | 3.727251000 |
| 1 | 2.247121000 | 5.136552000 | 3.896168000 |
| 1 | 1.154691000 | 5.974951000 | 2.780205000 |
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| 44 | -0.639621000 | 8.184179000 | 4.719594000 |
| 6 | -3.789289000 | 8.832885000 | 3.082051000 |
| 6 | -4.625885000 | 8.943557000 | 1.969249000 |
| 6 | -4.105677000 | 9.555063000 | 4.229976000 |
| 6 | -5.735216000 | 9.769946000 | 1.999054000 |
| 6 | -5.221844000 | 10.379325000 | 4.262098000 |
| 6 | -6.034480000 | 10.492035000 | 3.146740000 |
| 1 | -4.417549000 | 8.369487000 | 1.073462000 |
| 1 | -3.470112000 | 9.476093000 | 5.102502000 |
| 1 | -6.372411000 | 9.846656000 | 1.127084000 |
| 1 | -5.452185000 | 10.933959000 | 5.162726000 |
| 1 | -6.903291000 | 11.137550000 | 3.169578000 |
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| 6 | 1.346936000 | 6.881010000 | 7.599179000 |
| 6 | 2.012724000 | 4.751988000 | 6.716828000 |
| 6 | 2.079844000 | 6.626837000 | 8.750292000 |
| 6 | 2.751615000 | 4.503599000 | 7.859510000 |
| 6 | 2.786031000 | 5.443140000 | 8.881133000 |
| 1 | 0.809104000 | 7.813811000 | 7.493232000 |
| 1 | 1.977220000 | 4.003186000 | 5.932713000 |
| 1 | 2.098528000 | 7.361818000 | 9.544878000 |
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| 1 | 3.361432000 | 5.248674000 | 9.777367000 |
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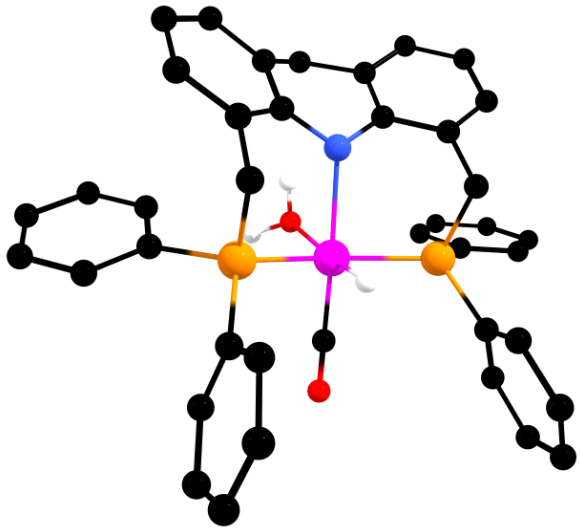
| 6 | -0.673194000 | 3.958234000 | 3.710135000 |
| 6 | -1.208394000 | 4.188483000 | 6.039122000 |
| 6 | -1.399481000 | 2.777970000 | 3.663068000 |
| 6 | -1.937409000 | 3.012667000 | 5.989135000 |
| 6 | -2.027887000 | 2.299948000 | 4.802215000 |
| 1 | -0.190754000 | 4.317484000 | 2.809044000 |
| 1 | -1.128717000 | 4.729773000 | 6.975189000 |
| 1 | -1.474994000 | 2.232868000 | 2.730630000 |

| | | | |
|---|---|---|---|
| 1 | -2.431027000 | 2.649212000 | 6.881586000 |
| 1 | -2.593563000 | 1.377502000 | 4.763511000 |
| 6 | -3.176127000 | 6.111551000 | 2.852711000 |
| 6 | -3.222051000 | 5.420992000 | 1.643495000 |
| 6 | -3.841089000 | 5.578504000 | 3.959198000 |
| 6 | -3.934381000 | 4.234242000 | 1.538340000 |
| 6 | -4.557170000 | 4.400095000 | 3.849316000 |
| 6 | -4.608601000 | 3.726069000 | 2.636385000 |
| 1 | -2.706686000 | 5.805343000 | 0.772413000 |
| 1 | -3.800009000 | 6.098425000 | 4.910964000 |
| 1 | -3.963862000 | 3.709757000 | 0.591410000 |
| 1 | -5.070242000 | 4.001513000 | 4.715472000 |
| 1 | -5.167394000 | 2.802553000 | 2.551937000 |
| 1 | 0.611383000 | 8.734060000 | 5.617691000 |
| 8 | -1.179095000 | 10.463148000 | 4.524553000 |
| 1 | -1.312770000 | 10.681474000 | 3.588340000 |
| 1 | -0.325982000 | 10.860349000 | 4.741298000 |

**6b-*mer***



| | 1 | 2 | 3 |
|---|---|---|---|
| | ***A*** | A | A |
| Frequencies -- | ***18.7560*** | 19.9140 | 25.2603 |
| Red. masses -- | ***5.3349*** | 5.1423 | 5.7400 |
| Frc consts -- | ***0.0011*** | 0.0012 | 0.0022 |
| IR Inten -- | ***0.0338*** | 0.0355 | 0.1474 |

| | | | |
|---|---|---|---|
| 44 | 8.427193000 | 7.559182000 | 3.208217000 |
| 1 | 7.203414000 | 8.305532000 | 3.874654000 |
| 15 | 9.458869000 | 9.172187000 | 4.515465000 |
| 15 | 6.579477000 | 6.613084000 | 2.164198000 |
| 8 | 8.437999000 | 5.598754000 | 5.455880000 |
| 7 | 8.670008000 | 8.927417000 | 1.408827000 |
| 6 | 11.752922000 | 10.325862000 | 5.664357000 |
| 1 | 11.072483000 | 10.955165000 | 6.227747000 |

| | | | |
|---|---|---|---|
| 6 | 7.517197000 | 9.993046000 | 6.350851000 |
| 1 | 7.025646000 | 10.458610000 | 5.504636000 |
| 6 | 7.694995000 | 4.098381000 | -0.849180000 |
| 1 | 8.565401000 | 3.991595000 | -1.484003000 |
| 6 | 6.923781000 | 10.051757000 | 7.601286000 |
| 1 | 5.982027000 | 10.571468000 | 7.724260000 |
| 6 | 6.820873000 | 8.179138000 | -0.021452000 |
| 6 | 5.472527000 | 3.441824000 | -0.228349000 |
| 1 | 4.604551000 | 2.811045000 | -0.373113000 |
| 6 | 11.247495000 | 9.341105000 | 4.814088000 |
| 6 | 9.333242000 | 8.722820000 | 7.274025000 |
| 1 | 10.272966000 | 8.196597000 | 7.150893000 |
| 6 | 12.133923000 | 8.540289000 | 4.099835000 |
| 1 | 11.743293000 | 7.773163000 | 3.441933000 |
| 6 | 4.400143000 | 4.610385000 | 4.969281000 |
| 1 | 4.462687000 | 3.654272000 | 5.472930000 |
| 6 | 8.479454000 | 8.300118000 | -2.251026000 |
| 1 | 9.143737000 | 8.341792000 | -3.107709000 |
| 6 | 13.996356000 | 9.709128000 | 5.067084000 |
| 1 | 15.064740000 | 9.855281000 | 5.163961000 |
| 6 | 8.991095000 | 8.589551000 | -0.996801000 |
| 6 | 7.531464000 | 9.444693000 | 8.690228000 |
| 1 | 7.065397000 | 9.488190000 | 9.666257000 |
| 6 | 6.346364000 | 7.862166000 | -1.289014000 |
| 1 | 5.310846000 | 7.553458000 | -1.385269000 |
| 6 | 7.151782000 | 7.937286000 | -2.412443000 |
| 1 | 6.755095000 | 7.703796000 | -3.391452000 |
| 6 | 10.608070000 | 9.912600000 | 0.275261000 |
| 6 | 11.612691000 | 10.864123000 | 0.214642000 |
| 1 | 12.269077000 | 10.876016000 | -0.648871000 |
| 6 | 6.590247000 | 3.281131000 | -1.033480000 |
| 1 | 6.598116000 | 2.523378000 | -1.806488000 |
| 6 | 8.171073000 | 8.566360000 | 0.152834000 |
| 6 | 5.335321000 | 4.939694000 | 4.003518000 |
| 1 | 6.124551000 | 4.237296000 | 3.759361000 |
| 6 | 5.918391000 | 8.002232000 | 1.151526000 |
| 1 | 4.897404000 | 7.791202000 | 0.828988000 |
| 1 | 5.914606000 | 8.879549000 | 1.802431000 |
| 6 | 13.503179000 | 8.726044000 | 4.224882000 |
| 1 | 14.184145000 | 8.100883000 | 3.661462000 |
| 6 | 6.564818000 | 5.234993000 | 0.963800000 |
| 6 | 5.456309000 | 4.413857000 | 0.760135000 |
| 1 | 4.571906000 | 4.537229000 | 1.373423000 |
| 6 | 5.273218000 | 6.167730000 | 3.343681000 |
| 6 | 4.259830000 | 7.061699000 | 3.681081000 |
| 1 | 4.200352000 | 8.026371000 | 3.192368000 |
| 6 | 9.911297000 | 10.789789000 | 2.412808000 |
| 6 | 8.735612000 | 8.778007000 | 8.522999000 |
| 1 | 9.212619000 | 8.296161000 | 9.366922000 |
| 6 | 7.680728000 | 5.062155000 | 0.145002000 |
| 1 | 8.531188000 | 5.725204000 | 0.262594000 |

| | | | |
|---|---|---|---|
| 6 | 13.119414000 | 10.507592000 | 5.789794000 |
| 1 | 13.502543000 | 11.275164000 | 6.450405000 |
| 6 | 9.067652000 | 10.742945000 | 3.640120000 |
| 1 | 8.002587000 | 10.709095000 | 3.401196000 |
| 1 | 9.259680000 | 11.602087000 | 4.284615000 |
| 6 | 3.391707000 | 5.506198000 | 5.295203000 |
| 1 | 2.662412000 | 5.250460000 | 6.053068000 |
| 6 | 8.415613000 | 6.365336000 | 4.582799000 |
| 6 | 3.324703000 | 6.731008000 | 4.650562000 |
| 1 | 2.541898000 | 7.435372000 | 4.901793000 |
| 6 | 9.720127000 | 9.854693000 | 1.369481000 |
| 6 | 11.796043000 | 11.771679000 | 1.245312000 |
| 1 | 12.587719000 | 12.507751000 | 1.202027000 |
| 6 | 8.732655000 | 9.333248000 | 6.173994000 |
| 6 | 10.948623000 | 11.712336000 | 2.338308000 |
| 1 | 11.078175000 | 12.406307000 | 3.161744000 |
| 6 | 10.441109000 | 8.869698000 | -0.778641000 |
| 1 | 10.948770000 | 7.940754000 | -0.456990000 |
| 1 | 10.941383000 | 9.150458000 | -1.706464000 |
| 8 | 10.313928000 | 6.561785000 | 2.067919000 |
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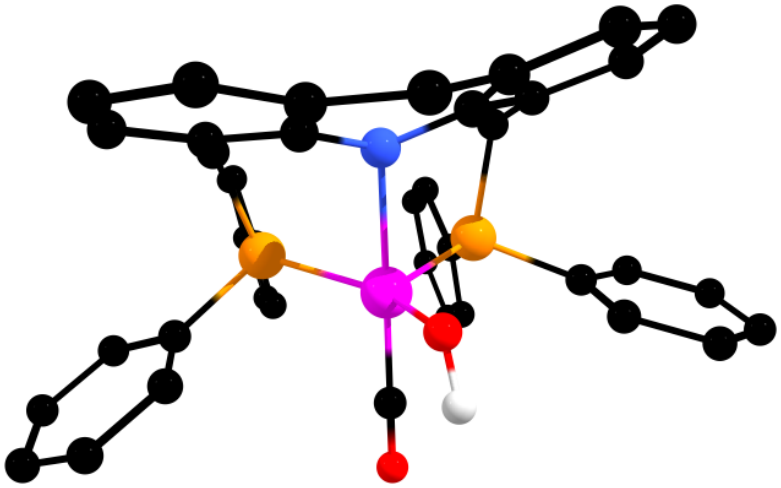
| 1 | 10.087634000 | 5.667676000 | 1.784576000 |

**6c**



| | 1 | 2 | 3 |
|---|---|---|---|
| | ***A*** | A | A |
| Frequencies -- | ***18.5371*** | 24.9666 | 34.5448 |
| Red. masses -- | ***5.0084*** | 4.7481 | 4.7718 |
| Frc consts -- | ***0.0010*** | 0.0017 | 0.0034 |
| IR Inten -- | ***0.0368*** | 0.0398 | 0.1963 |

| | | | |
|---|---|---|---|
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| 15 | -2.220312000 | 7.603224000 | 3.028310000 |

| | | | |
|---|---|---|---|
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| 8 | -2.543025000 | 7.731222000 | 6.906085000 |
| 7 | 0.701797000 | 8.464320000 | 2.914401000 |
| 6 | -1.562104000 | 8.140003000 | 1.394793000 |
| 1 | -0.837995000 | 7.372647000 | 1.102526000 |
| 1 | -2.382967000 | 8.140554000 | 0.675483000 |
| 6 | -0.882015000 | 9.469583000 | 1.446515000 |
| 6 | -1.351452000 | 10.569555000 | 0.742225000 |
| 1 | -2.281260000 | 10.488290000 | 0.189229000 |
| 6 | -0.622462000 | 11.749422000 | 0.714209000 |
| 1 | -0.986687000 | 12.600921000 | 0.154441000 |
| 6 | 0.589364000 | 11.824147000 | 1.391439000 |
| 1 | 1.169392000 | 12.740567000 | 1.355005000 |
| 6 | 1.065906000 | 10.757367000 | 2.137778000 |
| 6 | 0.311383000 | 9.574411000 | 2.191413000 |
| 6 | 2.336082000 | 10.832383000 | 2.936371000 |
| 1 | 3.076692000 | 11.451030000 | 2.422260000 |
| 1 | 2.127545000 | 11.350344000 | 3.880459000 |
| 6 | 2.903514000 | 9.476999000 | 3.251506000 |
| 6 | 4.232399000 | 9.288720000 | 3.598926000 |
| 1 | 4.902512000 | 10.142315000 | 3.595491000 |
| 6 | 4.710883000 | 8.040219000 | 3.979609000 |
| 1 | 5.747668000 | 7.917886000 | 4.264479000 |
| 6 | 3.852292000 | 6.950963000 | 3.987634000 |
| 1 | 4.216138000 | 5.969989000 | 4.274895000 |
| 6 | 2.526156000 | 7.098427000 | 3.604980000 |
| 6 | 2.035651000 | 8.373955000 | 3.260696000 |
| 6 | 1.577626000 | 5.945093000 | 3.546462000 |
| 1 | 2.086853000 | 4.993681000 | 3.711464000 |
| 1 | 1.070905000 | 5.916380000 | 2.576965000 |
| 6 | -1.817298000 | 7.897537000 | 6.017284000 |
| 44 | -0.661040000 | 8.149845000 | 4.599929000 |
| 1 | 0.000179000 | 10.008025000 | 6.201127000 |
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| 6 | -4.924257000 | 8.445572000 | 2.813420000 |
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| 6 | -5.939335000 | 9.383351000 | 2.923243000 |
| 6 | -4.392901000 | 10.956474000 | 3.865917000 |
| 6 | -5.676777000 | 10.638614000 | 3.450252000 |
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| 1 | -2.375157000 | 10.282059000 | 4.086019000 |
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| 6 | 1.716261000 | 7.171700000 | 6.958891000 |
| 6 | 1.657921000 | 4.770554000 | 6.846325000 |
| 6 | 2.582330000 | 7.095341000 | 8.039138000 |
| 6 | 2.520937000 | 4.699646000 | 7.927185000 |
| 6 | 2.982570000 | 5.862171000 | 8.527534000 |
| 1 | 1.422609000 | 8.138875000 | 6.563473000 |

| | | | |
|---|---|---|---|
| 1 | 1.313531000 | 3.855469000 | 6.379481000 |
| 1 | 2.948638000 | 8.006334000 | 8.494844000 |
| 1 | 2.834967000 | 3.732689000 | 8.299366000 |
| 1 | 3.656937000 | 5.804414000 | 9.372539000 |
| 6 | -0.677170000 | 4.568340000 | 4.823472000 |
| 6 | -0.694829000 | 3.714130000 | 3.722359000 |
| 6 | -1.412181000 | 4.224047000 | 5.960448000 |
| 6 | -1.411958000 | 2.528261000 | 3.768068000 |
| 6 | -2.123019000 | 3.037444000 | 6.004412000 |
| 6 | -2.119613000 | 2.184503000 | 4.909460000 |
| 1 | -0.138636000 | 3.965890000 | 2.827534000 |
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| 1 | -1.413360000 | 1.870244000 | 2.908316000 |
| 1 | -2.677794000 | 2.776397000 | 6.896591000 |
| 1 | -2.673411000 | 1.254809000 | 4.943740000 |
| 6 | -3.032430000 | 6.011697000 | 2.716301000 |
| 6 | -2.947299000 | 5.347952000 | 1.493828000 |
| 6 | -3.790309000 | 5.441980000 | 3.742878000 |
| 6 | -3.621520000 | 4.150888000 | 1.296355000 |
| 6 | -4.468383000 | 4.254047000 | 3.539864000 |
| 6 | -4.387765000 | 3.606681000 | 2.313649000 |
| 1 | -2.364191000 | 5.765729000 | 0.683311000 |
| 1 | -3.861154000 | 5.944927000 | 4.701273000 |
| 1 | -3.552349000 | 3.649509000 | 0.339314000 |
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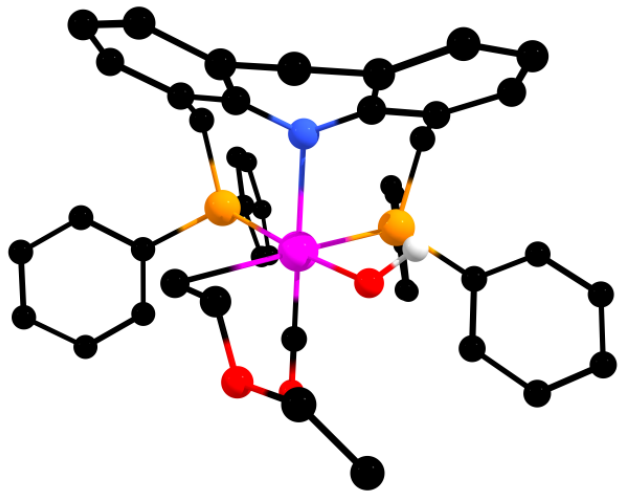
| 1 | -4.918918000 | 2.676579000 | 2.155646000 |

**6d**



| | 1 | 2 | 3 |
|---|---|---|---|
| | ***A*** | A | A |
| Frequencies -- | ***15.3859*** | 21.6111 | 31.1717 |
| Red. masses -- | ***4.2502*** | 5.1767 | 4.7998 |
| Frc consts -- | ***0.0006*** | 0.0014 | 0.0027 |
| IR Inten -- | ***0.1896*** | 0.0591 | 0.2068 |

| | | | |
|---|---|---|---|
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| 15 | 0.263586000 | 6.067193000 | 4.873882000 |
| 8 | -2.611896000 | 7.641954000 | 6.923526000 |
| 7 | 0.647012000 | 8.445507000 | 2.902016000 |
| 6 | -1.607278000 | 7.997900000 | 1.340169000 |
| 1 | -0.903739000 | 7.173543000 | 1.176463000 |
| 1 | -2.376735000 | 7.933498000 | 0.569621000 |
| 6 | -0.864255000 | 9.291660000 | 1.247511000 |
| 6 | -1.234669000 | 10.285194000 | 0.351199000 |
| 1 | -2.117108000 | 10.140955000 | -0.263384000 |
| 6 | -0.468601000 | 11.431142000 | 0.194437000 |
| 1 | -0.764832000 | 12.192766000 | -0.514557000 |
| 6 | 0.694813000 | 11.576233000 | 0.937786000 |
| 1 | 1.310322000 | 12.460815000 | 0.811308000 |
| 6 | 1.086943000 | 10.610627000 | 1.852254000 |
| 6 | 0.298439000 | 9.458619000 | 2.030172000 |
| 6 | 2.318824000 | 10.753739000 | 2.698255000 |
| 1 | 3.067074000 | 11.370095000 | 2.194617000 |
| 1 | 2.071635000 | 11.305890000 | 3.618030000 |
| 6 | 2.887023000 | 9.419083000 | 3.077957000 |
| 6 | 4.229000000 | 9.236204000 | 3.371392000 |
| 1 | 4.905939000 | 10.079462000 | 3.281488000 |
| 6 | 4.709998000 | 8.006555000 | 3.802269000 |
| 1 | 5.757242000 | 7.882510000 | 4.044220000 |
| 6 | 3.836837000 | 6.934236000 | 3.904272000 |
| 1 | 4.204964000 | 5.960953000 | 4.210142000 |
| 6 | 2.493942000 | 7.077521000 | 3.579183000 |
| 6 | 1.994919000 | 8.339299000 | 3.193299000 |
| 6 | 1.555589000 | 5.918620000 | 3.578069000 |
| 1 | 2.082938000 | 4.970137000 | 3.681526000 |
| 1 | 1.001554000 | 5.900153000 | 2.634417000 |
| 6 | -1.892098000 | 7.807211000 | 6.024912000 |
| 44 | -0.753173000 | 8.098275000 | 4.626758000 |
| 1 | 1.621449000 | 8.408353000 | 5.632278000 |
| 6 | -1.794753000 | 10.392538000 | 4.413646000 |
| 6 | -0.730492000 | 10.860955000 | 5.112359000 |
| 1 | -1.779500000 | 10.498160000 | 3.338734000 |
| 1 | -2.758999000 | 10.305077000 | 4.895876000 |
| 8 | -0.788907000 | 11.081733000 | 6.405287000 |
| 1 | 0.212563000 | 11.078138000 | 4.617570000 |
| 6 | 0.430636000 | 11.467100000 | 7.079937000 |
| 6 | 0.503448000 | 10.743943000 | 8.388851000 |
| 1 | 0.386531000 | 12.551784000 | 7.213936000 |
| 1 | 1.276548000 | 11.215359000 | 6.440071000 |
| 1 | -0.363959000 | 10.960820000 | 9.011592000 |
| 1 | 1.394317000 | 11.052522000 | 8.934890000 |
| 1 | 0.557783000 | 9.671275000 | 8.211110000 |
| 6 | 1.176396000 | 5.849313000 | 6.445016000 |
| 6 | 0.833892000 | 6.563191000 | 7.591450000 |
| 6 | 2.186508000 | 4.889564000 | 6.528312000 |

| | | | |
|---|---|---|---|
| 6 | 1.493321000 | 6.328715000 | 8.788705000 |
| 6 | 2.852195000 | 4.665302000 | 7.721871000 |
| 6 | 2.506968000 | 5.386379000 | 8.855427000 |
| 1 | 0.068373000 | 7.322386000 | 7.534941000 |
| 1 | 2.452840000 | 4.300378000 | 5.658952000 |
| 1 | 1.215879000 | 6.893815000 | 9.669699000 |
| 1 | 3.637964000 | 3.921984000 | 7.766495000 |
| 1 | 3.027149000 | 5.211511000 | 9.788750000 |
| 6 | -3.889472000 | 8.569652000 | 3.057873000 |
| 6 | -4.287615000 | 9.433928000 | 2.041732000 |
| 6 | -4.694293000 | 8.466358000 | 4.194164000 |
| 6 | -5.457177000 | 10.173096000 | 2.157525000 |
| 6 | -5.865164000 | 9.195257000 | 4.304917000 |
| 6 | -6.250045000 | 10.055344000 | 3.286017000 |
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| 1 | -5.743842000 | 10.844425000 | 1.357932000 |
| 1 | -6.473662000 | 9.097700000 | 5.194930000 |
| 1 | -7.161278000 | 10.632694000 | 3.375126000 |
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| 6 | -3.091663000 | 5.302878000 | 1.508646000 |
| 6 | -3.631864000 | 5.305122000 | 3.845574000 |
| 6 | -3.732976000 | 4.080071000 | 1.366421000 |
| 6 | -4.289309000 | 4.097208000 | 3.698036000 |
| 6 | -4.343786000 | 3.481356000 | 2.455208000 |
| 1 | -2.639992000 | 5.759598000 | 0.638226000 |
| 1 | -3.571230000 | 5.761896000 | 4.826970000 |
| 1 | -3.762514000 | 3.602544000 | 0.395096000 |
| 1 | -4.747324000 | 3.627594000 | 4.559253000 |
| 1 | -4.853073000 | 2.532836000 | 2.340460000 |
| 6 | -0.617578000 | 4.473013000 | 4.812450000 |
| 6 | -0.624271000 | 3.672265000 | 3.671485000 |
| 6 | -1.274300000 | 4.018767000 | 5.957716000 |
| 6 | -1.251109000 | 2.435472000 | 3.685220000 |
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| 6 | -1.884071000 | 1.986184000 | 4.833498000 |
| 1 | -0.131917000 | 4.004519000 | 2.765941000 |
| 1 | -1.277248000 | 4.628602000 | 6.854298000 |
| 1 | -1.242869000 | 1.822572000 | 2.792688000 |
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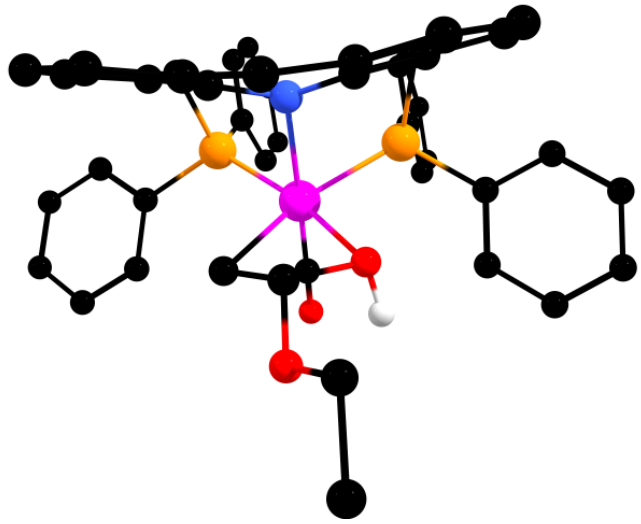
**6e**



| | 1 | 2 | 3 |
|---|---|---|---|
| | ***A*** | A | A |
| Frequencies -- | ***21.6110*** | 27.6777 | 31.5533 |
| Red. masses -- | ***5.2637*** | 4.6383 | 4.7016 |
| Frc consts -- | ***0.0014*** | 0.0021 | 0.0028 |
| IR Inten -- | ***0.0289*** | 0.6375 | 0.3845 |

| | | | |
|---|---|---|---|
| 8 | 0.811335000 | 8.853268000 | 5.982376000 |
| 15 | -2.079401000 | 7.295239000 | 2.975099000 |
| 15 | 0.598413000 | 5.699157000 | 4.754360000 |
| 8 | -2.605328000 | 6.944013000 | 6.723607000 |
| 7 | 0.848124000 | 8.330703000 | 2.993026000 |
| 6 | -1.359355000 | 7.888945000 | 1.397249000 |
| 1 | -0.576705000 | 7.159890000 | 1.164979000 |
| 1 | -2.120408000 | 7.837365000 | 0.617574000 |
| 6 | -0.745117000 | 9.244605000 | 1.460508000 |
| 6 | -1.261312000 | 10.313188000 | 0.744609000 |
| 1 | -2.189260000 | 10.182814000 | 0.197909000 |
| 6 | -0.581718000 | 11.522412000 | 0.690276000 |
| 1 | -0.986134000 | 12.353498000 | 0.127780000 |
| 6 | 0.642780000 | 11.636212000 | 1.330617000 |
| 1 | 1.205695000 | 12.561210000 | 1.256021000 |
| 6 | 1.171013000 | 10.592795000 | 2.080270000 |
| 6 | 0.445015000 | 9.396040000 | 2.206095000 |
| 6 | 2.504020000 | 10.724486000 | 2.760878000 |
| 1 | 3.225376000 | 11.181748000 | 2.075278000 |
| 1 | 2.438057000 | 11.442484000 | 3.590138000 |
| 6 | 3.040869000 | 9.408937000 | 3.253129000 |
| 6 | 4.370183000 | 9.291206000 | 3.633309000 |
| 1 | 5.003499000 | 10.171713000 | 3.589997000 |
| 6 | 4.898782000 | 8.082703000 | 4.060061000 |
| 1 | 5.934999000 | 8.011595000 | 4.363147000 |
| 6 | 4.090877000 | 6.956311000 | 4.048047000 |
| 1 | 4.504903000 | 5.989708000 | 4.313613000 |
| 6 | 2.762443000 | 7.032650000 | 3.653819000 |
| 6 | 2.195110000 | 8.283291000 | 3.315769000 |

| | | | |
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| 1 | 1.420398000 | 5.811289000 | 2.543253000 |
| 6 | -1.830802000 | 7.244188000 | 5.907270000 |
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| 6 | -1.073225000 | 9.837952000 | 4.890306000 |
| 6 | 0.275361000 | 10.145369000 | 5.439915000 |
| 1 | -1.300513000 | 10.428739000 | 4.003459000 |
| 1 | -1.835022000 | 10.025694000 | 5.647410000 |
| 8 | 0.288202000 | 11.085294000 | 6.448482000 |
| 1 | 1.004621000 | 10.382524000 | 4.665421000 |
| 6 | 1.589959000 | 11.614993000 | 6.727134000 |
| 6 | 1.483334000 | 12.558823000 | 7.886870000 |
| 1 | 1.961558000 | 12.126473000 | 5.830730000 |
| 1 | 2.285186000 | 10.795856000 | 6.941276000 |
| 1 | 0.792795000 | 13.372401000 | 7.668517000 |
| 1 | 2.456503000 | 12.992232000 | 8.112046000 |
| 1 | 1.128512000 | 12.046106000 | 8.780176000 |
| 6 | -2.583184000 | 5.581954000 | 2.596613000 |
| 6 | -2.375615000 | 4.983055000 | 1.355326000 |
| 6 | -3.249970000 | 4.857678000 | 3.587159000 |
| 6 | -2.836546000 | 3.697150000 | 1.107341000 |
| 6 | -3.709635000 | 3.577297000 | 3.337878000 |
| 6 | -3.507199000 | 2.994545000 | 2.093964000 |
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| 1 | -2.672260000 | 3.248521000 | 0.135606000 |
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| 6 | -0.472549000 | 1.980005000 | 3.358276000 |
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| 6 | -4.159512000 | 8.861857000 | 4.090488000 |
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| 6 | -5.414818000 | 9.453976000 | 4.077338000 |
| 6 | -6.250209000 | 9.292115000 | 2.985453000 |
| 1 | -4.277288000 | 7.316836000 | 1.081911000 |
| 1 | -3.510566000 | 8.999184000 | 4.943063000 |
| 1 | -6.481486000 | 8.388944000 | 1.050965000 |
| 1 | -5.735847000 | 10.044733000 | 4.925746000 |

| | | | |
|---|---|---|---|
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| 6 | 1.500543000 | 5.521423000 | 6.340302000 |
| 6 | 1.003816000 | 6.088277000 | 7.511798000 |
| 6 | 2.676190000 | 4.774055000 | 6.413918000 |
| 6 | 1.666934000 | 5.928380000 | 8.719368000 |
| 6 | 3.346451000 | 4.622139000 | 7.615887000 |
| 6 | 2.845298000 | 5.202225000 | 8.772028000 |
| 1 | 0.075766000 | 6.646266000 | 7.484520000 |
| 1 | 3.070894000 | 4.295606000 | 5.525995000 |
| 1 | 1.260403000 | 6.373548000 | 9.618585000 |
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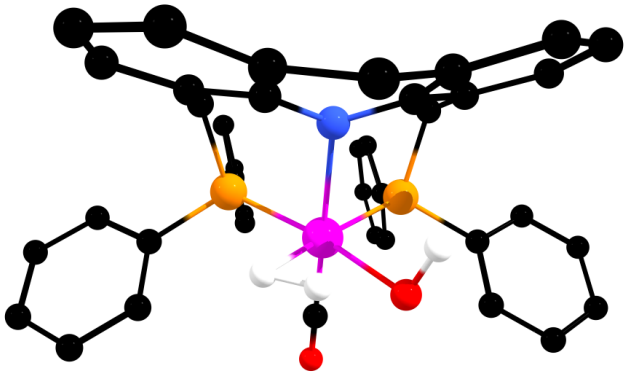
**6TS1**



| | 1 | 2 | 3 |
|---|---|---|---|
| | ***A*** | A | A |
| Frequencies -- | ***-938.8164*** | 17.9175 | 30.7460 |
| Red. masses -- | ***1.0705*** | 5.4051 | 4.3382 |
| Frc consts -- | ***0.5559*** | 0.0010 | 0.0024 |
| IR Inten -- | ***799.4021*** | 0.0317 | 0.2938 |

| | | | |
|---|---|---|---|
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| 15 | -2.309487000 | 7.814363000 | 3.053171000 |
| 15 | 0.258924000 | 6.327680000 | 4.984123000 |
| 8 | -2.528432000 | 8.201342000 | 6.909862000 |
| 7 | 0.667312000 | 8.512097000 | 2.800300000 |
| 6 | -1.641691000 | 8.048091000 | 1.356779000 |
| 1 | -0.962705000 | 7.201709000 | 1.207987000 |
| 1 | -2.460222000 | 7.963447000 | 0.640264000 |
| 6 | -0.887197000 | 9.321123000 | 1.169516000 |
| 6 | -1.298876000 | 10.296758000 | 0.272530000 |
| 1 | -2.234536000 | 10.163898000 | -0.259994000 |
| 6 | -0.507642000 | 11.409383000 | 0.025149000 |
| 1 | -0.828875000 | 12.159044000 | -0.685903000 |
| 6 | 0.706120000 | 11.544521000 | 0.685469000 |

| | | | |
|---|---|---|---|
| 1 | 1.333994000 | 12.407481000 | 0.489819000 |
| 6 | 1.124019000 | 10.607237000 | 1.618489000 |
| 6 | 0.316923000 | 9.489845000 | 1.880962000 |
| 6 | 2.380360000 | 10.771857000 | 2.422603000 |
| 1 | 3.136667000 | 11.322327000 | 1.858417000 |
| 1 | 2.162020000 | 11.405418000 | 3.295043000 |
| 6 | 2.923401000 | 9.454754000 | 2.899075000 |
| 6 | 4.263682000 | 9.267063000 | 3.204358000 |
| 1 | 4.956928000 | 10.087402000 | 3.051354000 |
| 6 | 4.720275000 | 8.063977000 | 3.724537000 |
| 1 | 5.765446000 | 7.938948000 | 3.974643000 |
| 6 | 3.827458000 | 7.019151000 | 3.913771000 |
| 1 | 4.176992000 | 6.068159000 | 4.300611000 |
| 6 | 2.487815000 | 7.160179000 | 3.579911000 |
| 6 | 2.015431000 | 8.397877000 | 3.093961000 |
| 6 | 1.524754000 | 6.024285000 | 3.686649000 |
| 1 | 2.036112000 | 5.082060000 | 3.887175000 |
| 1 | 0.966665000 | 5.924049000 | 2.750490000 |
| 6 | -1.814226000 | 8.278728000 | 6.000902000 |
| 44 | -0.682707000 | 8.396896000 | 4.551690000 |
| 1 | 1.605142000 | 9.603440000 | 5.101455000 |
| 1 | -0.215296000 | 10.186133000 | 4.767057000 |
| 1 | -0.978294000 | 10.167743000 | 4.229512000 |
| 6 | -3.106741000 | 6.178881000 | 2.991608000 |
| 6 | -3.101672000 | 5.371913000 | 1.855413000 |
| 6 | -3.806531000 | 5.747473000 | 4.120627000 |
| 6 | -3.796967000 | 4.170416000 | 1.843047000 |
| 6 | -4.499746000 | 4.551122000 | 4.105192000 |
| 6 | -4.501109000 | 3.761391000 | 2.962875000 |
| 1 | -2.566793000 | 5.678361000 | 0.966022000 |
| 1 | -3.817382000 | 6.362016000 | 5.014346000 |
| 1 | -3.790062000 | 3.558002000 | 0.950172000 |
| 1 | -5.040627000 | 4.233080000 | 4.987384000 |
| 1 | -5.046039000 | 2.825911000 | 2.951199000 |
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| 6 | -5.935693000 | 9.470233000 | 2.124594000 |
| 6 | -5.005003000 | 10.822199000 | 3.872841000 |
| 6 | -6.027597000 | 10.562241000 | 2.976831000 |
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| 1 | -3.092280000 | 10.216063000 | 4.615780000 |
| 1 | -6.732765000 | 9.258064000 | 1.423417000 |
| 1 | -5.069995000 | 11.669714000 | 4.542973000 |
| 1 | -6.897376000 | 11.205806000 | 2.941845000 |
| 6 | 1.221074000 | 6.258257000 | 6.533380000 |
| 6 | 1.154926000 | 7.273344000 | 7.482903000 |
| 6 | 2.032684000 | 5.147989000 | 6.780893000 |
| 6 | 1.891421000 | 7.180715000 | 8.656259000 |
| 6 | 2.769237000 | 5.062105000 | 7.948361000 |
| 6 | 2.699419000 | 6.081121000 | 8.889413000 |

| | | | |
|---|---|---|---|
| 1 | 0.556016000 | 8.152130000 | 7.287973000 |
| 1 | 2.078654000 | 4.337095000 | 6.061993000 |
| 1 | 1.834232000 | 7.978573000 | 9.385556000 |
| 1 | 3.394895000 | 4.196971000 | 8.127581000 |
| 1 | 3.275494000 | 6.013736000 | 9.803644000 |
| 6 | -0.686518000 | 4.779308000 | 5.107349000 |
| 6 | -0.772450000 | 3.874379000 | 4.051476000 |
| 6 | -1.339608000 | 4.483683000 | 6.305797000 |
| 6 | -1.475271000 | 2.688045000 | 4.200532000 |
| 6 | -2.042665000 | 3.300297000 | 6.450334000 |
| 6 | -2.106198000 | 2.396206000 | 5.399516000 |
| 1 | -0.280467000 | 4.084997000 | 3.109678000 |
| 1 | -1.278197000 | 5.177496000 | 7.137078000 |
| 1 | -1.526629000 | 1.989728000 | 3.374673000 |
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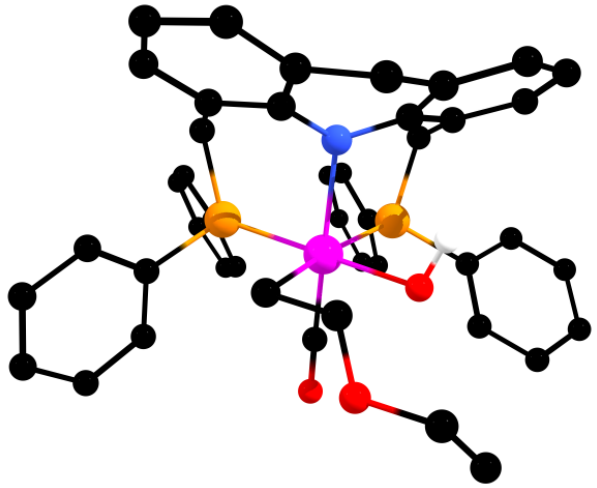
**6TS2**



| | 1 | 2 | 3 |
|---|---|---|---|
| | ***A*** | A | A |
| Frequencies -- | ***-242.6559*** | 15.8925 | 19.2440 |
| Red. masses -- | ***6.6320*** | 4.2141 | 5.3308 |
| Frc consts -- | ***0.2301*** | 0.0006 | 0.0012 |
| IR Inten -- | ***27.3568*** | 0.5908 | 0.2023 |

| | | | |
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| 15 | 0.296123000 | 5.962464000 | 4.848045000 |
| 8 | -2.645370000 | 7.565509000 | 6.872671000 |
| 7 | 0.648573000 | 8.373103000 | 2.865623000 |
| 6 | -1.650407000 | 7.833159000 | 1.315034000 |
| 1 | -1.005464000 | 6.960679000 | 1.156318000 |
| 1 | -2.451378000 | 7.788677000 | 0.575204000 |
| 6 | -0.853313000 | 9.086308000 | 1.129072000 |
| 6 | -1.192790000 | 9.995359000 | 0.133840000 |
| 1 | -2.074181000 | 9.803692000 | -0.469879000 |
| 6 | -0.413060000 | 11.112107000 | -0.123178000 |

| | | | |
|---|---|---|---|
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| 1 | 1.348788000 | 12.195220000 | 0.451308000 |
| 6 | 1.088291000 | 10.448356000 | 1.647748000 |
| 6 | 0.304290000 | 9.305817000 | 1.905533000 |
| 6 | 2.271069000 | 10.705294000 | 2.533469000 |
| 1 | 3.030145000 | 11.291217000 | 2.009980000 |
| 1 | 1.960148000 | 11.343131000 | 3.375051000 |
| 6 | 2.853532000 | 9.429895000 | 3.062519000 |
| 6 | 4.185488000 | 9.321221000 | 3.435326000 |
| 1 | 4.832934000 | 10.184851000 | 3.324380000 |
| 6 | 4.690420000 | 8.139311000 | 3.957861000 |
| 1 | 5.726406000 | 8.072946000 | 4.262784000 |
| 6 | 3.858361000 | 7.034153000 | 4.057744000 |
| 1 | 4.250719000 | 6.089796000 | 4.418969000 |
| 6 | 2.531104000 | 7.100696000 | 3.656461000 |
| 6 | 1.993234000 | 8.324762000 | 3.200611000 |
| 6 | 1.665342000 | 5.889096000 | 3.623833000 |
| 1 | 2.245626000 | 4.976526000 | 3.762141000 |
| 1 | 1.169253000 | 5.832690000 | 2.650873000 |
| 6 | -1.933031000 | 7.730810000 | 5.967549000 |
| 44 | -0.792479000 | 8.018511000 | 4.575614000 |
| 1 | 1.516987000 | 8.979178000 | 5.371641000 |
| 6 | -1.378186000 | 10.174563000 | 4.485911000 |
| 6 | -0.357340000 | 10.681733000 | 5.328933000 |
| 1 | -1.296394000 | 10.517577000 | 3.458090000 |
| 1 | -2.376174000 | 10.301295000 | 4.894970000 |
| 8 | -0.676850000 | 11.071984000 | 6.536087000 |
| 1 | 0.567298000 | 11.077104000 | 4.912780000 |
| 6 | 0.398478000 | 11.478262000 | 7.412833000 |
| 6 | 0.422771000 | 10.589876000 | 8.619806000 |
| 1 | 0.197185000 | 12.518611000 | 7.675039000 |
| 1 | 1.338788000 | 11.434902000 | 6.860121000 |
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| 1 | 1.190170000 | 10.928834000 | 9.315051000 |
| 1 | 0.643671000 | 9.565781000 | 8.326081000 |
| 6 | 1.156961000 | 5.750170000 | 6.448118000 |
| 6 | 0.822484000 | 6.522662000 | 7.557014000 |
| 6 | 2.139094000 | 4.767053000 | 6.587838000 |
| 6 | 1.458622000 | 6.321299000 | 8.774014000 |
| 6 | 2.778937000 | 4.572091000 | 7.799441000 |
| 6 | 2.439795000 | 5.351661000 | 8.896755000 |
| 1 | 0.075425000 | 7.296522000 | 7.460650000 |
| 1 | 2.397635000 | 4.134589000 | 5.746320000 |
| 1 | 1.185273000 | 6.929089000 | 9.627494000 |
| 1 | 3.539228000 | 3.806483000 | 7.889221000 |
| 1 | 2.938934000 | 5.199122000 | 9.845405000 |
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| 6 | -4.716069000 | 8.423871000 | 4.163277000 |
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| 1 | -5.324255000 | 11.303373000 | 1.684083000 |

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| 6 | -3.453123000 | 5.314352000 | 1.612452000 |
| 6 | -3.552712000 | 5.240032000 | 4.007679000 |
| 6 | -4.138443000 | 4.109918000 | 1.550458000 |
| 6 | -4.256721000 | 4.050018000 | 3.944302000 |
| 6 | -4.551142000 | 3.480951000 | 2.713878000 |
| 1 | -3.157886000 | 5.795982000 | 0.689670000 |
| 1 | -3.297395000 | 5.658239000 | 4.974391000 |
| 1 | -4.357146000 | 3.668360000 | 0.586304000 |
| 1 | -4.560693000 | 3.557968000 | 4.859390000 |
| 1 | -5.093081000 | 2.544955000 | 2.663781000 |
| 6 | -0.489425000 | 4.325338000 | 4.670908000 |
| 6 | -0.600886000 | 3.708252000 | 3.424380000 |
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| 6 | -1.621385000 | 2.435468000 | 5.664352000 |
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| 1 | -0.952257000 | 4.145438000 | 6.763305000 |
| 1 | -1.272318000 | 1.997985000 | 2.329068000 |
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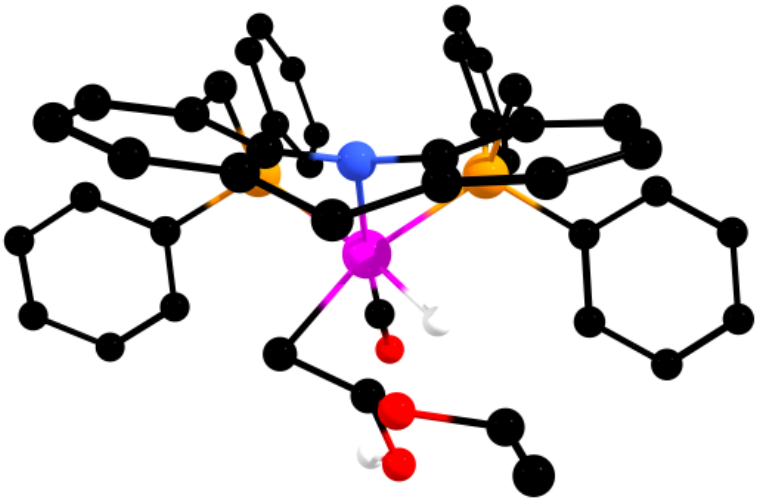
**6TS3**



| | 1 | 2 | 3 |
|---|---|---|---|
| | ***A*** | A | A |
| Frequencies -- | ***-625.0786*** | 27.4760 | 33.3881 |
| Red. masses -- | ***1.7755*** | 5.3906 | 5.3993 |
| Frc consts -- | ***0.4087*** | 0.0024 | 0.0035 |
| IR Inten -- | ***433.0749*** | 0.0180 | 0.2669 |

| | | | |
|---|---|---|---|
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| 15 | -2.126318000 | 7.233580000 | 2.813252000 |
| 15 | 0.710272000 | 5.880885000 | 4.702617000 |
| 8 | -2.246411000 | 6.989759000 | 6.797300000 |
| 7 | 0.810695000 | 8.335984000 | 2.751540000 |

| | | | |
|---|---|---|---|
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| 1 | -2.078414000 | 7.348544000 | 0.374404000 |
| 6 | -0.764059000 | 8.896127000 | 1.023696000 |
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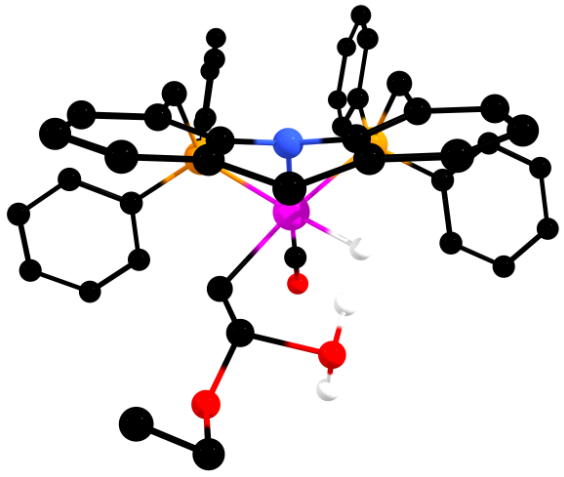
| 6 | 0.529980000 | 11.307977000 | 0.560571000 |
| 1 | 1.047697000 | 12.243646000 | 0.376386000 |
| 6 | 1.022666000 | 10.453142000 | 1.534604000 |
| 6 | 0.365603000 | 9.236421000 | 1.797594000 |
| 6 | 2.218071000 | 10.809376000 | 2.366738000 |
| 1 | 2.913534000 | 11.432356000 | 1.798423000 |
| 1 | 1.889029000 | 11.432473000 | 3.208597000 |
| 6 | 2.911914000 | 9.591447000 | 2.898868000 |
| 6 | 4.254109000 | 9.604506000 | 3.249660000 |
| 1 | 4.822447000 | 10.518371000 | 3.107989000 |
| 6 | 4.870399000 | 8.485363000 | 3.792808000 |
| 1 | 5.912461000 | 8.518790000 | 4.082571000 |
| 6 | 4.144664000 | 7.309671000 | 3.917093000 |
| 1 | 4.626251000 | 6.408286000 | 4.281167000 |
| 6 | 2.814210000 | 7.249211000 | 3.524144000 |
| 6 | 2.157499000 | 8.416696000 | 3.074187000 |
| 6 | 2.079061000 | 5.951862000 | 3.482130000 |
| 1 | 2.751373000 | 5.106163000 | 3.632728000 |
| 1 | 1.600703000 | 5.843364000 | 2.504287000 |
| 6 | -1.621599000 | 7.305753000 | 5.863601000 |
| 44 | -0.574372000 | 7.810598000 | 4.460454000 |
| 1 | -1.322115000 | 9.513081000 | 6.962455000 |
| 6 | -1.110648000 | 9.928398000 | 4.541787000 |
| 6 | -0.097397000 | 9.927944000 | 5.557880000 |
| 1 | -0.849915000 | 10.457692000 | 3.632354000 |
| 1 | -2.116012000 | 10.139904000 | 4.888620000 |
| 8 | 1.012292000 | 10.660122000 | 5.355132000 |
| 1 | 0.575774000 | 8.575808000 | 5.456506000 |
| 6 | 2.162513000 | 10.328219000 | 6.158852000 |
| 6 | 3.155229000 | 11.442357000 | 6.030840000 |
| 1 | 2.562067000 | 9.375582000 | 5.788318000 |
| 1 | 1.855637000 | 10.185887000 | 7.196685000 |
| 1 | 3.415538000 | 11.623137000 | 4.989375000 |
| 1 | 4.069697000 | 11.183385000 | 6.562412000 |
| 1 | 2.766617000 | 12.368249000 | 6.453215000 |
| 6 | -2.827572000 | 5.550574000 | 2.679696000 |
| 6 | -2.969350000 | 4.884394000 | 1.463333000 |
| 6 | -3.288672000 | 4.927780000 | 3.840568000 |
| 6 | -3.565912000 | 3.632959000 | 1.409746000 |
| 6 | -3.892745000 | 3.683927000 | 3.784166000 |
| 6 | -4.034021000 | 3.032716000 | 2.567021000 |
| 1 | -2.619247000 | 5.336112000 | 0.544534000 |
| 1 | -3.175190000 | 5.422125000 | 4.798255000 |
| 1 | -3.667079000 | 3.129433000 | 0.456453000 |
| 1 | -4.245007000 | 3.217642000 | 4.695572000 |
| 1 | -4.501637000 | 2.057177000 | 2.523506000 |
| 6 | 0.025226000 | 4.202121000 | 4.528650000 |
| 6 | -0.059643000 | 3.579269000 | 3.283282000 |

| | | | |
|---|---|---|---|
| 6 | -0.495765000 | 3.542990000 | 5.643887000 |
| 6 | -0.622962000 | 2.318860000 | 3.162182000 |
| 6 | -1.059690000 | 2.283896000 | 5.520444000 |
| 6 | -1.118672000 | 1.665386000 | 4.280382000 |
| 1 | 0.319527000 | 4.076690000 | 2.398397000 |
| 1 | -0.447173000 | 4.014915000 | 6.618912000 |
| 1 | -0.675155000 | 1.847155000 | 2.188931000 |
| 1 | -1.451259000 | 1.783676000 | 6.397311000 |
| 1 | -1.556264000 | 0.679792000 | 4.183626000 |
| 6 | -3.668185000 | 8.222738000 | 2.805955000 |
| 6 | -4.296057000 | 8.607440000 | 1.622471000 |
| 6 | -4.271174000 | 8.560194000 | 4.017073000 |
| 6 | -5.483491000 | 9.322244000 | 1.650602000 |
| 6 | -5.465418000 | 9.261276000 | 4.046051000 |
| 6 | -6.072030000 | 9.650229000 | 2.861438000 |
| 1 | -3.862393000 | 8.350382000 | 0.665018000 |
| 1 | -3.800567000 | 8.270683000 | 4.948458000 |
| 1 | -5.949793000 | 9.621459000 | 0.720470000 |
| 1 | -5.919083000 | 9.509373000 | 4.997227000 |
| 1 | -6.999685000 | 10.207679000 | 2.882114000 |
| 6 | 1.620764000 | 5.727459000 | 6.285007000 |
| 6 | 1.461810000 | 6.637771000 | 7.324666000 |
| 6 | 2.536767000 | 4.684449000 | 6.445670000 |
| 6 | 2.208145000 | 6.522131000 | 8.489368000 |
| 6 | 3.284766000 | 4.570578000 | 7.604042000 |
| 6 | 3.123808000 | 5.493232000 | 8.629271000 |
| 1 | 0.752214000 | 7.449840000 | 7.226429000 |
| 1 | 2.662866000 | 3.951466000 | 5.656100000 |
| 1 | 2.069398000 | 7.241379000 | 9.286720000 |
| 1 | 3.995085000 | 3.760178000 | 7.708049000 |
| 1 | 3.709467000 | 5.405010000 | 9.535472000 |

**6TS4**

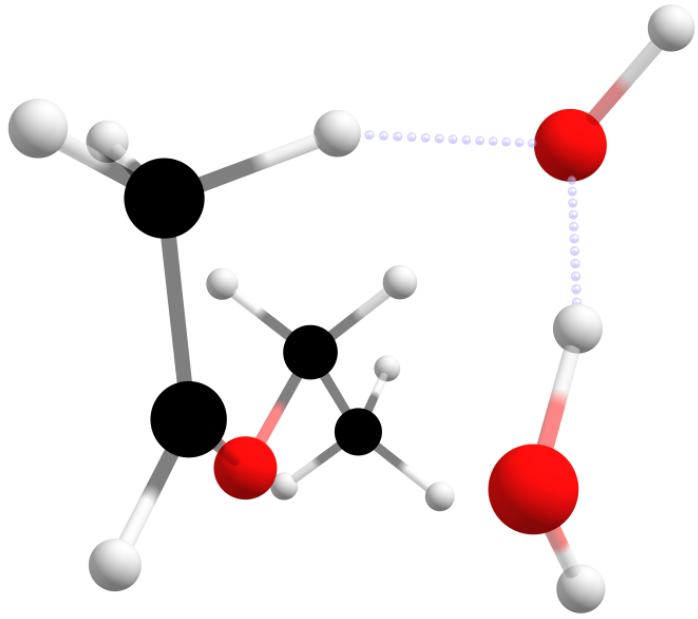


| | 1 | 2 | 3 |
|---|---|---|---|
| | ***A*** | A | A |
| Frequencies -- | ***-294.3637*** | 18.2594 | 27.5718 |
| Red. masses -- | ***5.5148*** | 5.2248 | 4.6669 |
| Frc consts -- | ***0.2815*** | 0.0010 | 0.0021 |
| IR Inten -- | ***219.6098*** | 0.0771 | 1.0755 |

| | | | |
|---|---|---|---|
| 44 | 0.246606000 | -0.428552000 | 0.959866000 |
| 15 | -1.097979000 | -1.807971000 | -0.373358000 |
| 15 | 2.331457000 | -0.654247000 | -0.045994000 |
| 7 | -0.126749000 | 1.221290000 | -0.595062000 |
| 6 | -1.616254000 | -0.797644000 | -1.817891000 |
| 1 | -0.676446000 | -0.597471000 | -2.342512000 |
| 1 | -2.252941000 | -1.379321000 | -2.485603000 |
| 6 | -2.248675000 | 0.506378000 | -1.458192000 |
| 6 | -3.582933000 | 0.760431000 | -1.740868000 |
| 1 | -4.189984000 | -0.030749000 | -2.167151000 |
| 6 | -4.133374000 | 2.017658000 | -1.536120000 |
| 1 | -5.171926000 | 2.206746000 | -1.773010000 |
| 6 | -3.321269000 | 3.036682000 | -1.060743000 |
| 1 | -3.728591000 | 4.034611000 | -0.929329000 |
| 6 | -1.989646000 | 2.812302000 | -0.739294000 |
| 6 | -1.437594000 | 1.524521000 | -0.900162000 |
| 6 | -1.126914000 | 3.916799000 | -0.195877000 |
| 1 | -1.369629000 | 4.108154000 | 0.862222000 |
| 1 | -1.369713000 | 4.861541000 | -0.691988000 |
| 6 | 0.337921000 | 3.621247000 | -0.333125000 |
| 6 | 1.284598000 | 4.633066000 | -0.244465000 |
| 1 | 0.946574000 | 5.649566000 | -0.069341000 |
| 6 | 2.639666000 | 4.367684000 | -0.366220000 |
| 1 | 3.366601000 | 5.164038000 | -0.275519000 |
| 6 | 3.046727000 | 3.072065000 | -0.650764000 |
| 1 | 4.096775000 | 2.855243000 | -0.816747000 |
| 6 | 2.122505000 | 2.045978000 | -0.777557000 |
| 6 | 0.750845000 | 2.293647000 | -0.542198000 |
| 6 | 2.533610000 | 0.699666000 | -1.267864000 |
| 1 | 3.562053000 | 0.719819000 | -1.631194000 |
| 1 | 1.883048000 | 0.410320000 | -2.100871000 |
| 6 | 0.570190000 | -1.693547000 | 2.221725000 |
| 8 | 0.771731000 | -2.491935000 | 3.048153000 |
| 6 | -1.712751000 | 1.568604000 | 2.497664000 |
| 1 | 1.140887000 | 0.767605000 | 1.765972000 |
| 1 | -1.673937000 | 2.350321000 | 1.740603000 |
| 8 | -0.215769000 | 1.931585000 | 3.220731000 |
| 1 | 0.412153000 | 1.371095000 | 2.566717000 |
| 1 | -0.229109000 | 1.420922000 | 4.046435000 |
| 6 | -1.641652000 | 0.196337000 | 1.994202000 |
| 1 | -2.457036000 | 0.132616000 | 1.265490000 |
| 1 | -1.901893000 | -0.480700000 | 2.811025000 |
| 8 | -2.585812000 | 1.798190000 | 3.490881000 |
| 6 | -2.915537000 | 3.190296000 | 3.705977000 |
| 1 | -1.996479000 | 3.782103000 | 3.675354000 |
| 1 | -3.301206000 | 3.232368000 | 4.723761000 |
| 6 | -3.928539000 | 3.668982000 | 2.706234000 |
| 1 | -4.850506000 | 3.093590000 | 2.775642000 |
| 1 | -3.557066000 | 3.581937000 | 1.684057000 |

| | | | |
|---|---|---|---|
| 1 | -4.167009000 | 4.716922000 | 2.884643000 |
| 6 | -0.486464000 | -3.358102000 | -1.124504000 |
| 6 | -0.474066000 | -4.527638000 | -0.361794000 |
| 6 | -0.012880000 | -3.412524000 | -2.434680000 |
| 6 | -0.032358000 | -5.722464000 | -0.903657000 |
| 6 | 0.430008000 | -4.610336000 | -2.975597000 |
| 6 | 0.413962000 | -5.769220000 | -2.216198000 |
| 1 | -0.828699000 | -4.508238000 | 0.662452000 |
| 1 | 0.004872000 | -2.520118000 | -3.047803000 |
| 1 | -0.040571000 | -6.620620000 | -0.298919000 |
| 1 | 0.788823000 | -4.634203000 | -3.997037000 |
| 1 | 0.755451000 | -6.703920000 | -2.642823000 |
| 6 | 2.869467000 | -2.134248000 | -0.974495000 |
| 6 | 2.871782000 | -3.357650000 | -0.300353000 |
| 6 | 3.325873000 | -2.097806000 | -2.290952000 |
| 6 | 3.341499000 | -4.503928000 | -0.915303000 |
| 6 | 3.791422000 | -3.250580000 | -2.909321000 |
| 6 | 3.807858000 | -4.452703000 | -2.222329000 |
| 1 | 2.510661000 | -3.406151000 | 0.721739000 |
| 1 | 3.332487000 | -1.167235000 | -2.843713000 |
| 1 | 3.339336000 | -5.442258000 | -0.374979000 |
| 1 | 4.147412000 | -3.202913000 | -3.931007000 |
| 1 | 4.174443000 | -5.350448000 | -2.704076000 |
| 6 | 3.808261000 | -0.449257000 | 1.028939000 |
| 6 | 3.706111000 | -0.303166000 | 2.408317000 |
| 6 | 5.080159000 | -0.446253000 | 0.451777000 |
| 6 | 4.841849000 | -0.149351000 | 3.191070000 |
| 6 | 6.212916000 | -0.282631000 | 1.229365000 |
| 6 | 6.095874000 | -0.133655000 | 2.604597000 |
| 1 | 2.729135000 | -0.303270000 | 2.871817000 |
| 1 | 5.186850000 | -0.583690000 | -0.618913000 |
| 1 | 4.742186000 | -0.040401000 | 4.263702000 |
| 1 | 7.189799000 | -0.277214000 | 0.762483000 |
| 1 | 6.981554000 | -0.009909000 | 3.214837000 |
| 6 | -2.664935000 | -2.420706000 | 0.351550000 |
| 6 | -3.827769000 | -2.554829000 | -0.405394000 |
| 6 | -2.693516000 | -2.821624000 | 1.686905000 |
| 6 | -4.988015000 | -3.059878000 | 0.160585000 |
| 6 | -3.848010000 | -3.340903000 | 2.249850000 |
| 6 | -5.001279000 | -3.454999000 | 1.489146000 |
| 1 | -3.834465000 | -2.270326000 | -1.449397000 |
| 1 | -1.801414000 | -2.723598000 | 2.292632000 |
| 1 | -5.883387000 | -3.147379000 | -0.441827000 |
| 1 | -3.846795000 | -3.649539000 | 3.287542000 |
| 1 | -5.907593000 | -3.850097000 | 1.930087000 |

**TS5**



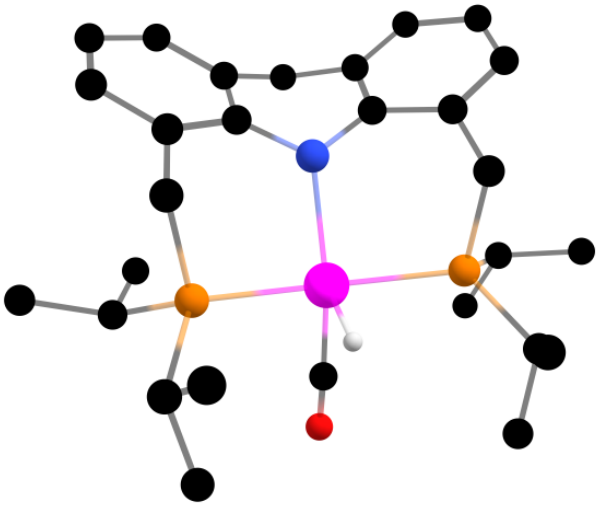
First three frequencies

| | 1 | 2 | 3 |
|---|---|---|---|
| | ***A*** | A | A |
| Frequencies -- | ***-289.2022*** | 60.1964 | 76.8902 |
| Red. masses -- | ***2.7477*** | 3.1875 | 3.4374 |
| Frc consts -- | ***0.1354*** | 0.0068 | 0.0120 |
| IR Inten -- | ***13.3802*** | 0.9123 | 0.9275 |

Coordinates

| | | | |
|---|---|---|---|
| 6 | -1.639497000 | -0.373674000 | 0.474704000 |
| 6 | -2.658458000 | 0.175644000 | 1.419964000 |
| 6 | -0.233377000 | 0.546578000 | -1.199366000 |
| 1 | -2.038284000 | -1.185551000 | -0.136804000 |
| 1 | -2.970847000 | -0.611217000 | 2.104101000 |
| 1 | -3.542360000 | 0.540077000 | 0.898616000 |
| 1 | -0.014162000 | 1.430316000 | -1.786467000 |
| 1 | -0.726191000 | -0.716886000 | 0.972128000 |
| 8 | 1.441214000 | 1.437416000 | 0.134864000 |
| 1 | 0.971321000 | 2.019628000 | 0.739853000 |
| 1 | 1.546992000 | 0.525393000 | 0.649126000 |
| 8 | 1.429275000 | -0.861430000 | 1.107915000 |
| 1 | 2.264399000 | -1.266659000 | 1.354933000 |
| 1 | 0.972911000 | -0.986265000 | -0.450928000 |
| 6 | 0.405460000 | -0.713940000 | -1.425104000 |
| 1 | -0.323582000 | -1.515833000 | -1.547858000 |
| 1 | 1.090514000 | -0.673235000 | -2.265188000 |
| 8 | -1.258456000 | 0.712846000 | -0.437678000 |
| 1 | -2.246906000 | 0.989056000 | 2.015164000 |

**1-*mer***



First three frequencies

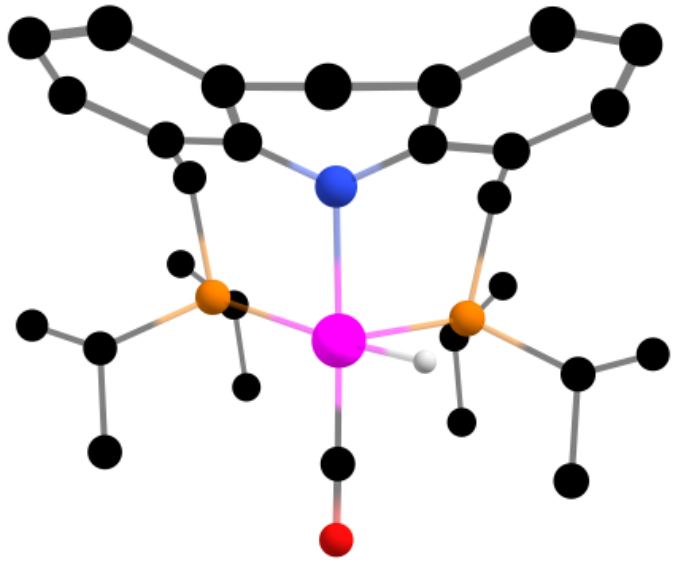
| | 1 | 2 | 3 |
|---|---|---|---|
| | ***A*** | A | A |
| Frequencies -- | ***24.1877*** | 38.2323 | 47.2942 |
| Red. masses -- | ***4.2569*** | 3.4034 | 3.2571 |
| Frc consts -- | ***0.0015*** | 0.0029 | 0.0043 |
| IR Inten -- | ***0.0266*** | 0.2258 | 0.7127 |

Coordinates

| | | | |
|---|---|---|---|
| 44 | -0.217375000 | 6.355775000 | 1.344339000 |
| 15 | -1.832412000 | 7.534745000 | 0.169300000 |
| 15 | 1.691341000 | 5.987845000 | 2.623814000 |
| 8 | -2.160231000 | 5.207239000 | 3.282007000 |
| 7 | 0.952229000 | 6.119283000 | -0.475762000 |
| 6 | -1.391028000 | 5.707331000 | 2.560150000 |
| 6 | -1.637562000 | 10.108312000 | 1.277586000 |
| 6 | -3.247848000 | 8.530175000 | 2.364352000 |
| 6 | -2.613944000 | 8.965192000 | 1.052658000 |
| 6 | -4.053614000 | 7.458776000 | -1.615136000 |
| 6 | -2.956844000 | 5.268193000 | -1.048278000 |
| 6 | -3.302177000 | 6.667658000 | -0.557375000 |
| 6 | 3.526360000 | 4.210755000 | 3.885355000 |
| 6 | 1.189899000 | 3.356261000 | 3.457058000 |
| 6 | 2.306329000 | 4.274739000 | 2.983166000 |
| 6 | 0.705580000 | 6.599447000 | 5.172430000 |
| 6 | 1.935293000 | 8.427901000 | 3.991932000 |
| 6 | 1.839952000 | 6.926774000 | 4.215226000 |
| 6 | 0.357304000 | 6.183708000 | -1.753902000 |
| 6 | 2.200107000 | 5.459872000 | -0.475533000 |
| 6 | -0.894794000 | 8.320234000 | -1.196074000 |
| 6 | -0.455271000 | 7.268125000 | -2.156764000 |
| 6 | -0.936769000 | 7.322058000 | -3.461552000 |
| 6 | -0.673101000 | 6.328302000 | -4.387307000 |
| 6 | 0.069756000 | 5.232581000 | -3.982004000 |

| | | | |
|---|---|---|---|
| 6 | 0.564224000 | 5.151092000 | -2.691136000 |
| 6 | 1.304078000 | 3.954789000 | -2.202907000 |
| 6 | 2.458106000 | 4.410997000 | -1.380114000 |
| 6 | 3.706728000 | 3.817558000 | -1.464779000 |
| 6 | 4.737350000 | 4.215628000 | -0.630264000 |
| 6 | 4.479815000 | 5.194407000 | 0.313496000 |
| 6 | 3.238809000 | 5.816050000 | 0.415184000 |
| 6 | 2.998266000 | 6.732383000 | 1.563694000 |
| 1 | -0.769211000 | 9.782593000 | 1.853404000 |
| 1 | -1.276724000 | 10.543802000 | 0.347192000 |
| 1 | -2.120244000 | 10.906349000 | 1.843686000 |
| 1 | -3.827151000 | 9.348719000 | 2.794083000 |
| 1 | -3.920984000 | 7.680226000 | 2.252039000 |
| 1 | -2.484278000 | 8.250490000 | 3.091631000 |
| 1 | -3.404065000 | 9.318961000 | 0.382013000 |
| 1 | -4.979021000 | 6.946968000 | -1.884713000 |
| 1 | -4.326853000 | 8.461310000 | -1.286692000 |
| 1 | -3.463650000 | 7.552533000 | -2.527123000 |
| 1 | -2.390347000 | 5.296686000 | -1.979137000 |
| 1 | -2.367939000 | 4.714355000 | -0.314499000 |
| 1 | -3.868212000 | 4.699656000 | -1.239960000 |
| 1 | -3.948151000 | 6.558361000 | 0.322689000 |
| 1 | 3.951719000 | 3.205865000 | 3.875910000 |
| 1 | 4.314811000 | 4.896389000 | 3.572501000 |
| 1 | 3.275611000 | 4.439865000 | 4.922374000 |
| 1 | 0.816244000 | 3.626589000 | 4.445095000 |
| 1 | 0.343040000 | 3.366519000 | 2.770853000 |
| 1 | 1.550705000 | 2.328639000 | 3.522154000 |
| 1 | 2.601994000 | 3.934373000 | 1.985178000 |
| 1 | -0.247052000 | 6.962249000 | 4.783663000 |
| 1 | 0.598429000 | 5.531564000 | 5.358270000 |
| 1 | 0.871110000 | 7.083837000 | 6.136101000 |
| 1 | 2.014464000 | 8.940008000 | 4.952163000 |
| 1 | 2.803626000 | 8.713377000 | 3.400284000 |
| 1 | 1.046465000 | 8.815755000 | 3.491718000 |
| 1 | 2.785200000 | 6.592803000 | 4.654592000 |
| 1 | -0.046944000 | 8.810941000 | -0.708350000 |
| 1 | -1.480139000 | 9.089257000 | -1.705097000 |
| 1 | -1.535416000 | 8.179927000 | -3.747584000 |
| 1 | -1.051855000 | 6.401519000 | -5.398118000 |
| 1 | 0.266275000 | 4.416411000 | -4.668435000 |
| 1 | 0.630490000 | 3.354107000 | -1.570944000 |
| 1 | 1.617954000 | 3.308201000 | -3.022328000 |
| 1 | 3.859504000 | 3.024059000 | -2.187938000 |
| 1 | 5.715527000 | 3.758137000 | -0.697281000 |
| 1 | 5.258430000 | 5.494772000 | 1.006189000 |
| 1 | 3.923268000 | 6.914595000 | 2.115163000 |
| 1 | 2.596414000 | 7.700327000 | 1.250871000 |
| 1 | -0.251497000 | 7.656077000 | 2.234239000 |

**1-*fac***



First three frequencies

| | 1 | 2 | 3 |
|---|---|---|---|
| | ***A*** | A | A |
| Frequencies -- | ***23.9063*** | 54.6100 | 58.1459 |
| Red. masses -- | ***4.2423*** | 5.0247 | 4.1572 |
| Frc consts -- | ***0.0014*** | 0.0088 | 0.0083 |
| IR Inten -- | ***0.0237*** | 0.2670 | 0.6636 |

Coordinates

| | | | |
|---|---|---|---|
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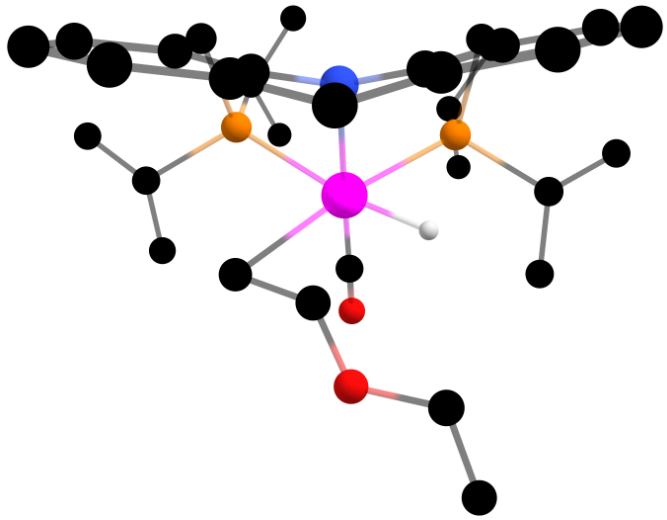
| 15 | 0.627060000 | 6.127333000 | 4.870198000 |
| 8 | -1.817884000 | 8.186142000 | 6.934558000 |
| 7 | 0.866239000 | 8.227722000 | 2.528550000 |
| 6 | -1.601703000 | 7.846892000 | 1.155263000 |
| 1 | -1.018043000 | 6.925925000 | 1.049834000 |
| 1 | -2.416817000 | 7.808133000 | 0.431336000 |
| 6 | -0.740524000 | 9.038288000 | 0.901271000 |
| 6 | -1.117455000 | 9.996919000 | -0.032801000 |
| 1 | -2.068288000 | 9.880206000 | -0.542875000 |
| 6 | -0.286015000 | 11.058916000 | -0.351486000 |
| 1 | -0.587834000 | 11.787314000 | -1.092522000 |
| 6 | 0.946742000 | 11.163065000 | 0.278242000 |
| 1 | 1.616763000 | 11.978887000 | 0.028457000 |
| 6 | 1.334645000 | 10.249290000 | 1.244381000 |
| 6 | 0.486004000 | 9.178402000 | 1.585562000 |
| 6 | 2.627654000 | 10.363081000 | 1.992284000 |
| 1 | 3.355083000 | 10.958211000 | 1.437561000 |
| 1 | 2.447780000 | 10.911888000 | 2.929510000 |
| 6 | 3.171346000 | 9.010977000 | 2.337565000 |
| 6 | 4.526795000 | 8.742400000 | 2.440089000 |
| 1 | 5.238679000 | 9.521212000 | 2.187739000 |

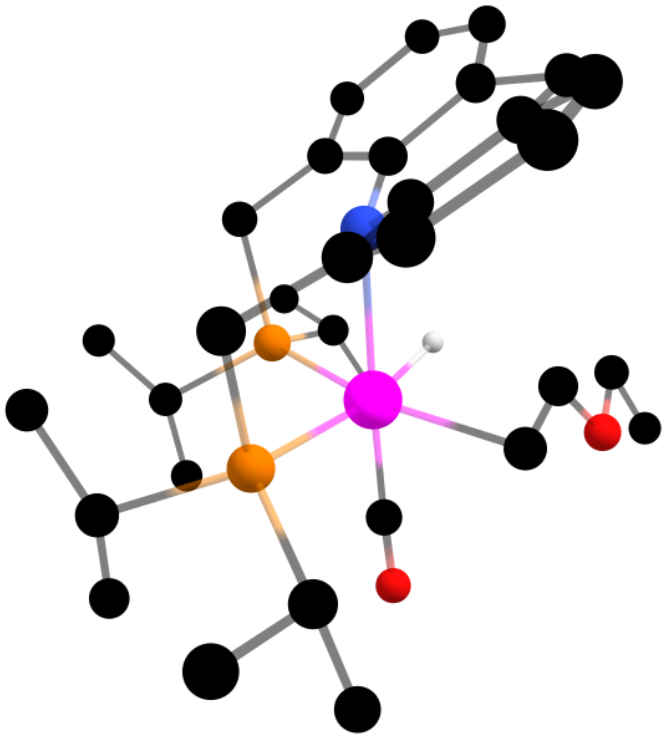
| | | | |
|---|---|---|---|
| 6 | 4.977078000 | 7.509255000 | 2.891451000 |
| 1 | 6.037201000 | 7.310966000 | 2.979141000 |
| 6 | 4.052103000 | 6.533992000 | 3.233445000 |
| 1 | 4.391628000 | 5.564614000 | 3.583558000 |
| 6 | 2.686913000 | 6.761125000 | 3.107949000 |
| 6 | 2.232167000 | 8.016728000 | 2.657318000 |
| 6 | 1.696494000 | 5.693638000 | 3.437167000 |
| 1 | 2.203777000 | 4.748137000 | 3.634810000 |
| 1 | 1.004398000 | 5.533259000 | 2.603646000 |
| 6 | -3.228216000 | 6.236410000 | 2.927511000 |
| 1 | -2.416136000 | 5.501091000 | 2.870533000 |
| 6 | -4.166092000 | 5.937587000 | 1.767490000 |
| 1 | -5.068158000 | 6.544387000 | 1.794481000 |
| 1 | -4.484820000 | 4.894788000 | 1.820289000 |
| 1 | -3.695458000 | 6.076619000 | 0.795551000 |
| 6 | -3.924463000 | 6.068936000 | 4.268974000 |
| 1 | -3.266491000 | 6.298662000 | 5.108020000 |
| 1 | -4.280353000 | 5.044699000 | 4.394747000 |
| 1 | -4.796172000 | 6.720452000 | 4.344853000 |
| 6 | -3.366891000 | 9.287680000 | 2.893682000 |
| 1 | -2.702550000 | 10.046478000 | 2.460748000 |
| 6 | -3.722054000 | 9.740116000 | 4.301870000 |
| 1 | -4.283747000 | 8.984162000 | 4.851823000 |
| 1 | -4.341956000 | 10.637345000 | 4.262833000 |
| 1 | -2.837028000 | 9.980769000 | 4.888847000 |
| 6 | -4.601838000 | 9.201493000 | 2.011947000 |
| 1 | -4.388990000 | 8.817865000 | 1.014392000 |
| 1 | -5.041115000 | 10.193111000 | 1.889567000 |
| 1 | -5.368625000 | 8.569063000 | 2.459923000 |
| 6 | 1.835530000 | 6.130106000 | 6.275223000 |
| 1 | 2.614877000 | 6.776536000 | 5.853641000 |
| 6 | 1.328608000 | 6.798411000 | 7.542173000 |
| 1 | 0.999633000 | 7.818037000 | 7.354991000 |
| 1 | 2.132547000 | 6.842191000 | 8.278540000 |
| 1 | 0.502880000 | 6.254990000 | 8.000669000 |
| 6 | 2.459226000 | 4.775133000 | 6.576382000 |
| 1 | 1.756403000 | 4.098773000 | 7.063416000 |
| 1 | 3.297298000 | 4.906049000 | 7.262766000 |
| 1 | 2.849436000 | 4.276057000 | 5.689899000 |
| 6 | -0.518203000 | 4.676176000 | 5.060149000 |
| 1 | -1.304915000 | 4.928930000 | 4.344458000 |
| 6 | -1.158811000 | 4.619101000 | 6.438938000 |
| 1 | -0.452613000 | 4.280889000 | 7.197601000 |
| 1 | -1.987673000 | 3.909208000 | 6.436080000 |
| 1 | -1.555767000 | 5.581224000 | 6.759743000 |
| 6 | 0.046631000 | 3.322467000 | 4.650765000 |
| 1 | 0.402928000 | 3.311646000 | 3.622128000 |
| 1 | -0.737625000 | 2.566900000 | 4.726371000 |
| 1 | 0.863781000 | 2.997033000 | 5.291932000 |
| 6 | -1.230910000 | 8.118028000 | 5.929202000 |
| 44 | -0.296628000 | 8.073018000 | 4.356984000 |

**1a-*fac***

**(Front view)**



(side view)



First three frequencies

| | 1 | 2 | 3 |
|---|---|---|---|
| | ***A*** | A | A |
| Frequencies -- | ***24.5626*** | 39.9359 | 51.3588 |
| Red. masses -- | ***4.1235*** | 4.1763 | 3.8543 |

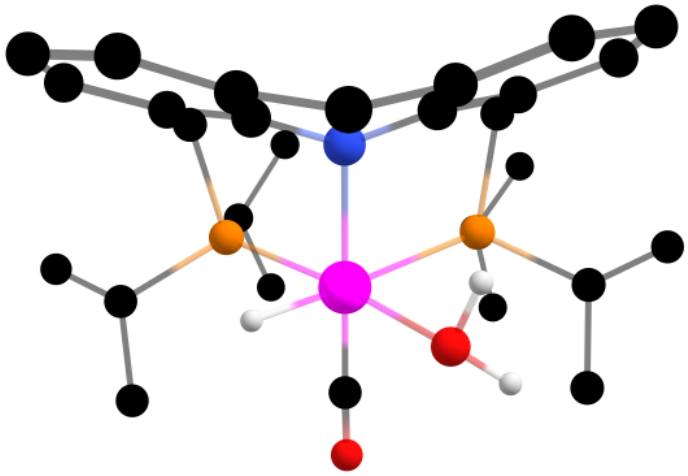
| | | | |
|---|---|---|---|
| Frc consts -- | ***0.0015*** | 0.0039 | 0.0060 |
| IR Inten -- | ***0.4610*** | 0.2133 | 0.8690 |

## Coordinates

| | | | |
|---|---|---|---|
| 15 | -2.447668000 | 7.586813000 | 2.729536000 |
| 15 | 0.333082000 | 6.007598000 | 4.853276000 |
| 8 | -2.578115000 | 7.704959000 | 6.813191000 |
| 7 | 0.653776000 | 8.350455000 | 2.704956000 |
| 6 | -1.601378000 | 7.906689000 | 1.125990000 |
| 1 | -0.876345000 | 7.093508000 | 1.038502000 |
| 1 | -2.314864000 | 7.809109000 | 0.305529000 |
| 6 | -0.870137000 | 9.201577000 | 1.051997000 |
| 6 | -1.291724000 | 10.222432000 | 0.211677000 |
| 1 | -2.202561000 | 10.086592000 | -0.362464000 |
| 6 | -0.546146000 | 11.383734000 | 0.065645000 |
| 1 | -0.878441000 | 12.169168000 | -0.600270000 |
| 6 | 0.646116000 | 11.508698000 | 0.762831000 |
| 1 | 1.252894000 | 12.400057000 | 0.640246000 |
| 6 | 1.079661000 | 10.521022000 | 1.636415000 |
| 6 | 0.306927000 | 9.359657000 | 1.821409000 |
| 6 | 2.345597000 | 10.679072000 | 2.426303000 |
| 1 | 3.099121000 | 11.207771000 | 1.835870000 |
| 1 | 2.166325000 | 11.339487000 | 3.287719000 |
| 6 | 2.884159000 | 9.361576000 | 2.902006000 |
| 6 | 4.220899000 | 9.212920000 | 3.241948000 |
| 1 | 4.884892000 | 10.064435000 | 3.132826000 |
| 6 | 4.713720000 | 8.009850000 | 3.725246000 |
| 1 | 5.757188000 | 7.910092000 | 3.993570000 |
| 6 | 3.851855000 | 6.929593000 | 3.838077000 |
| 1 | 4.226236000 | 5.971127000 | 4.182737000 |
| 6 | 2.513805000 | 7.036294000 | 3.481516000 |
| 6 | 1.998513000 | 8.274620000 | 3.035498000 |
| 6 | 1.615151000 | 5.846933000 | 3.542627000 |
| 1 | 2.195795000 | 4.936198000 | 3.694068000 |
| 1 | 1.058760000 | 5.743126000 | 2.605501000 |
| 6 | -3.201559000 | 5.914606000 | 2.418376000 |
| 1 | -3.988100000 | 6.069840000 | 1.675662000 |
| 6 | -3.855771000 | 5.379318000 | 3.686193000 |
| 1 | -3.206335000 | 5.463803000 | 4.558566000 |
| 1 | -4.124440000 | 4.327323000 | 3.571919000 |
| 1 | -4.770165000 | 5.920746000 | 3.924577000 |
| 6 | -2.178919000 | 4.963309000 | 1.798949000 |
| 1 | -2.108992000 | 5.102158000 | 0.721336000 |
| 1 | -2.453810000 | 3.922204000 | 1.976829000 |
| 1 | -1.173596000 | 5.111406000 | 2.196623000 |
| 6 | -3.899561000 | 8.749765000 | 2.650626000 |
| 1 | -3.403022000 | 9.711819000 | 2.488129000 |
| 6 | -4.675407000 | 8.832820000 | 3.956668000 |
| 1 | -5.306538000 | 7.956582000 | 4.105702000 |
| 1 | -5.337884000 | 9.699951000 | 3.948854000 |
| 1 | -4.029218000 | 8.919669000 | 4.827242000 |
| 6 | -4.847359000 | 8.518470000 | 1.484192000 |
| 1 | -4.337550000 | 8.431359000 | 0.525397000 |
| 1 | -5.544312000 | 9.354101000 | 1.400927000 |
| 1 | -5.450452000 | 7.620387000 | 1.625253000 |

| | | | |
|---|---|---|---|
| 6 | 1.392215000 | 6.059492000 | 6.383958000 |
| 1 | 2.093027000 | 6.852862000 | 6.096203000 |
| 6 | 0.678884000 | 6.528499000 | 7.641984000 |
| 1 | 0.134282000 | 7.456768000 | 7.482191000 |
| 1 | 1.410266000 | 6.710425000 | 8.432186000 |
| 1 | -0.025579000 | 5.790906000 | 8.024665000 |
| 6 | 2.203961000 | 4.801867000 | 6.652767000 |
| 1 | 1.584363000 | 3.984171000 | 7.021226000 |
| 1 | 2.949450000 | 5.004055000 | 7.423981000 |
| 1 | 2.742249000 | 4.445570000 | 5.775385000 |
| 6 | -0.572604000 | 4.379714000 | 4.865206000 |
| 1 | -1.352128000 | 4.547621000 | 4.124311000 |
| 6 | -1.281095000 | 4.133417000 | 6.189146000 |
| 1 | -0.588470000 | 3.837740000 | 6.976672000 |
| 1 | -2.003455000 | 3.322500000 | 6.078418000 |
| 1 | -1.829072000 | 5.008796000 | 6.539064000 |
| 6 | 0.215909000 | 3.162974000 | 4.405727000 |
| 1 | 0.610413000 | 3.281890000 | 3.397203000 |
| 1 | -0.440296000 | 2.290085000 | 4.390405000 |
| 1 | 1.049788000 | 2.923341000 | 5.063778000 |
| 6 | -1.880338000 | 7.805086000 | 5.887094000 |
| 44 | -0.779306000 | 8.021574000 | 4.451222000 |
| 6 | -1.503657000 | 10.194178000 | 4.234528000 |
| 6 | -0.338223000 | 10.268567000 | 4.977323000 |
| 1 | -1.460556000 | 10.485084000 | 3.195593000 |
| 1 | -2.442475000 | 10.369802000 | 4.743145000 |
| 8 | -0.380850000 | 10.557852000 | 6.293472000 |
| 1 | 0.617210000 | 10.437512000 | 4.488330000 |
| 6 | 0.867638000 | 10.435606000 | 6.973940000 |
| 6 | 0.640520000 | 10.678503000 | 8.435054000 |
| 1 | 1.581373000 | 11.150278000 | 6.547263000 |
| 1 | 1.270296000 | 9.430584000 | 6.788188000 |
| 1 | 0.249533000 | 11.678797000 | 8.616380000 |
| 1 | 1.576994000 | 10.577871000 | 8.981388000 |
| 1 | -0.068973000 | 9.959455000 | 8.843729000 |
| 1 | 0.548800000 | 8.299618000 | 5.356903000 |

**1b-*fac***



## First three frequencies

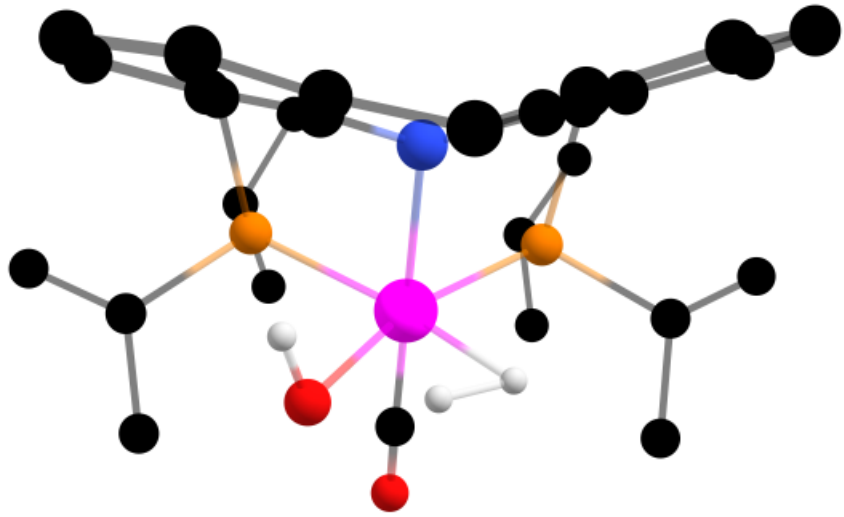
| | 1 | 2 | 3 |
|---|---|---|---|
| | ***A*** | A | A |
| Frequencies -- | ***33.2909*** | 52.1955 | 59.2400 |
| Red. masses -- | ***4.3635*** | 3.7402 | 4.6410 |
| Frc consts -- | ***0.0028*** | 0.0060 | 0.0096 |
| IR Inten -- | ***0.0207*** | 0.3881 | 0.6555 |

## Coordinates

| | | | |
|---|---|---|---|
| 8 | 1.018640000 | 9.292313000 | 5.530144000 |
| 15 | -2.362228000 | 7.880586000 | 2.868562000 |
| 15 | 0.373716000 | 6.068954000 | 4.881342000 |
| 8 | -2.569681000 | 8.082198000 | 6.727780000 |
| 7 | 0.705652000 | 8.377644000 | 2.675864000 |
| 6 | -1.613782000 | 8.039544000 | 1.194320000 |
| 1 | -0.978605000 | 7.157040000 | 1.086557000 |
| 1 | -2.403707000 | 7.978287000 | 0.442913000 |
| 6 | -0.786125000 | 9.262990000 | 1.013882000 |
| 6 | -1.129777000 | 10.255671000 | 0.106686000 |
| 1 | -2.051540000 | 10.155286000 | -0.457499000 |
| 6 | -0.296401000 | 11.343537000 | -0.111530000 |
| 1 | -0.567039000 | 12.104213000 | -0.832004000 |
| 6 | 0.891468000 | 11.440045000 | 0.599510000 |
| 1 | 1.551368000 | 12.286566000 | 0.440853000 |
| 6 | 1.240929000 | 10.482668000 | 1.540005000 |
| 6 | 0.401401000 | 9.381465000 | 1.763289000 |
| 6 | 2.453804000 | 10.605337000 | 2.410623000 |
| 1 | 3.230552000 | 11.204197000 | 1.930938000 |
| 1 | 2.177852000 | 11.164176000 | 3.318059000 |
| 6 | 2.983270000 | 9.257093000 | 2.803845000 |
| 6 | 4.328583000 | 9.035546000 | 3.058036000 |
| 1 | 5.027687000 | 9.855117000 | 2.929383000 |
| 6 | 4.782315000 | 7.796947000 | 3.488587000 |
| 1 | 5.832919000 | 7.635994000 | 3.690849000 |
| 6 | 3.871614000 | 6.762736000 | 3.644709000 |
| 1 | 4.216856000 | 5.783228000 | 3.958674000 |
| 6 | 2.520121000 | 6.936124000 | 3.370212000 |
| 6 | 2.049917000 | 8.205398000 | 2.952373000 |
| 6 | 1.567432000 | 5.793363000 | 3.500015000 |
| 1 | 2.111894000 | 4.857192000 | 3.629127000 |
| 1 | 0.952225000 | 5.707692000 | 2.598623000 |
| 6 | -3.297209000 | 6.285188000 | 2.714313000 |
| 1 | -4.120342000 | 6.488253000 | 2.024597000 |
| 6 | -3.891112000 | 5.879750000 | 4.053726000 |
| 1 | -3.125223000 | 5.782981000 | 4.823623000 |
| 1 | -4.408445000 | 4.921959000 | 3.973951000 |
| 1 | -4.613679000 | 6.610874000 | 4.416954000 |
| 6 | -2.426909000 | 5.201637000 | 2.085066000 |
| 1 | -2.386817000 | 5.298013000 | 1.001292000 |
| 1 | -2.821565000 | 4.208723000 | 2.308067000 |
| 1 | -1.395342000 | 5.232836000 | 2.441895000 |
| 6 | -3.658504000 | 9.213534000 | 2.811555000 |
| 1 | -3.063605000 | 10.048664000 | 2.422157000 |

| | | | |
|---|---|---|---|
| 6 | -4.203695000 | 9.635918000 | 4.164440000 |
| 1 | -4.744754000 | 8.831683000 | 4.664507000 |
| 1 | -4.906068000 | 10.461356000 | 4.036706000 |
| 1 | -3.414133000 | 9.977419000 | 4.829477000 |
| 6 | -4.790859000 | 8.937914000 | 1.833853000 |
| 1 | -4.444918000 | 8.596339000 | 0.858100000 |
| 1 | -5.364455000 | 9.850842000 | 1.667239000 |
| 1 | -5.488598000 | 8.193770000 | 2.221344000 |
| 6 | 1.546550000 | 6.178489000 | 6.327915000 |
| 1 | 2.236592000 | 6.949204000 | 5.961888000 |
| 6 | 0.902106000 | 6.700643000 | 7.606296000 |
| 1 | 0.195147000 | 7.512579000 | 7.428136000 |
| 1 | 1.665921000 | 7.061768000 | 8.298009000 |
| 1 | 0.348223000 | 5.924076000 | 8.131256000 |
| 6 | 2.385084000 | 4.941735000 | 6.608894000 |
| 1 | 1.788153000 | 4.138708000 | 7.041128000 |
| 1 | 3.170573000 | 5.176676000 | 7.330094000 |
| 1 | 2.875033000 | 4.552881000 | 5.717316000 |
| 6 | -0.565198000 | 4.470719000 | 5.062425000 |
| 1 | -1.399597000 | 4.612559000 | 4.375687000 |
| 6 | -1.169529000 | 4.333832000 | 6.452513000 |
| 1 | -0.424859000 | 4.049122000 | 7.195628000 |
| 1 | -1.932676000 | 3.553660000 | 6.452182000 |
| 1 | -1.647123000 | 5.253987000 | 6.792070000 |
| 6 | 0.158841000 | 3.207788000 | 4.624644000 |
| 1 | 0.455481000 | 3.246420000 | 3.577016000 |
| 1 | -0.504693000 | 2.347793000 | 4.736449000 |
| 1 | 1.050095000 | 3.002370000 | 5.215892000 |
| 6 | -1.866663000 | 8.118561000 | 5.798791000 |
| 44 | -0.726004000 | 8.190303000 | 4.376600000 |
| 1 | 1.233644000 | 8.917077000 | 6.392662000 |
| 1 | 1.816912000 | 9.160518000 | 4.992258000 |
| 1 | -1.199621000 | 9.700661000 | 3.973740000 |

**TS1**



## First three frequencies

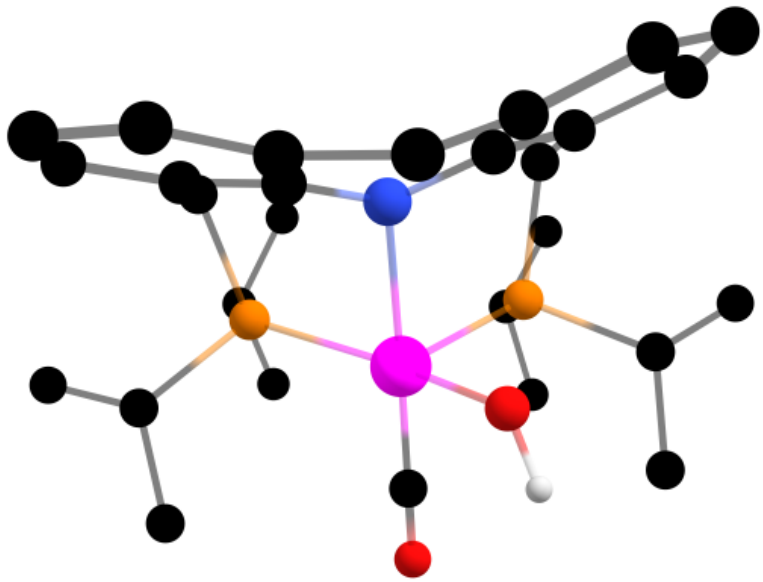
| | 1 | 2 | 3 |
|---|---|---|---|
| | ***A*** | A | A |
| Frequencies -- | ***-996.8853*** | 35.7060 | 57.3868 |
| Red. masses -- | ***1.0752*** | 4.2928 | 4.1858 |
| Frc consts -- | ***0.6295*** | 0.0032 | 0.0081 |
| IR Inten -- | ***713.6896*** | 0.0122 | 0.5383 |

## Coordinates

| | | | |
|---|---|---|---|
| 1 | 0.568318000 | 9.083049000 | 5.349118000 |
| 15 | -2.398034000 | 7.810724000 | 2.825286000 |
| 15 | 0.301121000 | 6.194320000 | 4.816850000 |
| 8 | -2.561651000 | 7.865278000 | 6.743395000 |
| 7 | 0.645516000 | 8.431645000 | 2.655912000 |
| 6 | -1.649781000 | 8.013806000 | 1.156859000 |
| 1 | -0.974285000 | 7.162339000 | 1.039012000 |
| 1 | -2.430480000 | 7.932555000 | 0.398064000 |
| 6 | -0.877736000 | 9.279260000 | 1.006724000 |
| 6 | -1.261644000 | 10.277380000 | 0.120968000 |
| 1 | -2.179710000 | 10.155027000 | -0.444246000 |
| 6 | -0.467979000 | 11.397882000 | -0.077824000 |
| 1 | -0.770378000 | 12.162624000 | -0.780970000 |
| 6 | 0.724188000 | 11.521779000 | 0.623004000 |
| 1 | 1.355507000 | 12.390277000 | 0.468362000 |
| 6 | 1.114977000 | 10.561884000 | 1.544710000 |
| 6 | 0.307206000 | 9.429881000 | 1.757371000 |
| 6 | 2.350629000 | 10.690638000 | 2.385600000 |
| 1 | 3.099026000 | 11.315131000 | 1.893893000 |
| 1 | 2.095026000 | 11.222284000 | 3.314793000 |
| 6 | 2.912262000 | 9.345968000 | 2.740322000 |
| 6 | 4.263636000 | 9.131161000 | 2.957431000 |
| 1 | 4.956721000 | 9.953686000 | 2.815472000 |
| 6 | 4.733635000 | 7.892916000 | 3.375403000 |
| 1 | 5.790253000 | 7.738810000 | 3.550448000 |
| 6 | 3.835302000 | 6.853002000 | 3.559594000 |
| 1 | 4.193121000 | 5.876474000 | 3.868687000 |
| 6 | 2.477817000 | 7.026861000 | 3.317454000 |
| 6 | 1.999433000 | 8.289837000 | 2.914964000 |
| 6 | 1.512018000 | 5.897264000 | 3.459573000 |
| 1 | 2.040578000 | 4.958908000 | 3.628944000 |
| 1 | 0.913491000 | 5.788677000 | 2.549423000 |
| 6 | -3.407704000 | 6.272587000 | 2.631780000 |
| 1 | -4.218751000 | 6.543323000 | 1.950184000 |
| 6 | -4.027188000 | 5.854472000 | 3.956351000 |
| 1 | -3.276993000 | 5.693585000 | 4.730710000 |
| 1 | -4.587686000 | 4.925372000 | 3.841146000 |
| 1 | -4.718206000 | 6.606056000 | 4.337129000 |
| 6 | -2.597464000 | 5.168055000 | 1.959876000 |
| 1 | -2.516542000 | 5.327979000 | 0.886067000 |
| 1 | -3.073826000 | 4.197965000 | 2.109821000 |
| 1 | -1.578956000 | 5.093670000 | 2.344031000 |
| 6 | -3.608714000 | 9.219786000 | 2.848816000 |
| 1 | -2.968386000 | 10.049444000 | 2.528250000 |

| | | | |
|---|---|---|---|
| 6 | -4.148225000 | 9.577821000 | 4.223089000 |
| 1 | -4.705302000 | 8.760745000 | 4.682508000 |
| 1 | -4.835849000 | 10.420753000 | 4.134969000 |
| 1 | -3.349808000 | 9.880220000 | 4.895430000 |
| 6 | -4.735952000 | 9.064792000 | 1.838652000 |
| 1 | -4.393333000 | 8.767819000 | 0.847512000 |
| 1 | -5.260889000 | 10.014253000 | 1.724592000 |
| 1 | -5.474478000 | 8.332792000 | 2.169931000 |
| 6 | 1.442560000 | 6.356035000 | 6.278076000 |
| 1 | 2.127889000 | 7.124762000 | 5.900821000 |
| 6 | 0.802495000 | 6.908767000 | 7.541725000 |
| 1 | 0.301340000 | 7.858479000 | 7.366268000 |
| 1 | 1.575314000 | 7.085875000 | 8.291426000 |
| 1 | 0.080908000 | 6.223560000 | 7.984338000 |
| 6 | 2.264575000 | 5.111115000 | 6.578838000 |
| 1 | 1.661020000 | 4.321873000 | 7.027388000 |
| 1 | 3.049676000 | 5.355497000 | 7.296355000 |
| 1 | 2.755517000 | 4.699585000 | 5.698013000 |
| 6 | -0.648843000 | 4.605595000 | 4.997569000 |
| 1 | -1.471759000 | 4.748542000 | 4.297047000 |
| 6 | -1.269195000 | 4.453260000 | 6.378897000 |
| 1 | -0.526637000 | 4.195039000 | 7.133307000 |
| 1 | -2.003561000 | 3.646084000 | 6.365733000 |
| 1 | -1.784350000 | 5.353598000 | 6.711809000 |
| 6 | 0.087248000 | 3.344880000 | 4.568958000 |
| 1 | 0.396249000 | 3.379281000 | 3.525198000 |
| 1 | -0.575573000 | 2.484405000 | 4.677975000 |
| 1 | 0.971265000 | 3.145534000 | 5.173041000 |
| 6 | -1.858444000 | 8.000779000 | 5.830222000 |
| 44 | -0.727258000 | 8.212270000 | 4.400114000 |
| 8 | -0.998608000 | 10.418238000 | 4.320044000 |
| 1 | 0.052908000 | 9.790937000 | 4.999669000 |
| 1 | -0.630913000 | 10.701594000 | 3.471652000 |

**1c**



## First three frequencies

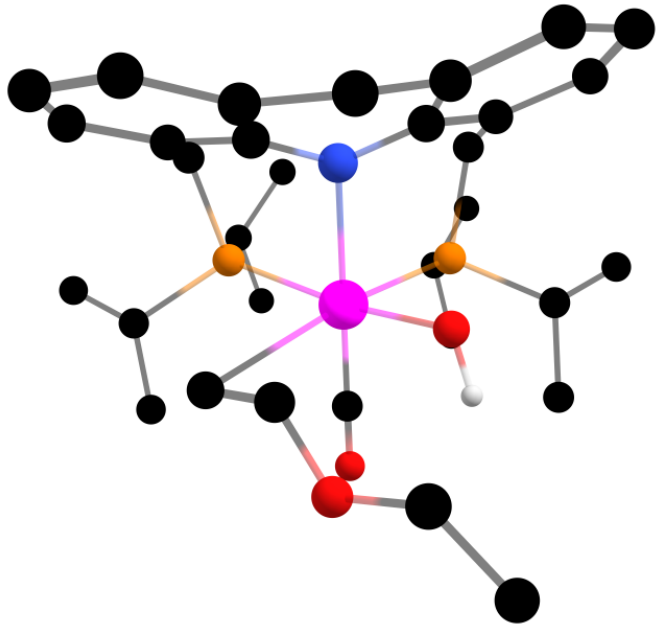
| | 1 | 2 | 3 |
|---|---|---|---|
| | ***A*** | A | A |
| Frequencies -- | ***27.0329*** | 48.2607 | 53.5414 |
| Red. masses -- | ***4.6814*** | 4.6039 | 3.3838 |
| Frc consts -- | ***0.0020*** | 0.0063 | 0.0057 |
| IR Inten -- | ***0.1746*** | 0.7314 | 0.5198 |

## Coordinates

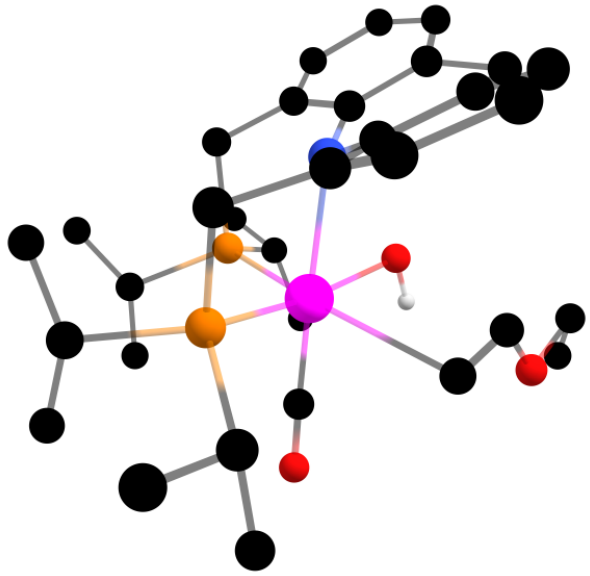
| | | | |
|---|---|---|---|
| 8 | 0.891427000 | 9.242364000 | 5.258426000 |
| 15 | -2.262880000 | 7.696581000 | 2.851652000 |
| 15 | 0.378643000 | 6.130185000 | 4.842061000 |
| 8 | -2.412442000 | 7.853323000 | 6.751284000 |
| 7 | 0.754674000 | 8.314795000 | 2.664580000 |
| 6 | -1.547114000 | 7.928002000 | 1.171745000 |
| 1 | -0.870209000 | 7.082084000 | 1.022353000 |
| 1 | -2.337704000 | 7.865548000 | 0.421154000 |
| 6 | -0.781834000 | 9.202011000 | 1.050801000 |
| 6 | -1.169467000 | 10.216449000 | 0.184447000 |
| 1 | -2.085569000 | 10.100608000 | -0.385842000 |
| 6 | -0.377961000 | 11.341698000 | 0.009051000 |
| 1 | -0.679908000 | 12.119348000 | -0.680278000 |
| 6 | 0.817551000 | 11.450545000 | 0.709244000 |
| 1 | 1.452081000 | 12.318298000 | 0.562477000 |
| 6 | 1.211831000 | 10.476321000 | 1.612390000 |
| 6 | 0.399206000 | 9.344776000 | 1.809096000 |
| 6 | 2.467082000 | 10.577267000 | 2.426673000 |
| 1 | 3.210700000 | 11.199359000 | 1.923936000 |
| 1 | 2.237696000 | 11.088799000 | 3.371131000 |
| 6 | 3.021897000 | 9.222473000 | 2.753200000 |
| 6 | 4.370319000 | 8.992961000 | 2.969030000 |
| 1 | 5.071553000 | 9.810169000 | 2.835582000 |
| 6 | 4.829740000 | 7.748708000 | 3.384532000 |
| 1 | 5.885240000 | 7.585546000 | 3.558756000 |
| 6 | 3.922969000 | 6.716627000 | 3.572167000 |
| 1 | 4.271904000 | 5.738045000 | 3.885219000 |
| 6 | 2.567919000 | 6.906836000 | 3.330148000 |
| 6 | 2.104542000 | 8.172183000 | 2.922611000 |
| 6 | 1.578698000 | 5.798419000 | 3.484360000 |
| 1 | 2.083279000 | 4.850300000 | 3.673046000 |
| 1 | 0.976564000 | 5.686654000 | 2.577344000 |
| 6 | -3.318048000 | 6.189010000 | 2.632207000 |
| 1 | -4.096877000 | 6.477226000 | 1.921551000 |
| 6 | -3.998115000 | 5.804777000 | 3.937607000 |
| 1 | -3.288066000 | 5.657202000 | 4.751721000 |
| 1 | -4.562765000 | 4.878356000 | 3.820046000 |
| 1 | -4.699635000 | 6.571388000 | 4.266906000 |
| 6 | -2.517932000 | 5.058825000 | 1.990294000 |
| 1 | -2.423315000 | 5.200140000 | 0.914895000 |
| 1 | -3.009848000 | 4.097960000 | 2.150019000 |
| 1 | -1.503947000 | 4.974965000 | 2.383934000 |
| 6 | -3.465215000 | 9.127807000 | 2.878446000 |
| 1 | -2.834755000 | 9.936440000 | 2.490397000 |

| | | | |
|---|---|---|---|
| 6 | -3.941682000 | 9.546949000 | 4.259268000 |
| 1 | -4.464249000 | 8.747817000 | 4.785384000 |
| 1 | -4.638491000 | 10.382127000 | 4.170759000 |
| 1 | -3.122769000 | 9.879815000 | 4.894377000 |
| 6 | -4.639617000 | 8.961836000 | 1.925845000 |
| 1 | -4.340885000 | 8.636431000 | 0.929373000 |
| 1 | -5.158622000 | 9.914375000 | 1.808995000 |
| 1 | -5.370774000 | 8.247027000 | 2.307137000 |
| 6 | 1.513845000 | 6.299859000 | 6.300926000 |
| 1 | 2.184982000 | 7.078384000 | 5.920713000 |
| 6 | 0.884098000 | 6.834855000 | 7.576293000 |
| 1 | 0.326092000 | 7.752842000 | 7.410266000 |
| 1 | 1.671041000 | 7.061156000 | 8.297405000 |
| 1 | 0.213561000 | 6.119468000 | 8.050300000 |
| 6 | 2.332822000 | 5.048589000 | 6.586758000 |
| 1 | 1.727948000 | 4.253011000 | 7.022878000 |
| 1 | 3.113927000 | 5.285744000 | 7.310959000 |
| 1 | 2.830063000 | 4.649020000 | 5.704438000 |
| 6 | -0.635493000 | 4.589149000 | 5.044490000 |
| 1 | -1.463813000 | 4.765420000 | 4.359145000 |
| 6 | -1.231064000 | 4.448608000 | 6.437623000 |
| 1 | -0.481240000 | 4.159578000 | 7.173276000 |
| 1 | -1.990247000 | 3.664718000 | 6.432122000 |
| 1 | -1.710756000 | 5.361276000 | 6.787817000 |
| 6 | 0.055957000 | 3.307932000 | 4.599745000 |
| 1 | 0.357735000 | 3.336947000 | 3.553959000 |
| 1 | -0.633782000 | 2.469542000 | 4.712117000 |
| 1 | 0.937967000 | 3.078991000 | 5.196556000 |
| 6 | -1.696289000 | 7.960010000 | 5.840178000 |
| 44 | -0.565760000 | 8.113910000 | 4.401946000 |
| 1 | 0.698360000 | 9.420408000 | 6.184401000 |

**1d**
**(front view)**



(side view)



First three frequencies

| | 1 | 2 | 3 |
|---|---|---|---|
| | ***A*** | A | A |
| Frequencies -- | ***19.3776*** | 37.5702 | 43.3288 |
| Red. masses -- | ***4.1303*** | 3.9021 | 3.6392 |
| Frc consts -- | ***0.0009*** | 0.0032 | 0.0040 |
| IR Inten -- | ***0.9564*** | 0.2178 | 0.2520 |

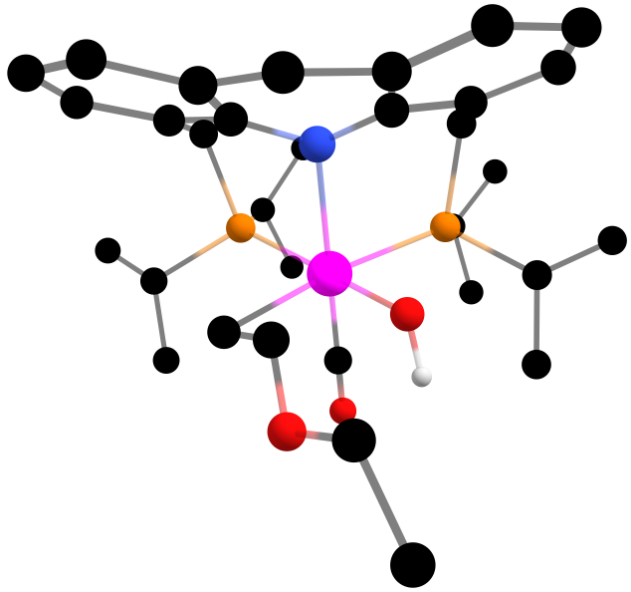
Coordinates

| | | | |
|---|---|---|---|
| 8 | 0.894275000 | 8.676134000 | 5.539120000 |
| 15 | -2.348390000 | 7.495335000 | 2.774169000 |

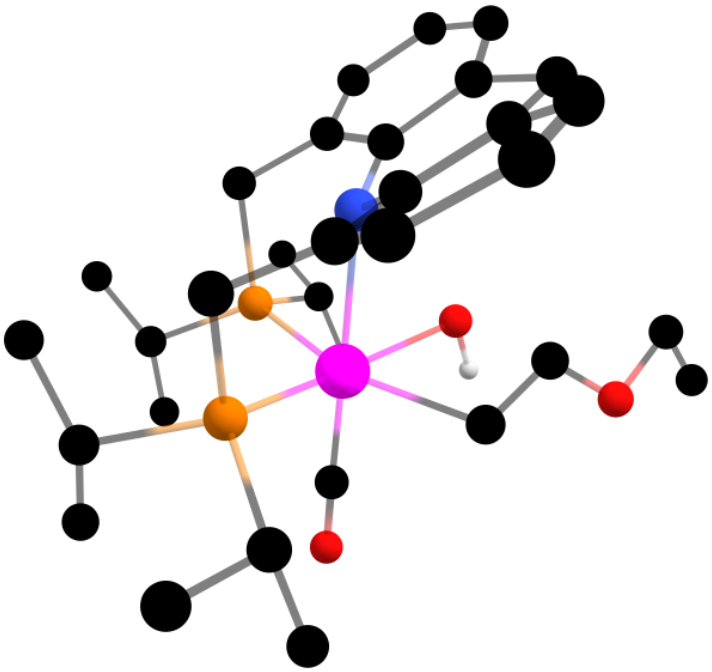
| | | | |
|---|---|---|---|
| 15 | 0.272840000 | 5.921370000 | 4.834165000 |
| 8 | -2.614732000 | 7.598783000 | 6.752054000 |
| 7 | 0.698505000 | 8.260065000 | 2.762094000 |
| 6 | -1.547640000 | 7.940915000 | 1.177552000 |
| 1 | -0.822274000 | 7.139597000 | 1.011265000 |
| 1 | -2.282100000 | 7.899890000 | 0.371416000 |
| 6 | -0.819114000 | 9.239617000 | 1.185892000 |
| 6 | -1.230826000 | 10.319571000 | 0.418015000 |
| 1 | -2.146456000 | 10.237115000 | -0.159112000 |
| 6 | -0.464321000 | 11.475022000 | 0.345181000 |
| 1 | -0.787287000 | 12.308981000 | -0.263927000 |
| 6 | 0.738758000 | 11.533080000 | 1.035236000 |
| 1 | 1.361847000 | 12.418409000 | 0.959282000 |
| 6 | 1.162929000 | 10.483013000 | 1.837813000 |
| 6 | 0.362182000 | 9.332740000 | 1.957426000 |
| 6 | 2.440004000 | 10.543518000 | 2.624353000 |
| 1 | 3.194903000 | 11.124094000 | 2.087374000 |
| 1 | 2.275198000 | 11.102542000 | 3.558704000 |
| 6 | 2.959256000 | 9.179074000 | 2.968163000 |
| 6 | 4.296976000 | 8.960003000 | 3.256553000 |
| 1 | 4.993625000 | 9.788063000 | 3.172800000 |
| 6 | 4.749731000 | 7.715655000 | 3.672753000 |
| 1 | 5.795593000 | 7.560271000 | 3.903058000 |
| 6 | 3.844976000 | 6.670086000 | 3.778375000 |
| 1 | 4.186657000 | 5.686045000 | 4.082536000 |
| 6 | 2.504605000 | 6.849986000 | 3.464672000 |
| 6 | 2.039713000 | 8.121332000 | 3.070605000 |
| 6 | 1.540682000 | 5.711534000 | 3.514468000 |
| 1 | 2.065396000 | 4.766388000 | 3.656885000 |
| 1 | 0.984096000 | 5.649366000 | 2.574769000 |
| 6 | -3.062437000 | 5.832634000 | 2.339807000 |
| 1 | -3.771279000 | 6.034976000 | 1.534024000 |
| 6 | -3.856378000 | 5.250228000 | 3.508950000 |
| 1 | -3.409737000 | 5.462549000 | 4.481943000 |
| 1 | -3.949191000 | 4.166150000 | 3.419665000 |
| 1 | -4.867770000 | 5.654051000 | 3.536775000 |
| 6 | -1.998978000 | 4.906037000 | 1.750602000 |
| 1 | -1.869588000 | 5.086240000 | 0.684595000 |
| 1 | -2.284185000 | 3.859366000 | 1.869765000 |
| 1 | -1.016702000 | 5.029561000 | 2.206304000 |
| 6 | -3.863383000 | 8.590287000 | 2.761404000 |
| 1 | -3.429217000 | 9.579074000 | 2.588423000 |
| 6 | -4.612110000 | 8.627858000 | 4.084142000 |
| 1 | -5.100053000 | 7.678174000 | 4.303315000 |
| 1 | -5.395868000 | 9.386546000 | 4.047667000 |
| 1 | -3.969824000 | 8.862596000 | 4.927200000 |
| 6 | -4.834487000 | 8.320111000 | 1.621035000 |
| 1 | -4.351380000 | 8.246971000 | 0.647314000 |
| 1 | -5.557777000 | 9.134660000 | 1.556770000 |
| 1 | -5.407001000 | 7.405709000 | 1.782523000 |
| 6 | 1.330865000 | 5.909558000 | 6.358010000 |
| 1 | 2.023432000 | 6.716689000 | 6.104086000 |
| 6 | 0.631290000 | 6.306237000 | 7.649642000 |
| 1 | -0.028457000 | 7.162716000 | 7.530003000 |
| 1 | 1.377522000 | 6.572889000 | 8.400390000 |
| 1 | 0.037205000 | 5.495255000 | 8.068922000 |

| | | | |
|---|---|---|---|
| 6 | 2.124522000 | 4.625758000 | 6.554807000 |
| 1 | 1.494004000 | 3.791621000 | 6.864018000 |
| 1 | 2.860049000 | 4.775101000 | 7.347531000 |
| 1 | 2.675545000 | 4.319512000 | 5.667001000 |
| 6 | -0.742368000 | 4.367489000 | 4.842845000 |
| 1 | -1.539597000 | 4.608323000 | 4.145497000 |
| 6 | -1.407398000 | 4.108939000 | 6.186674000 |
| 1 | -0.703191000 | 3.731681000 | 6.927518000 |
| 1 | -2.184428000 | 3.351074000 | 6.070201000 |
| 1 | -1.882593000 | 4.998769000 | 6.598822000 |
| 6 | -0.041439000 | 3.127124000 | 4.309284000 |
| 1 | 0.314123000 | 3.257690000 | 3.287971000 |
| 1 | -0.743780000 | 2.290932000 | 4.299529000 |
| 1 | 0.807163000 | 2.825289000 | 4.921548000 |
| 6 | -1.888920000 | 7.717121000 | 5.847972000 |
| 44 | -0.734426000 | 7.937811000 | 4.455173000 |
| 1 | 0.613720000 | 8.747844000 | 6.456467000 |
| 6 | -1.699882000 | 10.506238000 | 4.334351000 |
| 6 | -0.557108000 | 10.888702000 | 4.930537000 |
| 1 | -1.731457000 | 10.532956000 | 3.256541000 |
| 1 | -2.625471000 | 10.452315000 | 4.888606000 |
| 8 | -0.466450000 | 11.117548000 | 6.232346000 |
| 1 | 0.348796000 | 11.032309000 | 4.348773000 |
| 6 | 0.842101000 | 11.491195000 | 6.715955000 |
| 6 | 0.904819000 | 11.191917000 | 8.182200000 |
| 1 | 0.982179000 | 12.558425000 | 6.518379000 |
| 1 | 1.590235000 | 10.925341000 | 6.157234000 |
| 1 | 0.130207000 | 11.725296000 | 8.731563000 |
| 1 | 1.871352000 | 11.494240000 | 8.581993000 |
| 1 | 0.781620000 | 10.125698000 | 8.374449000 |

**TS2**
**(front view)**



(side view)



First three frequencies

| | 1 | 2 | 3 |
|---|---|---|---|
| | ***A*** | A | A |
| Frequencies -- | ***-219.2998*** | 29.6775 | 35.8700 |
| Red. masses -- | ***8.4659*** | 4.3995 | 3.2766 |
| Frc consts -- | ***0.2399*** | 0.0023 | 0.0025 |
| IR Inten -- | ***25.0695*** | 0.2509 | 0.5060 |

Coordinates

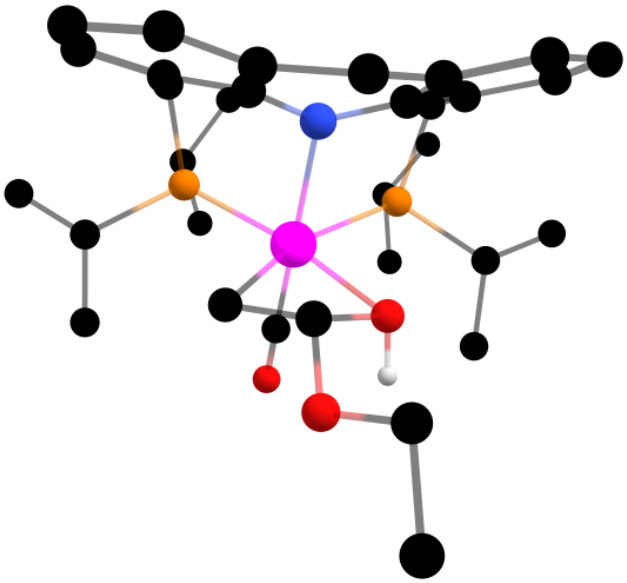
| | | | |
|---|---|---|---|
| 8 | 0.667697000 | 8.523640000 | 5.796182000 |
| 15 | -2.351913000 | 7.308741000 | 2.787537000 |
| 15 | 0.270014000 | 5.612420000 | 4.823284000 |
| 8 | -2.875640000 | 7.037822000 | 6.617326000 |
| 7 | 0.685078000 | 8.132180000 | 2.881805000 |
| 6 | -1.496700000 | 7.750666000 | 1.220903000 |
| 1 | -0.754622000 | 6.960009000 | 1.083867000 |
| 1 | -2.204261000 | 7.694069000 | 0.391629000 |
| 6 | -0.792006000 | 9.061702000 | 1.240147000 |
| 6 | -1.206099000 | 10.124666000 | 0.451022000 |
| 1 | -2.110309000 | 10.019617000 | -0.140257000 |
| 6 | -0.455474000 | 11.289984000 | 0.373504000 |
| 1 | -0.779947000 | 12.111737000 | -0.251129000 |
| 6 | 0.738098000 | 11.367950000 | 1.076068000 |
| 1 | 1.355646000 | 12.256696000 | 0.992674000 |
| 6 | 1.163732000 | 10.334937000 | 1.900668000 |
| 6 | 0.371588000 | 9.179451000 | 2.036748000 |
| 6 | 2.448303000 | 10.430858000 | 2.673287000 |
| 1 | 3.219732000 | 10.907381000 | 2.060510000 |

| | | | |
|---|---|---|---|
| 1 | 2.330153000 | 11.117303000 | 3.525400000 |
| 6 | 2.928257000 | 9.092018000 | 3.156143000 |
| 6 | 4.250429000 | 8.908921000 | 3.532680000 |
| 1 | 4.932502000 | 9.750954000 | 3.468546000 |
| 6 | 4.709179000 | 7.681881000 | 3.987698000 |
| 1 | 5.741915000 | 7.555258000 | 4.284931000 |
| 6 | 3.831297000 | 6.609499000 | 4.018505000 |
| 1 | 4.186052000 | 5.628902000 | 4.318212000 |
| 6 | 2.506675000 | 6.751690000 | 3.626901000 |
| 6 | 2.018605000 | 8.019315000 | 3.237194000 |
| 6 | 1.607029000 | 5.560762000 | 3.559581000 |
| 1 | 2.187579000 | 4.642781000 | 3.656928000 |
| 1 | 1.095340000 | 5.533884000 | 2.592123000 |
| 6 | -3.090478000 | 5.664083000 | 2.340567000 |
| 1 | -3.842803000 | 5.878070000 | 1.577340000 |
| 6 | -3.802751000 | 5.041053000 | 3.532962000 |
| 1 | -3.178602000 | 5.016321000 | 4.426243000 |
| 1 | -4.105990000 | 4.016032000 | 3.311366000 |
| 1 | -4.704242000 | 5.593917000 | 3.795466000 |
| 6 | -2.043558000 | 4.757832000 | 1.695783000 |
| 1 | -1.926457000 | 4.978257000 | 0.636015000 |
| 1 | -2.331950000 | 3.708428000 | 1.778736000 |
| 1 | -1.055885000 | 4.862721000 | 2.147285000 |
| 6 | -3.802611000 | 8.481372000 | 2.750524000 |
| 1 | -3.299839000 | 9.441806000 | 2.589778000 |
| 6 | -4.576882000 | 8.572656000 | 4.055091000 |
| 1 | -5.095163000 | 7.642801000 | 4.290750000 |
| 1 | -5.338838000 | 9.350518000 | 3.980451000 |
| 1 | -3.943440000 | 8.816978000 | 4.902379000 |
| 6 | -4.759411000 | 8.262040000 | 1.587465000 |
| 1 | -4.257282000 | 8.149420000 | 0.627226000 |
| 1 | -5.431970000 | 9.116577000 | 1.497458000 |
| 1 | -5.387637000 | 7.383509000 | 1.742488000 |
| 6 | 1.269743000 | 5.657761000 | 6.387657000 |
| 1 | 1.873905000 | 6.548521000 | 6.188473000 |
| 6 | 0.478679000 | 5.936383000 | 7.657952000 |
| 1 | -0.282057000 | 6.702359000 | 7.523018000 |
| 1 | 1.154558000 | 6.281519000 | 8.442801000 |
| 1 | -0.021367000 | 5.047815000 | 8.041002000 |
| 6 | 2.207710000 | 4.477553000 | 6.591894000 |
| 1 | 1.669874000 | 3.571232000 | 6.873159000 |
| 1 | 2.902627000 | 4.697233000 | 7.405126000 |
| 1 | 2.809999000 | 4.250464000 | 5.713506000 |
| 6 | -0.564038000 | 3.949270000 | 4.746891000 |
| 1 | -1.349607000 | 4.104465000 | 4.010383000 |
| 6 | -1.259773000 | 3.605494000 | 6.055867000 |
| 1 | -0.552600000 | 3.286222000 | 6.820773000 |
| 1 | -1.956937000 | 2.780025000 | 5.900348000 |
| 1 | -1.831690000 | 4.441901000 | 6.458960000 |
| 6 | 0.294048000 | 2.799398000 | 4.242212000 |
| 1 | 0.663188000 | 2.971689000 | 3.231800000 |
| 1 | -0.301441000 | 1.884424000 | 4.213492000 |
| 1 | 1.153953000 | 2.601138000 | 4.881002000 |
| 6 | -2.090464000 | 7.274445000 | 5.788031000 |
| 44 | -0.861481000 | 7.663240000 | 4.510860000 |
| 1 | 0.284383000 | 8.542723000 | 6.681278000 |

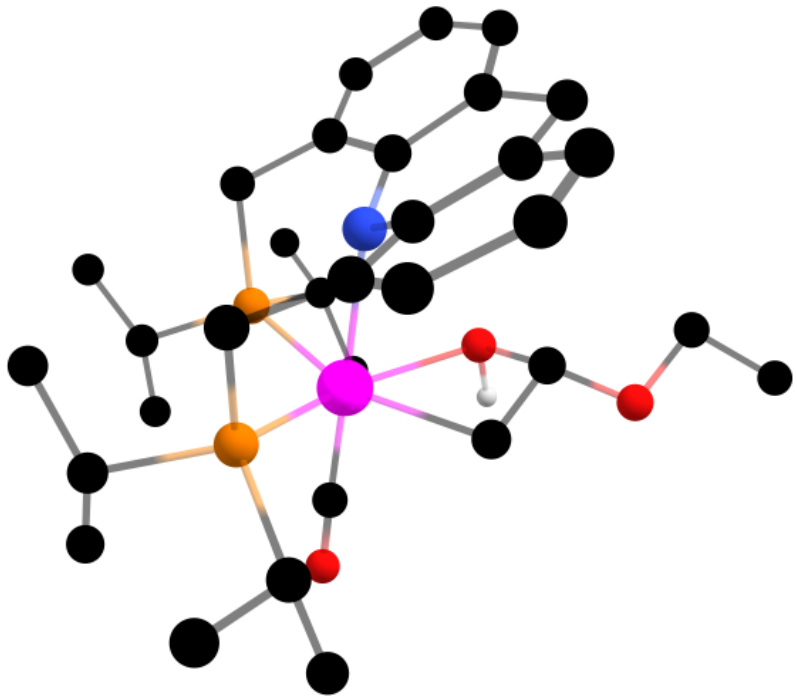
| | | | |
|---|---|---|---|
| 6 | -1.387279000 | 9.869280000 | 4.545708000 |
| 6 | -0.177079000 | 10.311714000 | 5.110289000 |
| 1 | -1.474758000 | 10.164309000 | 3.503661000 |
| 1 | -2.266635000 | 10.101530000 | 5.137358000 |
| 8 | -0.154819000 | 10.963926000 | 6.250606000 |
| 1 | 0.703508000 | 10.394120000 | 4.483807000 |
| 6 | 1.162986000 | 11.366091000 | 6.709487000 |
| 6 | 1.108028000 | 11.564070000 | 8.191802000 |
| 1 | 1.425581000 | 12.287115000 | 6.182937000 |
| 1 | 1.869555000 | 10.583968000 | 6.424866000 |
| 1 | 0.367350000 | 12.313529000 | 8.466822000 |
| 1 | 2.077691000 | 11.899192000 | 8.556002000 |
| 1 | 0.859886000 | 10.634842000 | 8.703541000 |

**1e**

**(front view)**



(side view)



## First three frequencies

| | 1 | 2 | 3 |
|---|---|---|---|
| | ***A*** | A | A |
| Frequencies -- | ***40.2807*** | 43.6344 | 52.0251 |
| Red. masses -- | ***3.7684*** | 3.6766 | 4.1007 |
| Frc consts -- | ***0.0036*** | 0.0041 | 0.0065 |
| IR Inten -- | ***0.3193*** | 0.2279 | 0.0206 |

## Coordinates

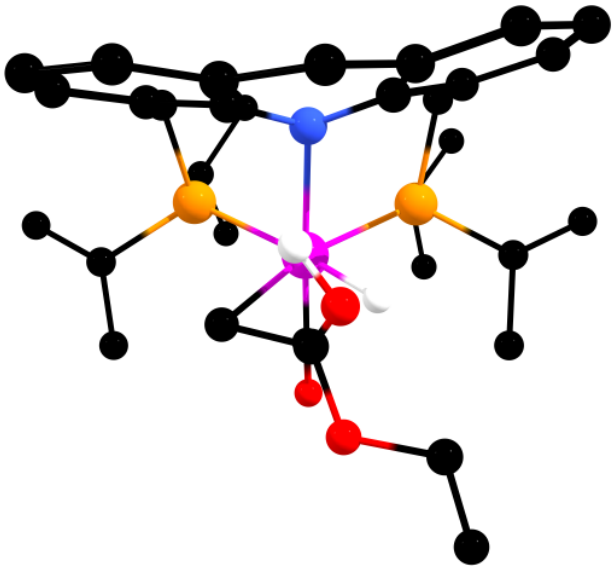
| | | | |
|---|---|---|---|
| 8 | 0.723346000 | 8.727313000 | 5.944643000 |
| 15 | -2.033656000 | 7.251731000 | 2.758893000 |
| 15 | 0.808519000 | 5.603960000 | 4.621498000 |
| 8 | -2.523643000 | 6.589877000 | 6.493181000 |
| 7 | 0.928285000 | 8.308657000 | 2.890144000 |
| 6 | -1.235317000 | 7.857625000 | 1.222223000 |
| 1 | -0.432209000 | 7.143331000 | 1.025965000 |
| 1 | -1.947438000 | 7.797723000 | 0.397157000 |
| 6 | -0.649534000 | 9.221165000 | 1.331709000 |
| 6 | -1.169963000 | 10.294434000 | 0.624101000 |
| 1 | -2.069089000 | 10.148428000 | 0.033838000 |
| 6 | -0.531024000 | 11.526452000 | 0.626802000 |
| 1 | -0.938617000 | 12.358231000 | 0.067582000 |
| 6 | 0.660318000 | 11.661300000 | 1.322804000 |
| 1 | 1.195128000 | 12.605447000 | 1.299251000 |
| 6 | 1.190481000 | 10.613959000 | 2.064927000 |
| 6 | 0.507950000 | 9.385732000 | 2.126315000 |
| 6 | 2.481984000 | 10.772879000 | 2.812408000 |
| 1 | 3.198139000 | 11.334122000 | 2.203858000 |
| 1 | 2.332832000 | 11.408029000 | 3.697204000 |

| | | | |
|---|---|---|---|
| 6 | 3.079749000 | 9.453701000 | 3.211819000 |
| 6 | 4.419927000 | 9.371895000 | 3.559168000 |
| 1 | 5.015248000 | 10.279422000 | 3.550431000 |
| 6 | 5.005731000 | 8.165222000 | 3.909011000 |
| 1 | 6.051570000 | 8.117783000 | 4.182355000 |
| 6 | 4.237434000 | 7.013478000 | 3.859892000 |
| 1 | 4.692078000 | 6.051064000 | 4.069836000 |
| 6 | 2.896267000 | 7.052983000 | 3.498652000 |
| 6 | 2.275193000 | 8.293654000 | 3.220058000 |
| 6 | 2.128241000 | 5.779781000 | 3.350162000 |
| 1 | 2.808266000 | 4.927748000 | 3.378610000 |
| 1 | 1.608949000 | 5.763030000 | 2.386440000 |
| 6 | -2.638905000 | 5.576664000 | 2.239401000 |
| 1 | -3.440908000 | 5.766351000 | 1.520863000 |
| 6 | -3.228420000 | 4.814166000 | 3.415080000 |
| 1 | -2.511850000 | 4.700963000 | 4.228982000 |
| 1 | -3.540773000 | 3.814629000 | 3.107277000 |
| 1 | -4.103454000 | 5.314834000 | 3.828553000 |
| 6 | -1.542031000 | 4.806039000 | 1.511549000 |
| 1 | -1.444432000 | 5.126260000 | 0.475627000 |
| 1 | -1.761838000 | 3.737111000 | 1.501360000 |
| 1 | -0.562595000 | 4.935533000 | 1.975922000 |
| 6 | -3.556716000 | 8.318446000 | 2.825170000 |
| 1 | -3.113822000 | 9.315348000 | 2.713580000 |
| 6 | -4.305877000 | 8.290343000 | 4.146522000 |
| 1 | -4.751945000 | 7.315794000 | 4.347552000 |
| 1 | -5.122495000 | 9.013859000 | 4.121898000 |
| 1 | -3.670389000 | 8.545906000 | 4.989033000 |
| 6 | -4.521026000 | 8.096473000 | 1.668563000 |
| 1 | -4.033823000 | 8.063262000 | 0.694723000 |
| 1 | -5.247979000 | 8.909325000 | 1.633908000 |
| 1 | -5.088097000 | 7.172297000 | 1.790827000 |
| 6 | 1.816850000 | 5.735781000 | 6.182012000 |
| 1 | 2.303812000 | 6.701574000 | 6.005649000 |
| 6 | 1.006510000 | 5.870270000 | 7.463823000 |
| 1 | 0.142400000 | 6.523545000 | 7.355189000 |
| 1 | 1.632945000 | 6.281219000 | 8.257677000 |
| 1 | 0.634173000 | 4.911020000 | 7.820450000 |
| 6 | 2.909117000 | 4.690583000 | 6.350354000 |
| 1 | 2.499216000 | 3.715681000 | 6.616517000 |
| 1 | 3.581750000 | 4.982573000 | 7.159459000 |
| 1 | 3.520427000 | 4.564842000 | 5.458024000 |
| 6 | 0.208839000 | 3.844008000 | 4.488955000 |
| 1 | -0.588984000 | 3.914358000 | 3.749524000 |
| 6 | -0.437387000 | 3.379620000 | 5.786170000 |
| 1 | 0.305959000 | 3.139893000 | 6.546195000 |
| 1 | -1.018438000 | 2.472592000 | 5.610634000 |
| 1 | -1.115518000 | 4.123475000 | 6.206794000 |
| 6 | 1.213075000 | 2.832313000 | 3.959882000 |
| 1 | 1.554066000 | 3.078212000 | 2.954774000 |
| 1 | 0.746827000 | 1.846345000 | 3.906734000 |
| 1 | 2.092032000 | 2.736815000 | 4.595802000 |
| 6 | -1.769747000 | 6.962182000 | 5.685315000 |
| 44 | -0.574810000 | 7.564395000 | 4.456497000 |
| 1 | 0.275275000 | 8.602382000 | 6.794664000 |
| 6 | -1.146293000 | 9.632848000 | 4.747287000 |

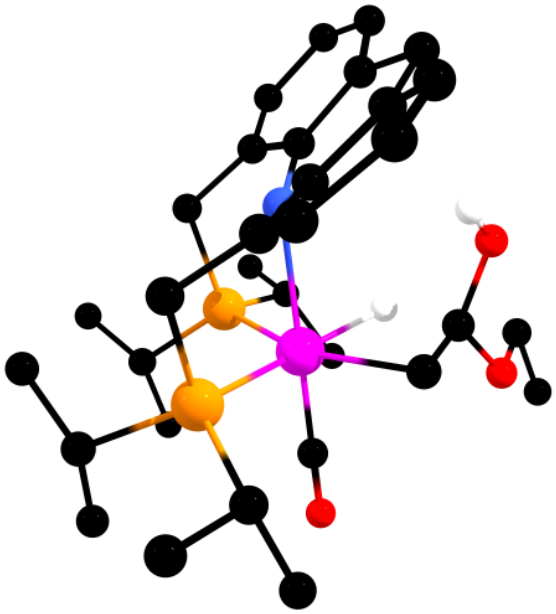
| | | | |
|---|---|---|---|
| 6 | 0.148348000 | 9.993743000 | 5.389963000 |
| 1 | -1.334612000 | 10.252171000 | 3.870170000 |
| 1 | -1.968166000 | 9.758756000 | 5.452657000 |
| 8 | 0.048688000 | 10.916993000 | 6.410679000 |
| 1 | 0.909477000 | 10.283776000 | 4.665021000 |
| 6 | 1.300875000 | 11.500305000 | 6.786591000 |
| 6 | 1.066966000 | 12.436903000 | 7.933585000 |
| 1 | 1.719979000 | 12.028702000 | 5.920963000 |
| 1 | 2.011607000 | 10.711011000 | 7.055316000 |
| 1 | 0.362659000 | 13.221966000 | 7.661546000 |
| 1 | 2.001272000 | 12.909313000 | 8.232909000 |
| 1 | 0.665101000 | 11.908277000 | 8.797179000 |

**TS3**

**(front view)**



(side view)



First three frequencies

| | 1 | 2 | 3 |
|---|---|---|---|
| | ***A*** | A | A |
| Frequencies -- | ***-671.9172*** | 30.5896 | 36.2743 |
| Red. masses -- | ***1.7784*** | 3.5684 | 4.2587 |
| Frc consts -- | ***0.4730*** | 0.0020 | 0.0033 |
| IR Inten -- | ***385.0465*** | 0.1264 | 0.0377 |

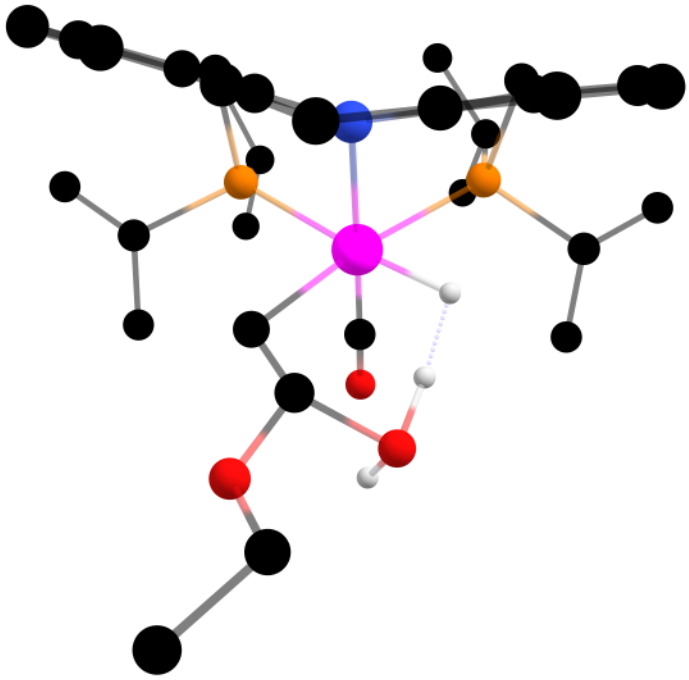
Coordinates

| | | | |
|---|---|---|---|
| 15 | -2.354928000 | 7.382052000 | 2.730746000 |
| 15 | 0.386581000 | 5.825210000 | 4.840940000 |
| 8 | -2.674687000 | 7.302212000 | 6.649554000 |
| 7 | 0.735512000 | 8.170032000 | 2.688698000 |
| 6 | -1.530192000 | 7.762216000 | 1.133101000 |
| 1 | -0.794064000 | 6.963709000 | 1.011919000 |
| 1 | -2.252671000 | 7.685306000 | 0.318290000 |
| 6 | -0.818581000 | 9.069652000 | 1.097524000 |
| 6 | -1.273619000 | 10.122173000 | 0.319917000 |
| 1 | -2.213538000 | 10.014226000 | -0.211813000 |
| 6 | -0.523852000 | 11.282362000 | 0.175604000 |
| 1 | -0.886641000 | 12.099171000 | -0.433155000 |
| 6 | 0.720584000 | 11.351311000 | 0.778438000 |
| 1 | 1.347508000 | 12.223371000 | 0.624123000 |
| 6 | 1.200123000 | 10.320940000 | 1.580472000 |
| 6 | 0.395960000 | 9.187859000 | 1.817285000 |
| 6 | 2.585581000 | 10.383635000 | 2.164773000 |
| 1 | 3.291521000 | 10.692728000 | 1.386671000 |
| 1 | 2.667942000 | 11.182844000 | 2.915265000 |
| 6 | 3.026705000 | 9.075733000 | 2.755284000 |
| 6 | 4.362704000 | 8.882804000 | 3.072310000 |
| 1 | 5.059192000 | 9.696288000 | 2.897746000 |
| 6 | 4.818090000 | 7.686732000 | 3.601671000 |
| 1 | 5.862402000 | 7.553998000 | 3.849738000 |
| 6 | 3.915878000 | 6.649843000 | 3.768583000 |
| 1 | 4.260003000 | 5.683849000 | 4.122883000 |

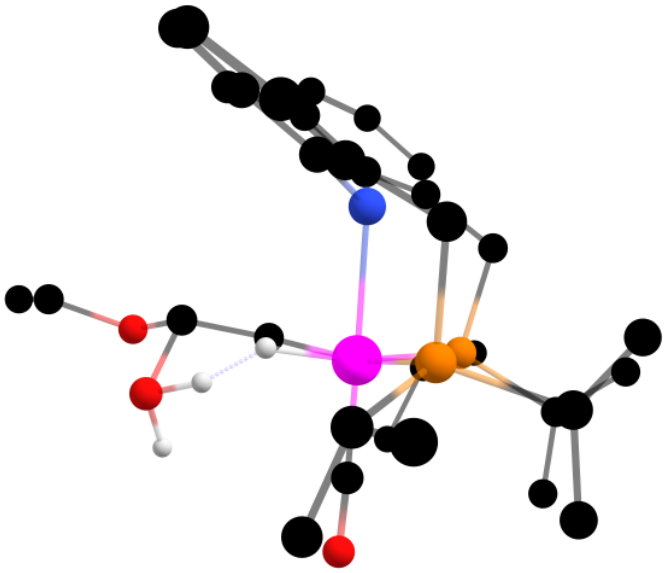
| | | | |
|---|---|---|---|
| 6 | 2.573991000 | 6.801857000 | 3.443477000 |
| 6 | 2.089711000 | 8.046781000 | 2.980060000 |
| 6 | 1.655010000 | 5.629459000 | 3.524148000 |
| 1 | 2.227903000 | 4.713899000 | 3.675075000 |
| 1 | 1.091254000 | 5.528532000 | 2.591129000 |
| 6 | -3.105340000 | 5.718303000 | 2.380704000 |
| 1 | -3.868546000 | 5.881622000 | 1.614792000 |
| 6 | -3.788828000 | 5.161683000 | 3.622664000 |
| 1 | -3.131436000 | 5.178099000 | 4.492664000 |
| 1 | -4.104070000 | 4.129513000 | 3.461767000 |
| 1 | -4.675724000 | 5.735216000 | 3.887458000 |
| 6 | -2.057953000 | 4.775478000 | 1.793899000 |
| 1 | -1.906337000 | 4.955742000 | 0.731395000 |
| 1 | -2.362862000 | 3.734338000 | 1.910260000 |
| 1 | -1.084848000 | 4.888461000 | 2.275179000 |
| 6 | -3.794080000 | 8.562710000 | 2.696926000 |
| 1 | -3.276049000 | 9.512375000 | 2.515764000 |
| 6 | -4.543737000 | 8.682136000 | 4.014987000 |
| 1 | -5.089626000 | 7.770429000 | 4.257425000 |
| 1 | -5.279553000 | 9.485069000 | 3.952468000 |
| 1 | -3.887247000 | 8.900414000 | 4.851705000 |
| 6 | -4.772881000 | 8.331138000 | 1.553965000 |
| 1 | -4.286409000 | 8.206698000 | 0.587576000 |
| 1 | -5.450319000 | 9.181409000 | 1.466386000 |
| 1 | -5.393320000 | 7.451548000 | 1.731750000 |
| 6 | 1.463505000 | 5.997769000 | 6.351801000 |
| 1 | 2.097324000 | 6.833262000 | 6.027321000 |
| 6 | 0.723876000 | 6.451758000 | 7.601997000 |
| 1 | 0.060356000 | 7.290517000 | 7.400543000 |
| 1 | 1.439614000 | 6.772231000 | 8.361703000 |
| 1 | 0.125757000 | 5.656184000 | 8.043267000 |
| 6 | 2.372110000 | 4.815372000 | 6.653789000 |
| 1 | 1.813334000 | 3.965118000 | 7.045625000 |
| 1 | 3.102757000 | 5.091946000 | 7.415622000 |
| 1 | 2.930413000 | 4.477514000 | 5.781783000 |
| 6 | -0.457177000 | 4.163652000 | 4.950061000 |
| 1 | -1.261176000 | 4.264762000 | 4.221220000 |
| 6 | -1.121473000 | 3.947669000 | 6.302851000 |
| 1 | -0.392283000 | 3.721721000 | 7.080422000 |
| 1 | -1.805513000 | 3.099134000 | 6.250288000 |
| 1 | -1.698378000 | 4.813560000 | 6.627364000 |
| 6 | 0.373097000 | 2.959922000 | 4.528119000 |
| 1 | 0.709253000 | 3.034952000 | 3.494896000 |
| 1 | -0.230094000 | 2.053485000 | 4.605759000 |
| 1 | 1.252257000 | 2.815033000 | 5.153896000 |
| 6 | -1.949186000 | 7.501422000 | 5.762704000 |
| 44 | -0.789265000 | 7.818215000 | 4.394347000 |
| 6 | -1.275674000 | 9.942179000 | 4.381108000 |
| 6 | -0.123023000 | 10.009493000 | 5.239560000 |
| 1 | -1.160624000 | 10.452445000 | 3.429276000 |
| 1 | -2.206914000 | 10.177973000 | 4.879131000 |
| 8 | -0.346688000 | 10.257880000 | 6.549934000 |
| 6 | 0.796582000 | 10.139642000 | 7.403080000 |
| 6 | 0.309240000 | 10.090803000 | 8.821465000 |
| 1 | 1.469362000 | 10.981870000 | 7.226586000 |
| 1 | 1.343195000 | 9.228205000 | 7.126458000 |

| | | | |
|---|---|---|---|
| 1 | -0.230832000 | 10.999622000 | 9.080780000 |
| 1 | 1.150279000 | 9.990783000 | 9.505382000 |
| 1 | -0.360282000 | 9.245694000 | 8.976087000 |
| 1 | 0.382294000 | 8.630515000 | 5.371570000 |
| 8 | 1.025961000 | 10.591979000 | 4.793429000 |
| 1 | 0.977755000 | 10.624288000 | 3.826586000 |

**TS4**
**(front view)**



(side view)



## First three frequencies

| | 1 | 2 | 3 |
|---|---|---|---|
| | ***A*** | A | A |
| Frequencies -- | ***-413.4617*** | 22.7420 | 27.4072 |
| Red. masses -- | ***3.0176*** | 4.0218 | 4.6734 |
| Frc consts -- | ***0.3039*** | 0.0012 | 0.0021 |
| IR Inten -- | ***743.4817*** | 0.5899 | 0.7344 |

## Coordinates

| | | | |
|---|---|---|---|
| 44 | 0.215609000 | -0.420775000 | 0.595603000 |
| 15 | -1.121175000 | -1.781075000 | -0.799047000 |
| 15 | 2.415130000 | -0.513036000 | -0.265515000 |
| 7 | -0.112466000 | 1.262705000 | -0.940610000 |
| 6 | -1.466057000 | -0.786962000 | -2.311618000 |
| 1 | -0.485242000 | -0.607260000 | -2.763755000 |
| 1 | -2.061713000 | -1.364460000 | -3.018958000 |
| 6 | -2.132833000 | 0.512644000 | -2.008074000 |
| 6 | -3.444329000 | 0.743459000 | -2.403580000 |
| 1 | -3.982775000 | -0.048681000 | -2.913589000 |
| 6 | -4.054457000 | 1.971234000 | -2.196404000 |
| 1 | -5.071757000 | 2.141423000 | -2.523375000 |
| 6 | -3.331261000 | 2.982376000 | -1.580456000 |
| 1 | -3.790151000 | 3.952181000 | -1.415678000 |
| 6 | -2.030811000 | 2.777441000 | -1.145566000 |
| 6 | -1.406865000 | 1.528322000 | -1.342952000 |
| 6 | -1.284091000 | 3.845442000 | -0.402636000 |
| 1 | -1.607559000 | 3.849141000 | 0.650150000 |
| 1 | -1.564345000 | 4.836345000 | -0.770940000 |
| 6 | 0.201576000 | 3.656448000 | -0.483714000 |
| 6 | 1.081536000 | 4.709978000 | -0.275749000 |
| 1 | 0.677240000 | 5.693629000 | -0.058284000 |
| 6 | 2.454889000 | 4.524657000 | -0.332385000 |
| 1 | 3.129312000 | 5.351689000 | -0.152918000 |
| 6 | 2.950431000 | 3.270811000 | -0.663619000 |
| 1 | 4.019990000 | 3.121404000 | -0.774365000 |
| 6 | 2.096289000 | 2.205666000 | -0.909838000 |
| 6 | 0.700325000 | 2.369895000 | -0.756491000 |
| 6 | 2.605245000 | 0.903404000 | -1.423662000 |
| 1 | 3.649891000 | 0.984119000 | -1.732423000 |
| 1 | 2.018121000 | 0.620147000 | -2.301509000 |
| 6 | -0.438567000 | -3.393748000 | -1.438106000 |
| 1 | 0.630187000 | -3.187827000 | -1.467766000 |
| 6 | -0.631224000 | -4.536271000 | -0.452640000 |
| 1 | -1.655604000 | -4.908062000 | -0.456444000 |
| 1 | -0.380944000 | -4.255066000 | 0.570595000 |
| 1 | 0.012635000 | -5.374476000 | -0.726031000 |
| 6 | -0.855957000 | -3.789570000 | -2.845820000 |
| 1 | -0.356050000 | -4.718933000 | -3.127615000 |
| 1 | -0.578114000 | -3.041210000 | -3.587096000 |
| 1 | -1.927754000 | -3.963351000 | -2.935795000 |
| 6 | -2.840836000 | -2.129193000 | -0.181704000 |
| 1 | -3.214389000 | -1.107950000 | -0.048611000 |
| 6 | -2.892452000 | -2.821702000 | 1.175848000 |
| 1 | -3.833963000 | -2.593171000 | 1.678193000 |

| | | | |
|---|---|---|---|
| 1 | -2.085053000 | -2.519367000 | 1.839612000 |
| 1 | -2.843137000 | -3.904921000 | 1.077045000 |
| 6 | -3.765226000 | -2.828246000 | -1.167430000 |
| 1 | -3.490453000 | -3.874644000 | -1.304820000 |
| 1 | -3.785492000 | -2.354265000 | -2.147684000 |
| 1 | -4.788708000 | -2.818389000 | -0.786890000 |
| 6 | 3.712881000 | -0.091013000 | 1.007173000 |
| 1 | 3.474688000 | 0.962331000 | 1.199489000 |
| 6 | 5.143219000 | -0.166913000 | 0.496823000 |
| 1 | 5.818311000 | 0.311887000 | 1.208111000 |
| 1 | 5.283410000 | 0.332070000 | -0.462004000 |
| 1 | 5.481139000 | -1.199055000 | 0.388782000 |
| 6 | 3.572903000 | -0.840205000 | 2.321740000 |
| 1 | 3.676062000 | -1.919091000 | 2.200128000 |
| 1 | 2.612600000 | -0.654465000 | 2.797175000 |
| 1 | 4.349868000 | -0.520076000 | 3.018461000 |
| 6 | 3.182228000 | -1.885174000 | -1.256586000 |
| 1 | 4.231081000 | -1.612395000 | -1.398204000 |
| 6 | 3.144312000 | -3.192236000 | -0.476269000 |
| 1 | 2.151536000 | -3.417374000 | -0.083334000 |
| 1 | 3.821293000 | -3.166705000 | 0.377669000 |
| 1 | 3.449974000 | -4.030818000 | -1.104909000 |
| 6 | 2.543967000 | -1.966468000 | -2.641960000 |
| 1 | 1.477514000 | -1.735102000 | -2.630676000 |
| 1 | 2.656334000 | -2.965011000 | -3.068653000 |
| 1 | 3.006754000 | -1.264095000 | -3.333567000 |
| 6 | 0.446019000 | -1.732948000 | 1.822755000 |
| 8 | 0.567964000 | -2.557540000 | 2.643586000 |
| 6 | -1.406470000 | 1.478937000 | 2.465185000 |
| 1 | 1.109131000 | 0.763723000 | 1.453931000 |
| 1 | -0.976396000 | 2.367726000 | 1.993830000 |
| 8 | -0.070091000 | 1.109115000 | 3.397636000 |
| 1 | 0.540930000 | 0.832790000 | 2.546243000 |
| 1 | -0.292667000 | 0.259416000 | 3.814722000 |
| 6 | -1.636967000 | 0.329697000 | 1.576460000 |
| 1 | -2.301164000 | 0.694047000 | 0.788493000 |
| 1 | -2.196745000 | -0.420592000 | 2.140316000 |
| 8 | -2.380545000 | 1.749461000 | 3.348287000 |
| 6 | -2.251075000 | 2.998697000 | 4.053311000 |
| 1 | -1.998816000 | 3.781802000 | 3.330363000 |
| 1 | -1.417789000 | 2.920932000 | 4.757193000 |
| 6 | -3.543806000 | 3.283129000 | 4.753786000 |
| 1 | -3.786922000 | 2.495988000 | 5.465977000 |
| 1 | -4.366222000 | 3.366386000 | 4.045095000 |
| 1 | -3.472248000 | 4.221142000 | 5.301640000 |

Energies of Computed Structures

| | $E^{\omega B97M\text{-}V}_{el/SMD}$ | $G^{o}\ corr^{M06\text{-}L}_{freq/SMD}$ (1 atm, 398.15 K) | **Imaginary Frequency** |
|---|---|---|---|
| **Main Cycle Intermediates and Transition States of complex 6** | | | |
| **6-*mer*** | -2451.812888950932 | 0.500451 | |
| **6-*fac*** | -2451.807880184399 | 0.504386 | |
| **6b-*fac*** | -2528.276789651755 | 0.526216 | |
| **6TS1** | -2528.236979945745 | 0.523622 | -938.8164 |
| **6c** | -2527.074177824430 | 0.508927 | |
| **6d** | -2759.510380012993 | 0.612153 | |
| **6TS2** | -2759.505730365457 | 0.611821 | -242.6559 |
| **6e** | -2759.521912974986 | 0.616558 | |
| **6TS3** | -2759.51053136025 | 0.613380 | - -625.0786 |
| **Alternate Reaction Pathway Intermediates and Transition States of complex 6** | | | |
| **6a-*fac*** | -2684.267631991996 | 0.609672 | |
| **6TS4** | -2760.661002441410 | 0.636184 | -294.3637 |
| **TS5** | -385.244326553544 | 0.109791 | -289.2022 |
| **Organics** | | | |
| Ethyl Vinyl Ether | -232.413491675489 | 0.069705 | |
| Water | -76.438317920532 | -0.00462 | |
| Hydrogen | -1.160713129166 | -0.006738 | |
| Ethyl Acetate | -307.712692350948 | 0.0722 | |
| **Main Cycle Intermediates and Transition States of complex 1** | | | |
| **1-*mer*** | -1999.28016801161 | 0.648033 | |
| **1-*fac*** | -1999.26335929438 | 0.529431 | |
| **1b-*fac*** | -2075.72834157513 | 0.554507 | |

| | | | |
|---|---|---|---|
| **TS1** | -2075.69360847472 | 0.551809 | -996.8853 |
| **1c** | -2074.52553654306 | 0.535057 | |
| **1d** | -2306.95759882973 | 0.637097 | |
| **TS2** | -2306.95536625218 | 0.641367 | -219.2998 |
| **1e** | -2306.97893888902 | 0.648033 | |
| **TS3** | -2306.97253807245 | 0.639521 | -671.9172 |
| **Alternate Reaction Pathway Intermediates and Transition States of complex 1** | | | |
| **1a-*fac*** | -2231.7212988878 | 0.640258 | |
| **TS4** | -2308.11567501238 | 0.655057 | -413.4617 |

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