

## Supporting Information

### **Mechanistic Insights and Comparative Analysis of Ru(II)-NNC Pincer Complexes with Anionic-, Protic-, and Classical-NHCs for Transfer Hydrogenation of Ketones**

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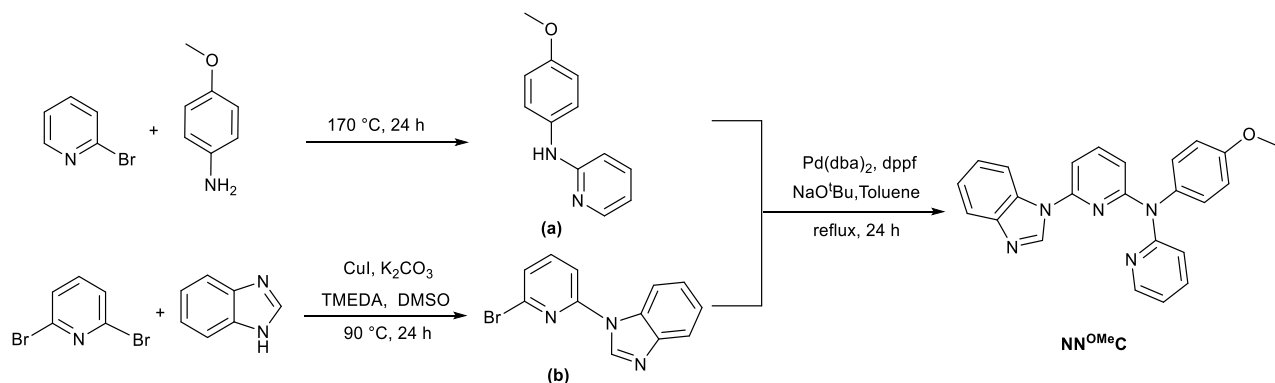
## Overview

Schemes for ligand synthesis.....	S4
$^1\text{H}$ and $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of $\text{NN}^{\text{OMe}}\text{C}$ .....	S5
LCMS of $\text{NN}^{\text{OMe}}\text{C}$ .....	S6
HRMS of $\text{NN}^{\text{OMe}}\text{C}$ .....	S7
$^1\text{H}$ and $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of <b>3</b> .....	S8
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of <b>3</b> .....	S9
LCMS of <b>3</b> .....	S10
HRMS of <b>3</b> .....	S11
$^1\text{H}$ and $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of <b>3'</b> .....	S12
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of <b>3'</b> and $^1\text{H}$ spectrum of <b>3'</b> after adding 10 equiv. $\text{PPh}_3$ .....	S13
$^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of <b>3'</b> after adding 10 equiv. $\text{PPh}_3$ .....	S14
HRMS of <b>3'</b> .....	S15
HRMS of <b>3b'</b> .....	S16
$^1\text{H}$ and $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of <b>4</b> .....	S17
LCMS of <b>4</b> .....	S18
HRMS of <b>4</b> .....	S19
$^1\text{H}$ and $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of $\text{NN}^{\text{Me}}\text{C}^{\text{Me}}\cdot\text{HI}$ .....	S20
LCMS of $\text{NN}^{\text{Me}}\text{C}^{\text{Me}}\cdot\text{HI}$ .....	S21
HRMS of $\text{NN}^{\text{Me}}\text{C}^{\text{Me}}\cdot\text{HI}$ .....	S22
$^1\text{H}$ and $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of <b>5</b> .....	S23
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of <b>5</b> .....	S24
$^1\text{H}$ NMR and $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of <b>5</b> after adding 10 equiv. $\text{PPh}_3$ .....	S25
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of <b>5</b> after adding 10 equiv. $\text{PPh}_3$ .....	S26
LCMS of <b>5</b> .....	S27
HRMS of <b>5</b> .....	S28
$^1\text{H}$ and $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of <b>6</b> .....	S29

$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of <b>6</b> .....	S30
LCMS of <b>6</b> .....	S31
HRMS of <b>6</b> .....	S32
$^1\text{H}$ and $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of $\text{NN}^{\text{OMe}}\text{C}^{\text{Me}}\cdot\text{HI}$ .....	S33
LCMS of $\text{NN}^{\text{OMe}}\text{C}^{\text{Me}}\cdot\text{HI}$ .....	S34
HRMS of $\text{NN}^{\text{OMe}}\text{C}^{\text{Me}}\cdot\text{HI}$ .....	S35
$^1\text{H}$ and $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of <b>7</b> .....	S36
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of <b>7</b> .....	S37
LCMS of <b>7</b> .....	S38
HRMS of <b>7</b> .....	S39
LCMS of <b>8</b> .....	S40
X-ray Diffraction Studies .....	S41
Crystallographic Data.....	S41-S42
General method for transfer hydrogenation of ketone.....	S42
General method for transfer hydrogenation of ketone using CuI as phosphine scavenger .....	S43
The molecular structure of CuI capped anionic NHC complex <b>1b</b> .....	S43
Mechanistic investigation of transfer hydrogenation reactions using Mass spectrometry .....	S44-S45
NMR experiments for the mechanistic investigation of transfer hydrogenation reactions .....	S46-S53
NMR tube experiments to evaluate the effect of excess triphenyl phosphine.....	S53-S55
Computational details .....	S56- S57
Calculated energy profile for TH using complex <b>5</b> .....	S58
References.....	S59
Calibration curve.....	S59
GCMS data.....	S60-S128
Computational data.....	S129-S336

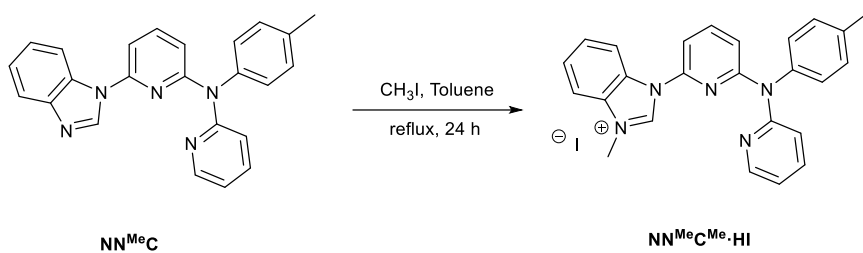
## Schemes for ligand synthesis

### a) Synthesis of $\text{NN}^{\text{OMeC}}$



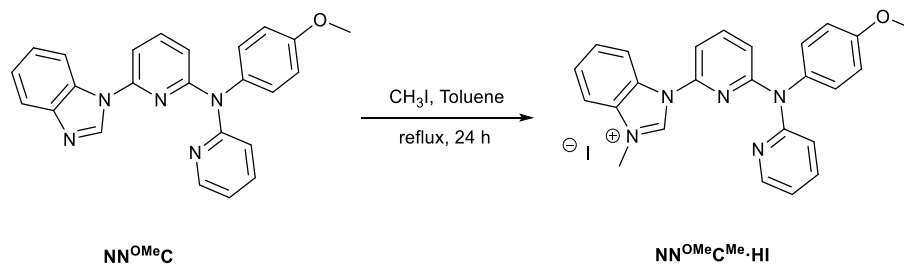
Scheme S1. The synthetic procedure for  $\text{NN}^{\text{OMeC}}$ .

### b) Synthesis of $\text{NN}^{\text{MeC}^{\text{Me}}\cdot\text{HI}}$



Scheme S2. The synthetic procedure for  $\text{NN}^{\text{MeC}^{\text{Me}}\cdot\text{HI}}$ .

### c) Synthesis of $\text{NN}^{\text{OMeC}^{\text{Me}}\cdot\text{HI}}$



Scheme S3. The synthetic procedure for  $\text{NN}^{\text{OMeC}^{\text{Me}}\cdot\text{HI}}$ .

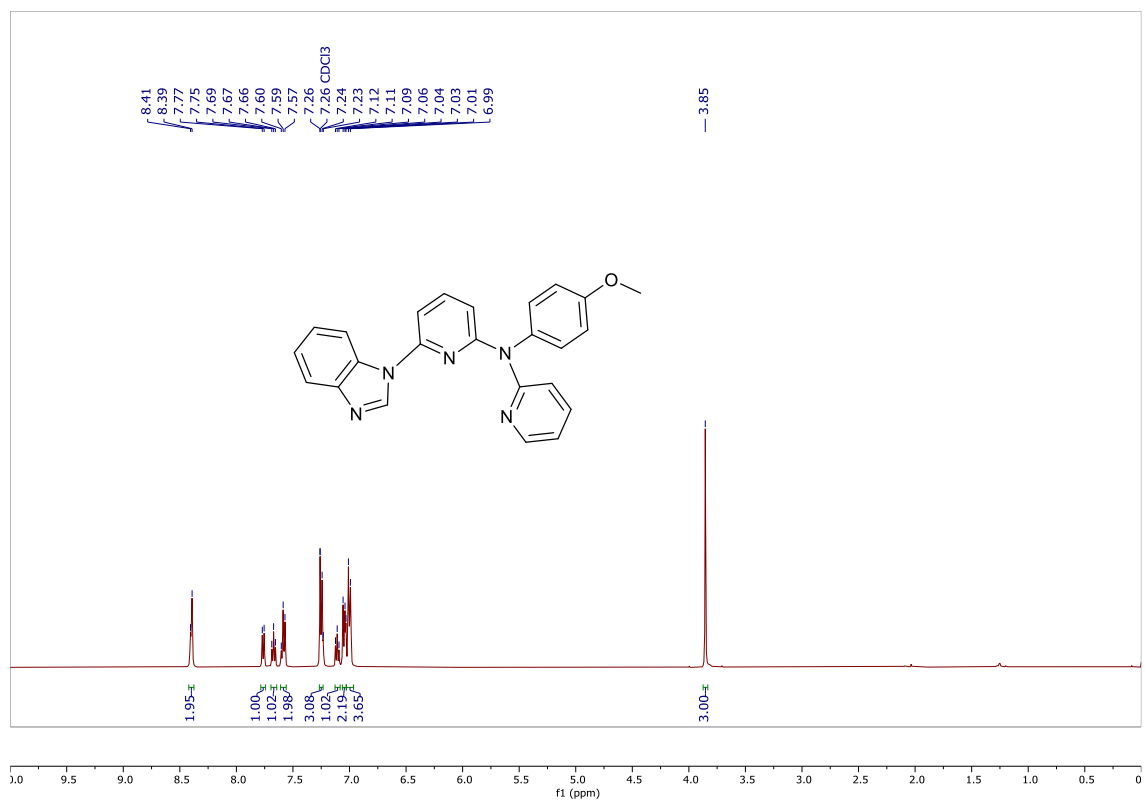


Figure S1. <sup>1</sup>H NMR of NN<sup>OMe</sup>C in CDCl<sub>3</sub>.

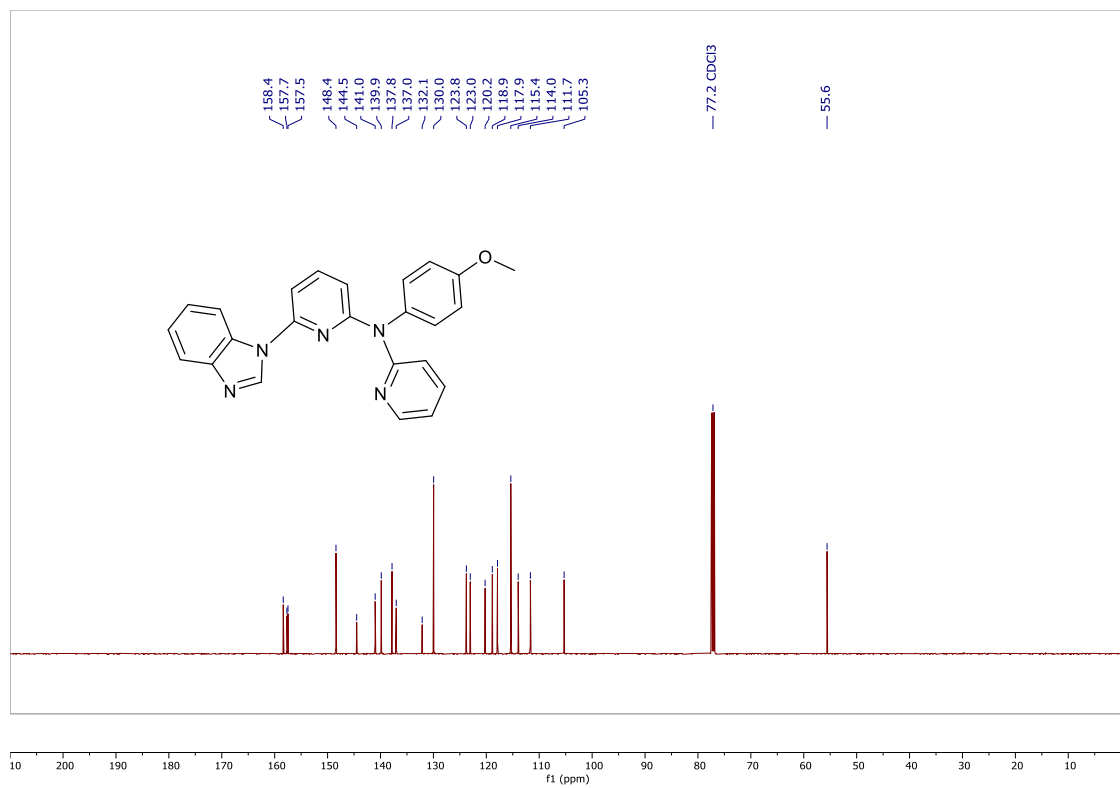


Figure S2. <sup>13</sup>C{<sup>1</sup>H} NMR of NN<sup>OMe</sup>C in CDCl<sub>3</sub>.

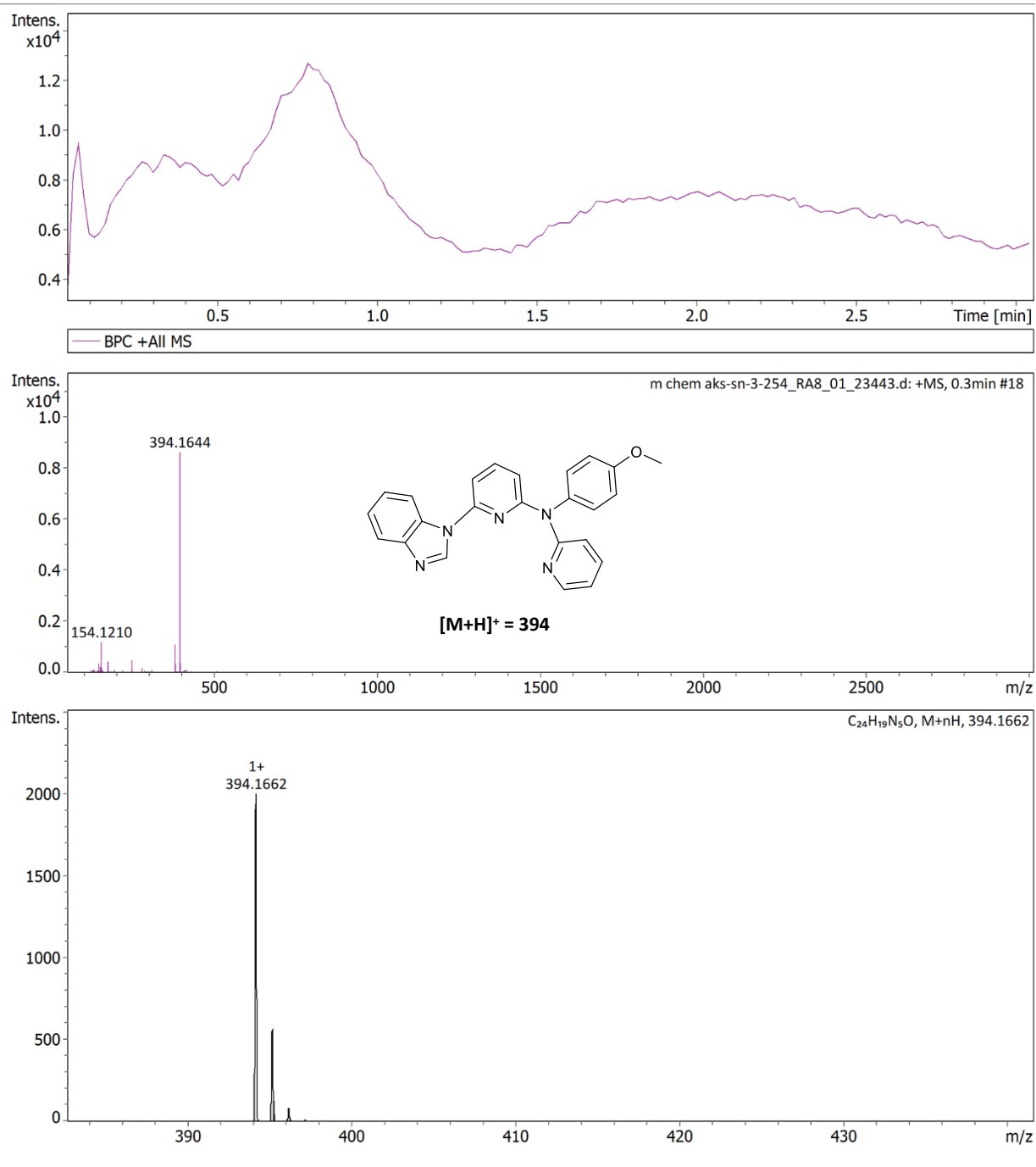
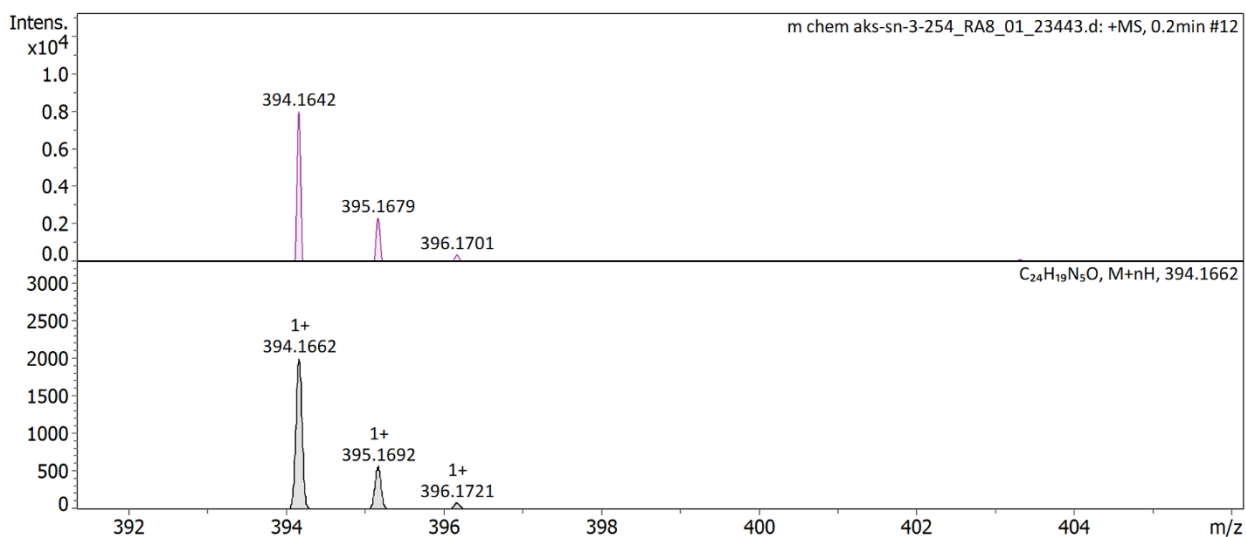
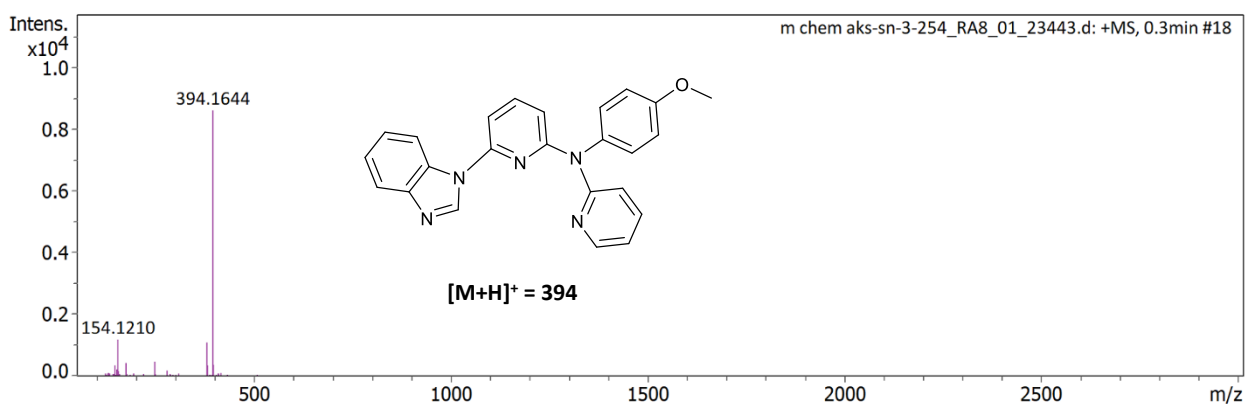
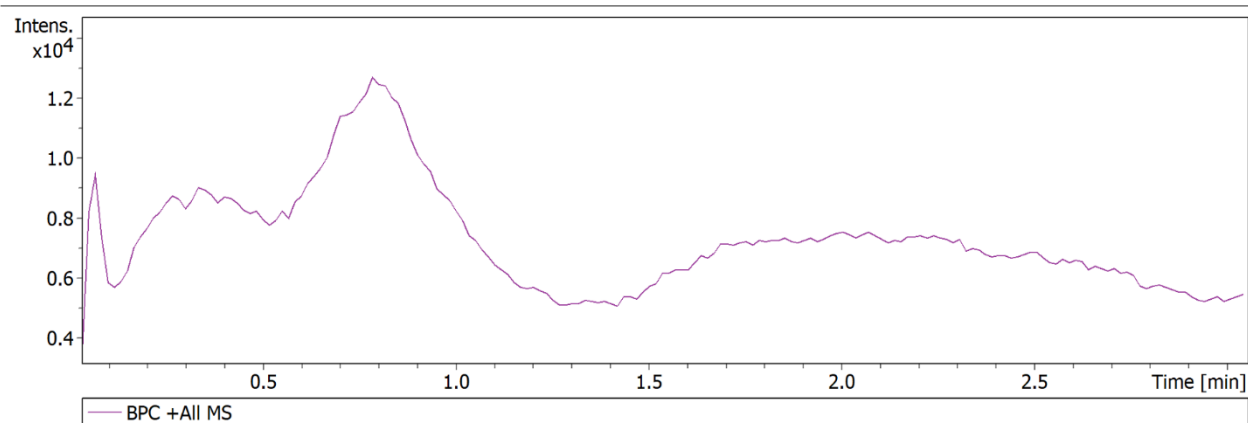


Figure S3. LCMS of NN<sup>OMe</sup>C.



**Figure S4.** HRMS of NN<sup>OMe</sup>C.

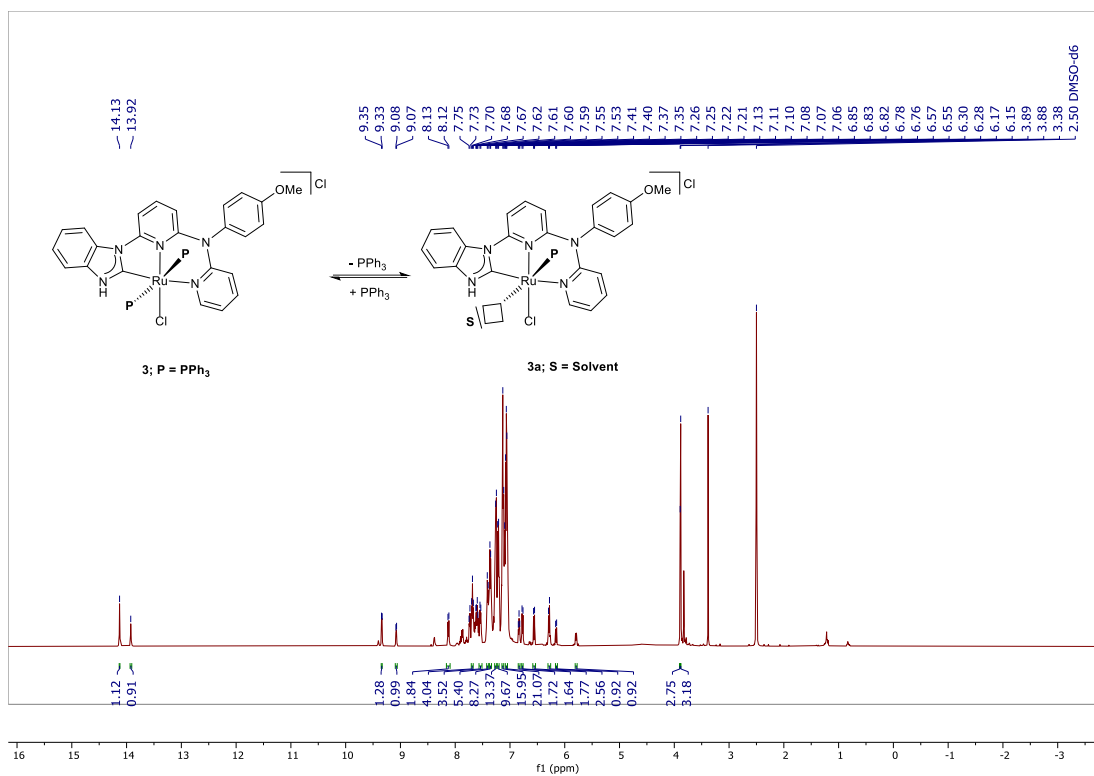


Figure S5. <sup>1</sup>H NMR spectrum of **3** in DMSO-d<sub>6</sub>.

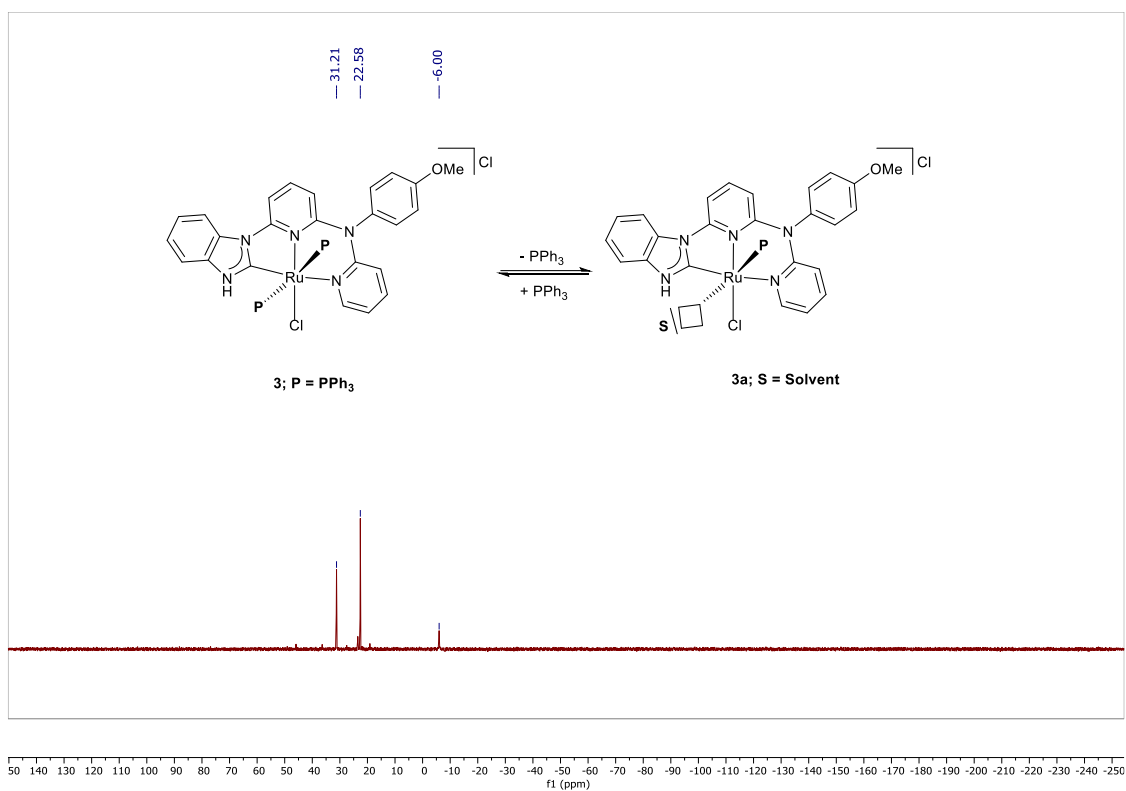
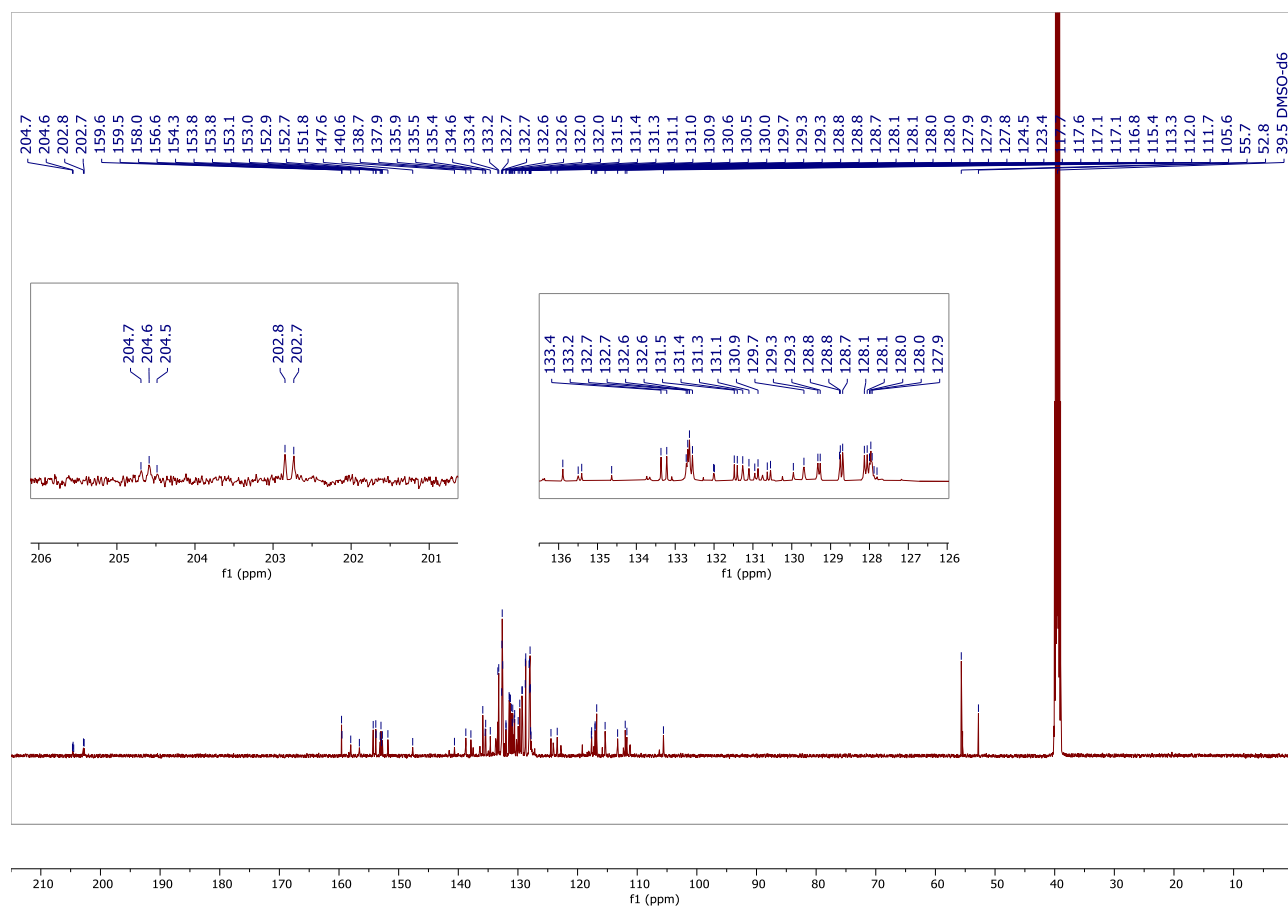


Figure S6. <sup>31</sup>P{<sup>1</sup>H} NMR spectrum of **3** in DMSO-d<sub>6</sub>.





**Figure S7.**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **3** in  $\text{DMSO-d}_6$ .

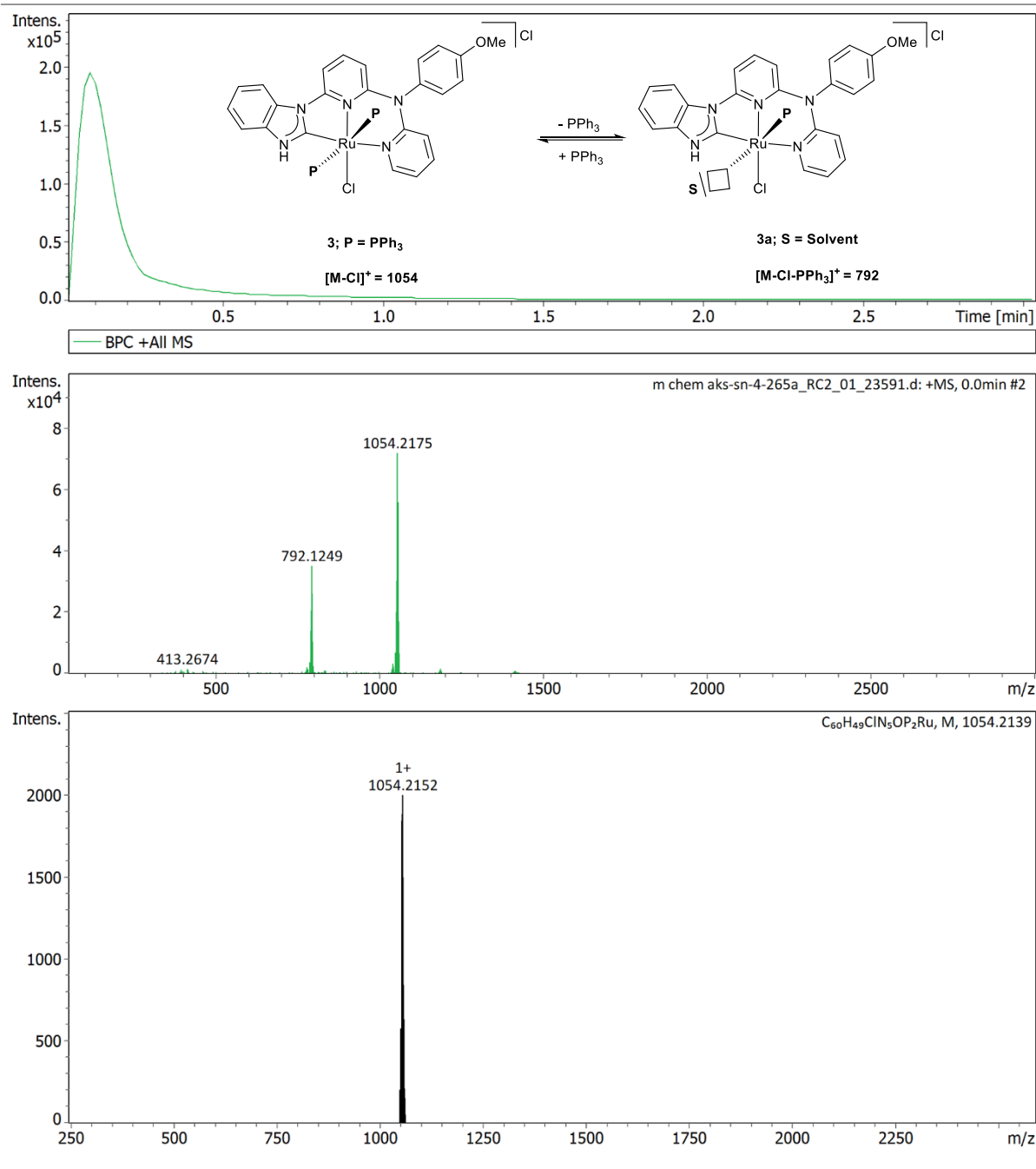


Figure S8. LCMS of **3**.

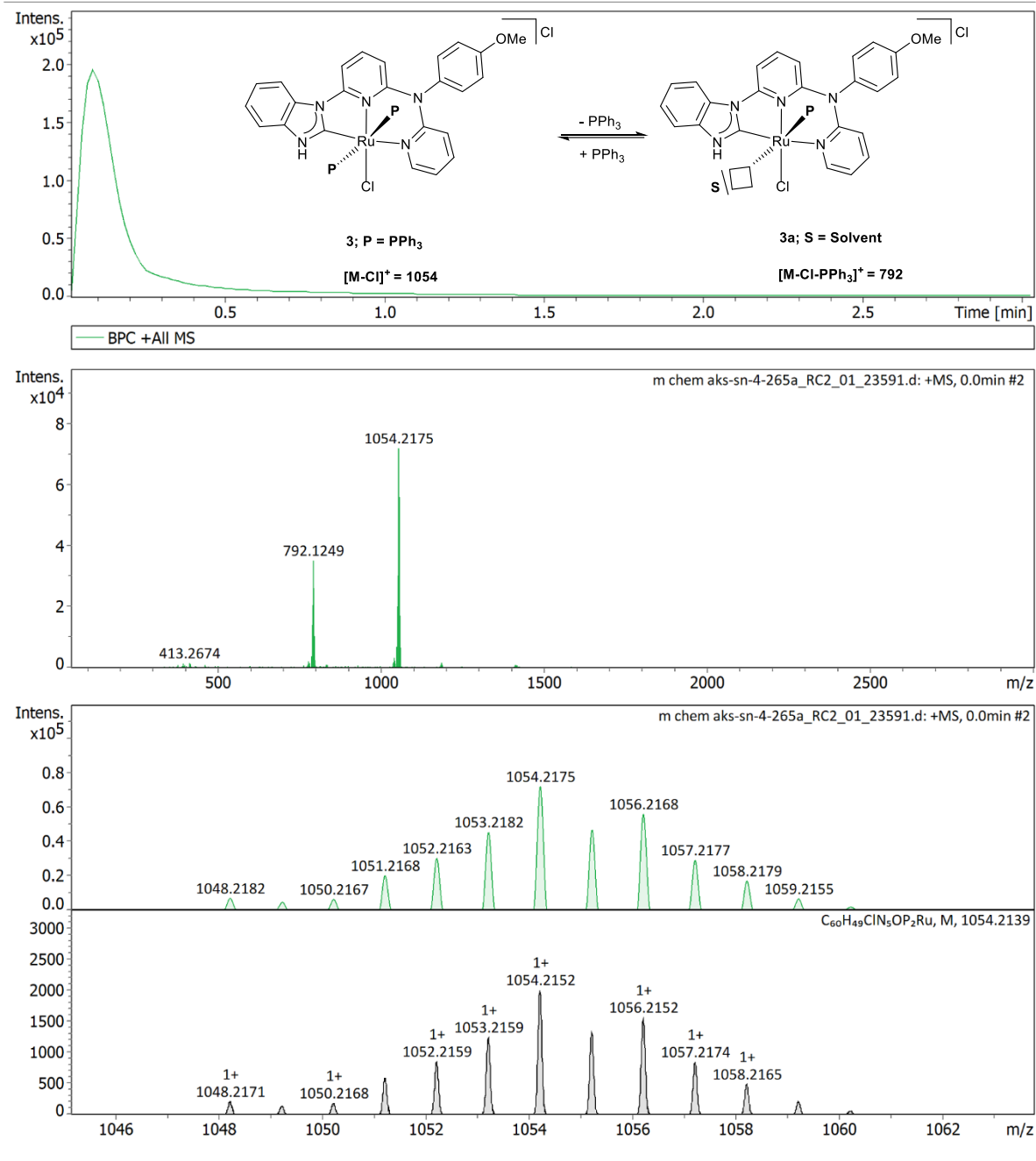
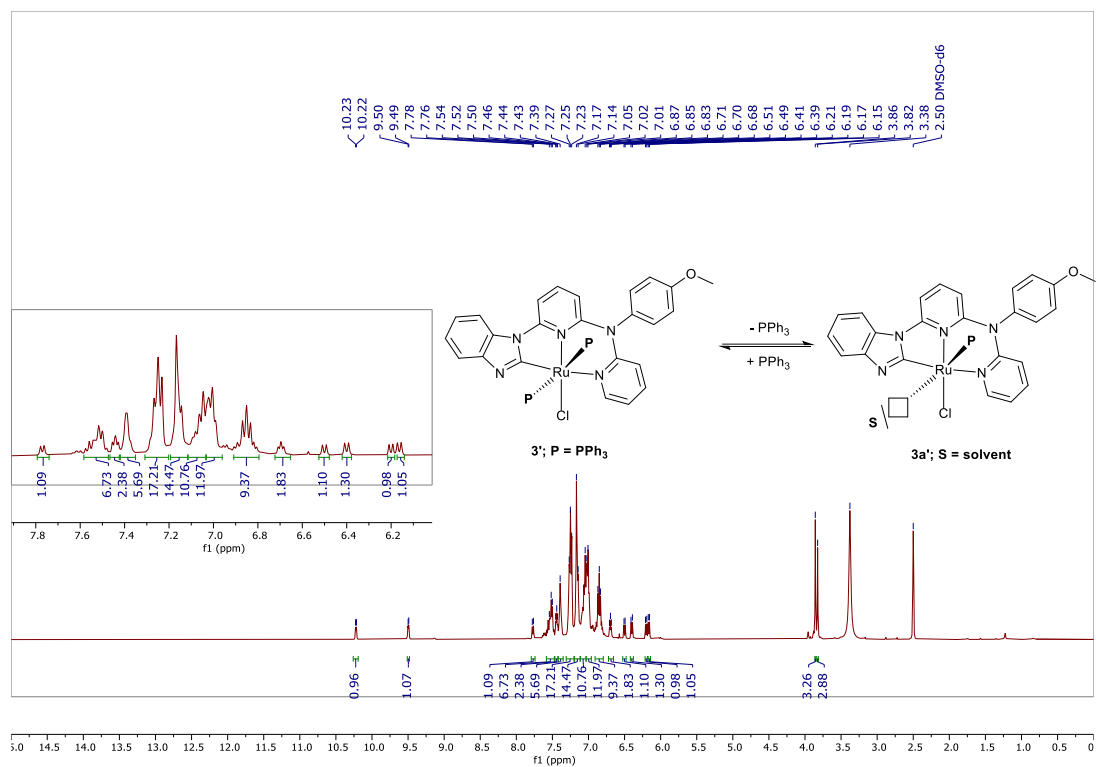
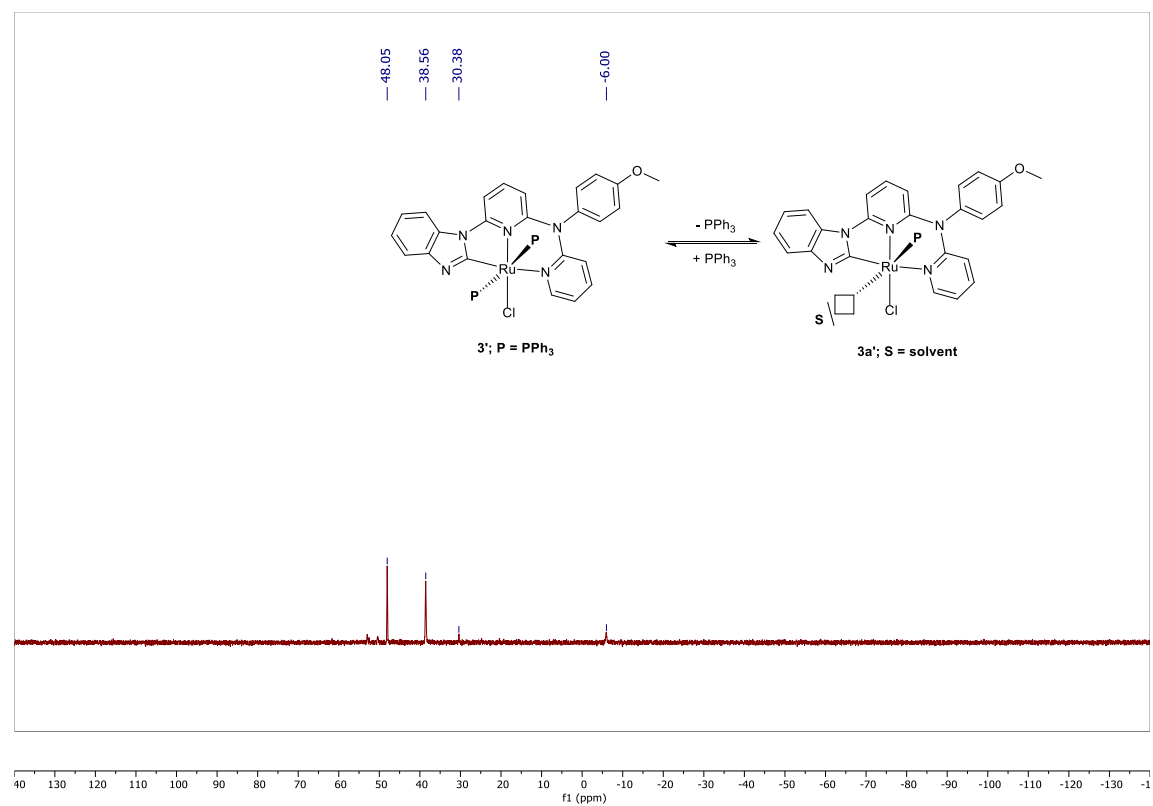


Figure S9. HRMS of 3.



**Figure S10.  $^1\text{H}$  NMR spectrum of  $\mathbf{3}'$  in  $\text{DMSO-d}_6$ .**



**Figure S11.  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum of  $\mathbf{3}'$  in  $\text{DMSO-d}_6$ .**

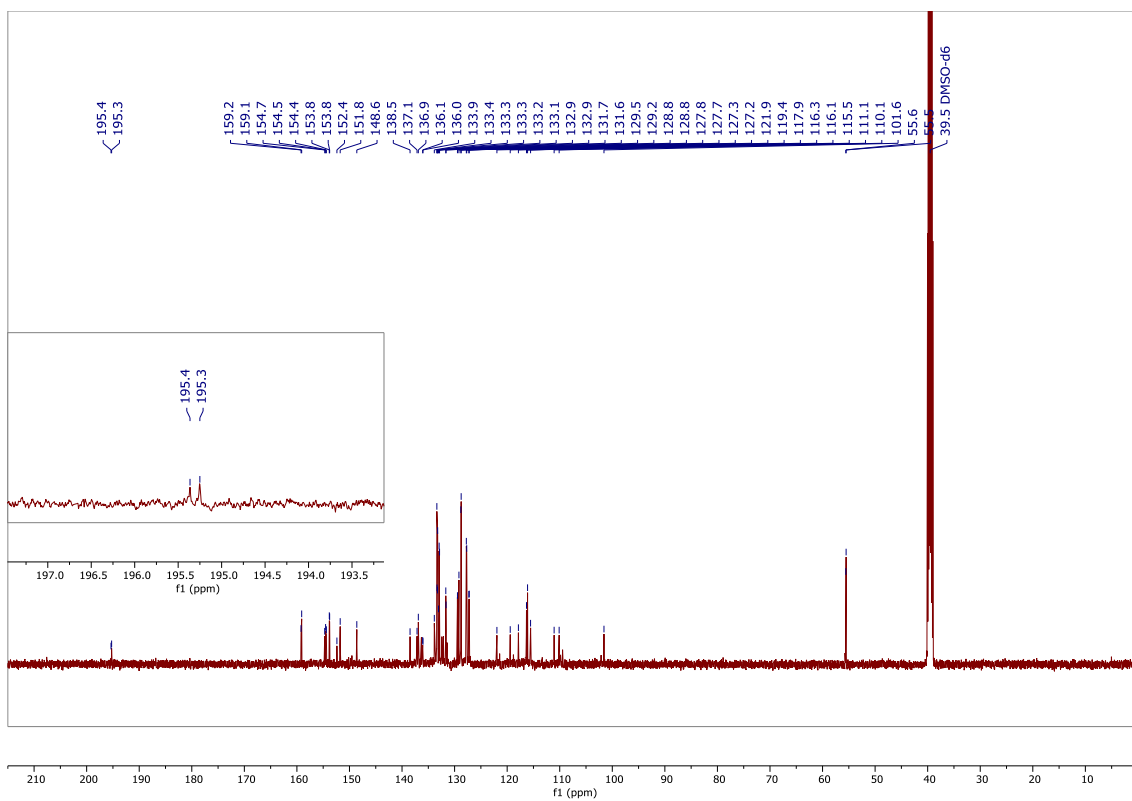


Figure S12.  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **3'** in  $\text{DMSO-d}_6$ .

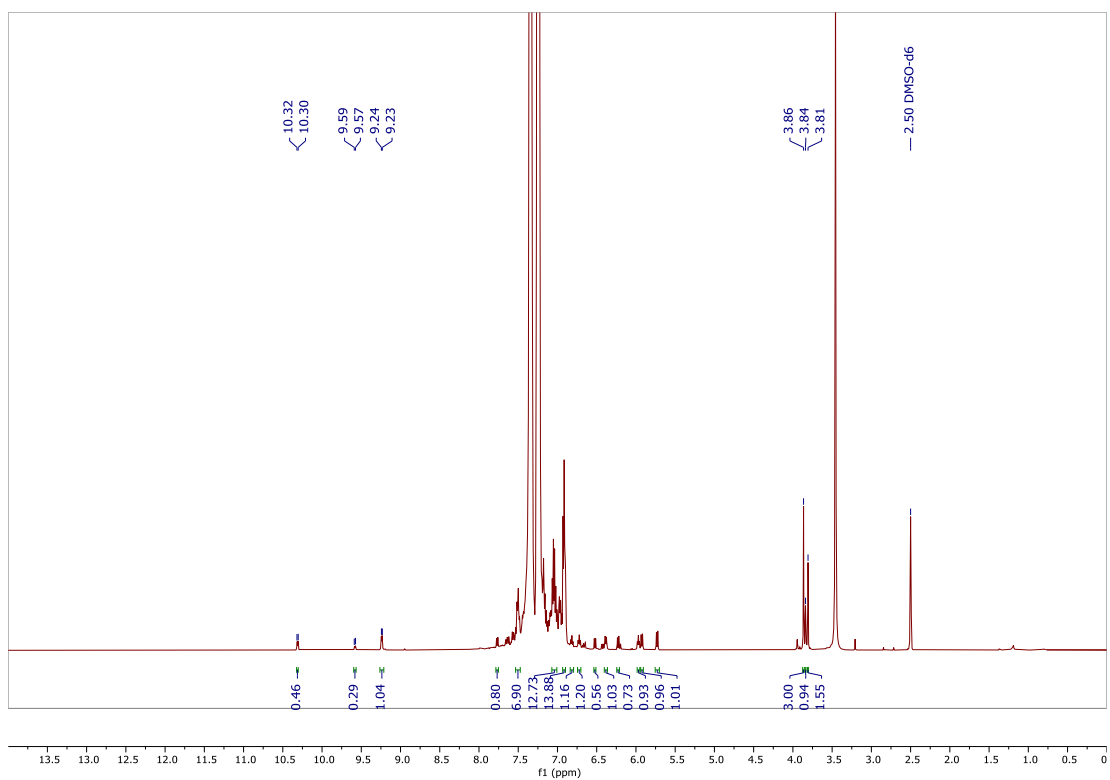
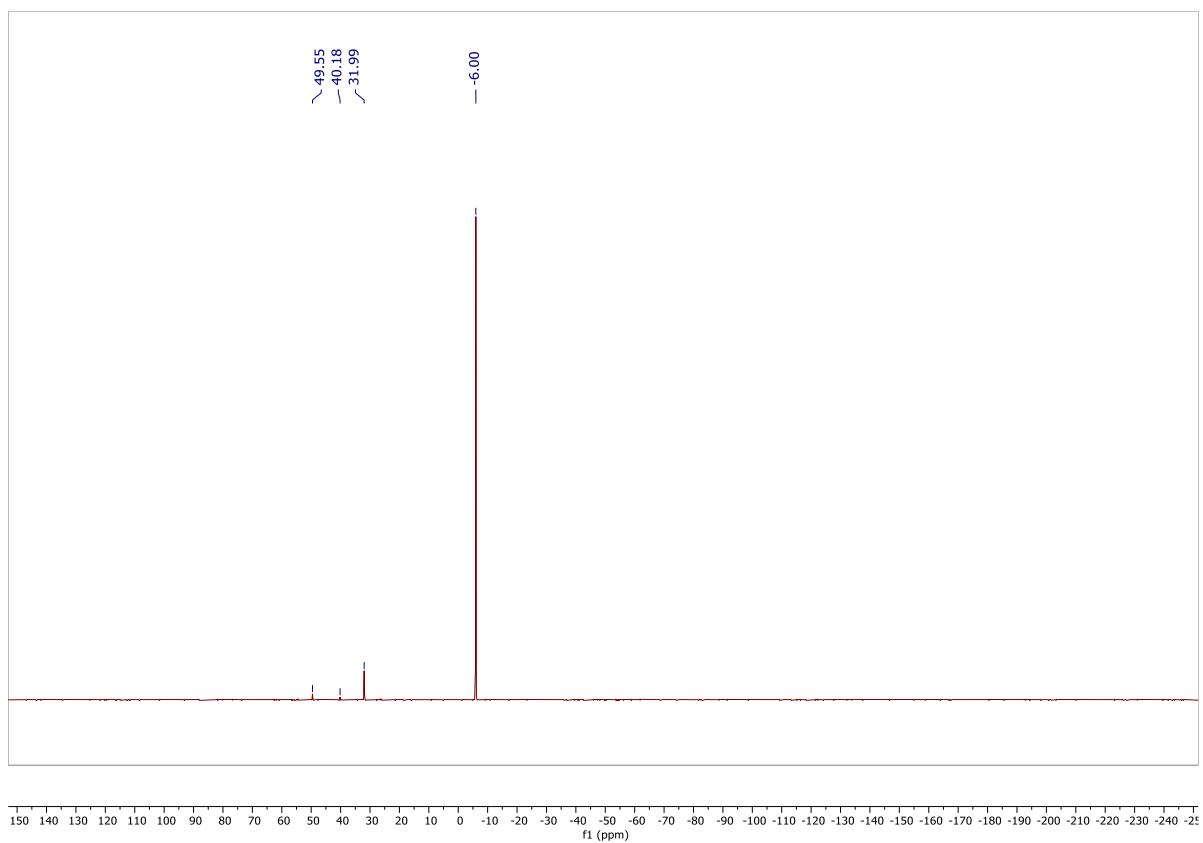


Figure S13.  $^1\text{H}$  NMR spectrum of **3'** after adding 10 equiv. of  $\text{PPh}_3$ .



**Figure S14.**  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum of **3'** after adding 10 equiv. of  $\text{PPh}_3$ .

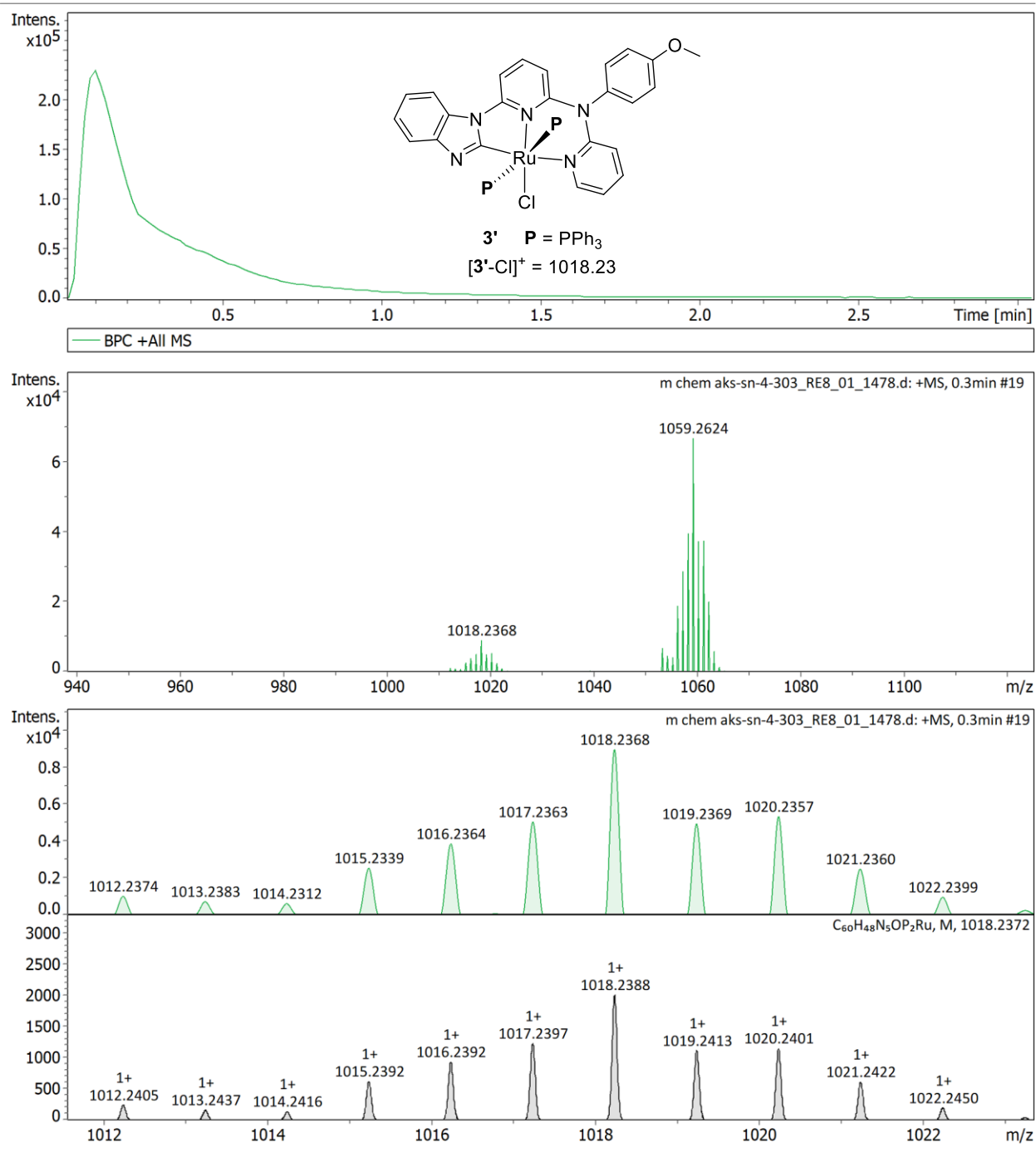


Figure S15. HRMS of 3'.

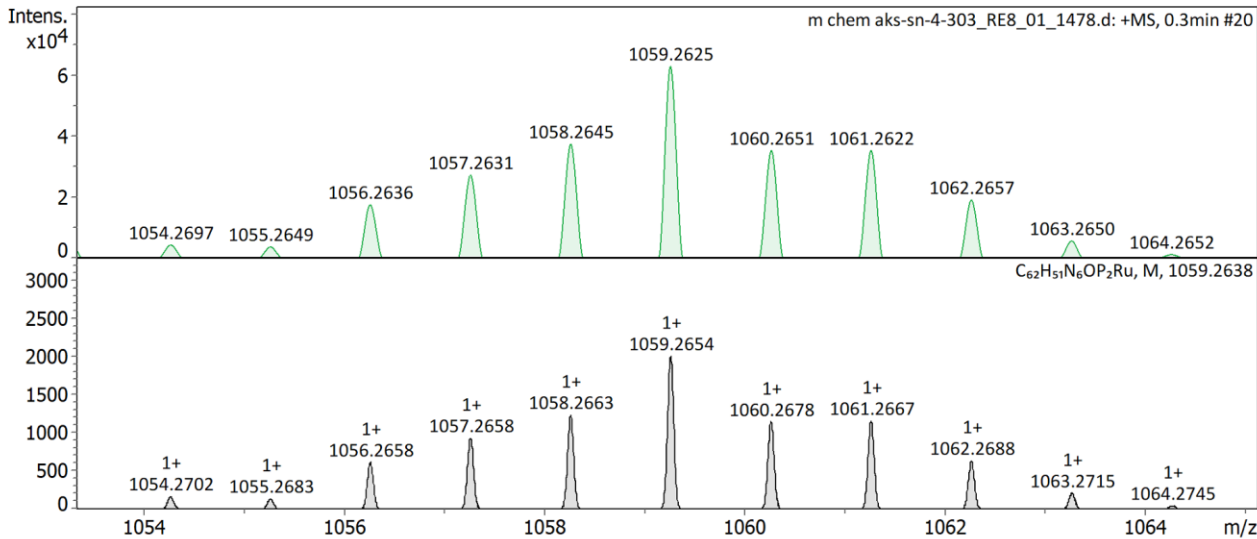
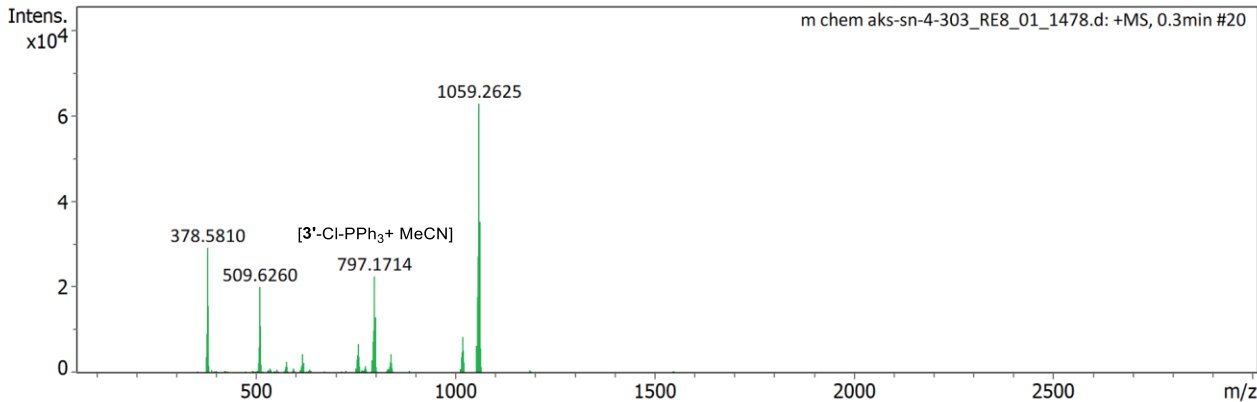
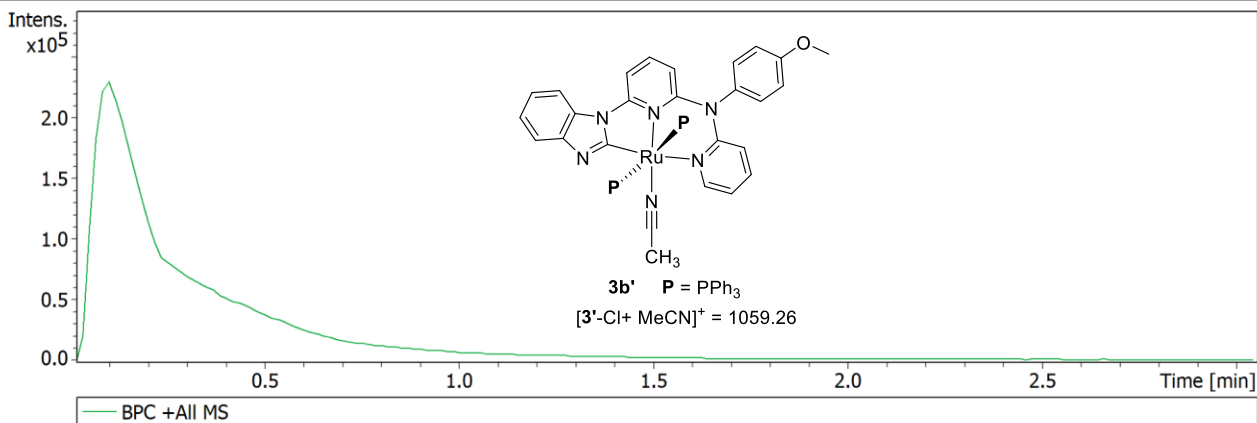
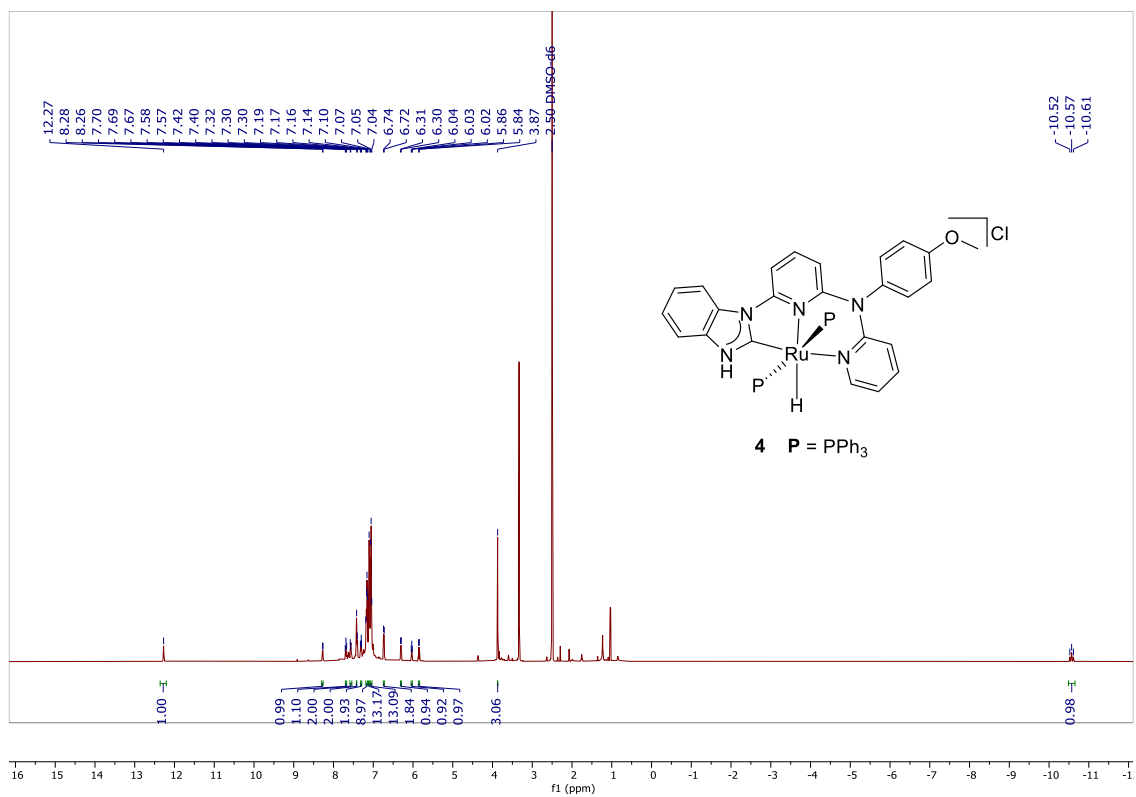
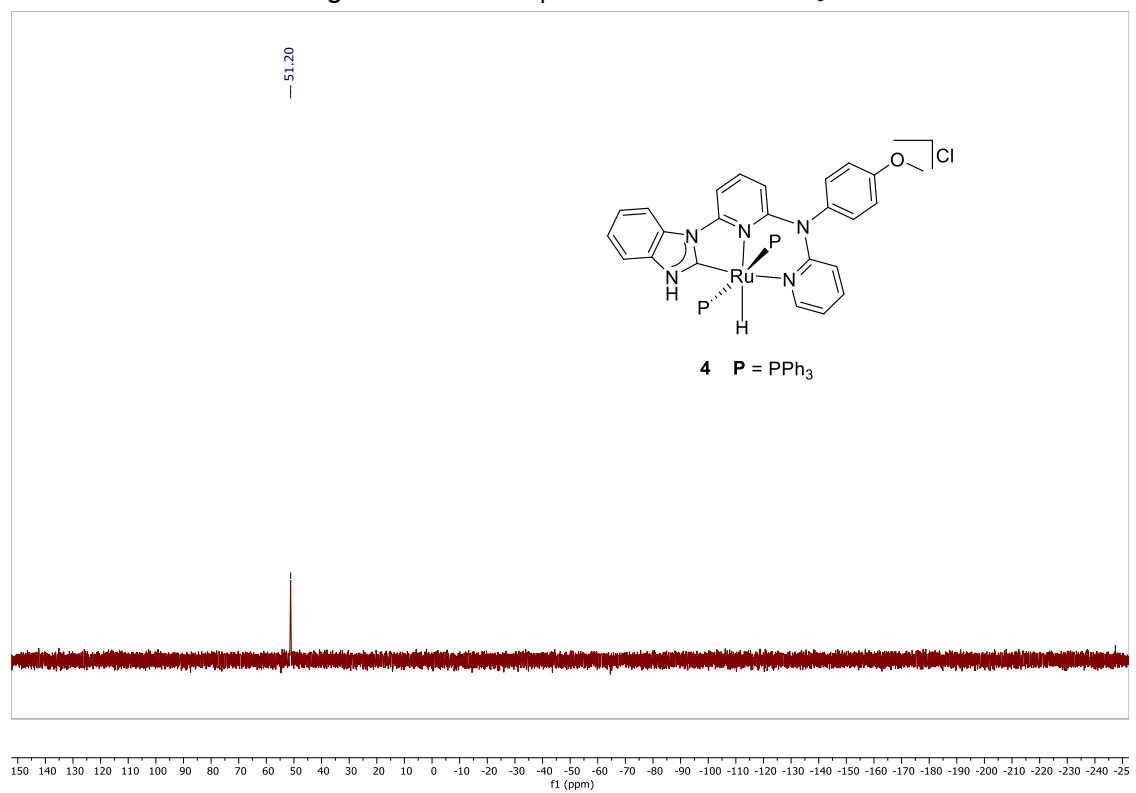


Figure S16. HRMS of 3b'.





**Figure S17.**  $^1\text{H}$  NMR spectrum of **4** in  $\text{DMSO-d}_6$ .



**Figure S18.**  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum of **4** in  $\text{DMSO-d}_6$ .

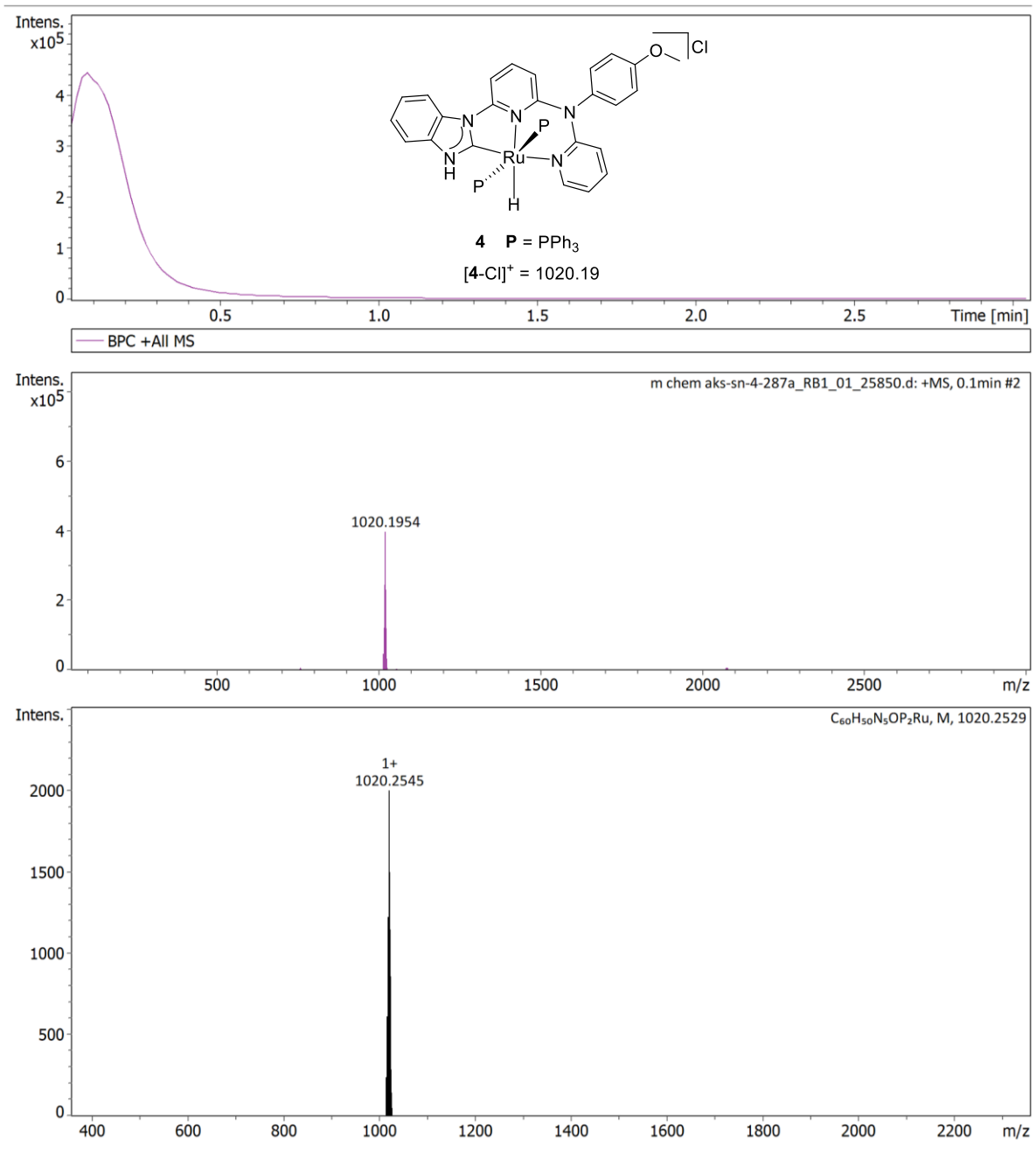


Figure S19 LCMS of 4.

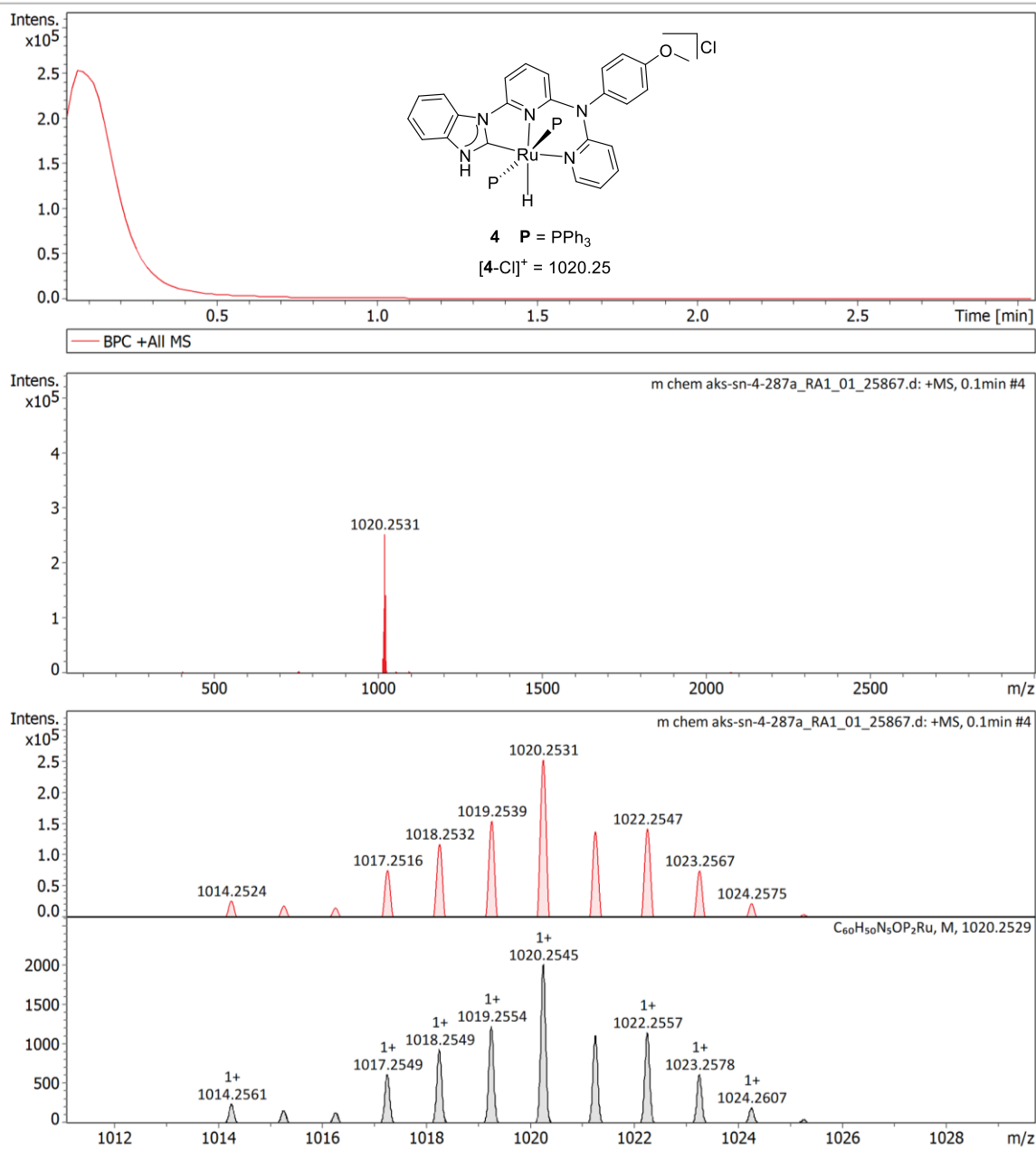


Figure S20. HRMS of 4.

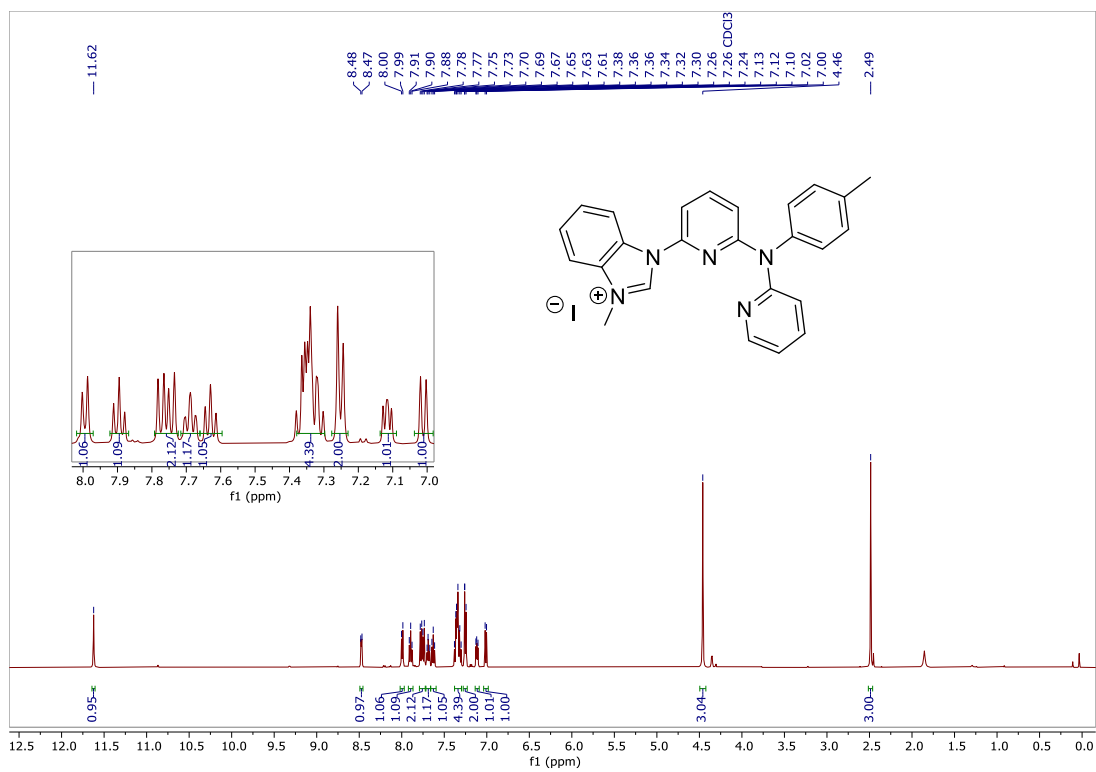


Figure S21.  $^1\text{H}$  NMR spectrum of  $\text{NN}^{\text{Me}}\text{C}^{\text{Me}}\cdot\text{HI}$  in  $\text{CDCl}_3$ .

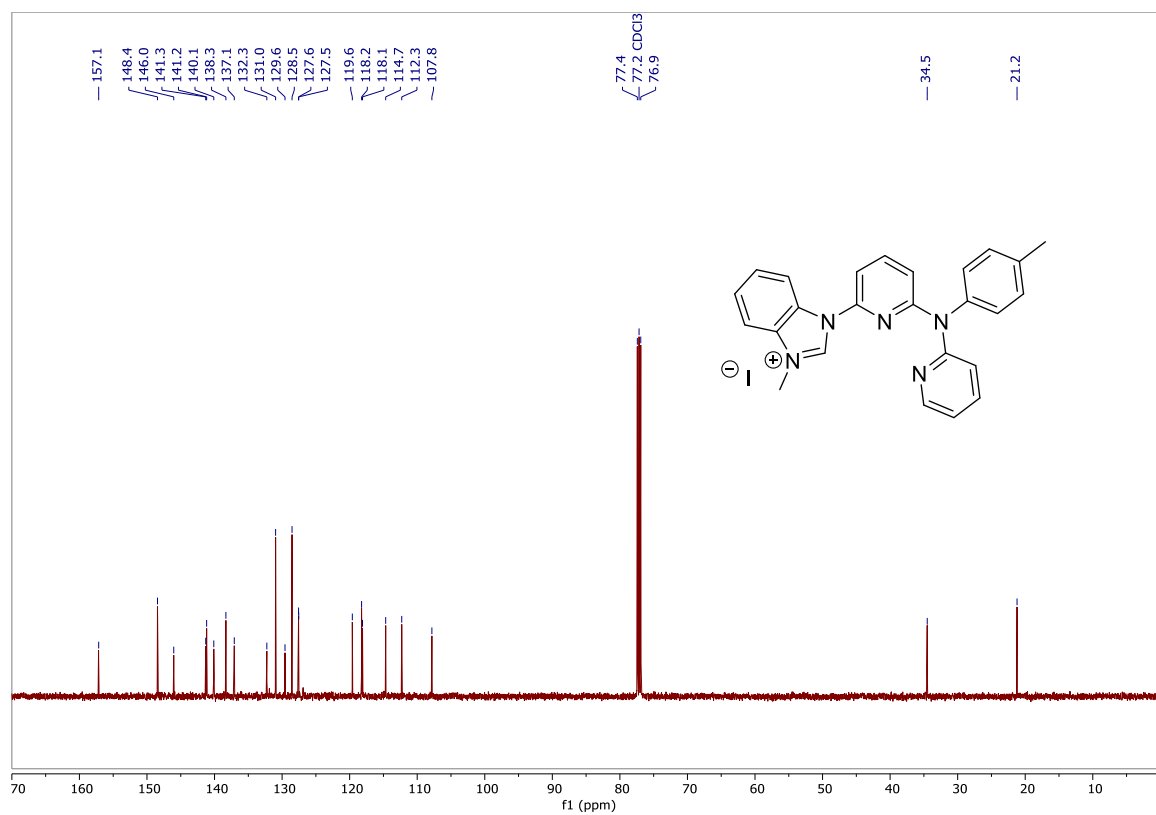


Figure S22.  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of ligand  $\text{NN}^{\text{Me}}\text{C}^{\text{Me}}\cdot\text{HI}$  in  $\text{CDCl}_3$ .

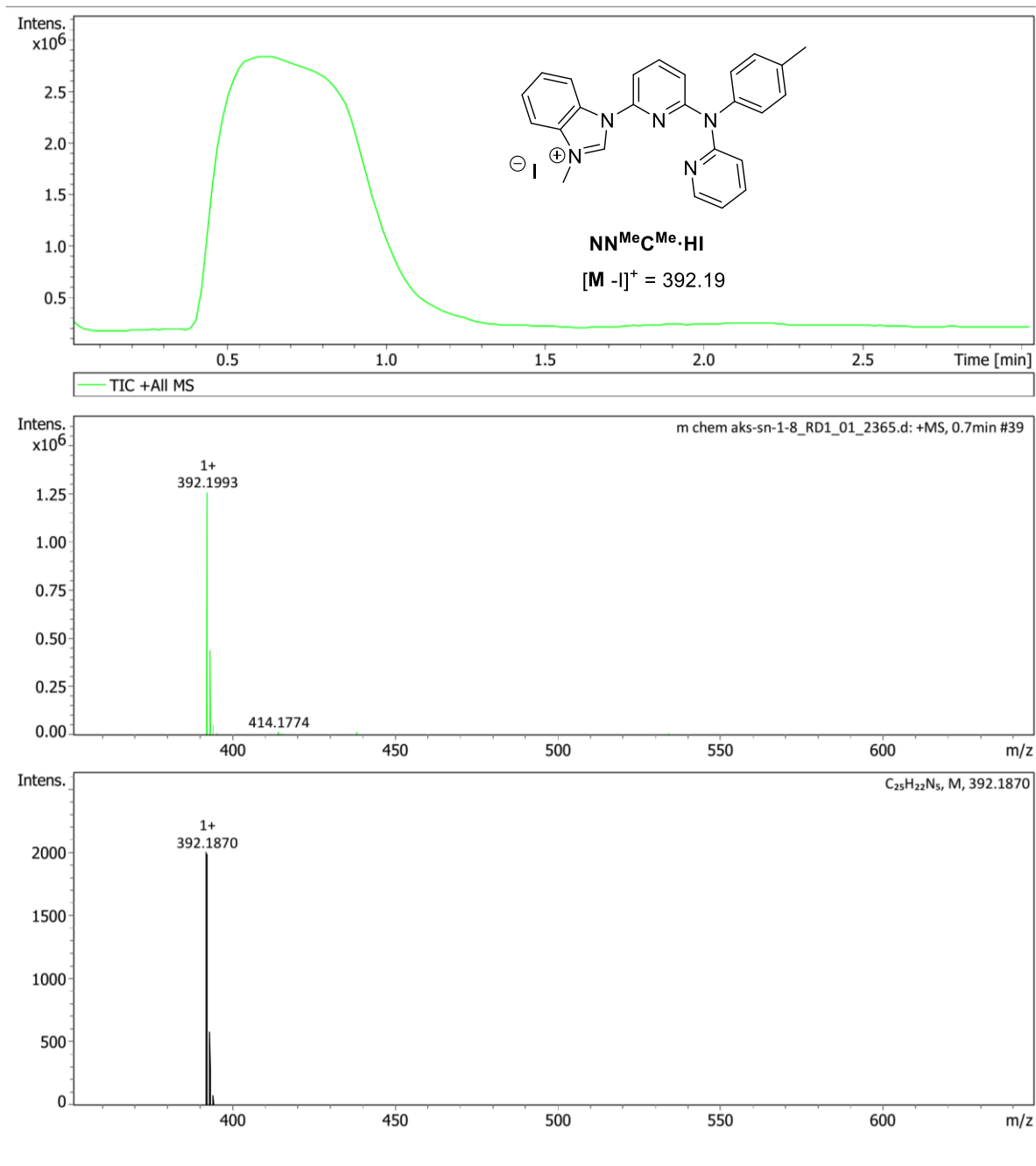


Figure S23. LC-MS of NN<sup>Me</sup>C<sup>Me</sup>.HI.

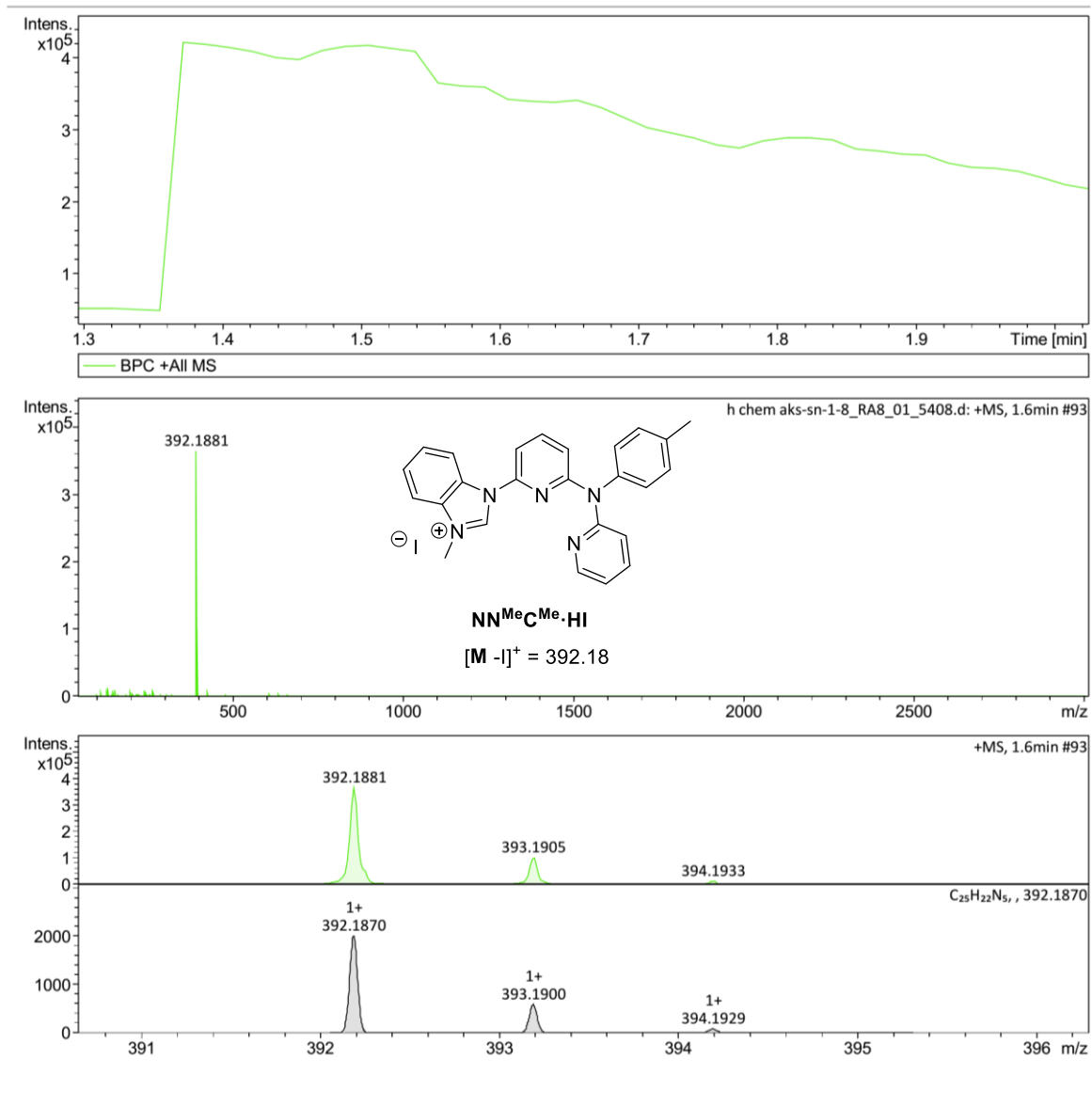


Figure S24. HRMS of NN<sup>Me</sup>C<sup>Me</sup>.HI.

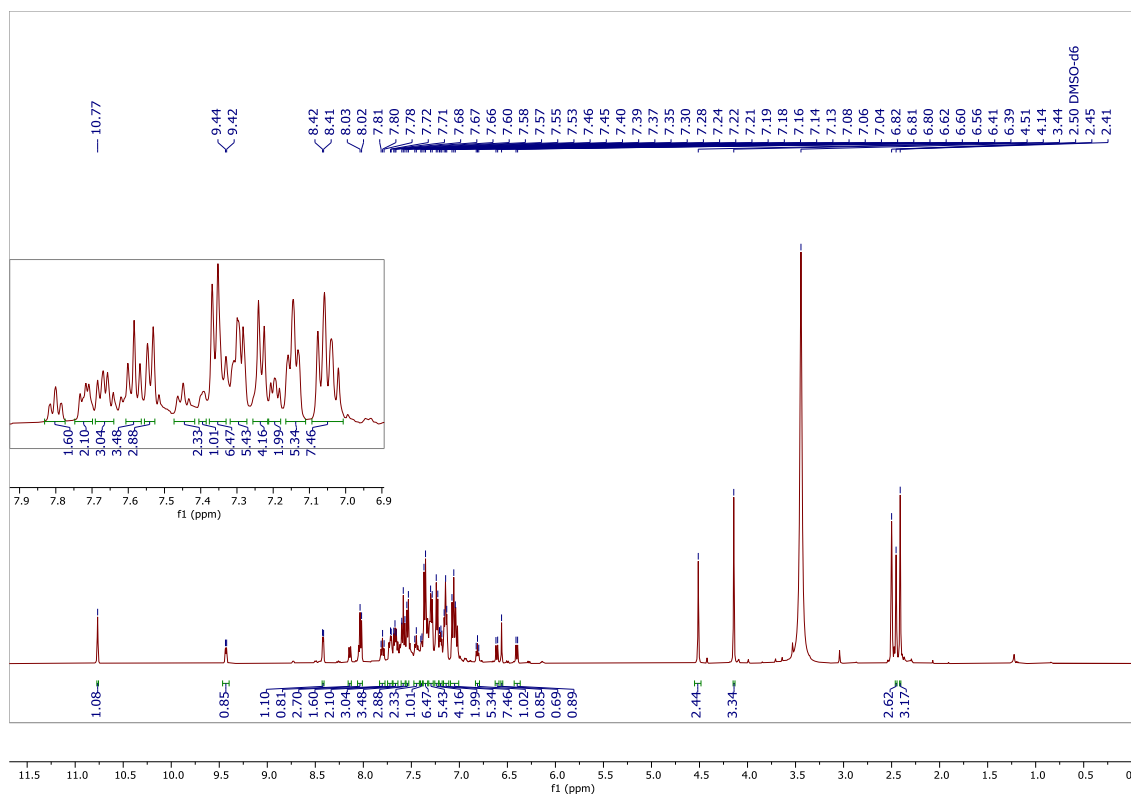


Figure S25.  $^1\text{H}$  NMR spectrum of **5** in  $\text{DMSO-d}_6$ .

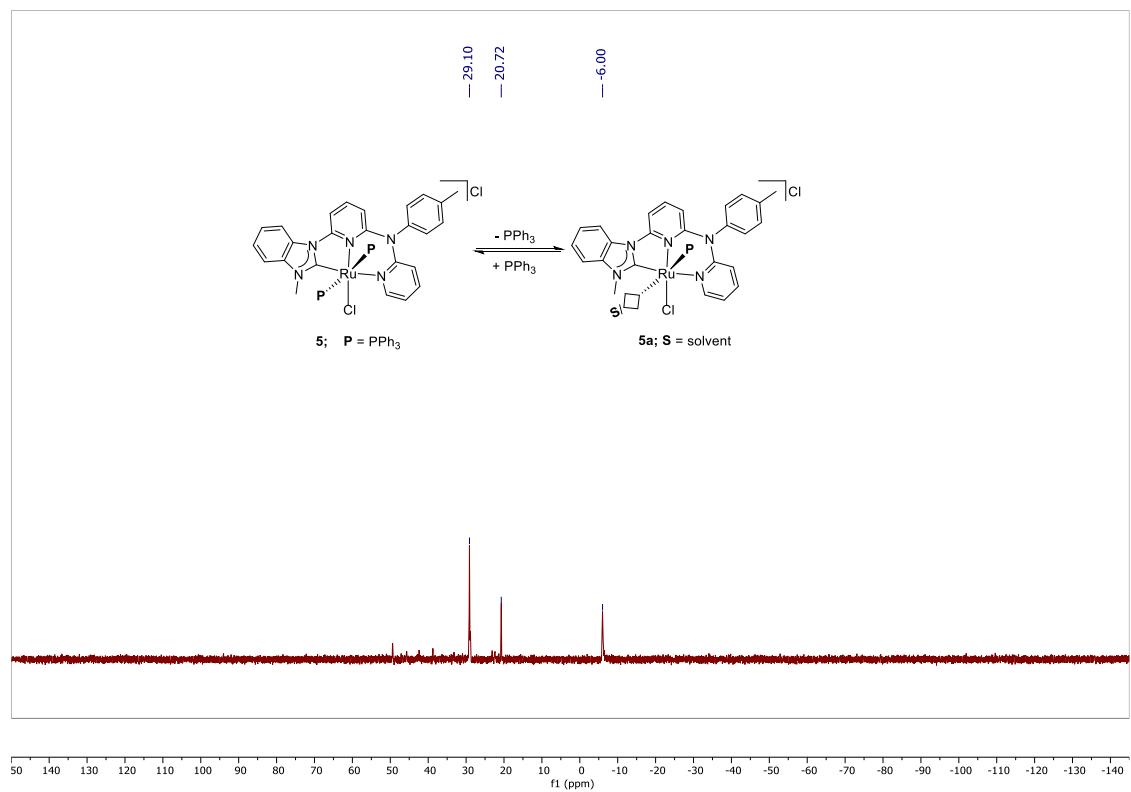


Figure S26.  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum of **5** in  $\text{DMSO-d}_6$ .

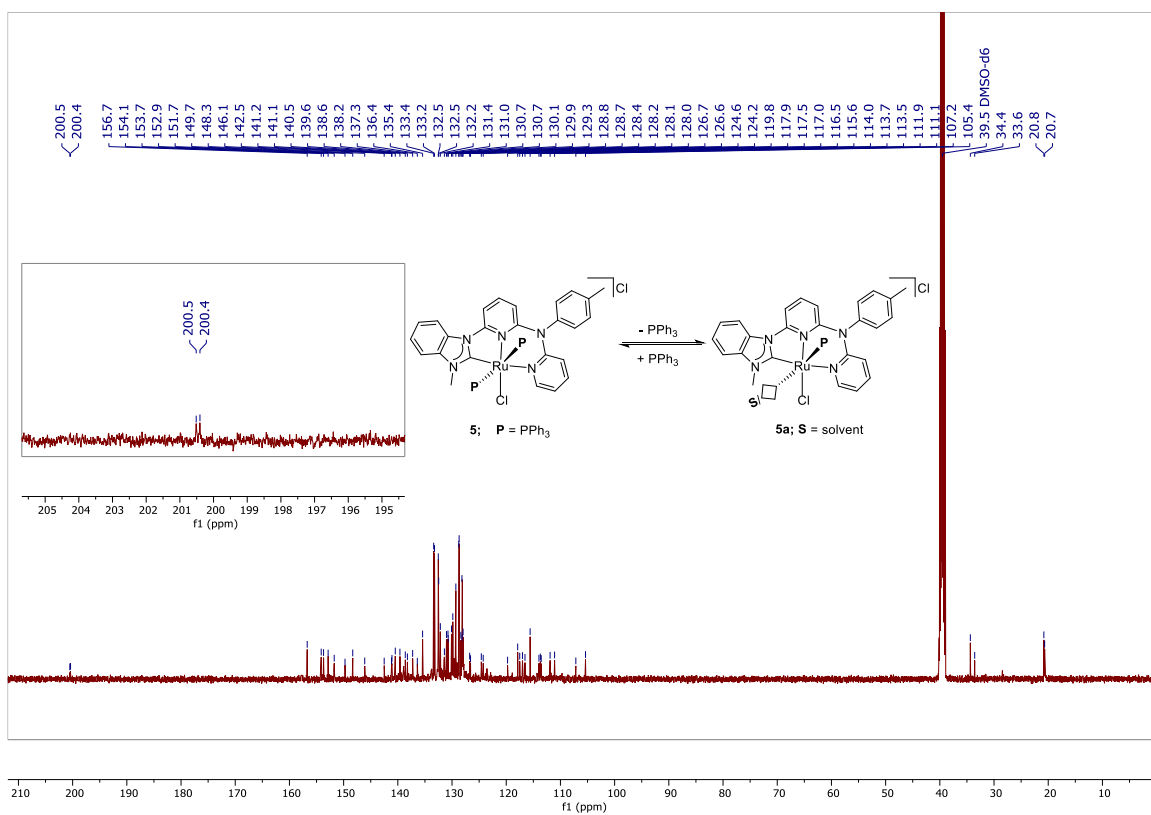
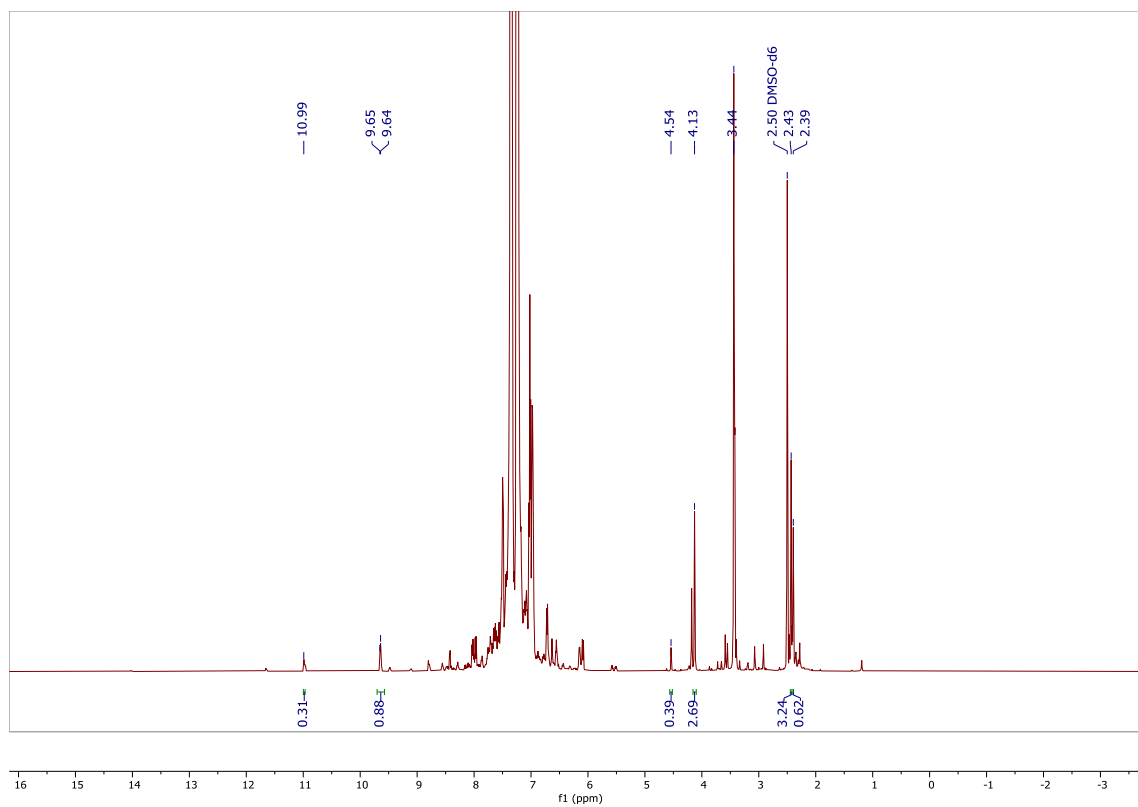
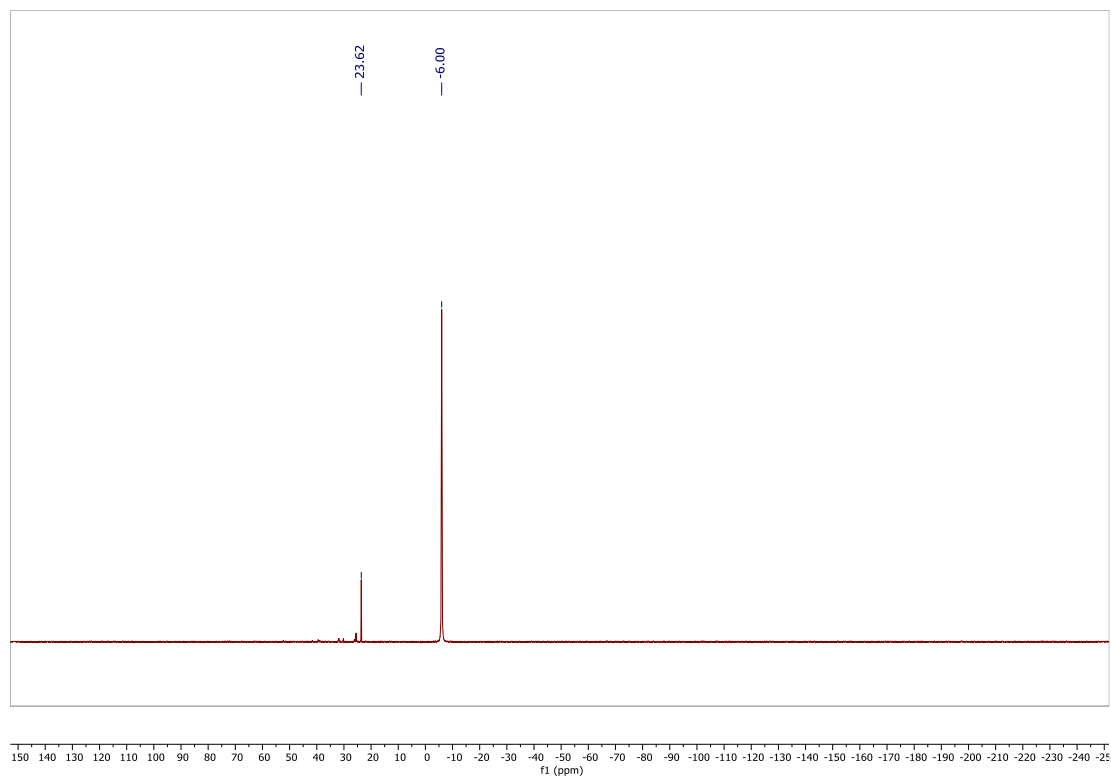


Figure S27.  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **5** in DMSO- $\text{d}_6$ .

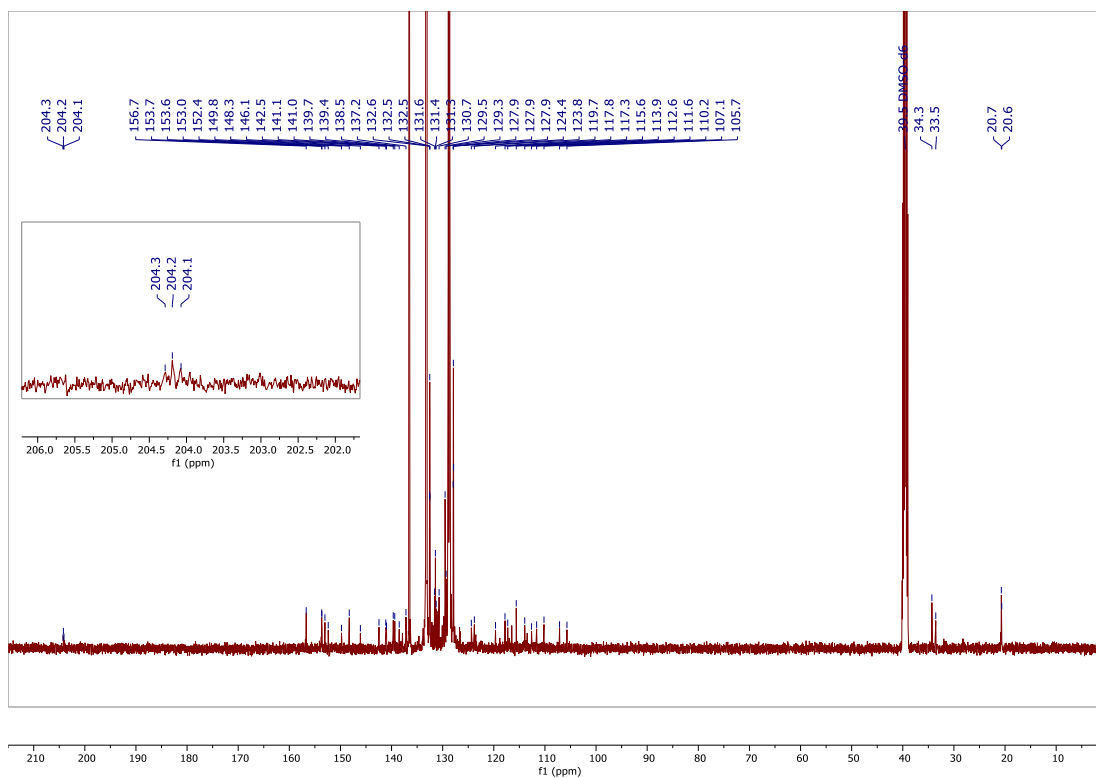




**Figure S28.**  $^1\text{H}$  NMR spectrum of **5** after adding 10 equiv. of  $\text{PPh}_3$  in  $\text{DMSO-d}_6$ .



**Figure S29.**  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum of **5** after adding 10 equiv. of  $\text{PPh}_3$  in  $\text{DMSO-d}_6$ .



**Figure S30.**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **5** after adding 10 equiv. of  $\text{PPh}_3$  in  $\text{DMSO-d}_6$ .

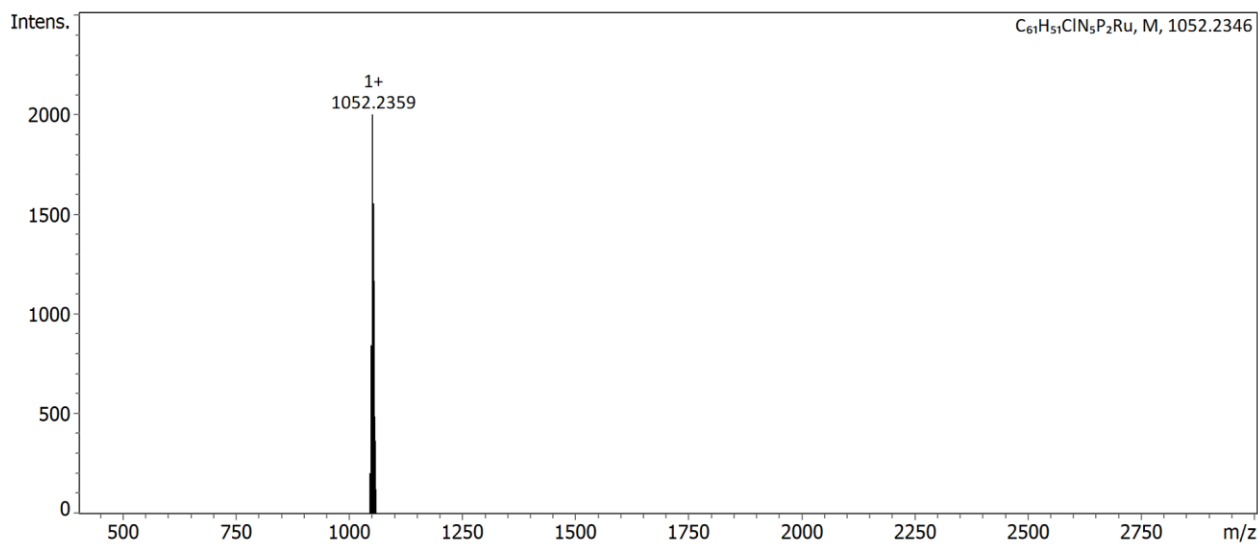
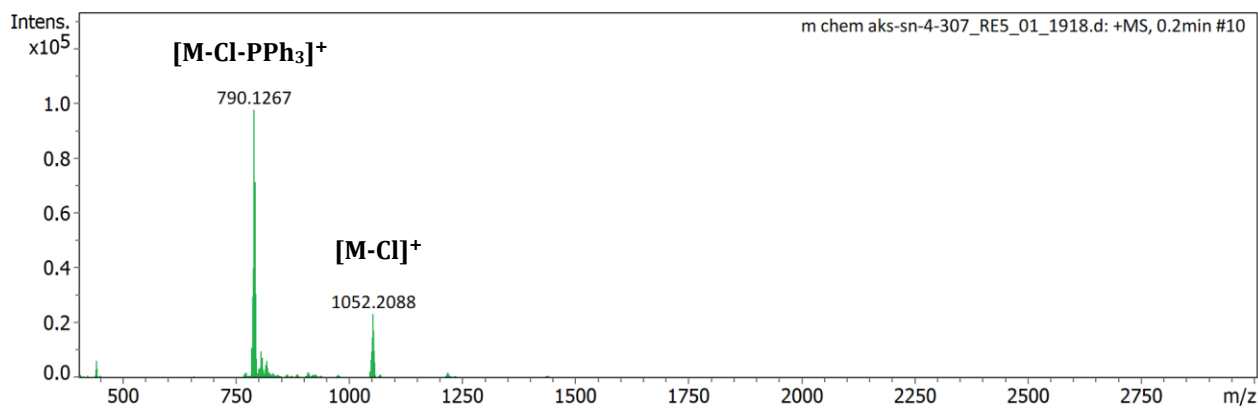
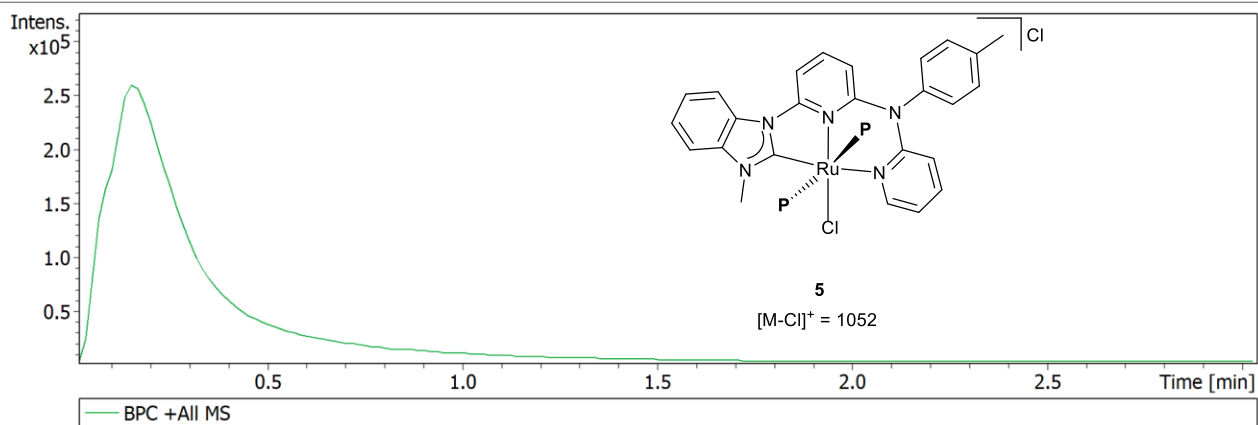


Figure S31. LC-MS of 5.

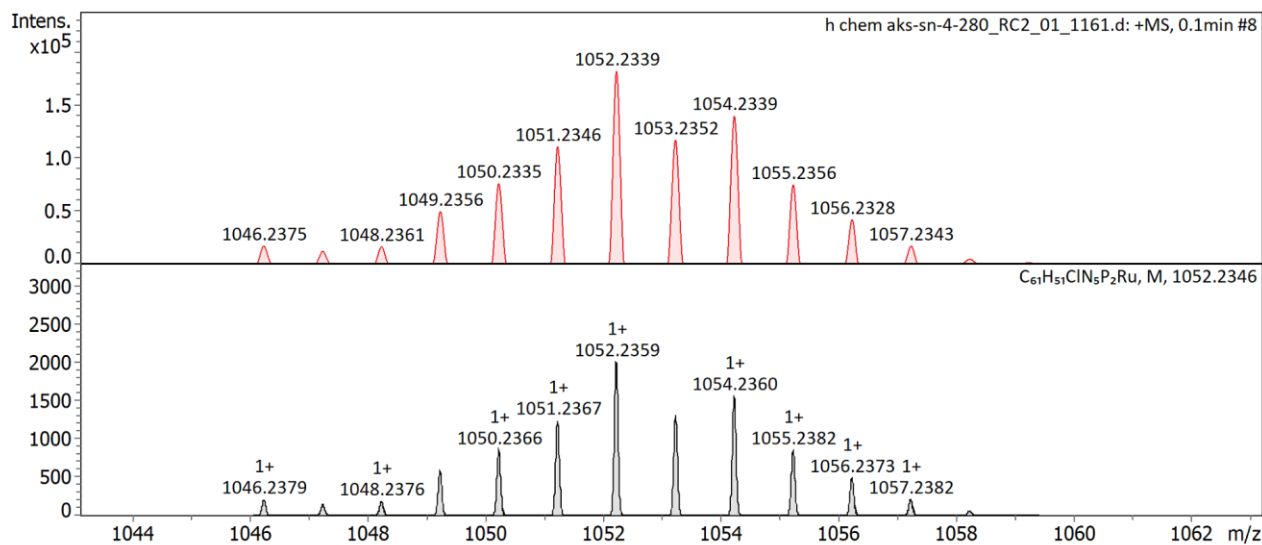
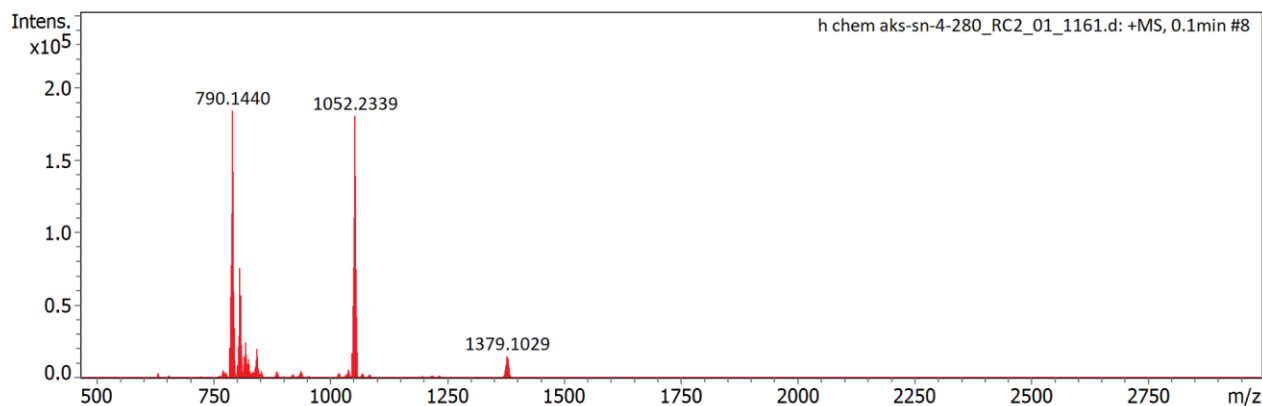
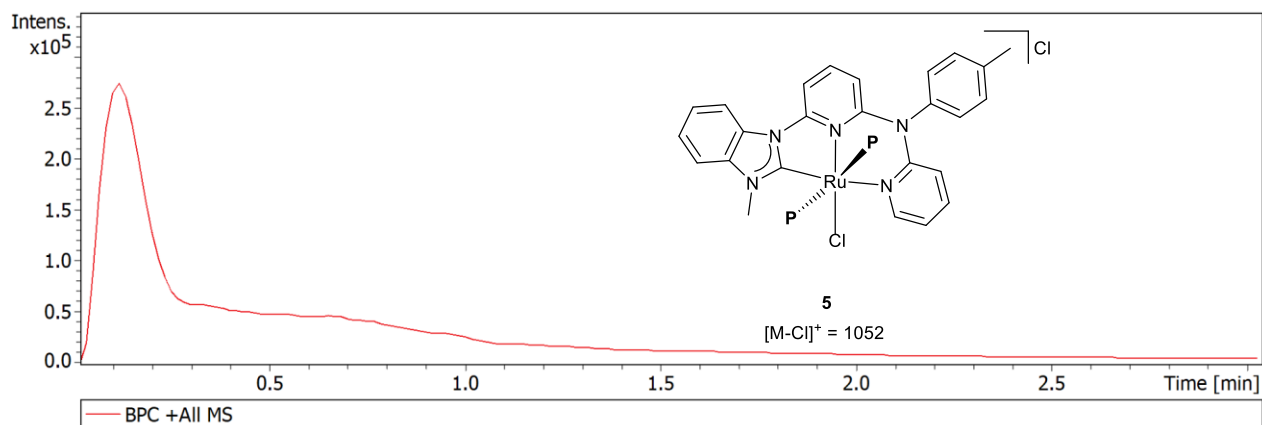
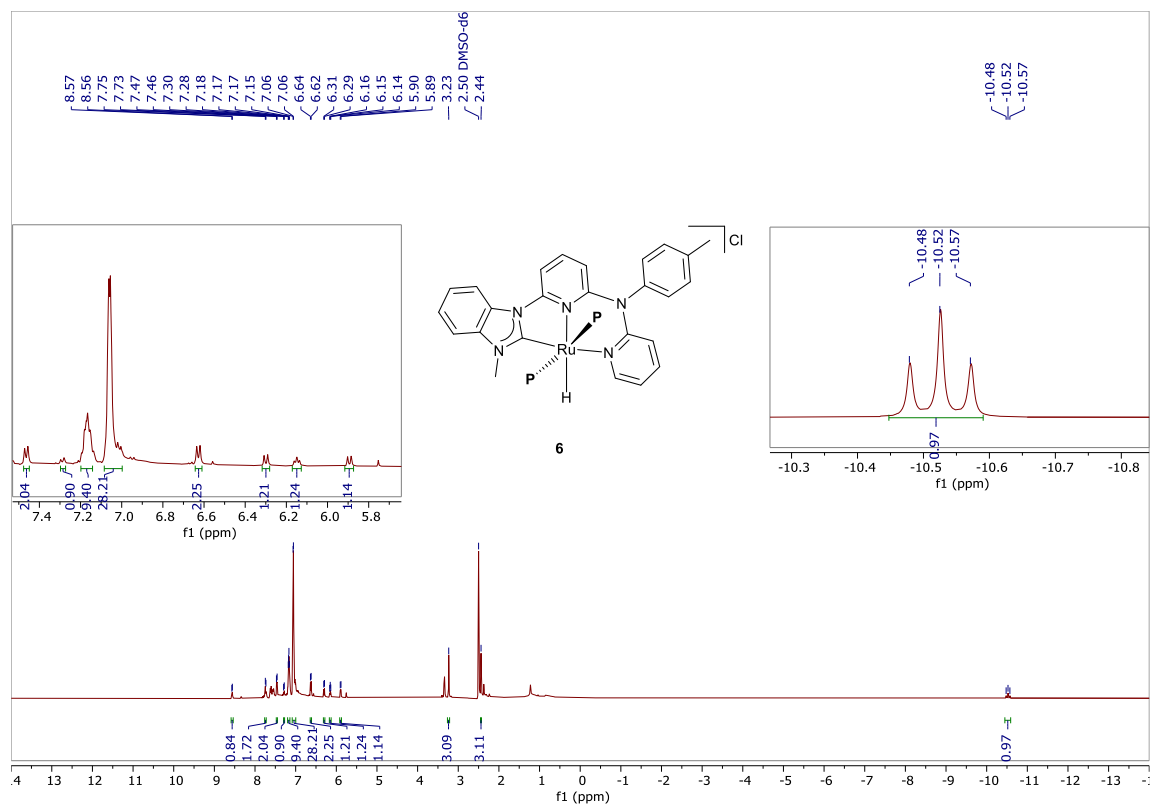
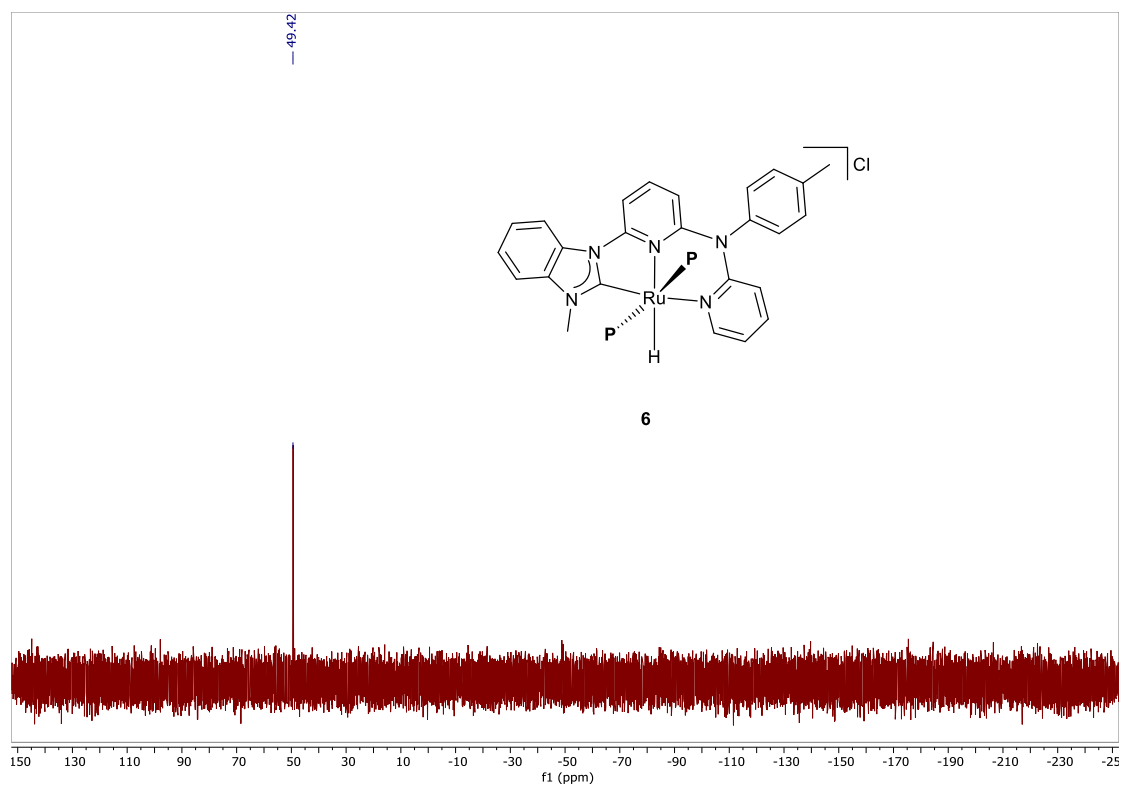


Figure S32. HRMS of 5.



**Figure S33.**  $^1\text{H}$  NMR spectrum of **6** in  $\text{DMSO-d}_6$ .



**Figure S34.**  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum of **6** in  $\text{DMSO-d}_6$ .

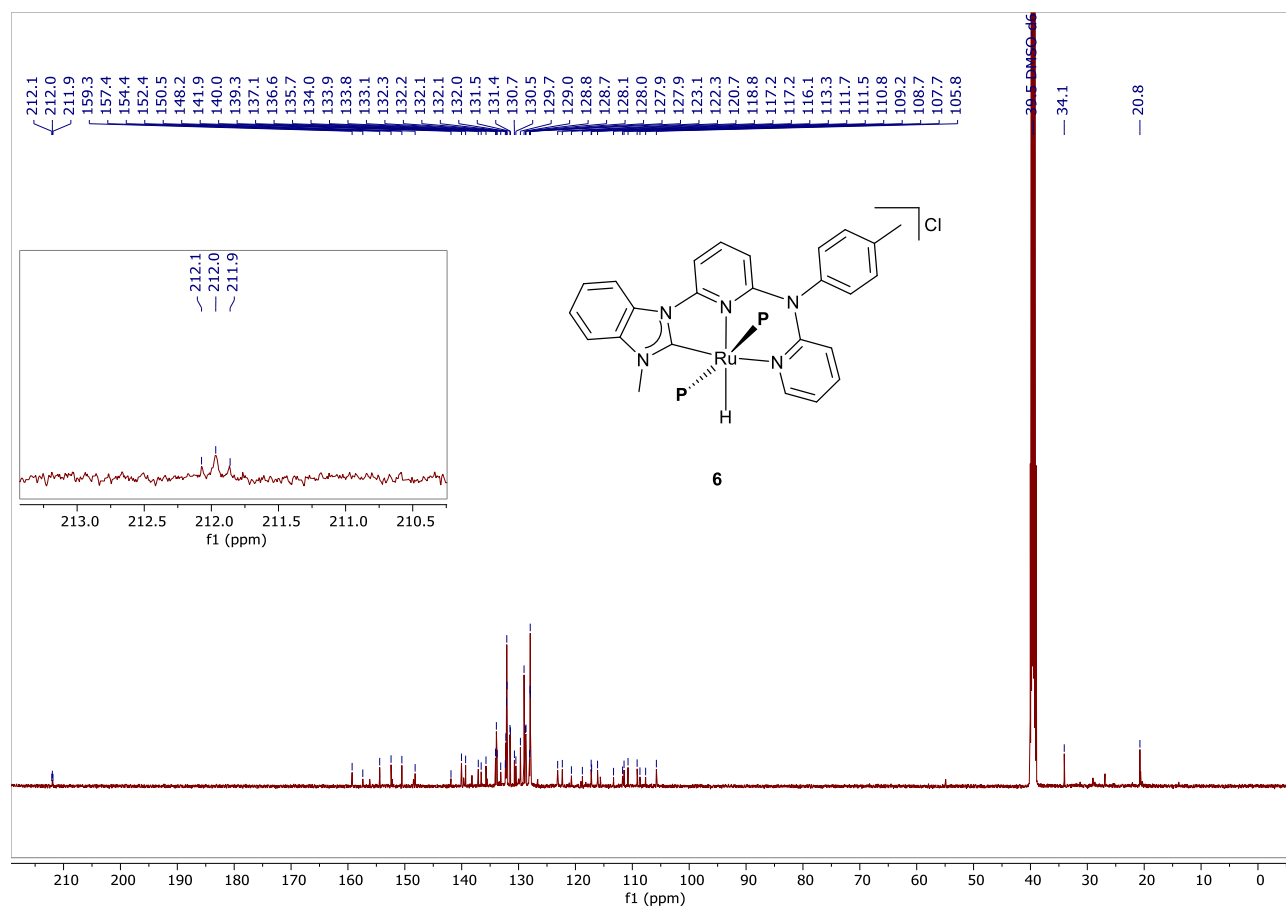


Figure S35.  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of 6 in  $\text{DMSO-d}_6$ .

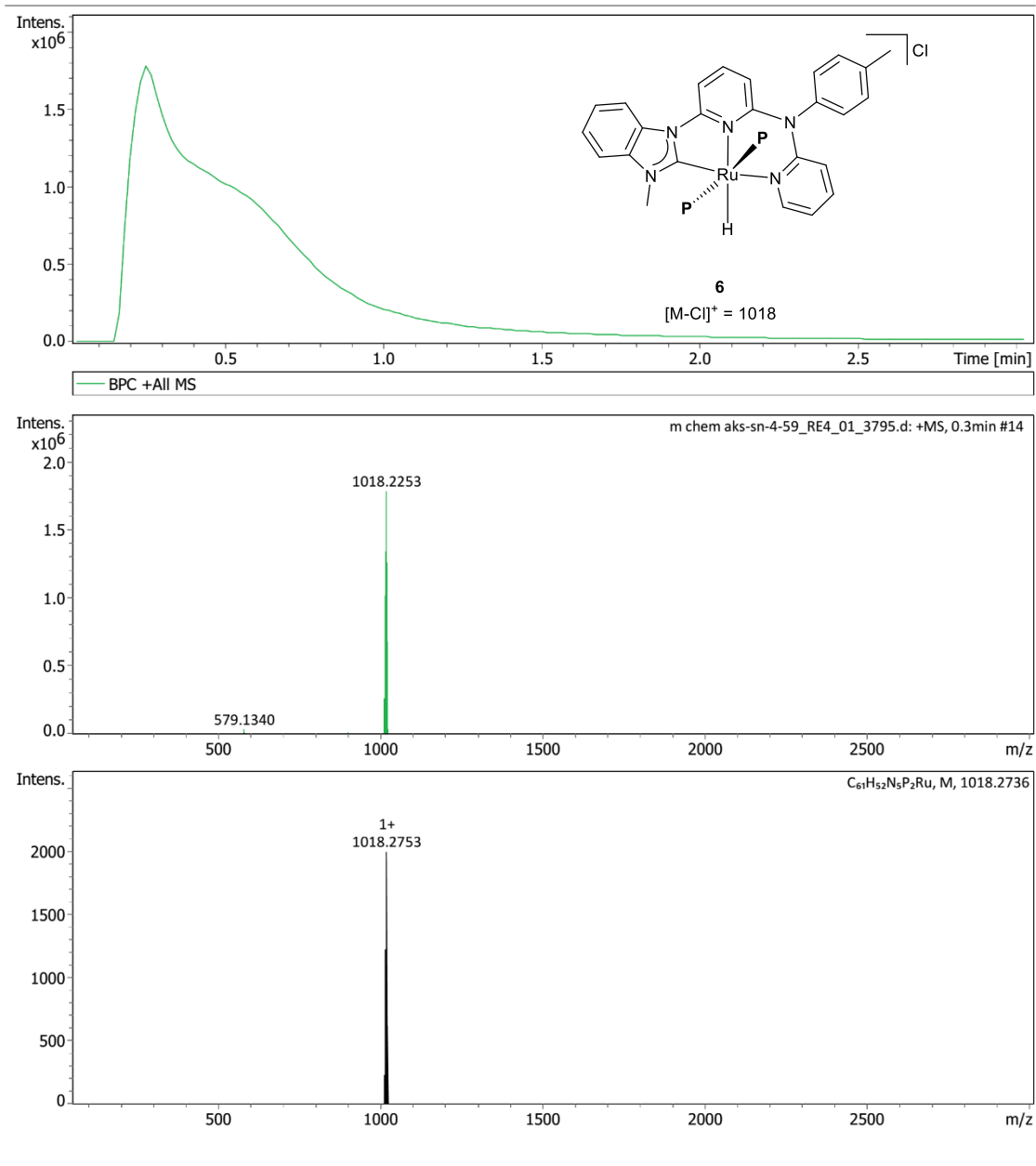


Figure S36. LC-MS of 6.

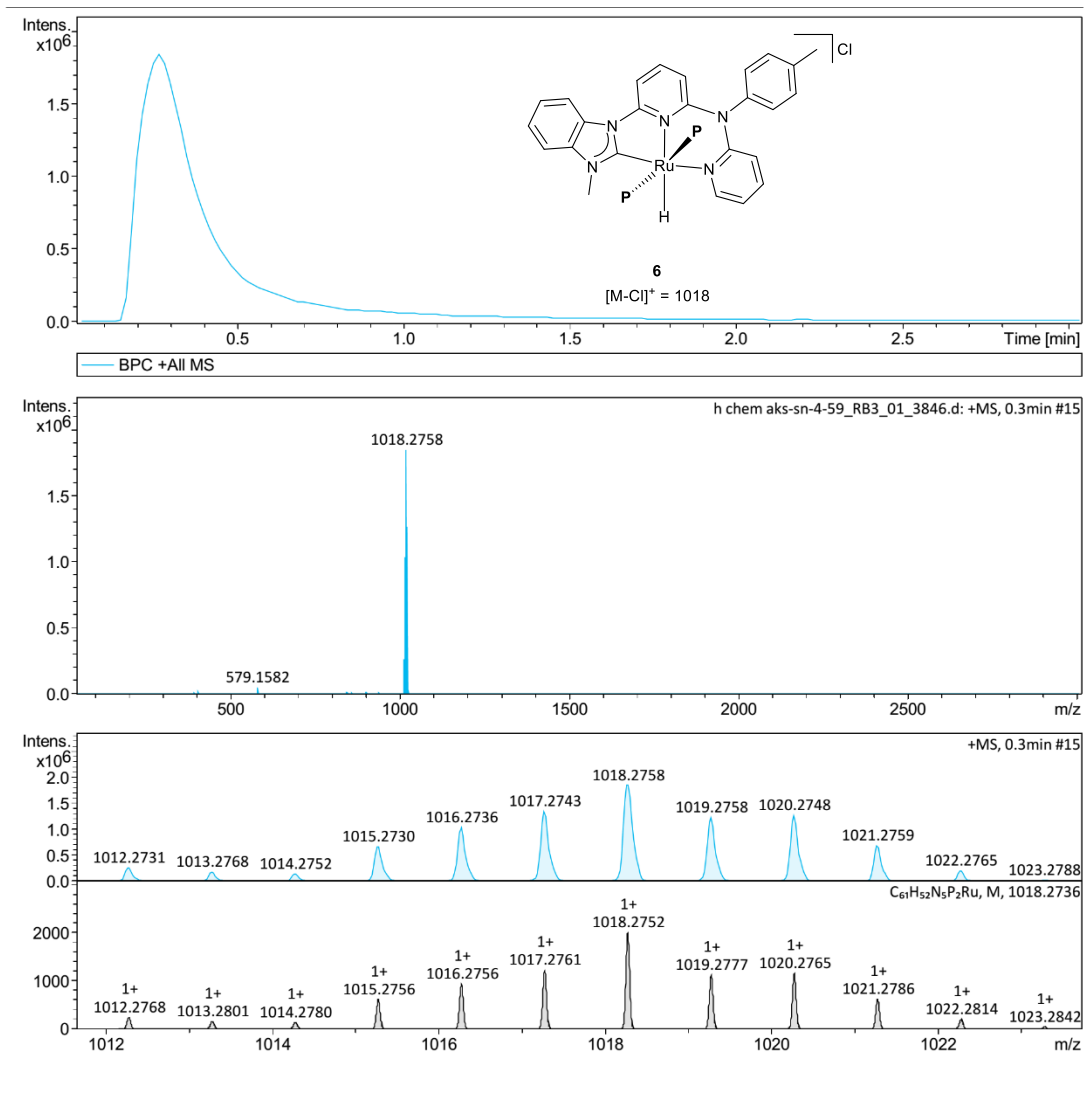
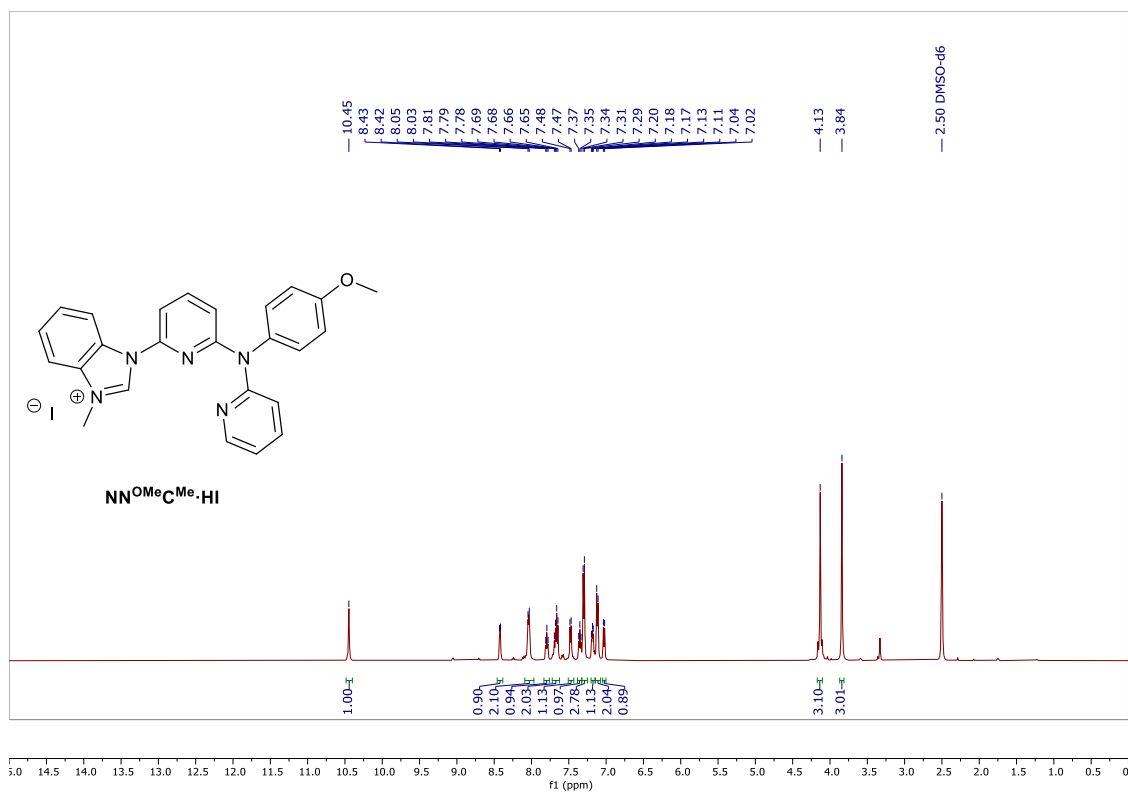
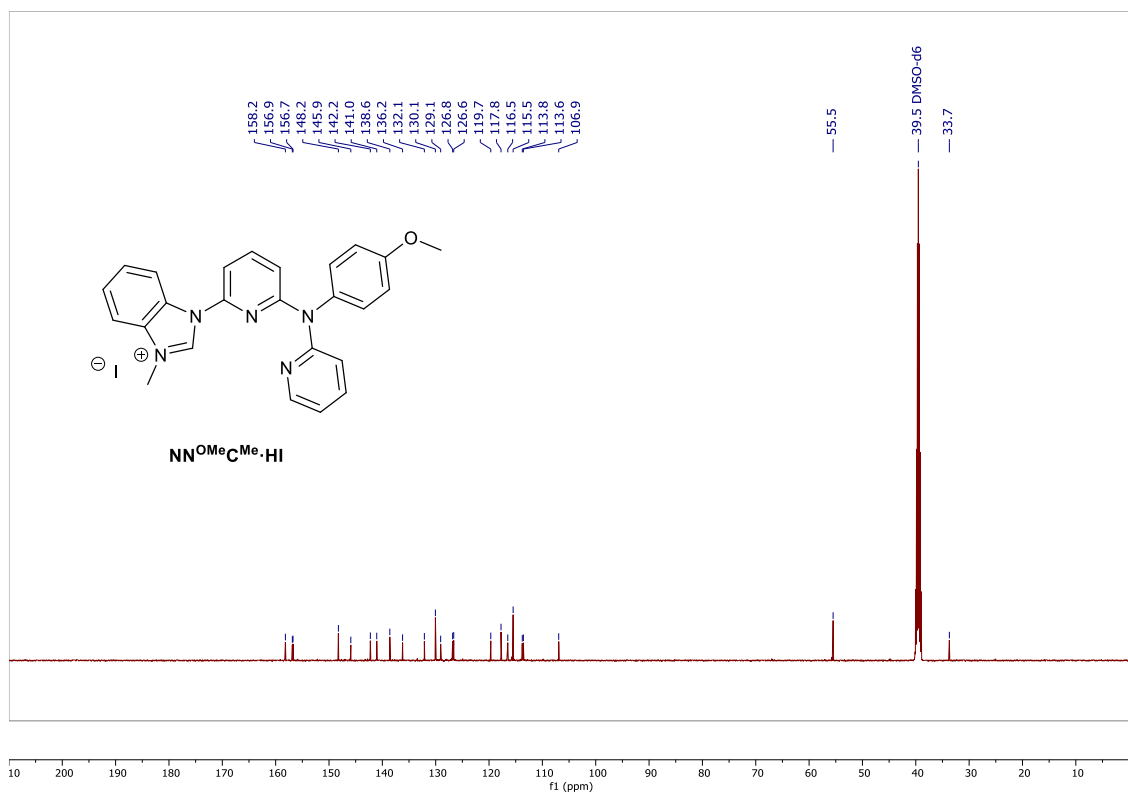


Figure S37. HRMS of 6.





**Figure S38.**  $^1\text{H}$  NMR spectrum of  $\text{NN}^{\text{OMe}}\text{C}^{\text{Me}}\cdot\text{HI}$  in  $\text{DMSO-d}_6$ .



**Figure S39.**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of  $\text{NN}^{\text{OMe}}\text{C}^{\text{Me}}\cdot\text{HI}$  in  $\text{DMSO-d}_6$ .

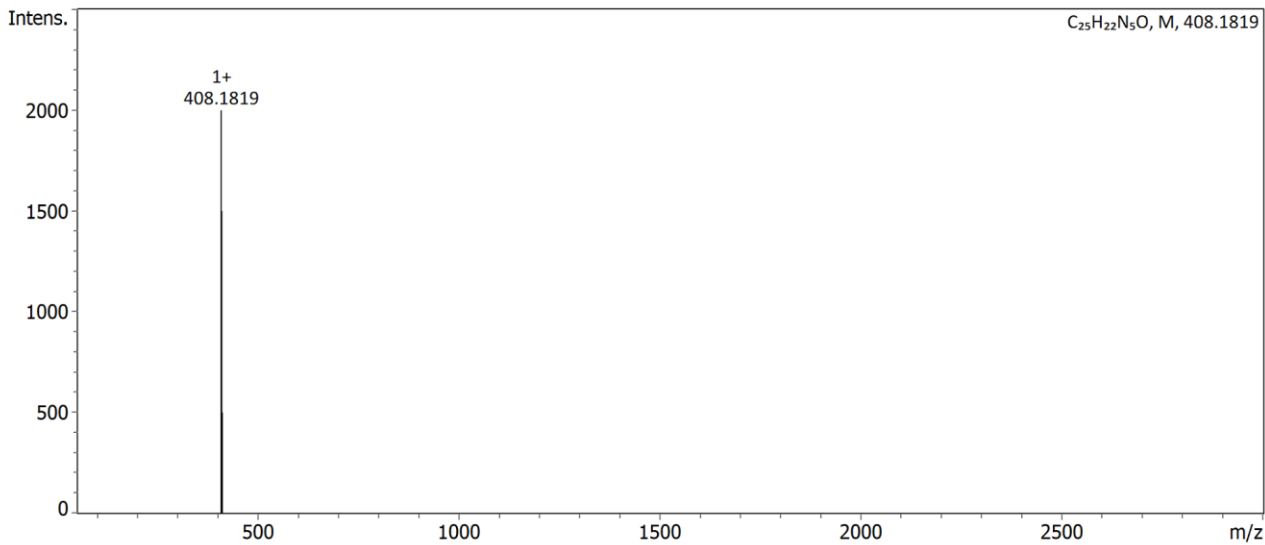
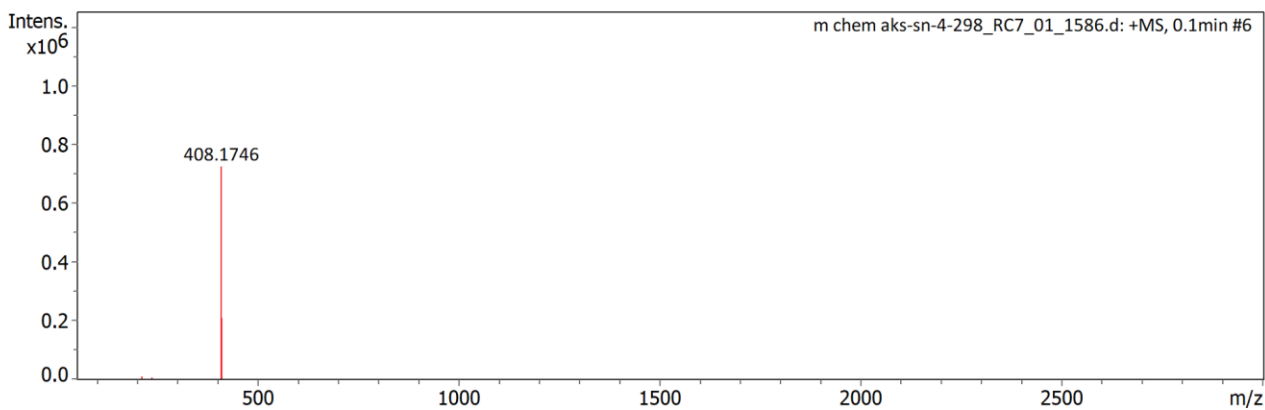
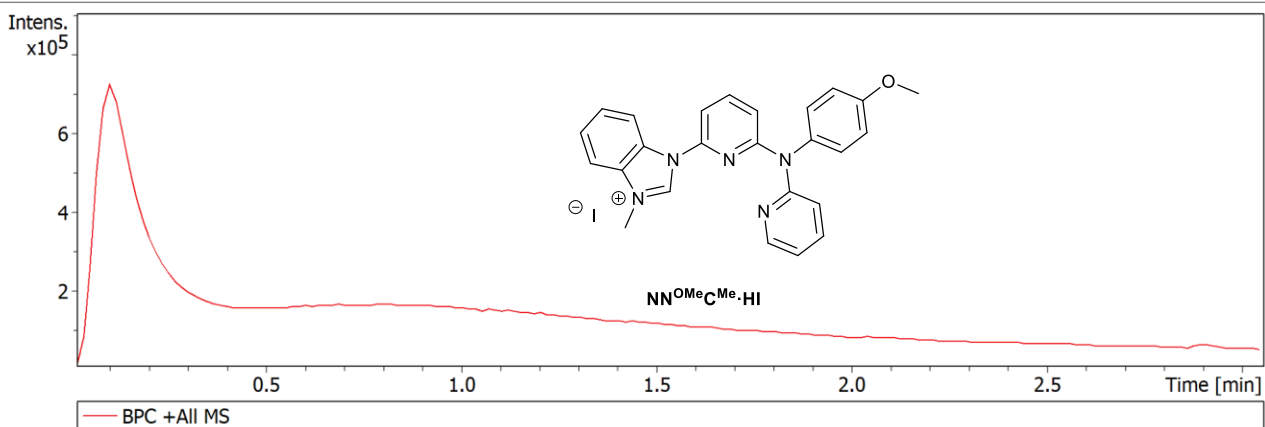


Figure S40. LCMS of NN<sup>OMe</sup>C<sup>Me</sup>.HI.

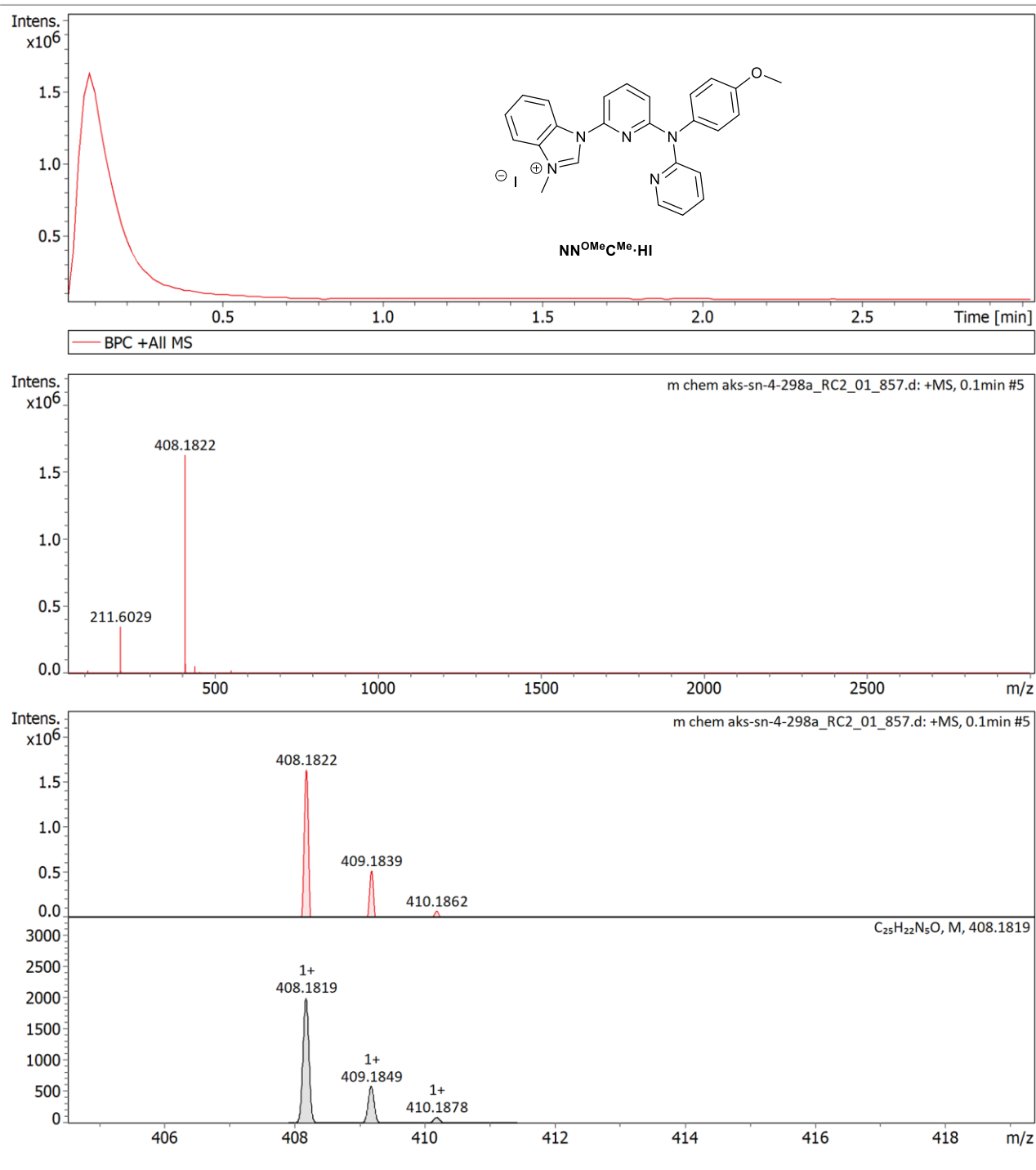


Figure S41. HRMS of  $NN^{OMe}C^{Me}.HI$ .

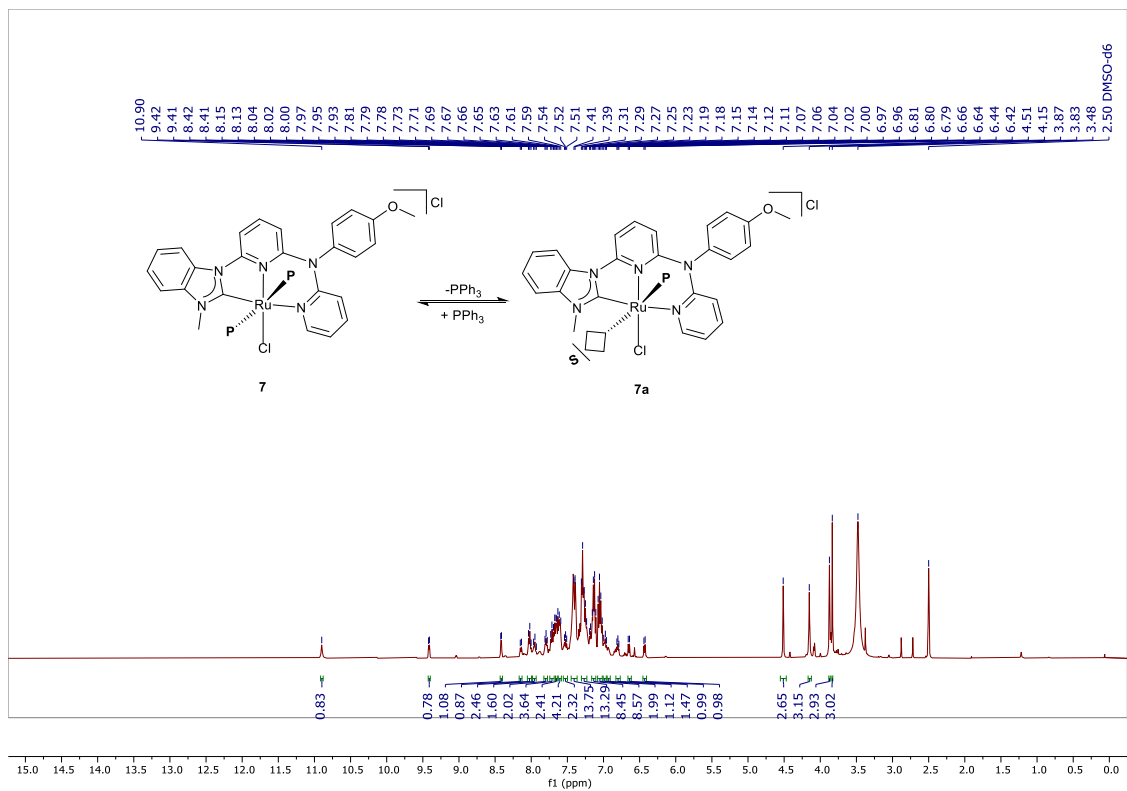


Figure S42.  $^1H$  NMR spectrum of **7** in DMSO- $d_6$ .

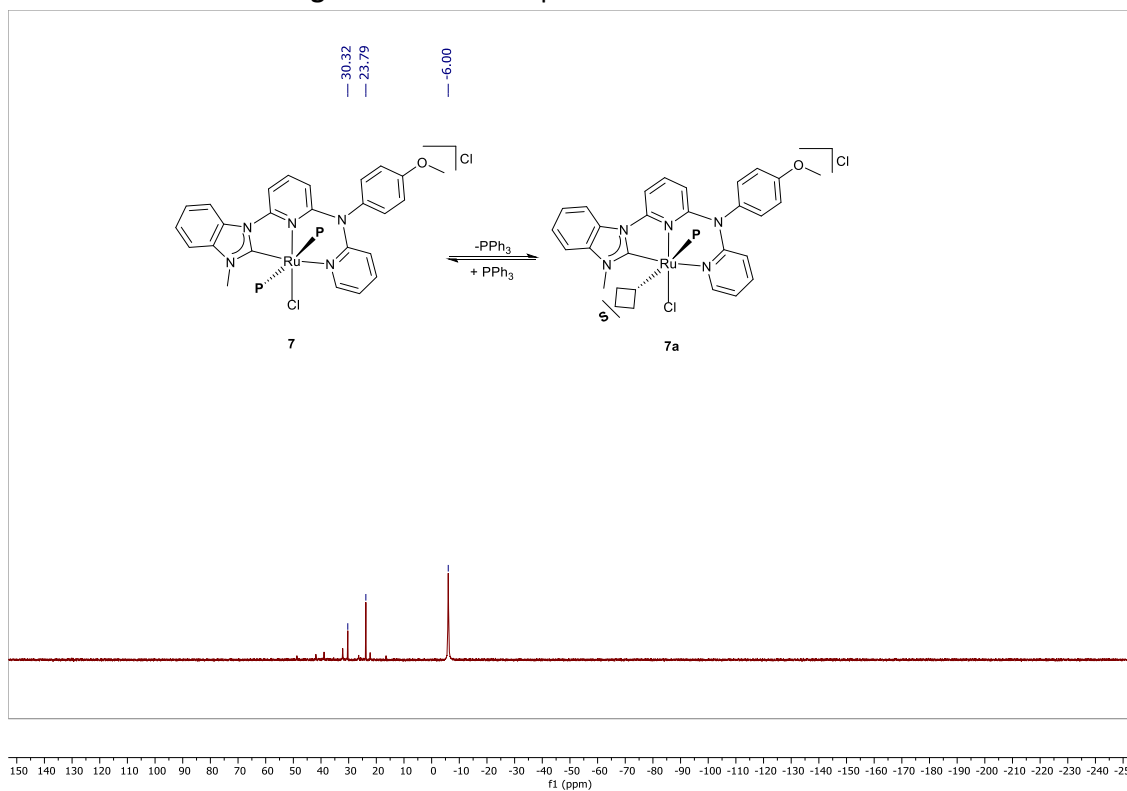


Figure S43.  $^{31}P\{^1H\}$  NMR spectrum of **7** in DMSO- $d_6$ .

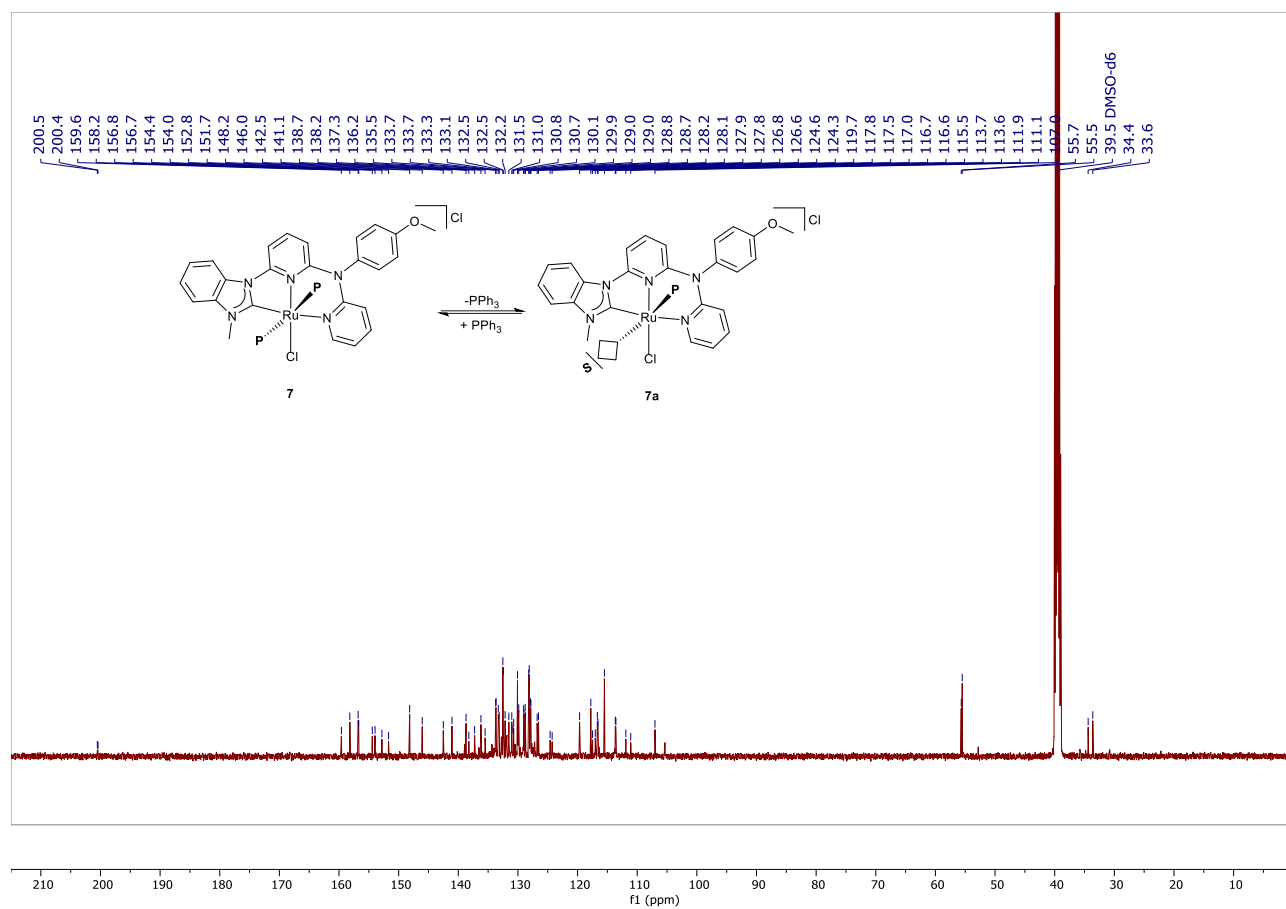


Figure S44.  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **7** in  $\text{DMSO-d}_6$ .

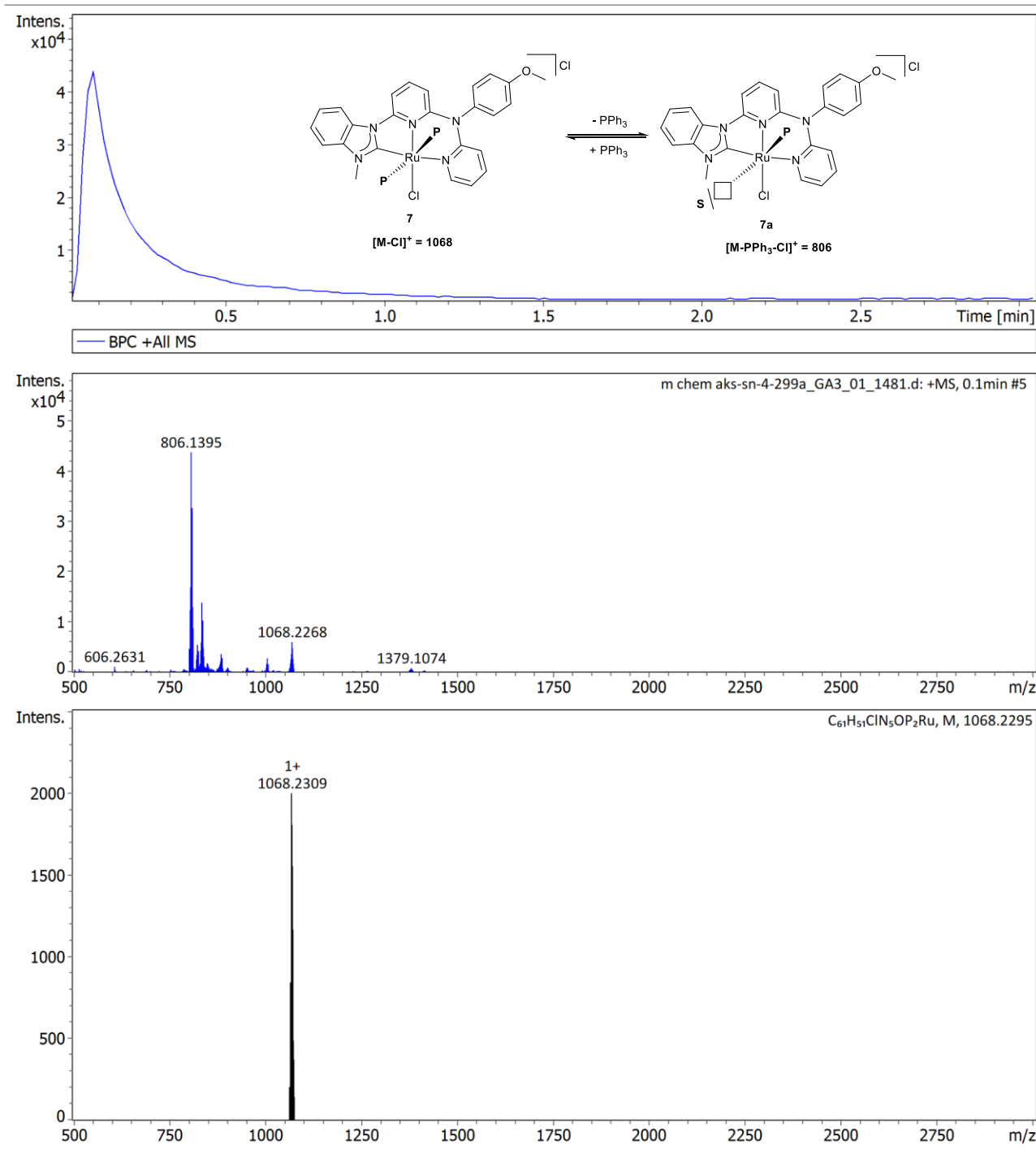


Figure S45. LCMS of **7**.

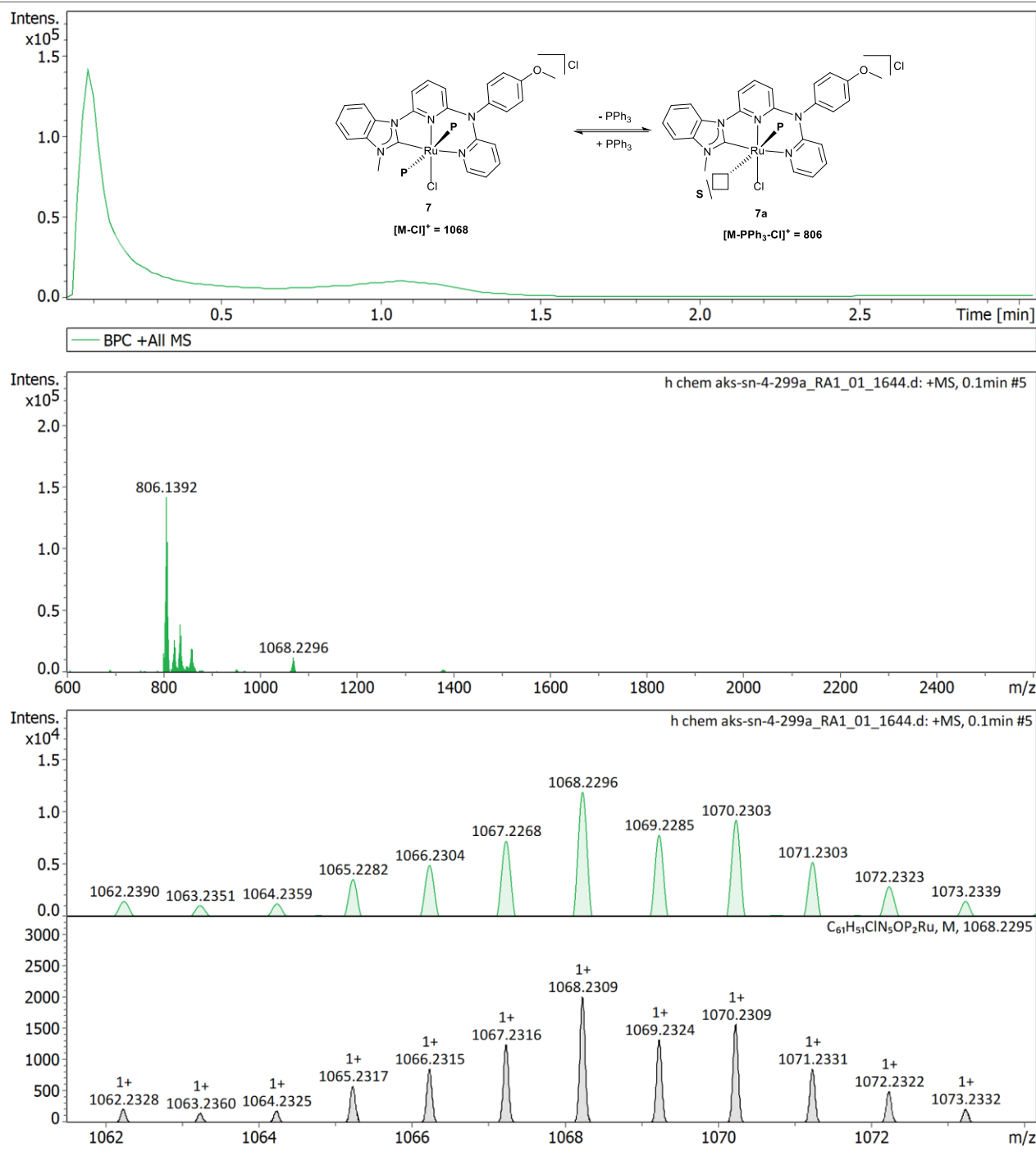


Figure S46. HRMS of **7**.

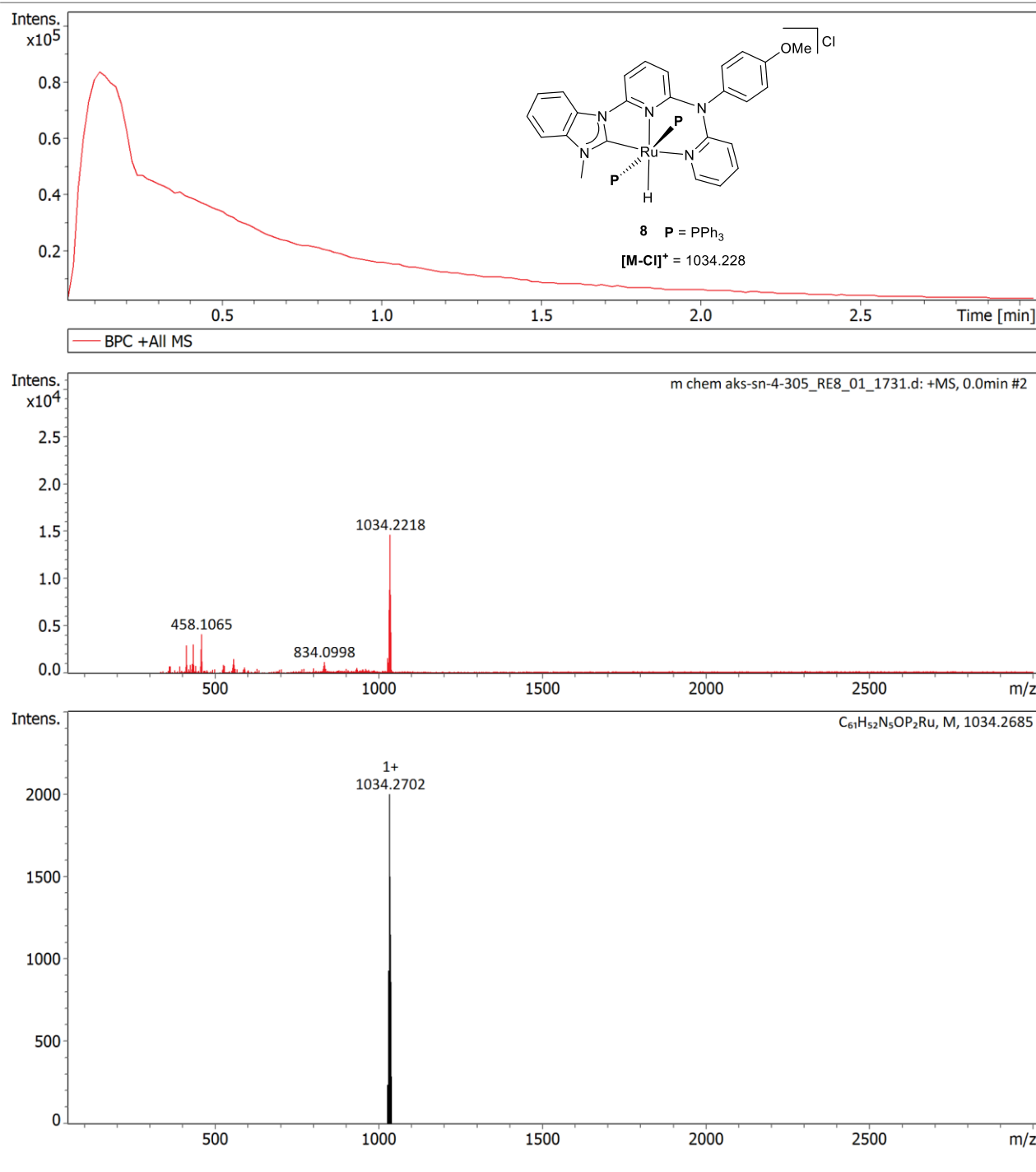


Figure S47. LCMS of **8**.



**X-ray Diffraction Studies:** Single crystals of complexes **3** suitable for X-ray crystallographic determination were obtained by layering a solution in MeOH with Ether (1/3, v/v) at -4 °C. Single crystal X-ray diffraction study for complex **3** was carried out using dual-core Agilent technology (Oxford diffraction) super Nova CCD system, with monochromated CuK $\alpha$  ( $\lambda = 1.54184 \text{ \AA}$ ). Unit cell determination, data collection and reduction, and empirical absorption correction were performed using the CrysAlisPro65 program. The Olex 2-1.5 program was used as the graphical interface.<sup>1</sup> The structure model was refined using full matrix least squares minimization on F<sup>2</sup> using ShelXL within Olex2 for a graphical interface.<sup>2</sup> The structures were solved by direct methods using SHELXT,<sup>3</sup> which revealed the positions of all not-disordered non-hydrogen atoms. The non-hydrogen atoms were refined anisotropically. All hydrogen positions were fixed in place for the final refinement cycles. CCDC 2299181 contains the supplementary crystallographic data for this paper.

**Crystallographic Data:** Table S1 Crystal data and structure refinement parameters.

<b>3</b>	
Empirical formula	C <sub>61</sub> H <sub>53</sub> P <sub>2</sub> Cl <sub>2</sub> N <sub>5</sub> O <sub>2</sub> Ru
Formula weight	1121.99
Temperature/K	298
Crystal system	Monoclinic
Space group	P21/c
a/ $\text{\AA}$	13.5479(11)
b/ $\text{\AA}$	22.1691(10)
c/ $\text{\AA}$	23.429(2)
$\alpha$ /°	90
$\beta$ /°	131.809(14)
$\gamma$ /°	90
Volume/ $\text{\AA}^3$	5245.0(11)
Z	4
$\rho_{\text{calc}}/\text{cm}^3$	1.421
$\mu/\text{mm}^{-1}$	4.327
F(000)	2312.0
Radiation	CuK $\alpha$ ( $\lambda = 1.54184$ )
2 $\theta$ range for data collection/°	7.808 to 142.392
Reflections collected	25346

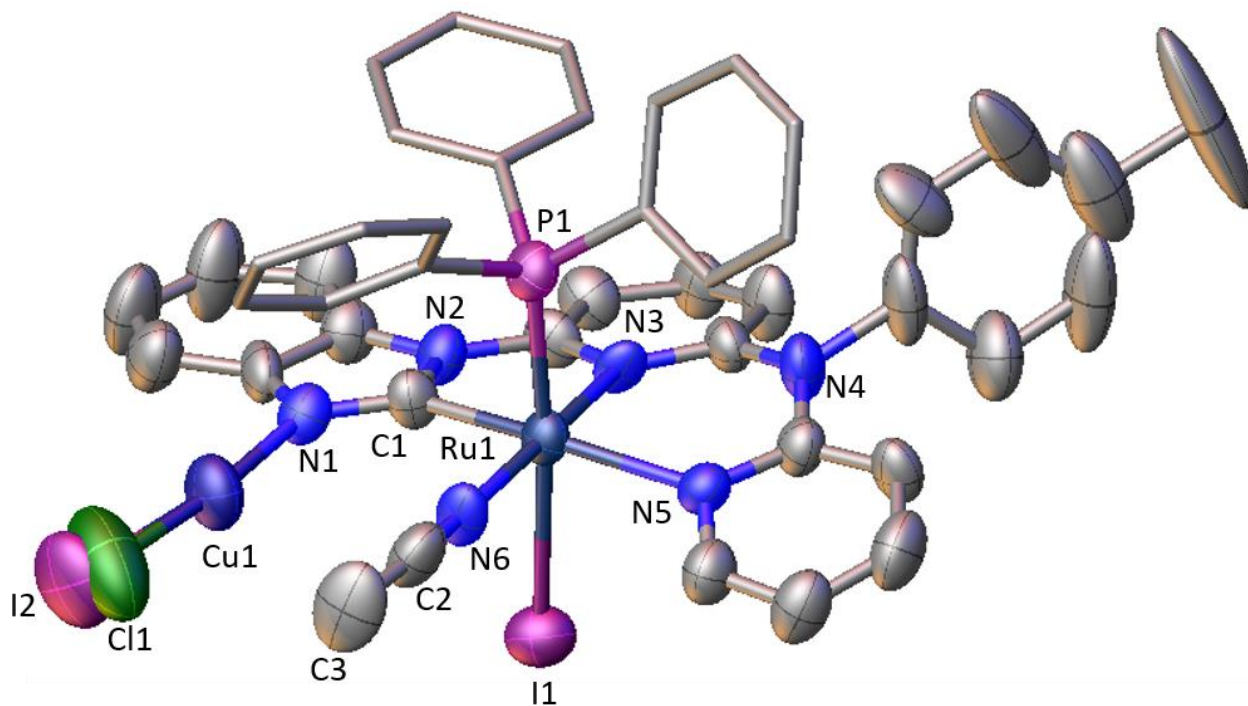
Independent reflections	9922 [Rint = 0.1173]
Data/restraints/parameters	9922/0/661
Goodness-of-fit on F2	1.116
Final R indexes [ $I \geq 2\sigma(I)$ ]	R1 = 0.0960, wR2 = 0.2217
Final R indexes [all data]	0.1479, wR2 = 0.2727

### General method for transfer hydrogenation of ketone

The general procedure for transfer hydrogenation: An oven-dried Schlenk tube equipped with a magnetic stirring bar was loaded with catalyst (1 – 0.01 mol%), base (10 mol%), and anhydrous 2-propanol (3 mL) to make it homogeneous. Next, add the substrate (1 mmol) to the reaction mixture. After that, the Schlenk tube was placed in a preheated oil bath ( 82 °C) with stirring at 350 rpm. At the end of the reaction, n-decane (0.1 mmol) was added to the catalytic solution as an internal standard, and a 0.1 mL sample was taken, added to a GC vial, and diluted with 2-PrOH (1.3 mL). The products were analyzed on a GC-MS QP 2010 ultra-mass spectrometer equipped with an FID detector. Products were identified using retention times and peak areas from analytically pure reference samples. The reaction yields were calculated by GC using n-decane as an internal standard.

### General method for transfer hydrogenation of ketone using CuI as phosphine scavenger.

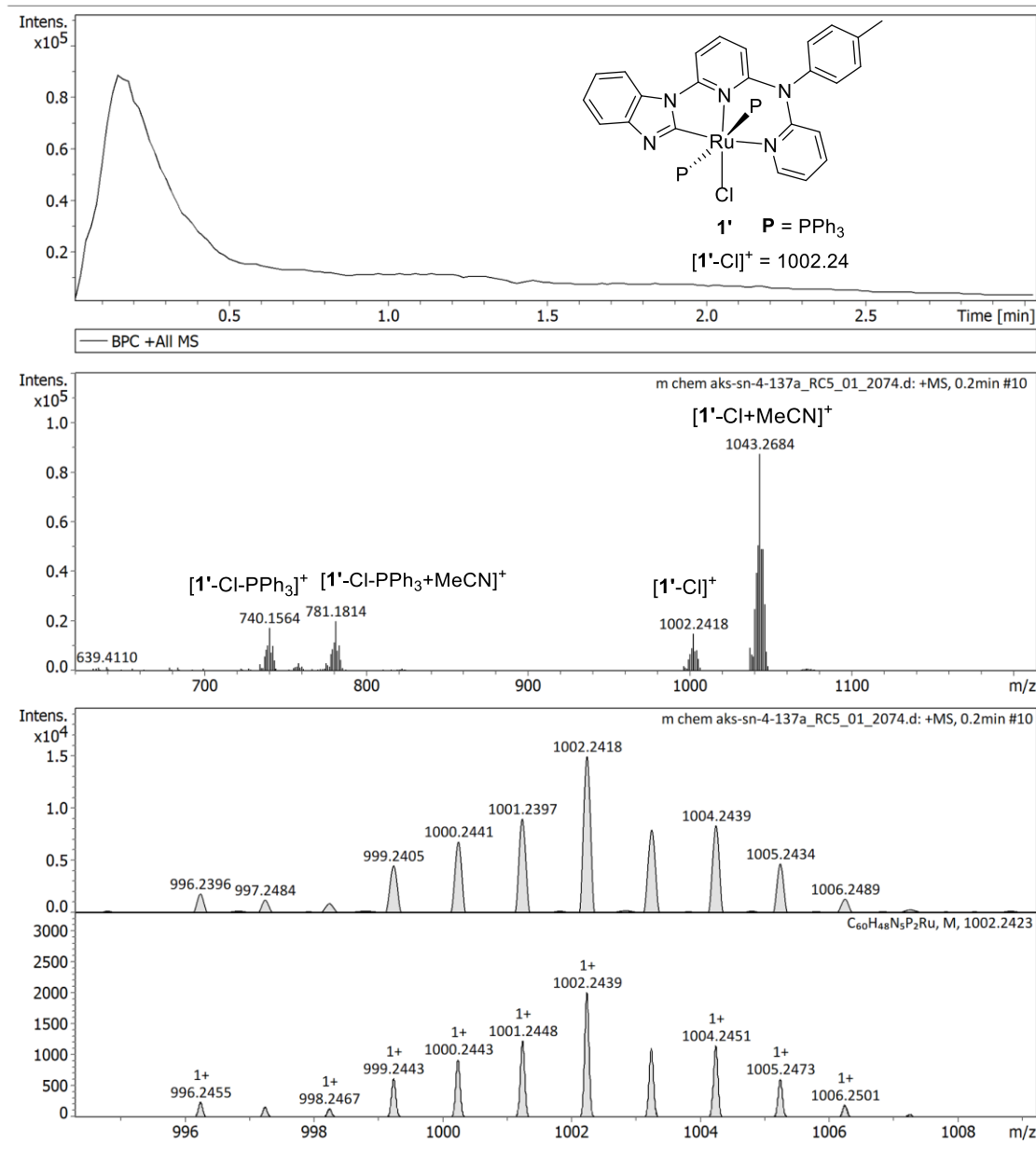
An oven-dried 50 mL Schlenk tube containing a stir bar was purged with nitrogen. Complex **1** (10.7 mg, 0.01 mmol, 1 mol%) or **5** (10.8 mg, 0.01 mmol, 1 mol%) and KO<sup>t</sup>Bu (11.2 mg, 0.1 mmol, 10 mol %) were added, followed by freshly-distilled 2-propanol (3 mL), cyclohexanone (103  $\mu$ L, 1.0 mmol) and CuI (9.5 mg, 5 mol%) were added to the reaction vessel, purged with inert gas, and sealed with a septum. The reaction vessel was placed in a preheated oil bath (85 °C) and stirred for 15 minutes. The results of catalysis were analyzed by GC-MS as described above. A pale-yellow precipitate appeared in the reaction with **1** which was filtered, washed with diethyl ether (3X10 mL), and dried under vacuum. The formation of CuI-capped anionic-NHC complex was confirmed by growing crystals of the precipitated complex from acetonitrile/diethyl ether solution (1:1, v/v). The data quality of this structure is not publishable (high Rint and other parameters probably due to mixed halides in the structure and disorder), however, it does confirm the formation of CuI capped anionic-NHC complex.



**Figure S48.** Molecular structure of CuI capped anionic NHC complex **1b**.

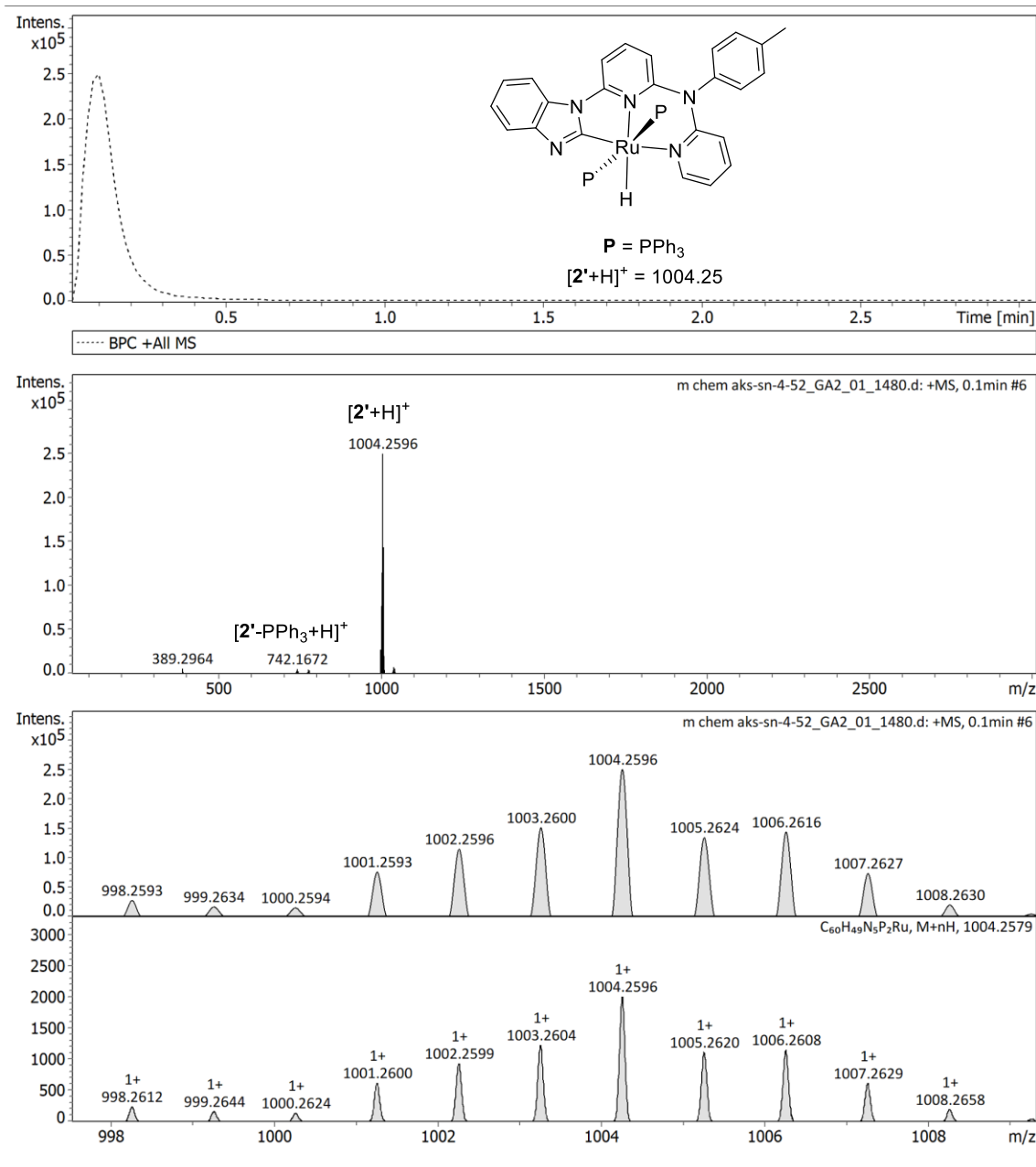
## Mechanistic investigation of transfer hydrogenation reactions using Mass spectrometry.

**Experiment A:** An oven-dried 50 mL Schlenk tube containing a stir bar was purged with nitrogen. Complex **1** (10.73 mg, 0.01 mmol, 1 mol %) and KO<sup>t</sup>Bu (11.2 mg, 0.1 mmol, 10 mol %) were added, followed by freshly-distilled 2-propanol (3 mL). After that, cyclohexanone (103  $\mu$ L, 1.0 mmol) was added to the reaction vessel, purged with inert gas, and sealed with a septum. The reaction mixture was stirred for 15 minutes at rt. An aliquot was taken at 10 minutes, and a mass spectrogram of the reaction mixture was recorded.



**Figure S49.** HRMS of the catalytic mixture of experiment **A** (MeCN was used for data collection).

**Experiment B:** An oven-dried 50 mL Schlenk tube containing a stir bar was purged with nitrogen. Complex **1** (10.73 mg, 0.01 mmol, 1 mol %) and  $\text{KO}^t\text{Bu}$  (11.2 mg, 0.1 mmol, 10 mol %) were added, followed by freshly-distilled 2-propanol (3 mL). After that, cyclohexanone (103  $\mu\text{L}$ , 1.0 mmol) was added to the reaction vessel and purged with inert gas, and sealed with a septum. The reaction vessel was placed in a preheated oil bath (85  $^\circ\text{C}$ ) and stirred for 15 minutes. An aliquot was taken during the reactions, and a mass spectrogram of the reaction mixture was recorded.



**Figure S50.** HRMS of the catalytic mixture of experiment **B** (MeCN was used for data collection).

## NMR tube experiments for mechanistic investigation of transfer hydrogenation reactions.

**Experiments:** All NMR tube studies were carried out using the glovebox under a nitrogen atmosphere. In situ, NMR reaction progress monitoring was performed in a J Young NMR tube charged with solid complex **1** (43.9 mg, 0.041 mmol) and dissolved in deuterated DMSO (0.5 mL). After that,  $^1\text{H}$  and  $^{31}\text{P}\{^1\text{H}\}$  were recorded using a 500 MHz NMR spectrometer.  $^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ , 25 °C)  $\delta$  14.14 (s, 1H), 13.96 (s, 1H), 9.34 (d,  $J = 5.9$  Hz, 1H), 9.07 (d,  $J = 7.8$  Hz, 1H), 8.13 (d,  $J = 8.4$  Hz, 1H), 7.86 (d,  $J = 8.4$  Hz, 1H), 7.74 (d,  $J = 8.0$  Hz, 1H), 7.72-7.64 (m, 3H), 7.59 (d,  $J = 8.0$  Hz, 1H), 7.52 (t,  $J = 8.2$  Hz, 4H), 7.44 -7.31 (m, 12H), 7.21 (q,  $J = 7.2$  Hz, 17H), 7.13 (s, 14H), 7.07 (d,  $J = 6.9$  Hz, 24H), 6.84 (t,  $J = 6.4$  Hz, 1H), 6.74 (d,  $J = 7.8$  Hz, 2H), 6.51 (d,  $J = 8.8$  Hz, 1H), 6.31- 6.21 (m, 2H), 6.12 (d,  $J = 9.0$  Hz, 1H), 5.75 (d,  $J = 7.2$  Hz, 1H), 2.45 (s, 6H).  $^{31}\text{P}\{^1\text{H}\}$  NMR (202 MHz, DMSO- $d_6$ , 25 °C)  $\delta$  33.65, 25.09, -6.00.

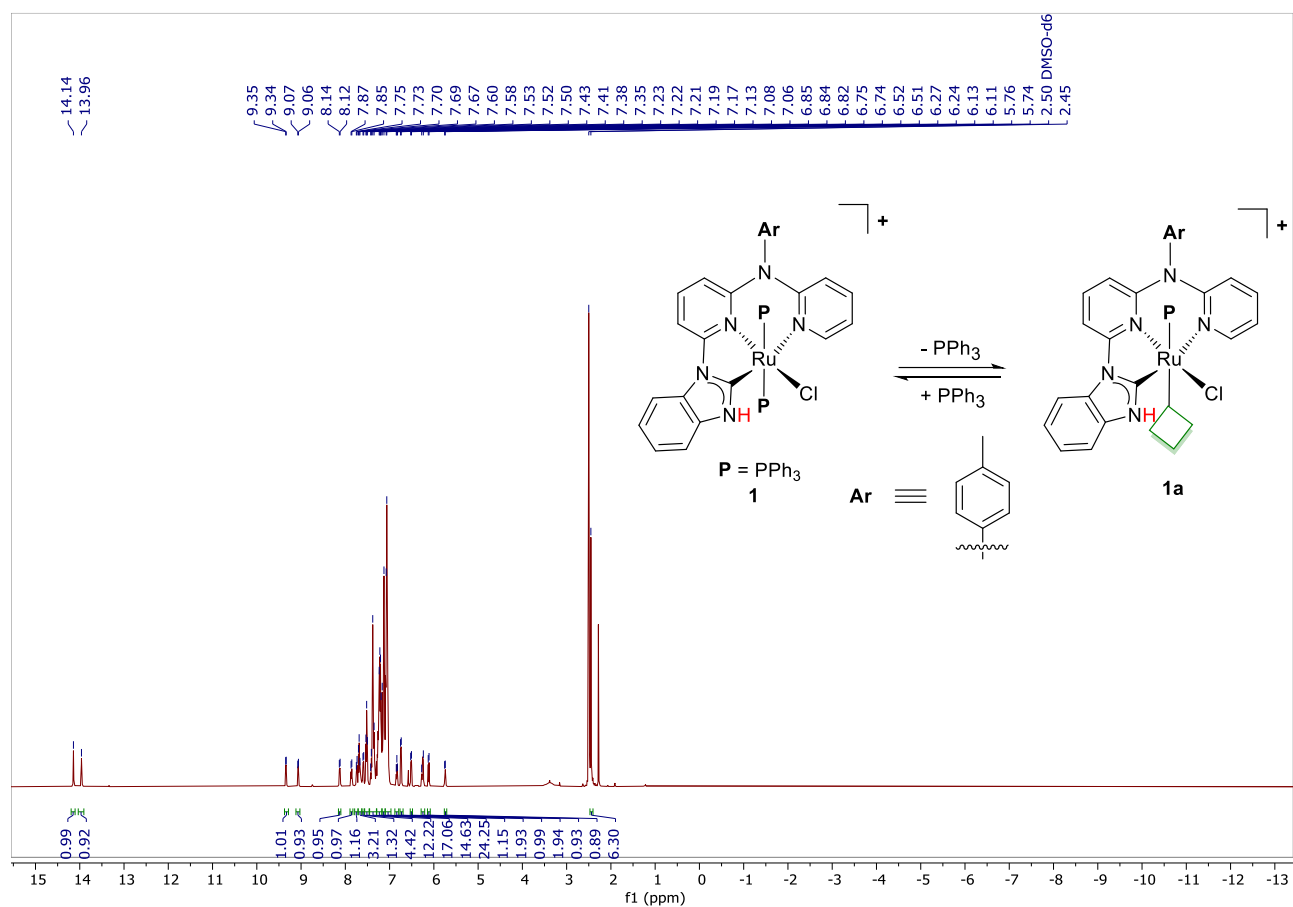


Figure S51.  $^1\text{H}$  NMR spectrum of **1** in DMSO- $d_6$  before adding a base.

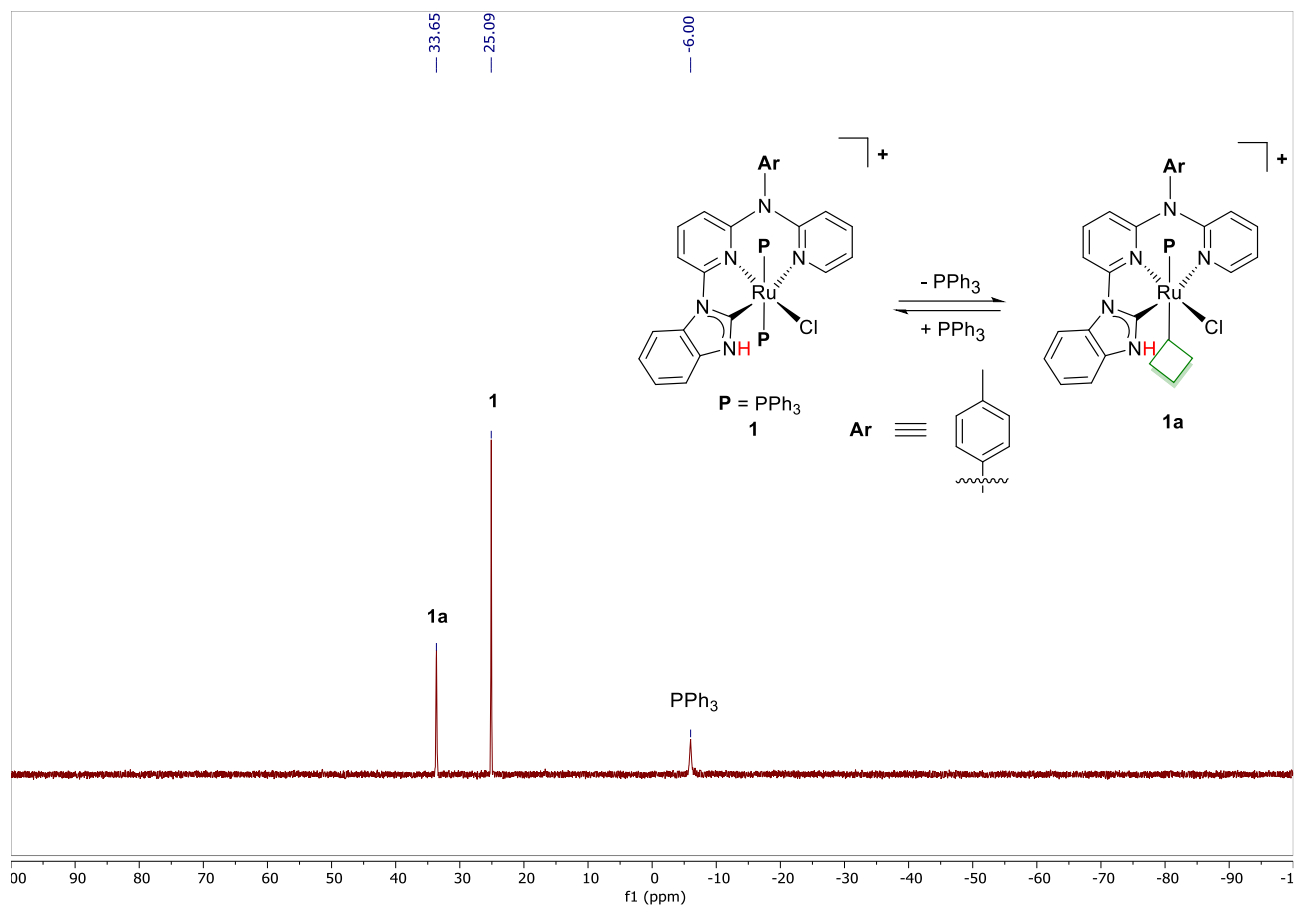
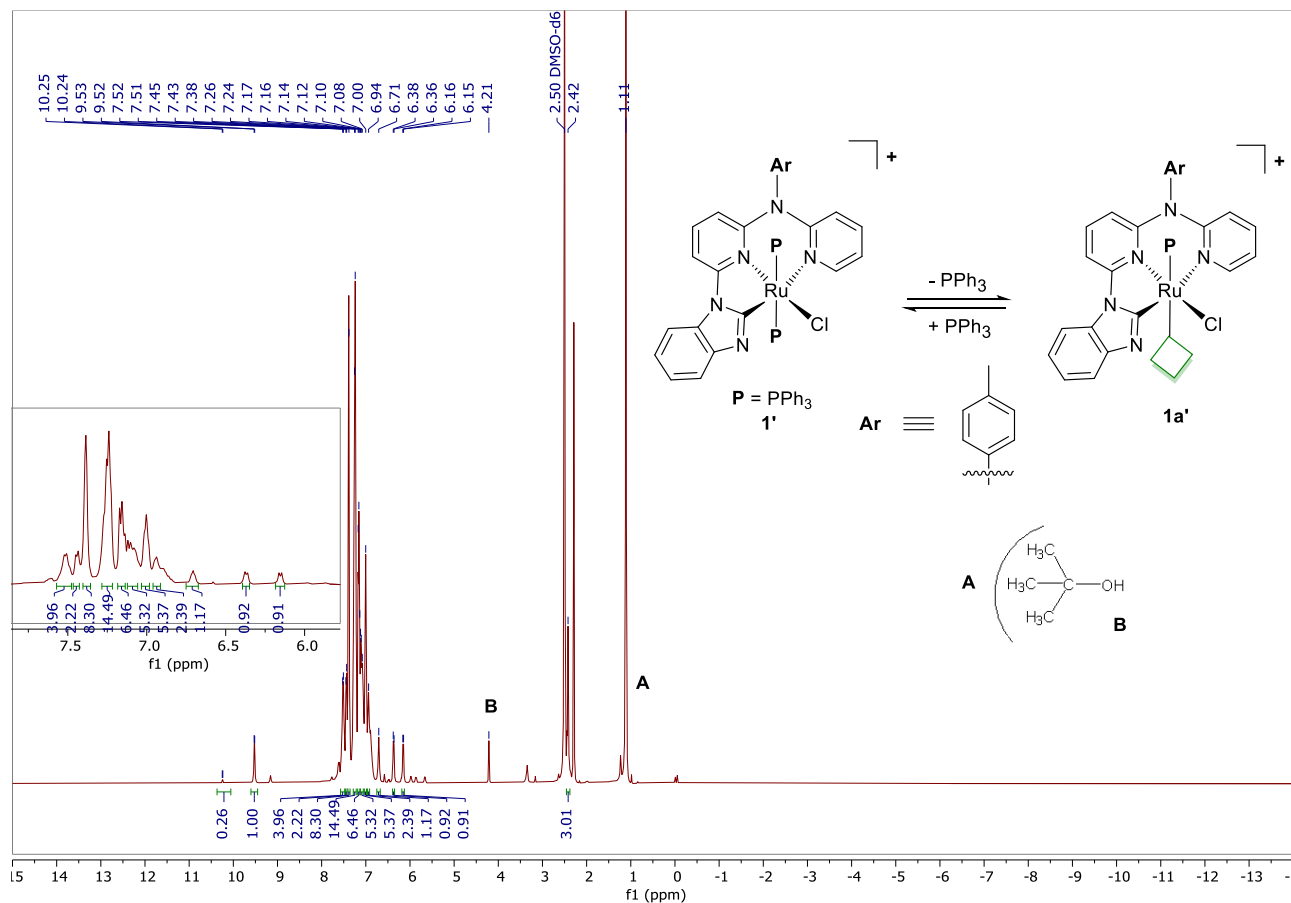


Figure S52.  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum of **1** in  $\text{DMSO-d}_6$  before adding base.

**Step 1: In situ generation of 1' and 1a':** After NMR analysis of complex **1**, the equimolar amount KO<sup>t</sup>Bu (4.59 mg, 0.041 mmol) was added to the J Young NMR tube, and an orange-red solution was formed immediately. The NMR tube was sealed with a Teflon screw-cap to ensure air tightness and shaken prior to recording the NMR.



**Figure S53.** <sup>1</sup>H NMR spectrum after adding 1 equiv. of KO<sup>t</sup>Bu.



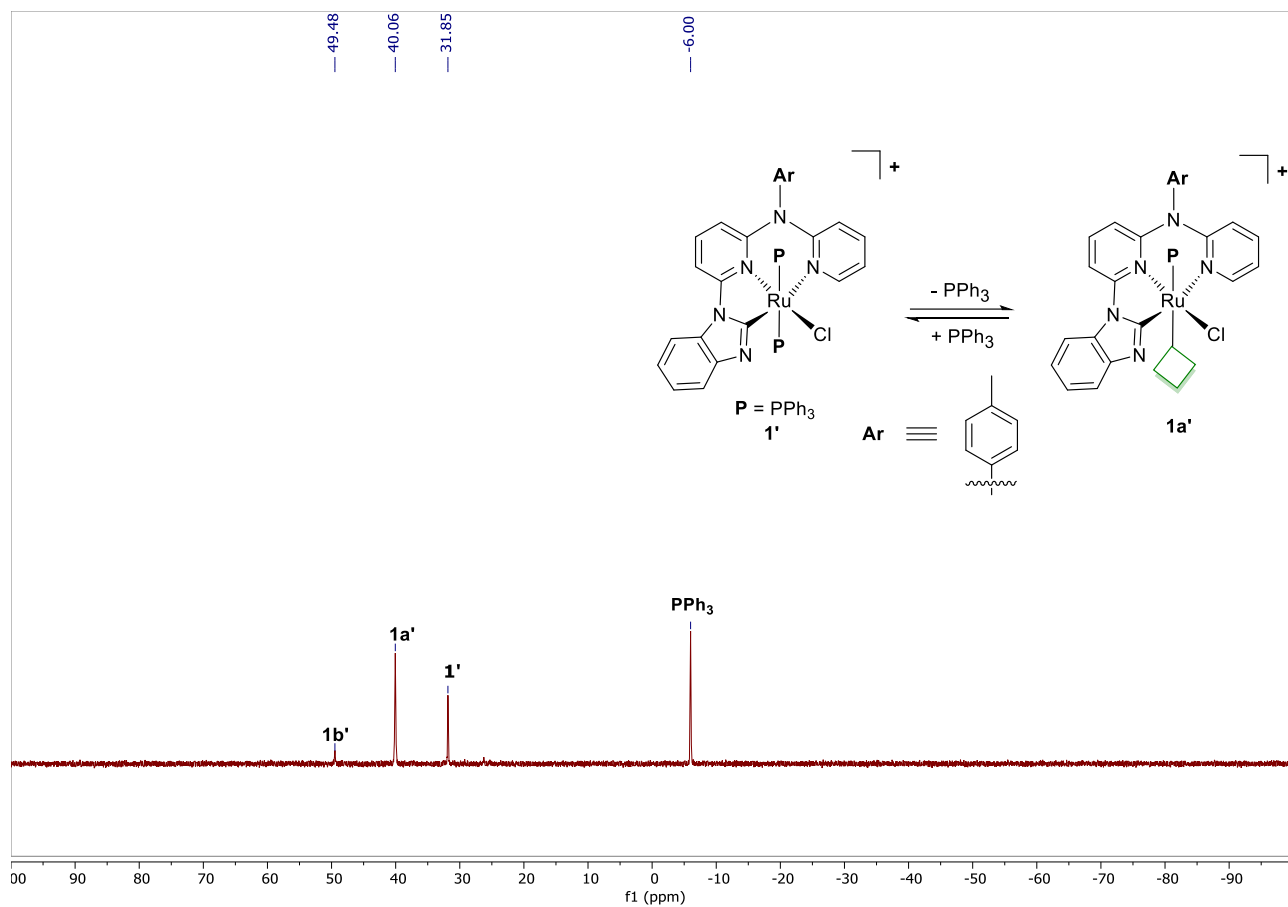
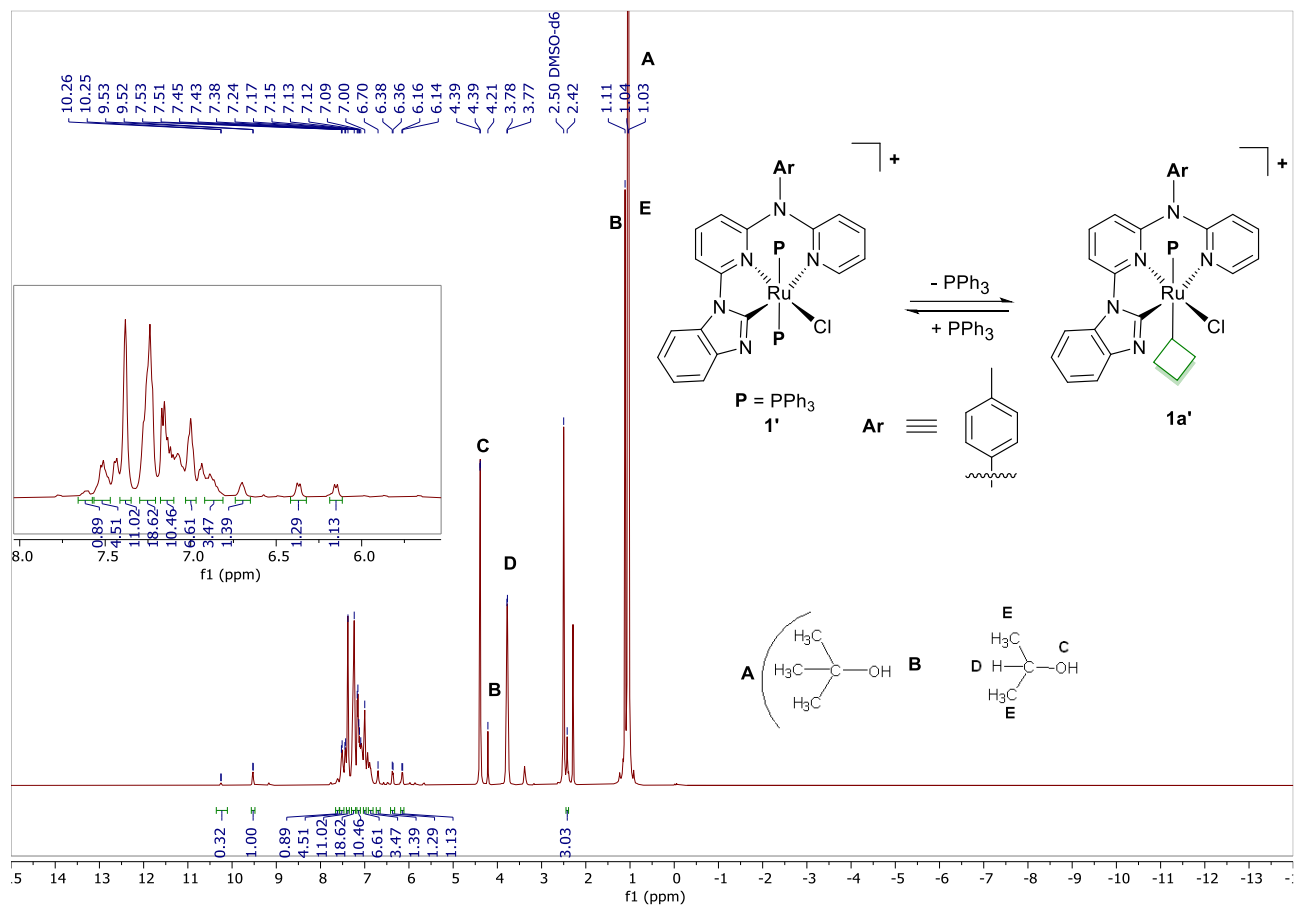
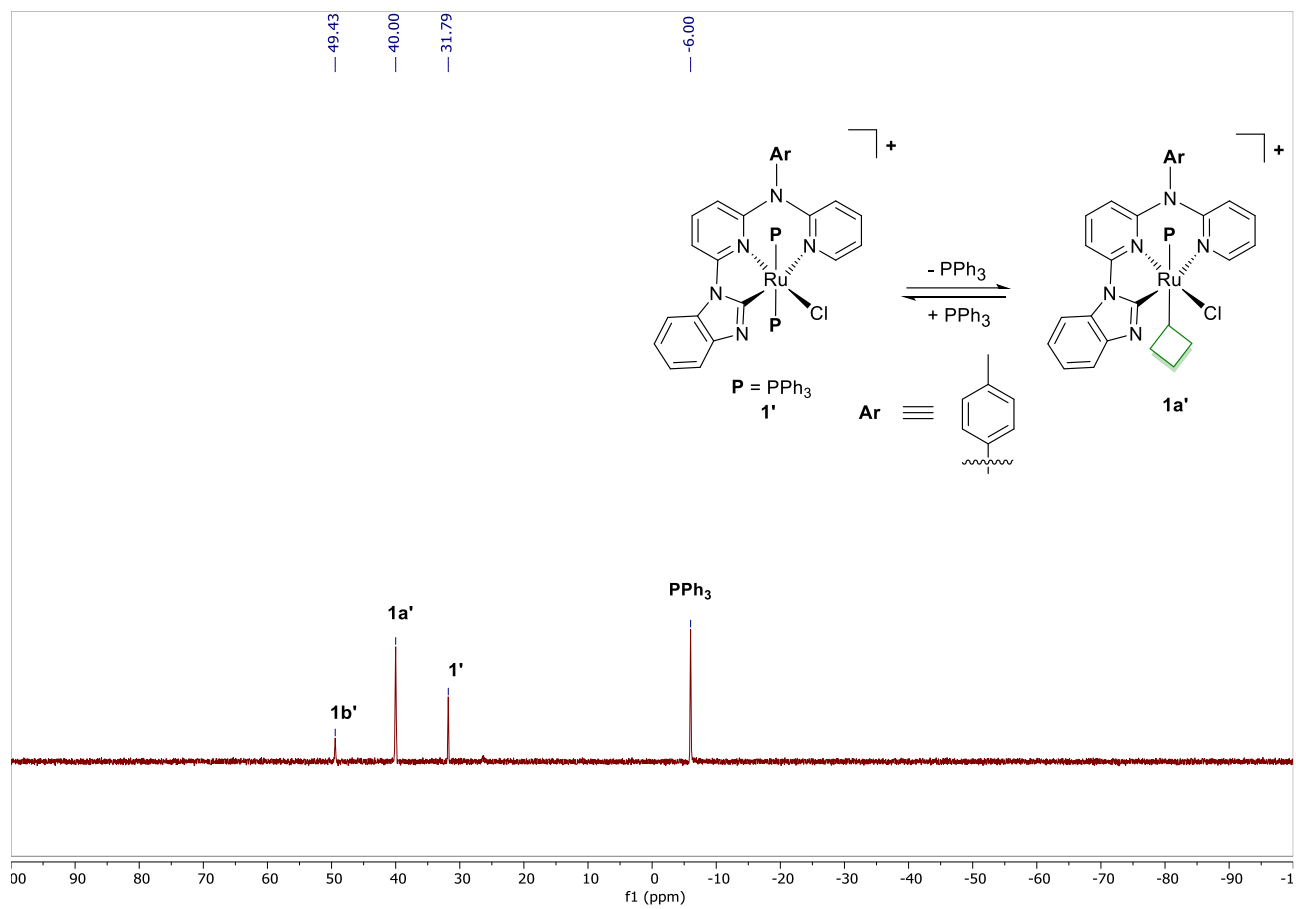


Figure S54.  $^{31}\text{P}$   $\{^1\text{H}\}$  NMR spectrum after adding 1 equiv.  $\text{KO}^t\text{Bu}$ .

**Step 2: In situ no regeneration of complex 1:** In the next step, 5 equiv. of 2-propanol was added to the J. Young NMR tube, The tube was sealed with a Teflon screw-cap to ensure air tightness and was vigorously shaken before being allowed to stand overnight at room temperature. The resulting reaction was monitored on a 500 MHz NMR spectrometer. The  $^1\text{H}$  NMR spectrum did not show any regeneration of the NH proton.  $^1\text{H}$  and  $^{31}\text{P}\{^1\text{H}\}$  NMR spectra showed no significant change in the chemical shifts of their respective signals.

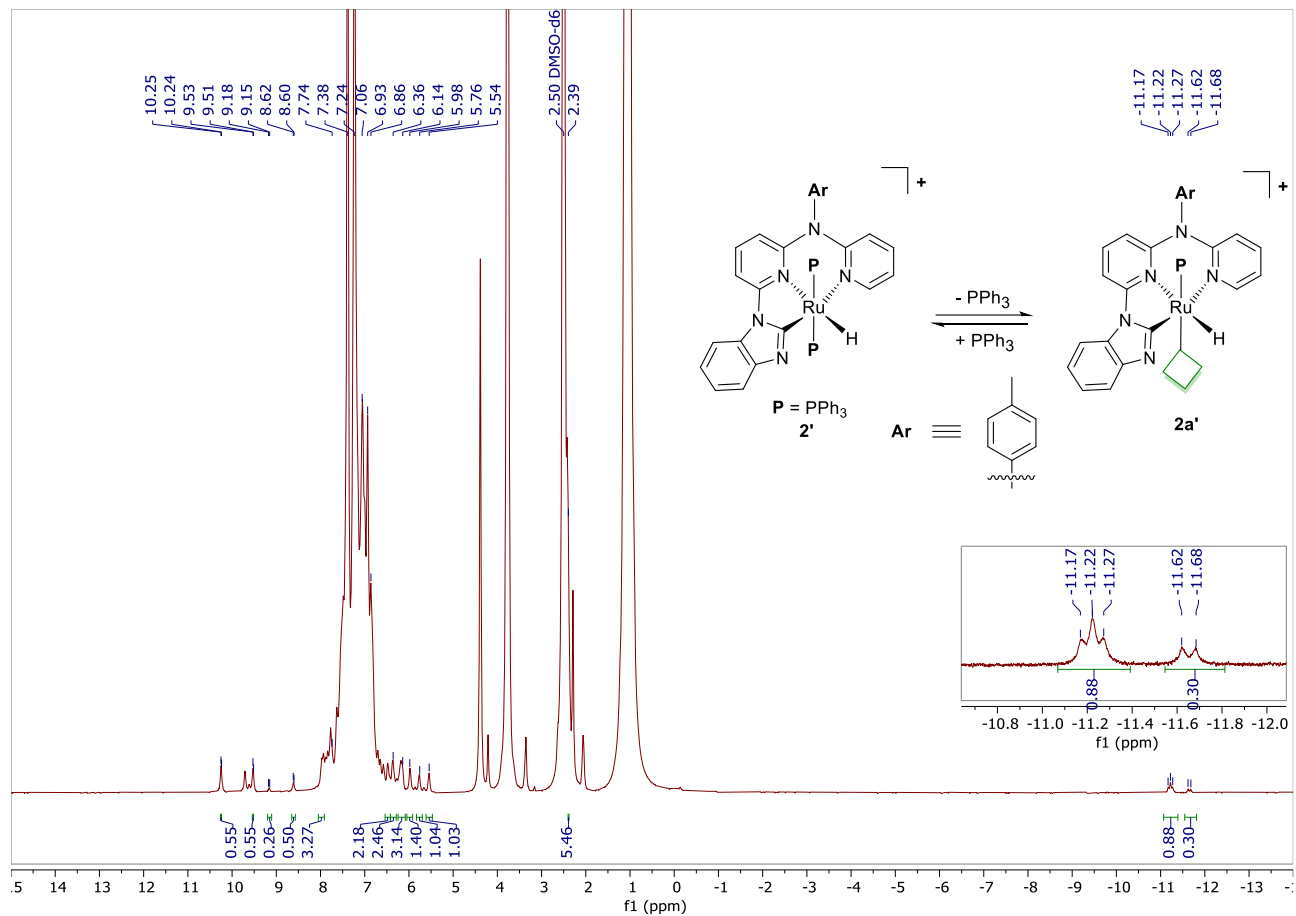


**Figure S55.**  $^1\text{H}$  NMR spectrum after adding 5 equiv. 2-propanol.

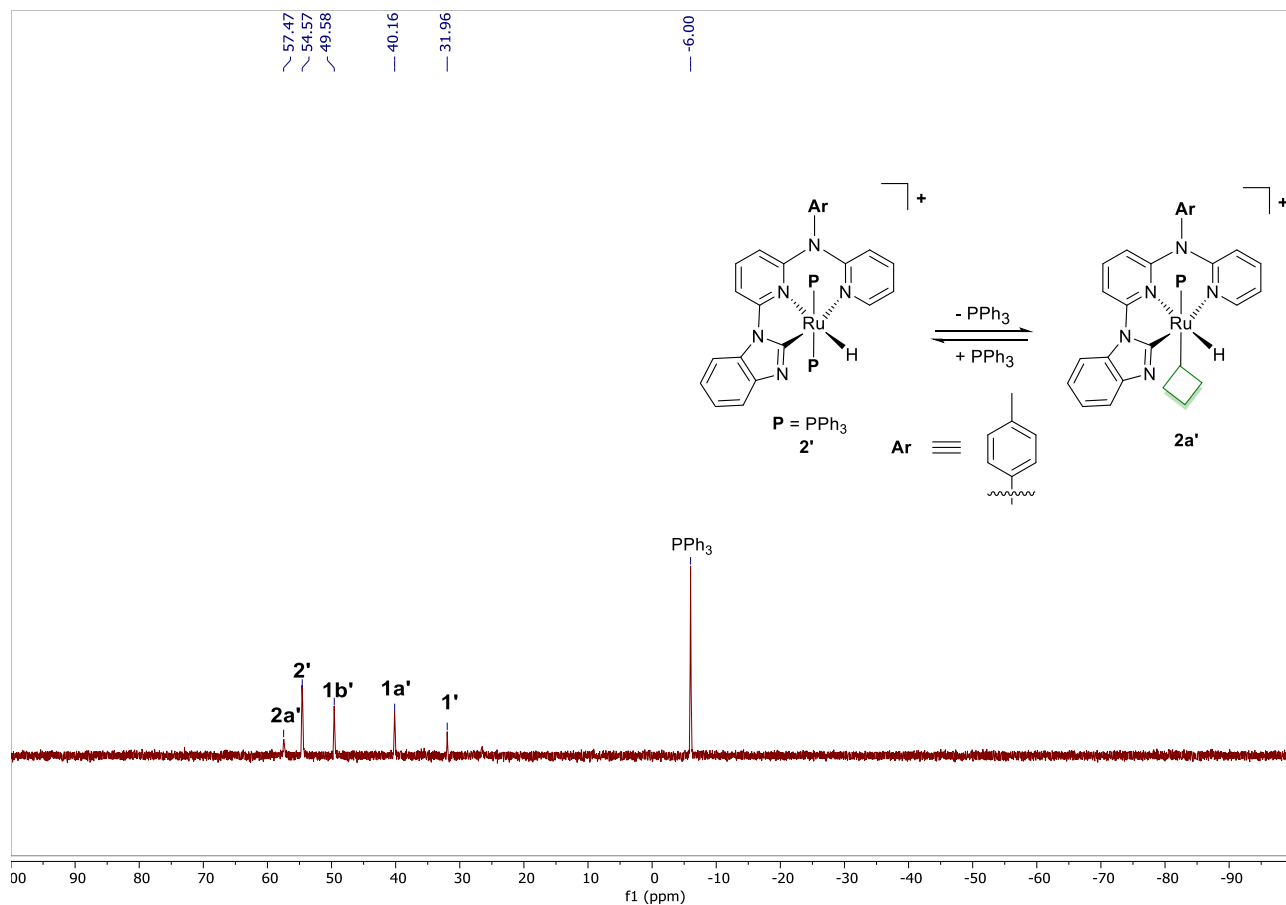


**Figure S56.**  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum after adding 5 equiv. 2-propanol.

**Step 3: In situ generation of 2' and 2a'.** In the J Young NMR tube, the mixture was heated at 82 °C for 1 h and allowed to cool to room temperature. The extent of the reaction was monitored by NMR analysis.



**Figure S57.** <sup>1</sup>H NMR spectrum after heating at 85 °C for 1 h.



**Figure S58.**  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum after heating at 85 °C for 1 h.

**NMR tube experiments to evaluate the effect of excess triphenyl phosphine:** In an  $\text{N}_2$  glovebox, a J-Young tube was charged with complex **1** (50.0 mg, 0.046 mmol) dissolved in  $\text{DMSO-d}_6$  (0.5 mL). Then, the J-Young tube was sealed, and the NMR data was analyzed. After that, the J-Young tube was returned to the glove box, and  $\text{PPh}_3$  (120.52 mg, 0.46 mmol, 10 equiv) was added to the solution. The tube was again sealed, and the mixture- was sonicated and NMR was recorded.

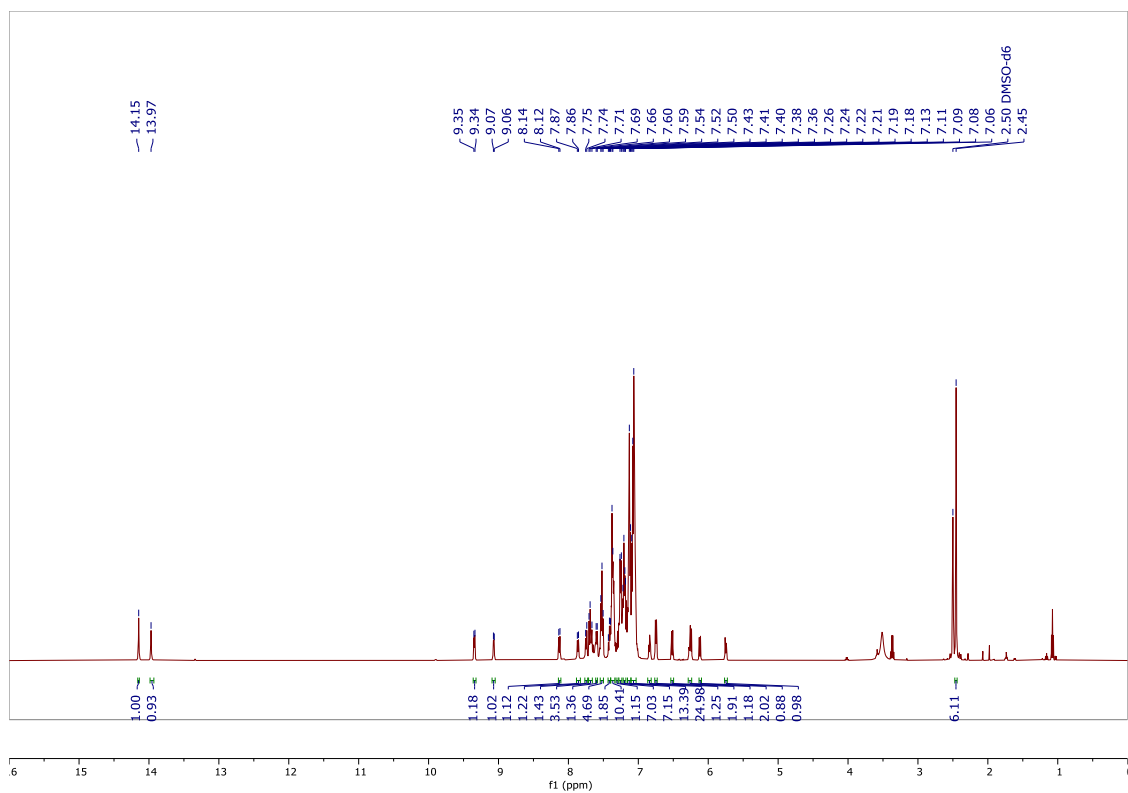


Figure S59.  $^1\text{H}$  NMR spectrum of **1** before adding 10 equiv. of  $\text{PPh}_3$ .

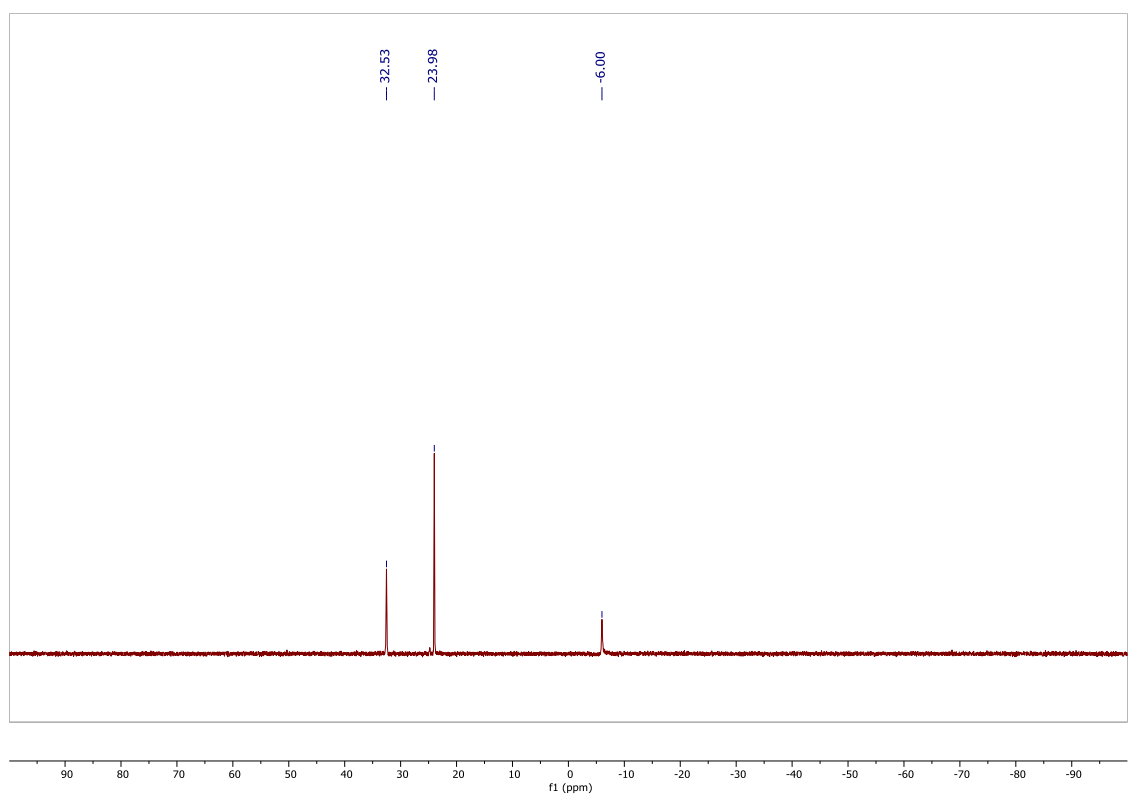


Figure S60.  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum **1** before adding 10 equiv. of  $\text{PPh}_3$ .

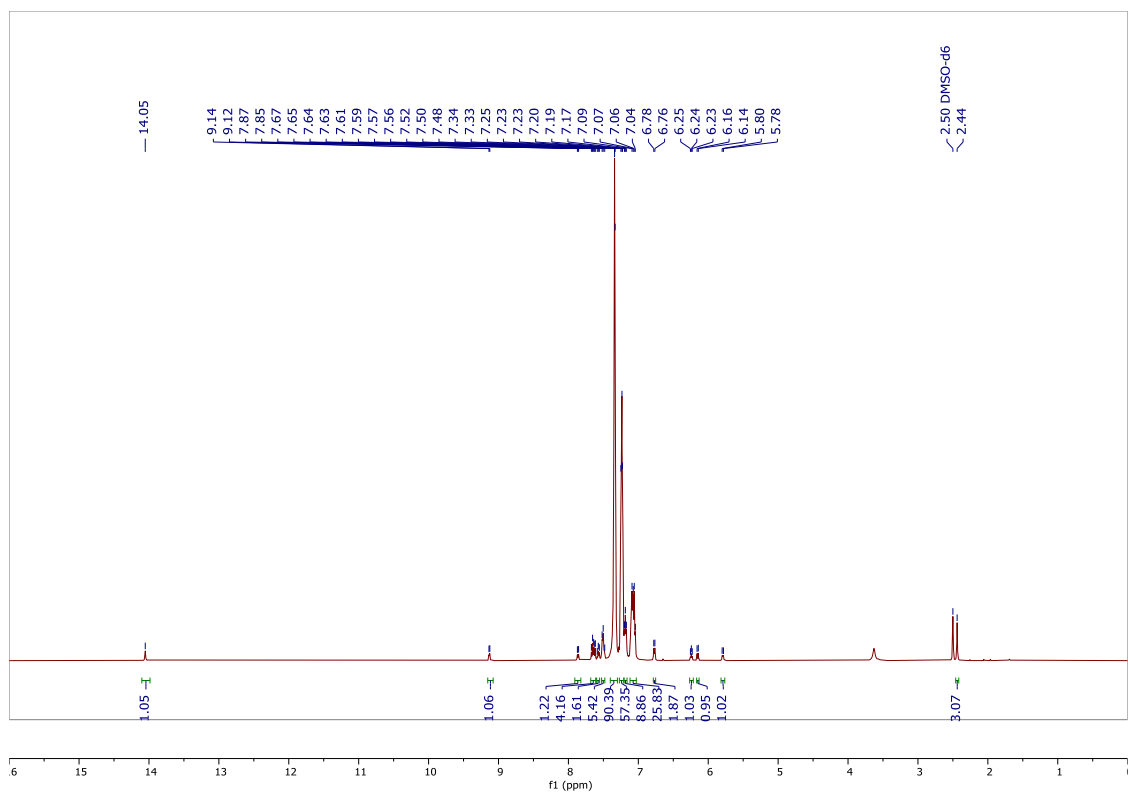


Figure S61.  $^1\text{H}$  NMR spectrum of **1** after adding 10 equiv. of  $\text{PPh}_3$ .

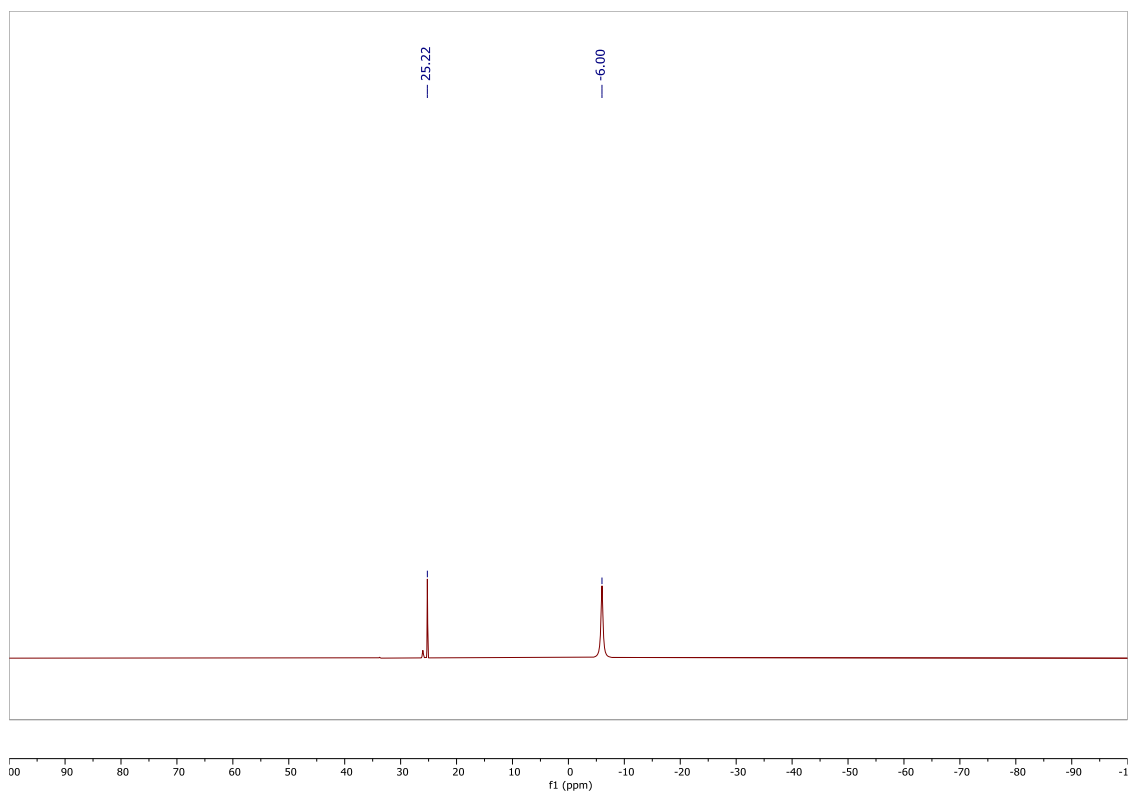


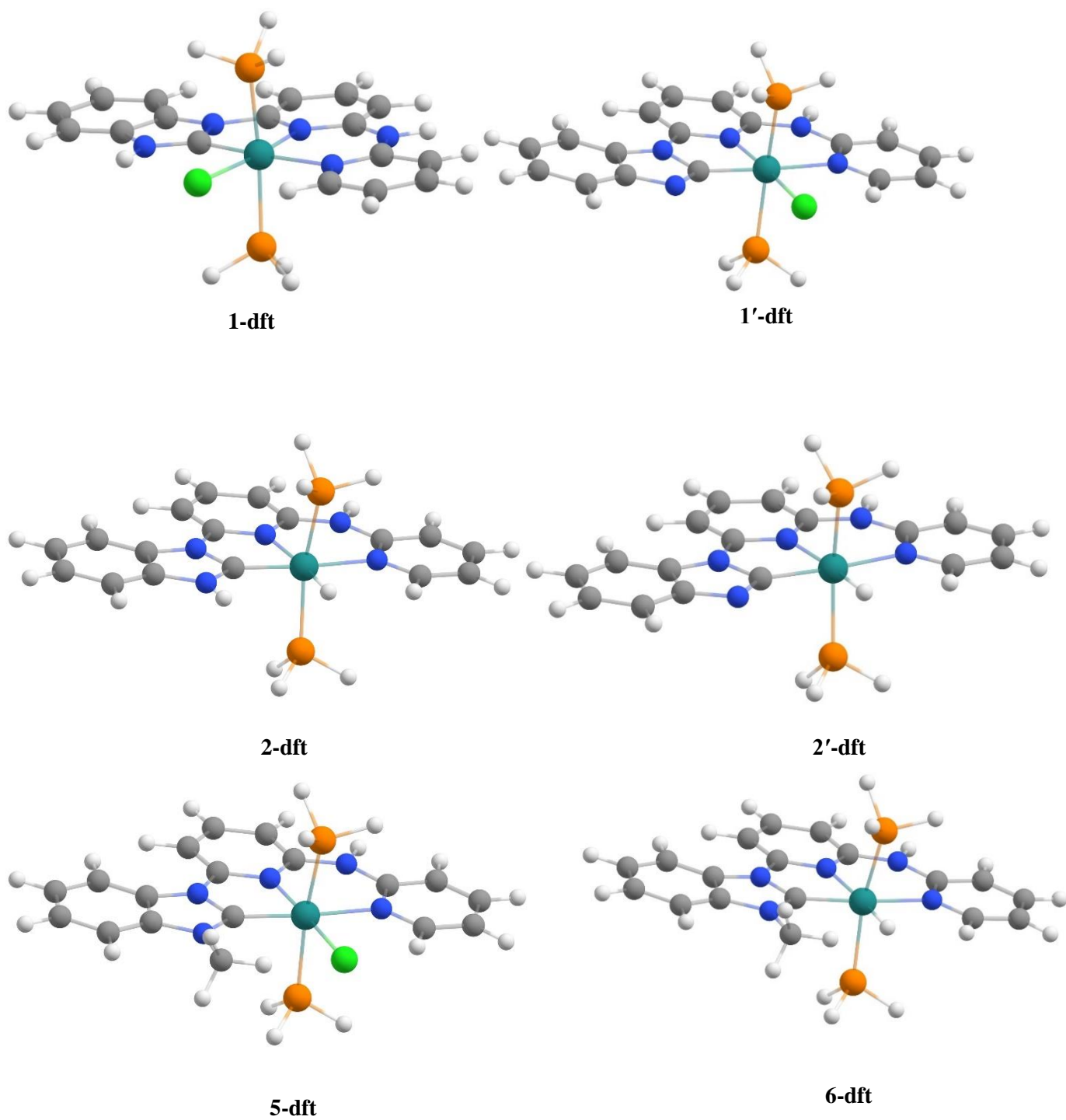
Figure S62.  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum of **1** after adding 10 equiv. of  $\text{PPh}_3$ .

**Computational investigation for the plausible mechanism of the transfer hydrogenation of ketone using Ru(II) complexes.** DFT calculations were carried out with the help of the ORCA 4.2.1 software package. Geometry optimizations were performed with the BP86 GGA functional and Ahlrichs def2-TZVP with def2 ECP on Ru, def2 -TZVP(-f) on P, and def2 SVP on all other atoms. Resolution of identity (RI) with their corresponding auxiliary basis set, def2/J, to speed up the calculation.<sup>4</sup> Dispersion corrections were applied in accordance with Grimme's D3 scheme and Beck-Johnson damping (D3BJ).<sup>5</sup> The grids used were "grid3", final grid 5, and "grid X5". By performing analytical frequency calculations at the same level as the DFT method, stationary points were confirmed to have either no imaginary frequency (for reactant and intermediate) or only one in imaginary frequency along with reaction coordinate (for TS). Following the frequency calculation, the thermochemical properties were calculated at 298.15K. To estimate the solvation energies, single-point calculation was performed according to the SMD model using 2-propanol.<sup>6</sup> For final energy calculation, single-point calculations were performed using a higher basis set def2-QZVP with def2 -ECP on Ru atom, def2-TZVP on P, and def2-TZVP(-f) on all other atoms (BS2) using the PBE0 hybrid GGA functional. For the final Gibbs free energy calculations, the electronic energy from the final single point calculation at PBE0/BS2 level was corrected for the total correction (G-Eel) obtained at BP86/BS1 level, solvation energy obtained at BP86(SMD)/BS1 level and standard state conversion from 1 atm pressure to 1M solution at 298.15 K. The Gibbs free energies are reported in kcal/mol.

### **DFT optimized structures**

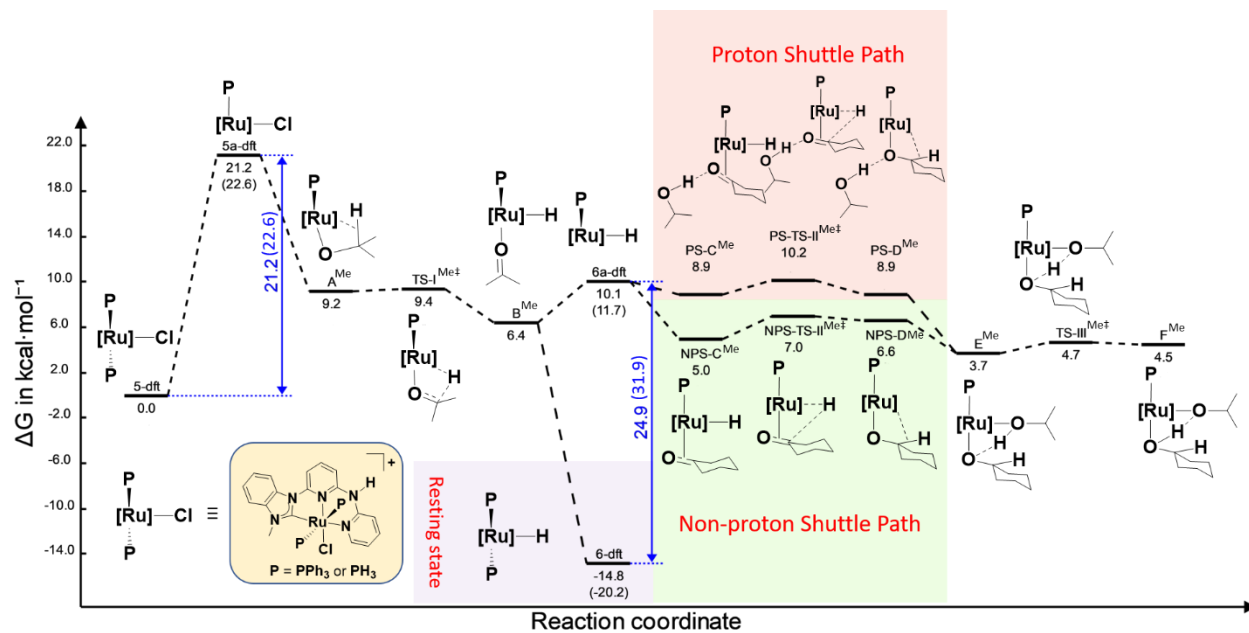
For the geometry optimization of complexes **1-2**(including its anionic complexes **1'-2'**) and **5-6**, the bulky p-tolyl group on nitrogen was replaced with hydrogen atom reduce the computational cost. The p-tolyl group being far away from the Ru center, is expected to have minimal effect on the catalyst. After the structural modifications, these optimized geometries were renamed as **1-dft**, **1'-dft**, **2-dft**, **2'-dft**, **5-dft** and **6-dft**. The structural parameters for these complexes were in good agreement with the X-ray diffraction structures.





**Figure S63.** The important optimized structure of 1-dft, 1'-dft, 2-dft, 2'-dft, 5-dft and 6-dft.

Calculated energy profile for TH using complex **5**:

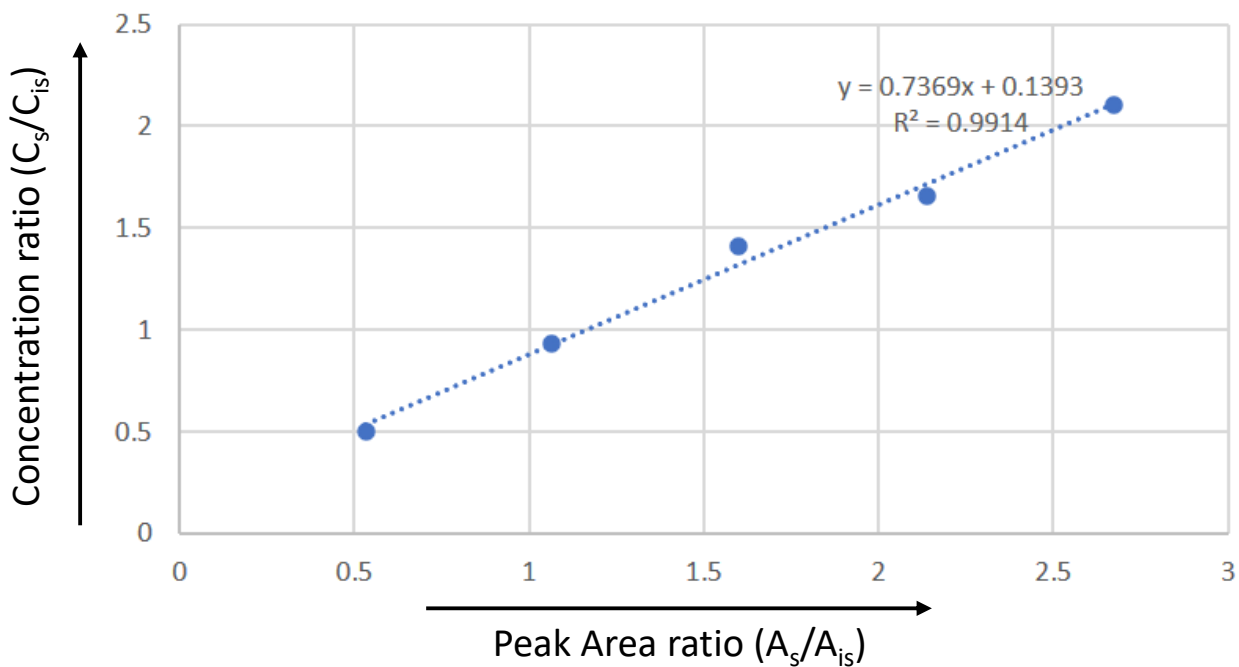


**Figure S64.** Calculated Gibbs free energy profile showing dissociation of phosphine ( $\text{PPh}_3$  and  $\text{PH}_3$  are displayed by **P** in the formula for clarity) and comparison between the energy of proton shuttle and non-proton shuttle paths in transfer hydrogenation of cyclohexanone to cyclohexanol by classical-NHC complex **5**. The values of Gibbs free energy (in  $\text{Kcal mol}^{-1}$ ) in brackets correspond to the calculation with the  $\text{PPh}_3$  ligand.

## References

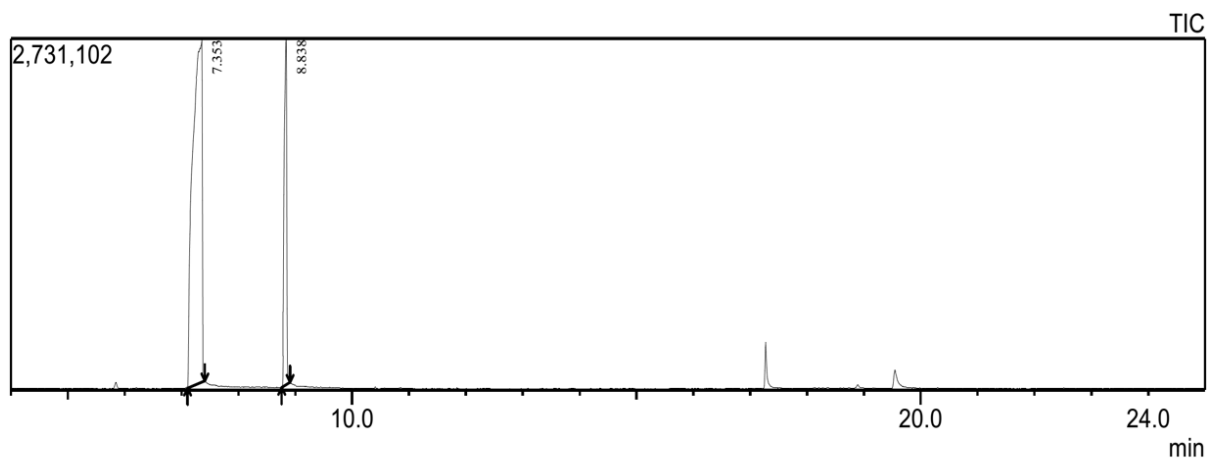
- 1 O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, *J. Appl. Cryst.*, 2009, **42**, 339-341.
- 2 G. M. Sheldrick, *Acta Cryst. A*, 2008, **64**, 112-122.
- 3 G. M. Sheldrick, *Acta Cryst. Sect. Found. Adv.*, 2015, **71**, 3-8.
- 4 J. M. Guevara-Vela, T. Rocha-Rinza and Á. M. Pendás, *Theor. Chem. Acc.*, 2017, **136**, 57.
- 5 L. Goerigk, in *Non-Covalent Interactions in Quantum Chemistry and Physics*, Elsevier, 2017, pp. 195-219.
- 6 J. Zhang, H. Zhang, T. Wu, Q. Wang and D. Van Der Spoel, *J. Chem. Theory Comput.*, 2017, **13**, 1034-1043.

## Calibration curve



**GCMS of data for catalyst screening for the transfer hydrogenation of cyclohexanone (Table 1)**

**Entry 1**



Peak Report TIC

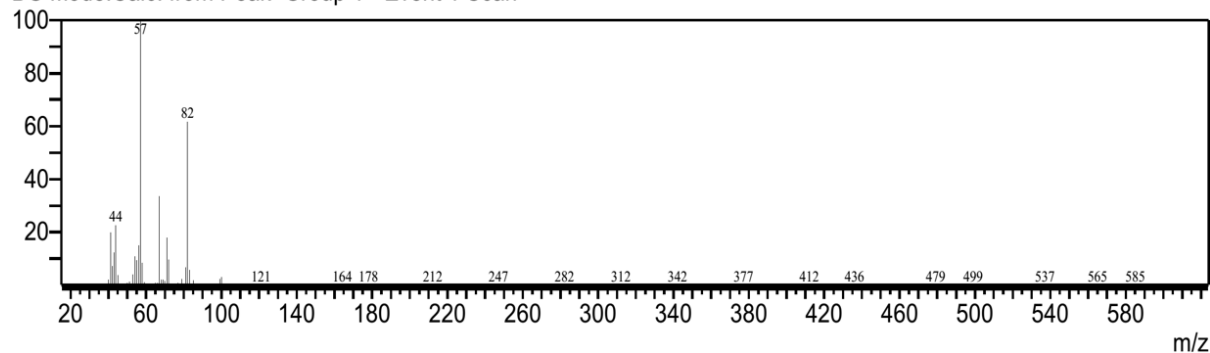
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	7.353	10404150	79.00	2657481	49.72	11.44	Cyclohexanol
2	8.838	8081406	21.00	2687791	50.28	3.01	Decane
		8485556	100.00	5345272	100.00		

Line#:1 R.Time:7.355(Scan#:672)

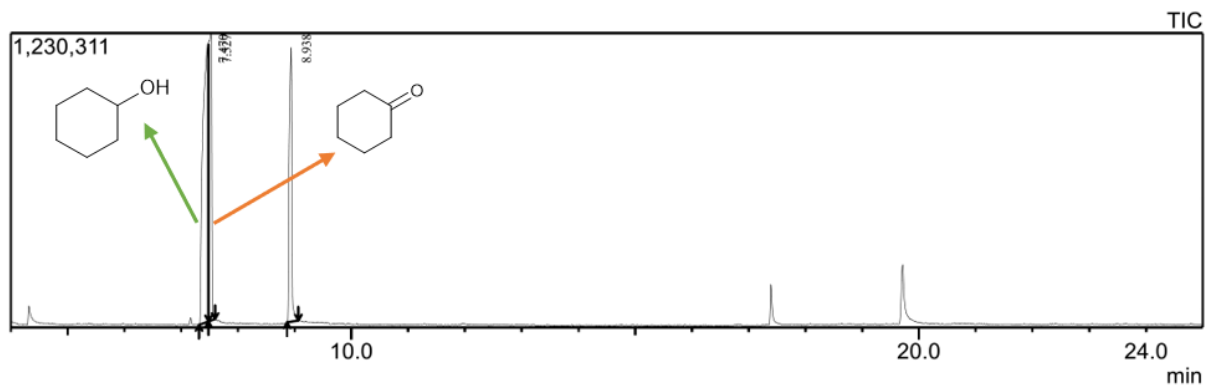
MassPeaks:307

RawMode:Averaged 7.350-7.360(671-673) BasePeak:57(683424)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan



Entry 2



Peak Report TIC

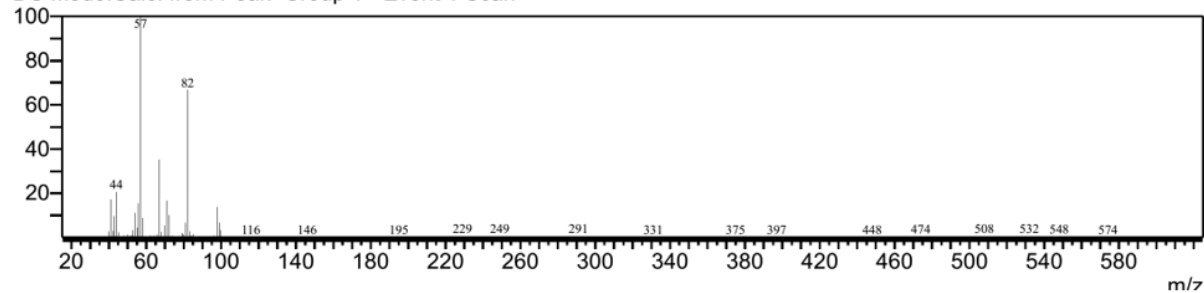
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	7.470	7766528	49.68	1162930	33.14	6.68	Cyclohexanol
2	7.527	4356119	27.87	1200477	34.21	3.63	Cyclohexanone
3	8.938	3509492	22.45	1145771	32.65	3.06	Decane
		5632139	100.00	3509178	100.00		

Line#:1 R.Time:7.470(Scan#:695)

MassPeaks:307

RawMode:Averaged 7.465-7.475(694-696) BasePeak:57(19096)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan

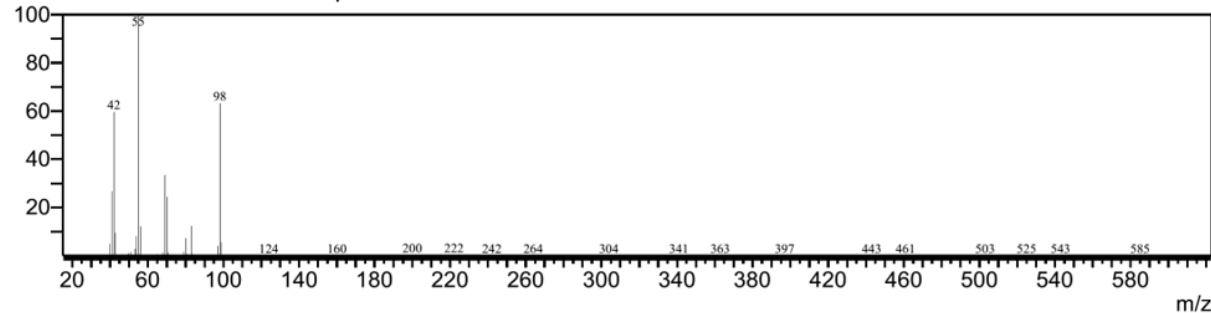


Line#:2 R.Time:7.525(Scan#:706)

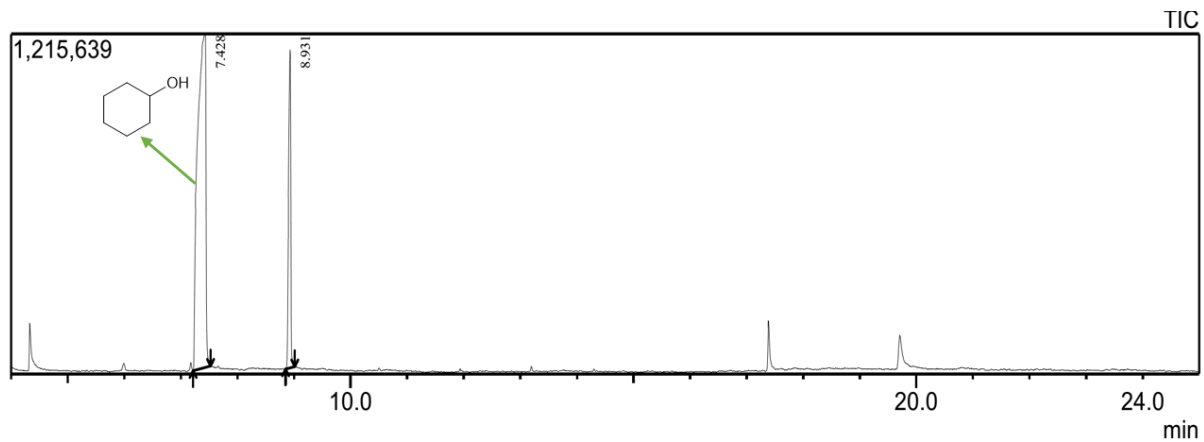
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Entry 3



Peak Report TIC

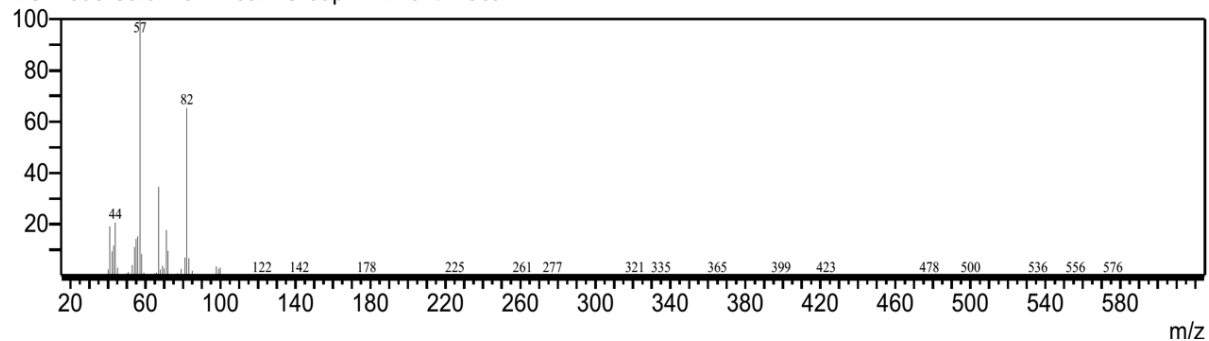
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	7.428	2045105	79.44	1190965	51.16	10.11	Cyclohexanol
2	8.931	3117356	20.56	1136795	48.84	2.74	Decane
		5162461	100.00	2327760	100.00		

Line#:1 R.Time:7.430(Scan#:687)

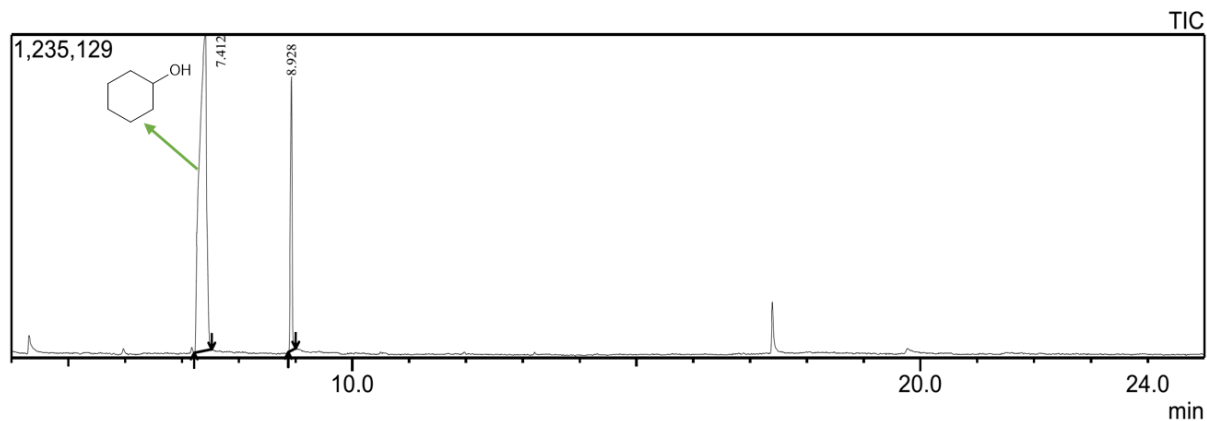
MassPeaks:285

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BG Mode:Calc. from Peak Group 1 - Event 1 Scan



Entry 4



Peak Report TIC

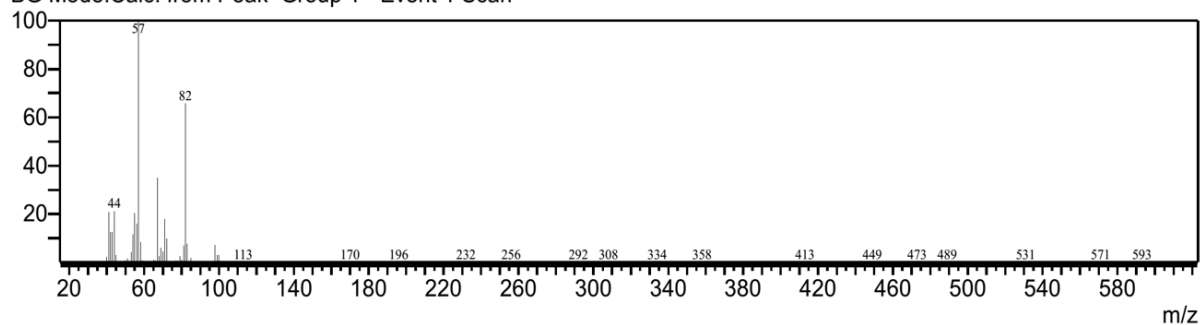
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	7.412	0635183	82.57	1206645	53.58	8.81	Cyclohexanol
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		2880120	100.00	2252123	100.00		

Line#:1 R.Time:7.410(Scan#:683)

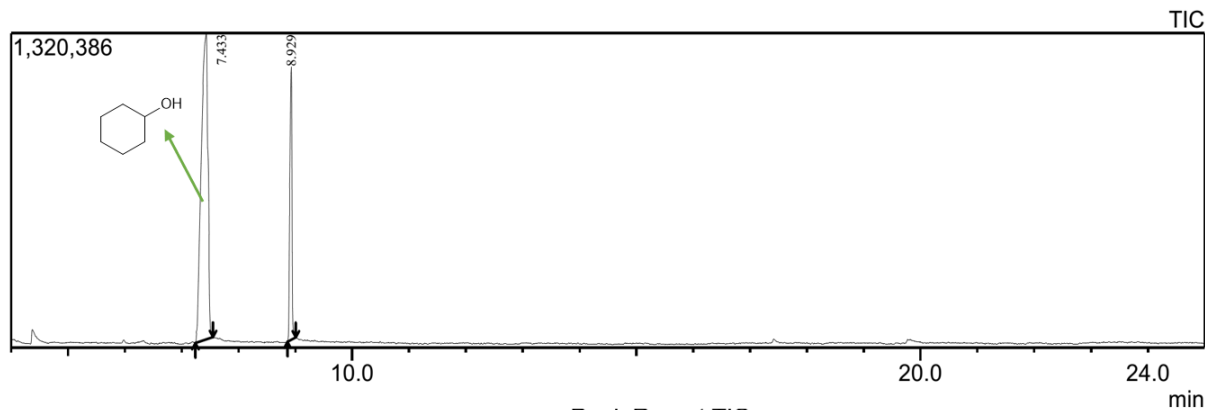
MassPeaks:226

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BG Mode:Calc. from Peak Group 1 - Event 1 Scan



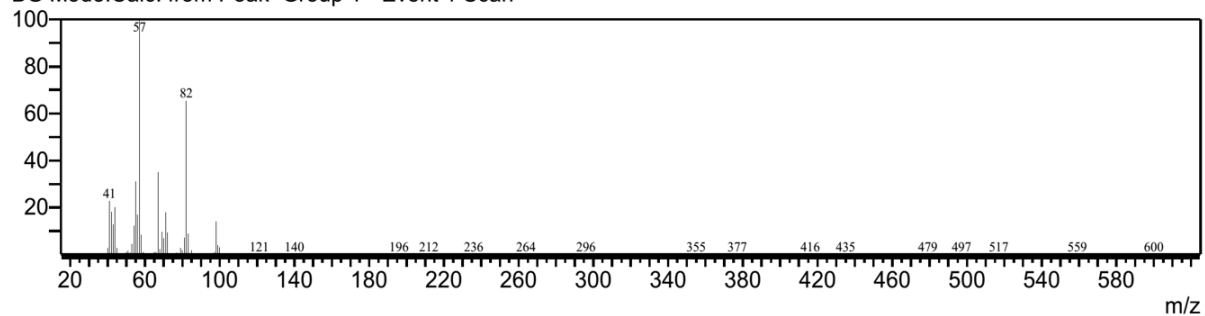
Entry 5



Peak Report TIC

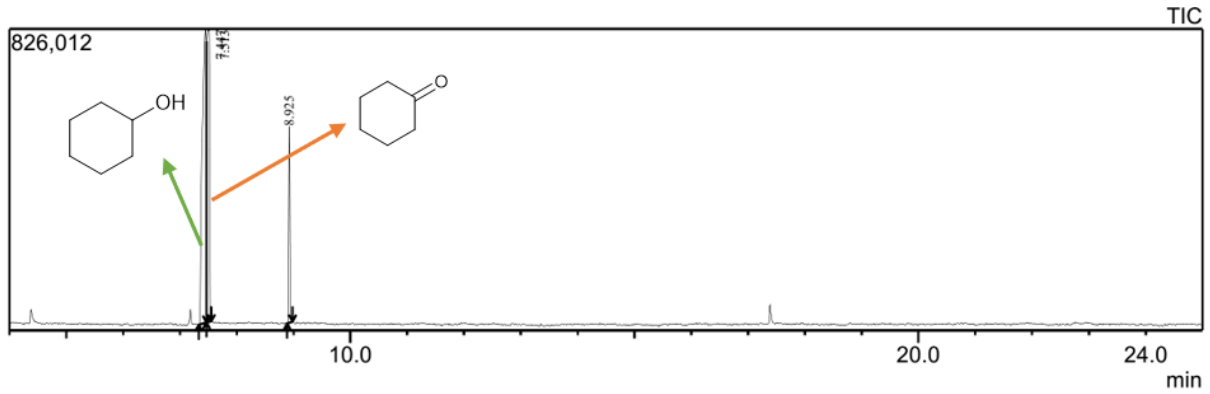
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	7.433	0484852	77.34	1284251	52.86	8.16	Cyclohexanol
2	8.929	3072818	22.66	1145472	47.14	2.68	Decane
		3557670	100.00	2429723	100.00		

Line#:1 R.Time:7.430(Scan#:687)  
 MassPeaks:318  
 RawMode:Averaged 7.425-7.435(686-688) BasePeak:57(283343)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Scan





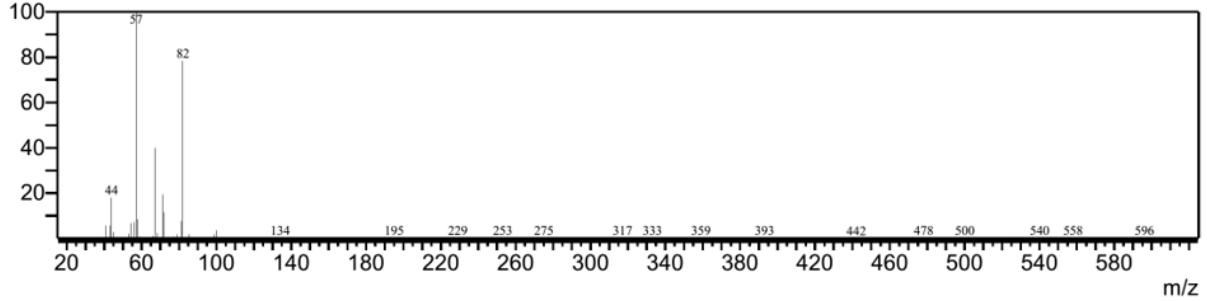
Entry 6



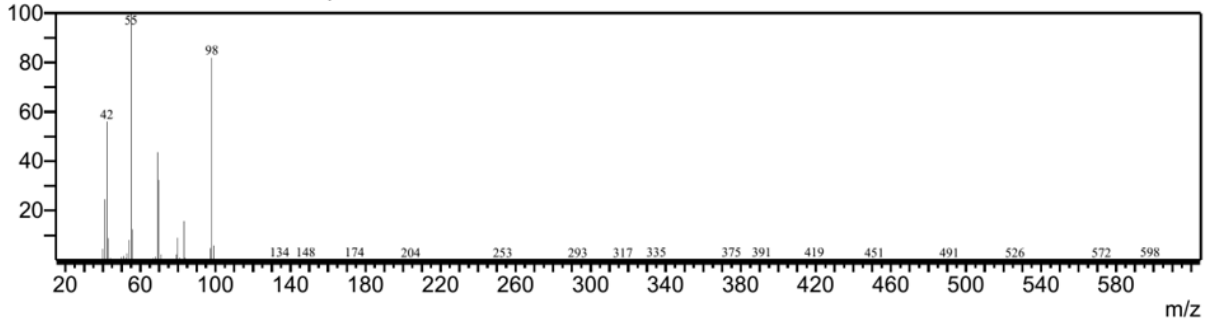
Peak Report TIC

Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	7.447	3938880	52.53	803580	37.49	4.90	Cyclohexanol
2	7.513	2798607	37.33	801603	37.40	3.49	Cyclohexanone
3	8.925	760347	10.14	538290	25.11	1.41	Decane
		7497834	100.00	2143473	100.00		

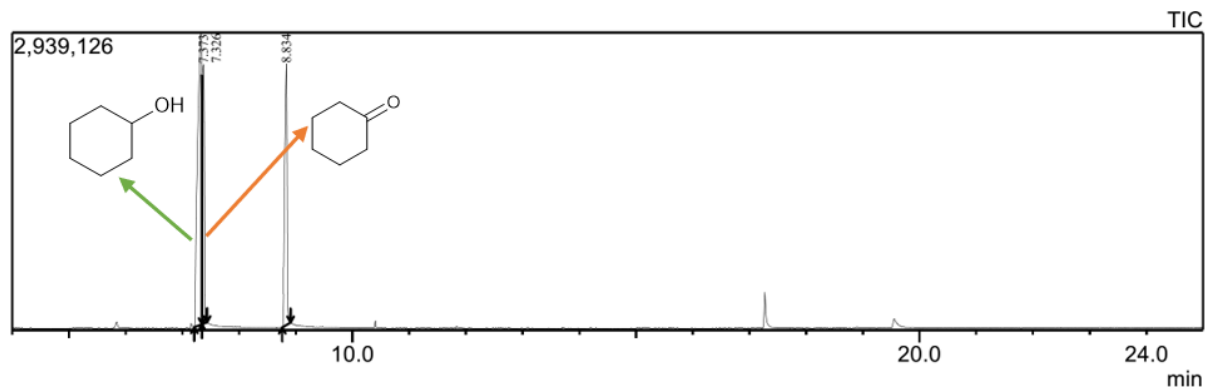
Line#:1 R.Time:7.445(Scan#:690)  
 MassPeaks:294  
 RawMode:Averaged 7.440-7.450(689-691) BasePeak:57(66930)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Scan



Line#:2 R.Time:7.515(Scan#:704)  
 MassPeaks:270  
 RawMode:Averaged 7.510-7.520(703-705) BasePeak:55(108652)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Scan



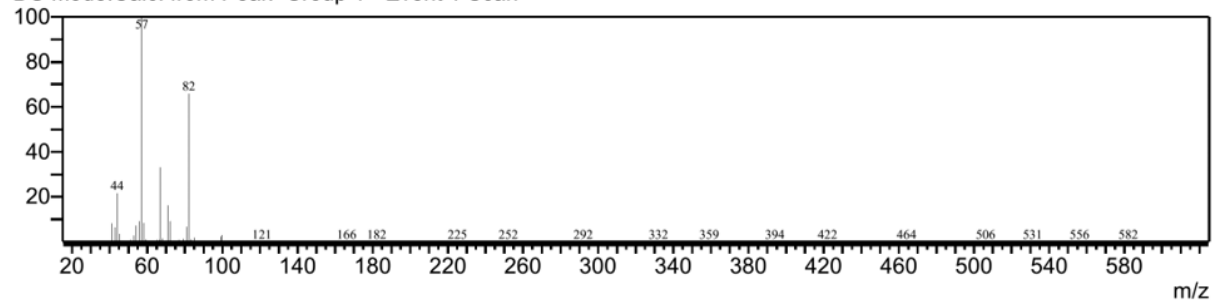
Entry 7



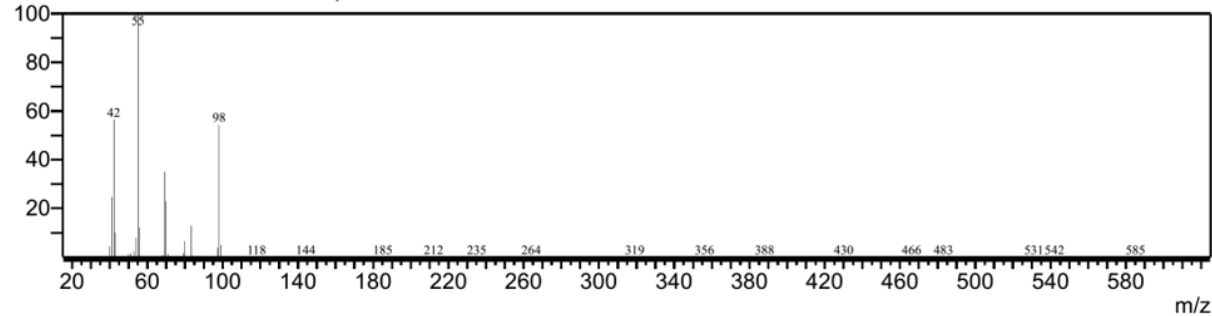
Peak Report TIC

Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	7.326	4904418	50.79	2883320	35.93	5.17	Cyclohexanol
2	7.373	7085261	24.14	2561137	31.92	2.77	Cyclohexanone
3	8.834	7355587	25.07	2579457	32.15	2.85	Decane
		9345266	100.00	8023914	100.00		

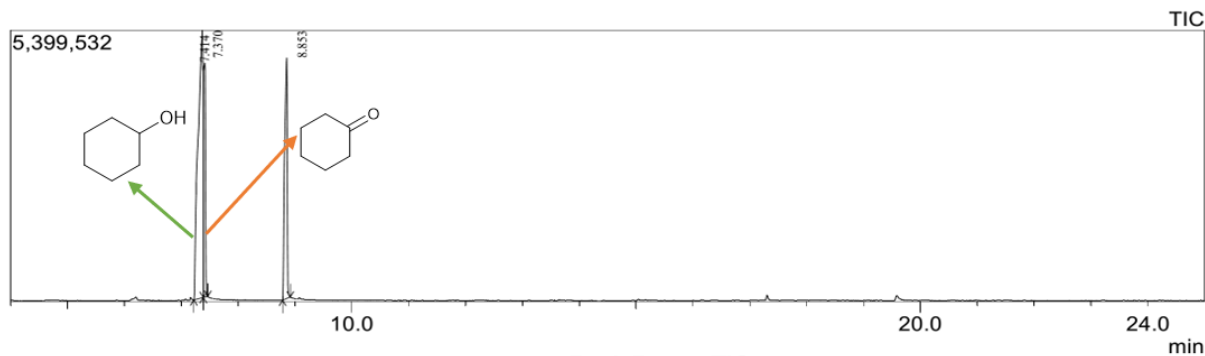
Line#:1 R.Time:7.325(Scan#:666)  
 MassPeaks:257  
 RawMode:Averaged 7.320-7.330(665-667) BasePeak:57(350605)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Scan



Line#:2 R.Time:7.370(Scan#:675)  
 MassPeaks:274  
 RawMode:Averaged 7.365-7.375(674-676) BasePeak:55(213232)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Scan



Entry 8



Peak Report TIC

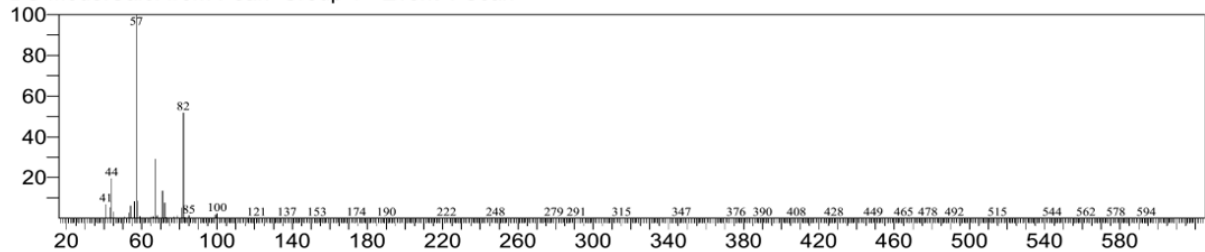
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	7.370	3557488	57.80	5323602	36.05	6.30	Cyclohexanol
2	7.414	0007548	17.24	4658970	31.55	2.15	Cyclohexanone
3	8.853	4496621	24.97	4786214	32.41	3.03	Decane
		8061657	100.00	14768786	100.00		

Line#:1 R.Time:7.370(Scan#:675)

MassPeaks:265

RawMode:Averaged 7.365-7.375(674-676) BasePeak:57(733423)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan

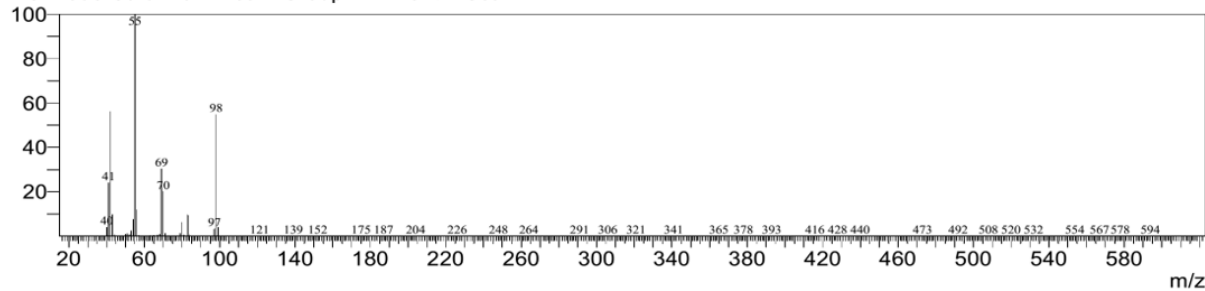


Line#:2 R.Time:7.415(Scan#:684)

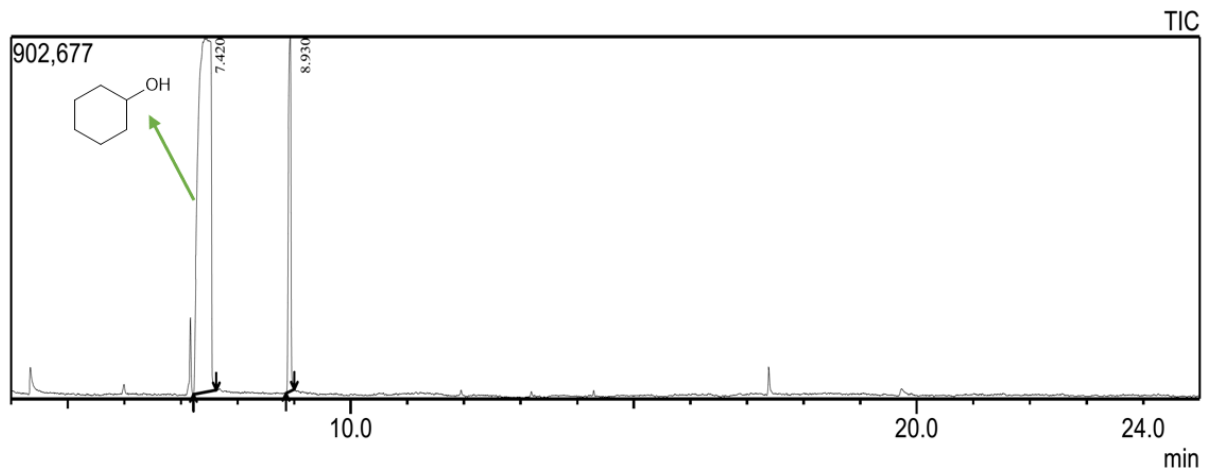
MassPeaks:305

RawMode:Averaged 7.410-7.420(683-685) BasePeak:55(456381)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan



Entry 9



Peak Report TIC

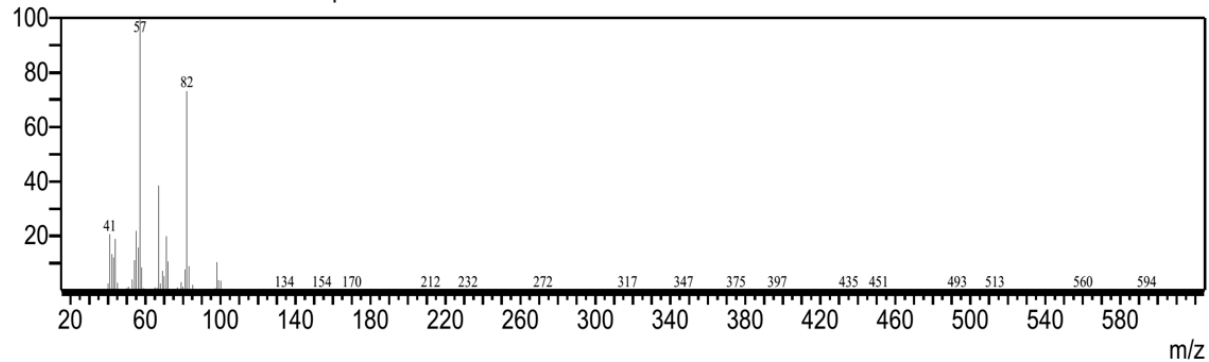
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	7.420	3675192	82.96	884264	50.04	15.47	Cyclohexanol
2	8.930	2807947	17.04	882892	49.96	3.18	Decane
		6483139	100.00	1767156	100.00		

Line#:1 R.Time:7.420(Scan#:685)

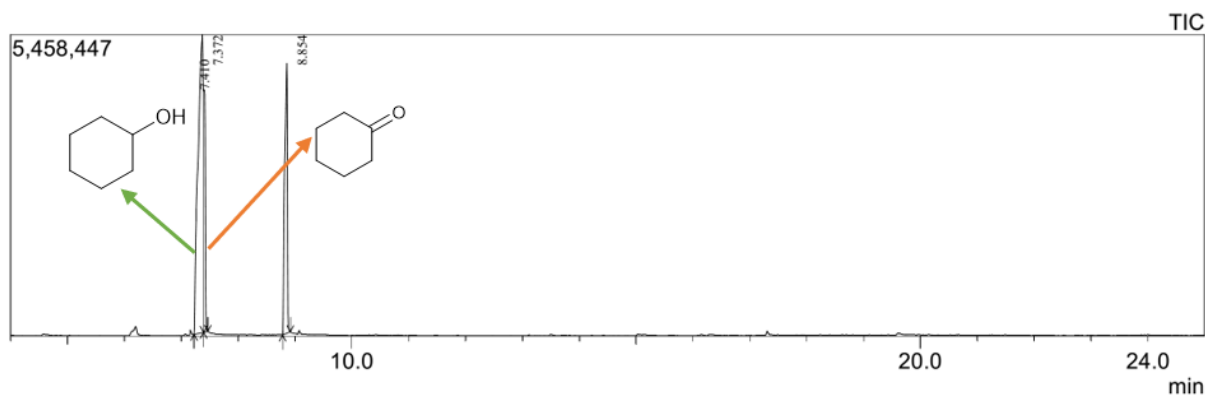
MassPeaks:311

RawMode:Averaged 7.415-7.425(684-686) BasePeak:57(202156)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan



Entry 10



Peak Report TIC

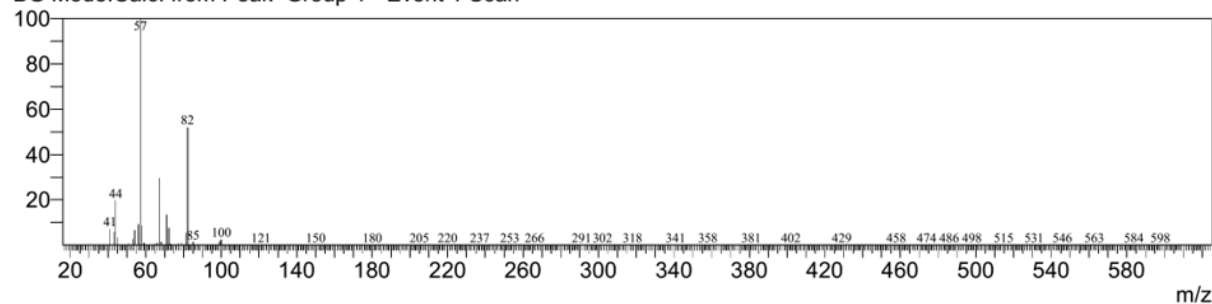
Peak#	R. Time	Area	Area%	Height	Height%	A/H	Name
1	7.372	5375207	61.43	5390310	36.81	6.56	Cyclohexanol
2	7.410	7348629	12.76	4369078	29.83	1.68	Cyclohexanone
3	8.854	4865728	25.81	4885581	33.36	3.04	Decane
		7589564	100.00	14644969	100.00		

Line#:1 R.Time:7.370(Scan#:675)

MassPeaks:286

RawMode:Averaged 7.365-7.375(674-676) BasePeak:57(865936)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan

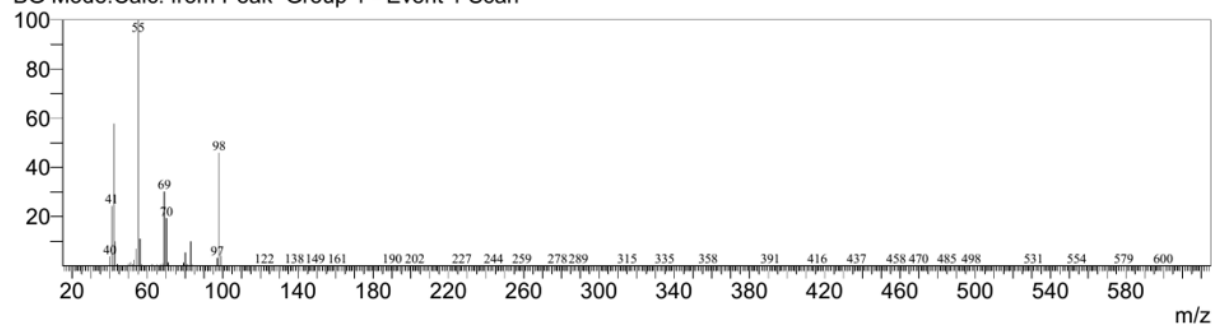


Line#:2 R.Time:7.410(Scan#:683)

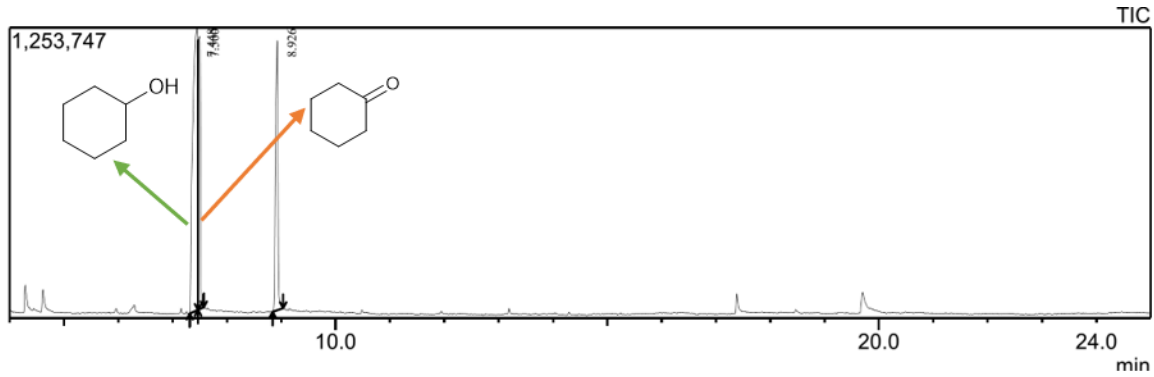
MassPeaks:282

RawMode:Averaged 7.405-7.415(682-684) BasePeak:55(266825)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan



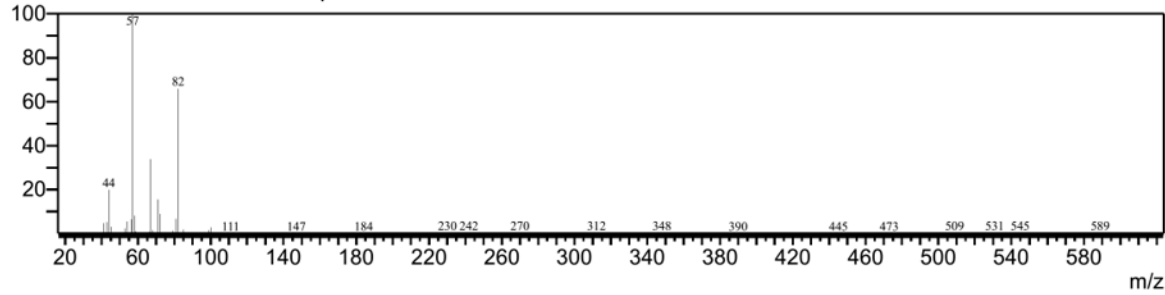
Entry 11



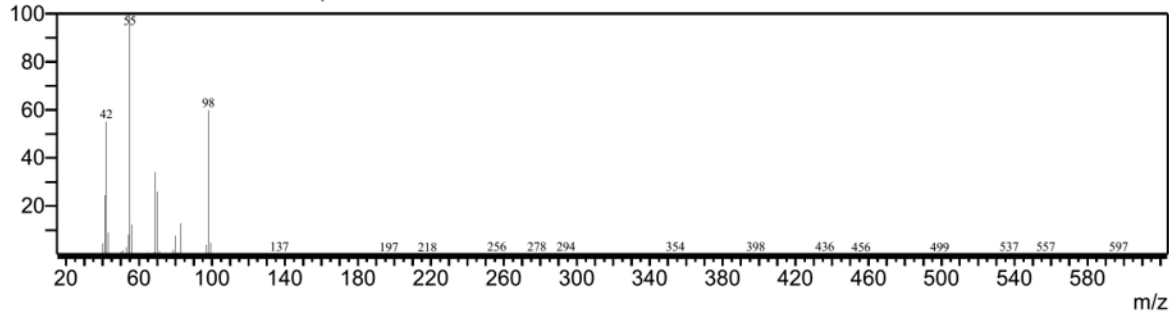
Peak Report TIC

Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	7.448	7882749	53.16	1218692	34.26	6.47	Cyclohexanol
2	7.500	3267537	22.04	1175706	33.05	2.78	Cyclohexanone
3	8.926	3676768	24.80	1162884	32.69	3.16	Decane
		4827054	100.00	3557282	100.00		

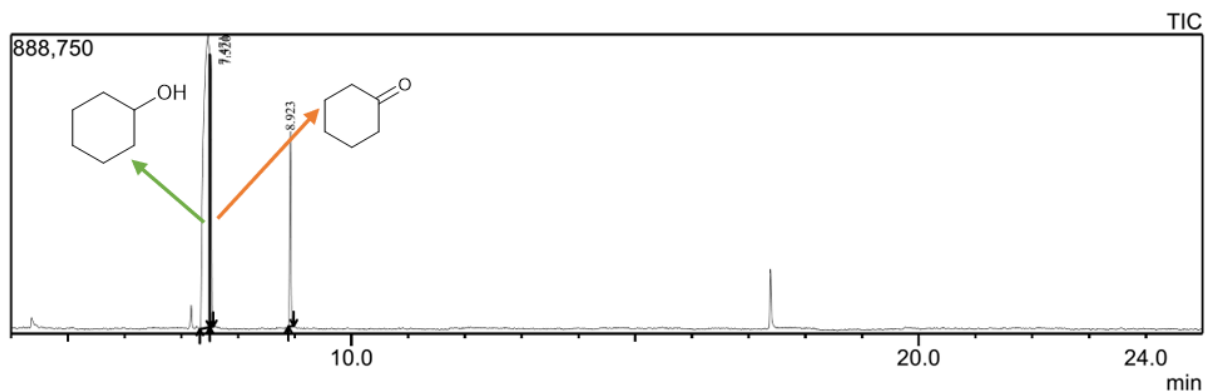
Line#:1 R.Time:7.445(Scan#:690)  
 MassPeaks:289  
 RawMode:Averaged 7.440-7.450(689-691) BasePeak:57(146557)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Scan



Line#:2 R.Time:7.500(Scan#:701)  
 MassPeaks:289  
 RawMode:Averaged 7.495-7.505(700-702) BasePeak:55(104862)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Scan



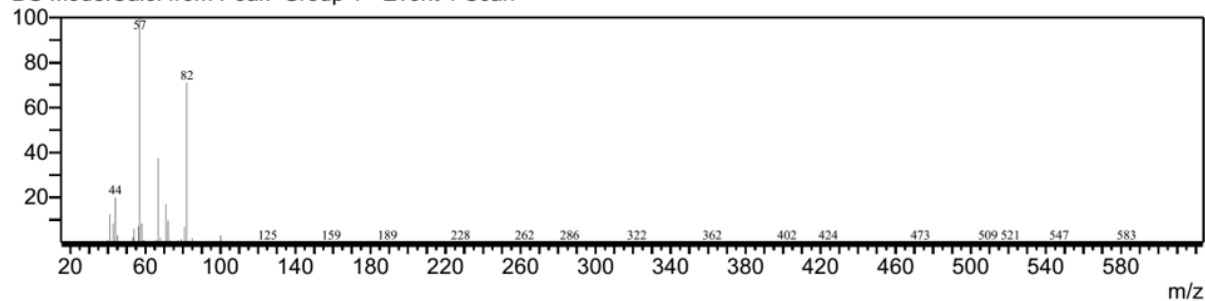
Entry 12



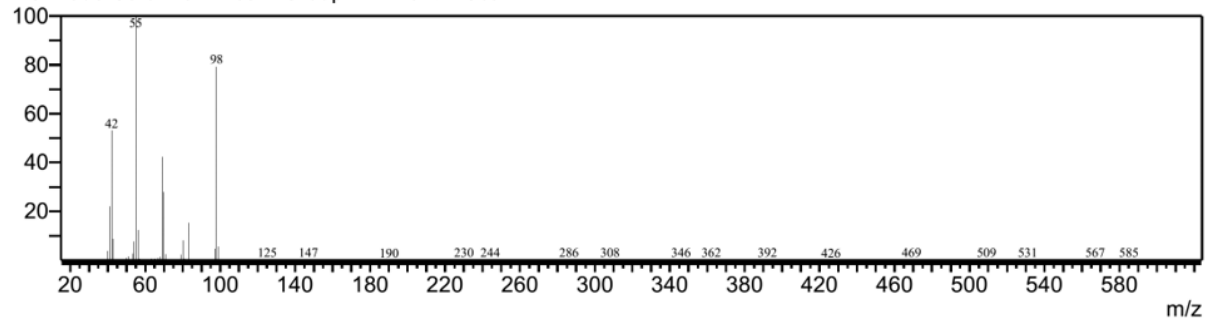
Peak Report TIC

Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	7.471	6603588	73.81	869848	38.53	7.59	Cyclohexanol
2	7.520	1450298	16.21	809008	35.83	1.79	Cyclohexanone
3	8.923	892504	9.98	578849	25.64	1.54	Decane
		8946390	100.00	2257705	100.00		

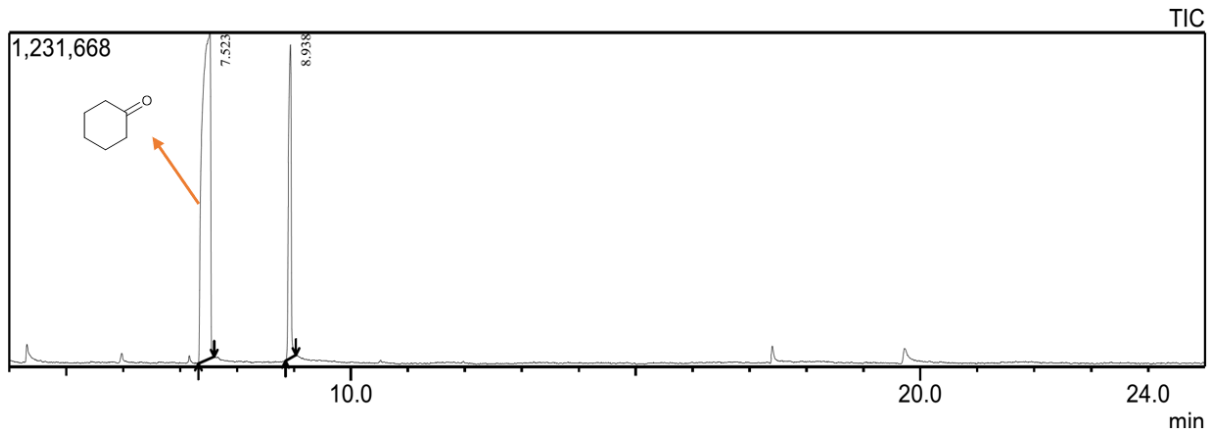
Line#:1 R.Time:7.470(Scan#:695)  
 MassPeaks:302  
 RawMode:Averaged 7.465-7.475(694-696) BasePeak:57(119335)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Scan



Line#:2 R.Time:7.520(Scan#:705)  
 MassPeaks:307  
 RawMode:Averaged 7.515-7.525(704-706) BasePeak:55(53656)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Scan



Entry 13



Peak Report TIC

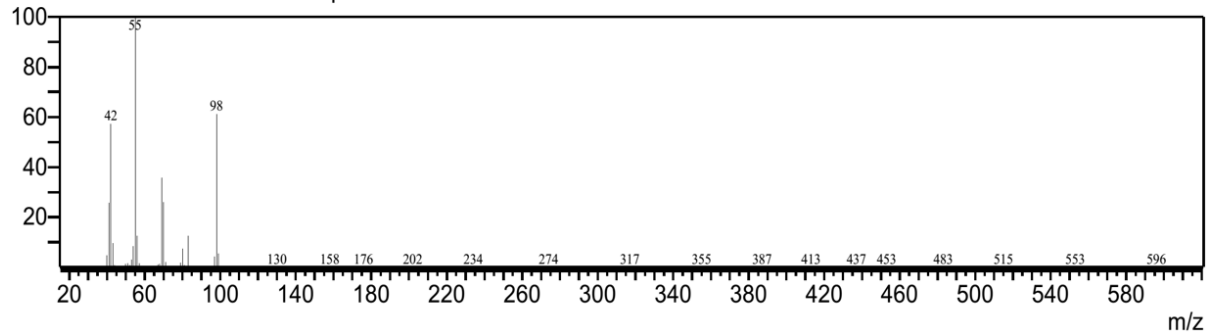
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	7.523	2271639	76.30	1199608	50.92	10.23	Cyclohexanone
2	8.938	3812559	23.70	1156046	49.08	3.30	Decane
		6084198	100.00	2355654	100.00		

Line#:1 R.Time:7.525(Scan#:706)

MassPeaks:265

RawMode:Averaged 7.520-7.530(705-707) BasePeak:55(307979)

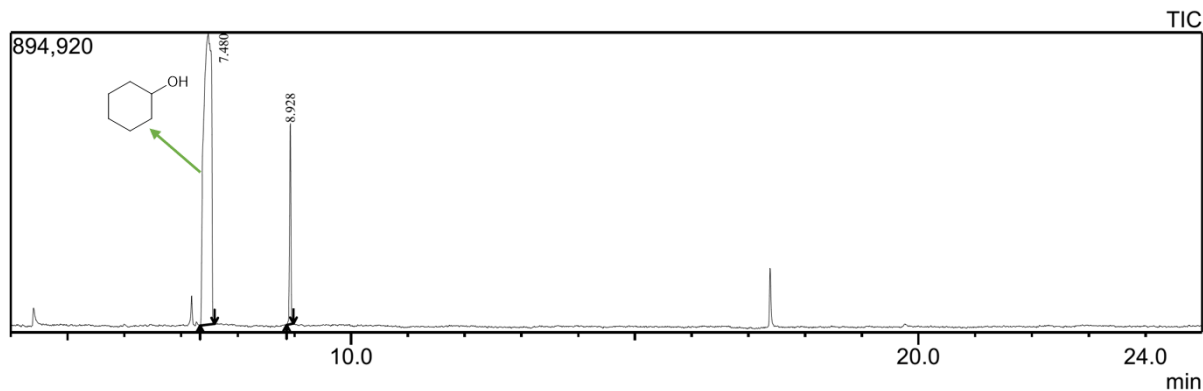
BG Mode:Calc. from Peak Group 1 - Event 1 Scan





## GCMS of Base optimization for the Transfer Hydrogenation of cyclohexanone (Table 2)

### Entry 1



Peak Report TIC

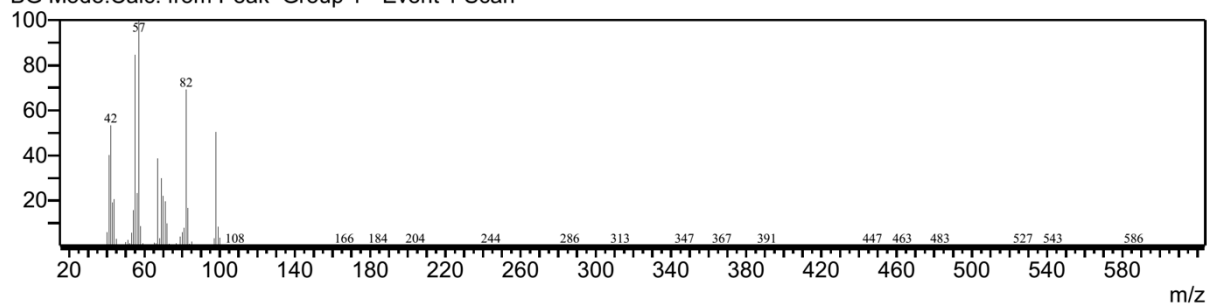
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	7.480	8297012	89.54	871051	59.27	9.53	Cyclohexanol
2	8.928	969652	10.46	598501	40.73	1.62	Decane
		9266664	100.00	1469552	100.00		

Line#:1 R.Time:7.480(Scan#:697)

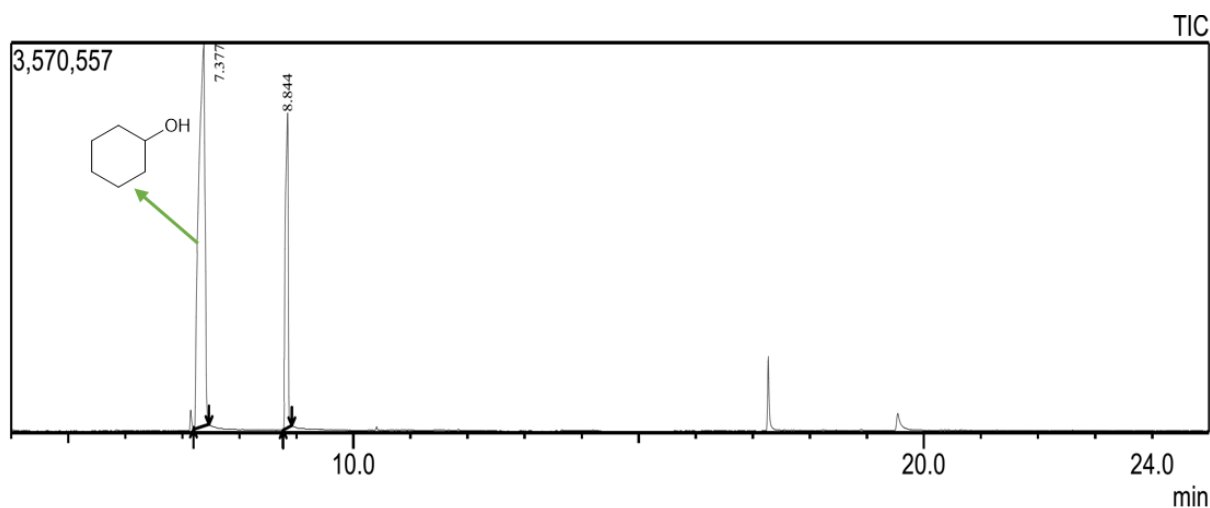
MassPeaks:339

RawMode:Averaged 7.475-7.485(696-698) BasePeak:57(125814)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan



**Entry 2**



Peak Report TIC

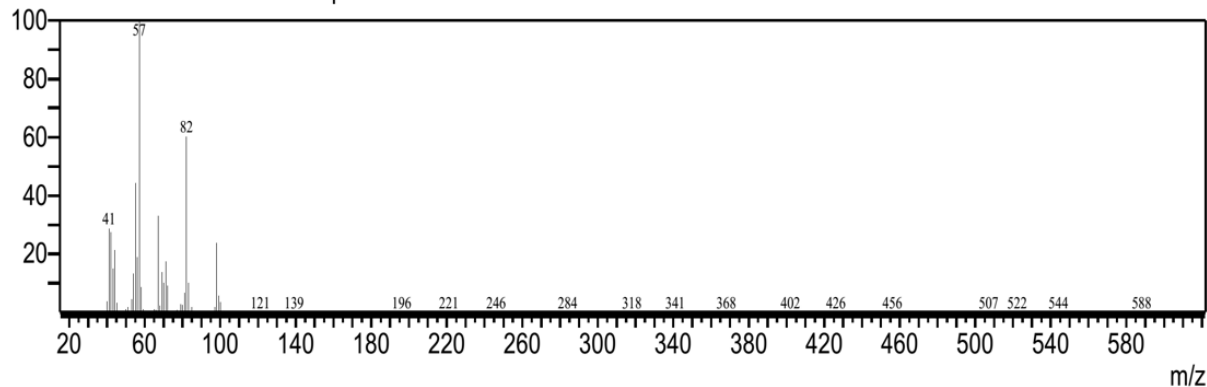
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	7.377	27160971	73.62	3505164	54.90	7.75	Cyclohexanol
2	8.844	9730795	26.38	2879758	45.10	3.38	Decane
		36891766	100.00	6384922	100.00		

Line#:1 R.Time:7.375(Scan#:676)

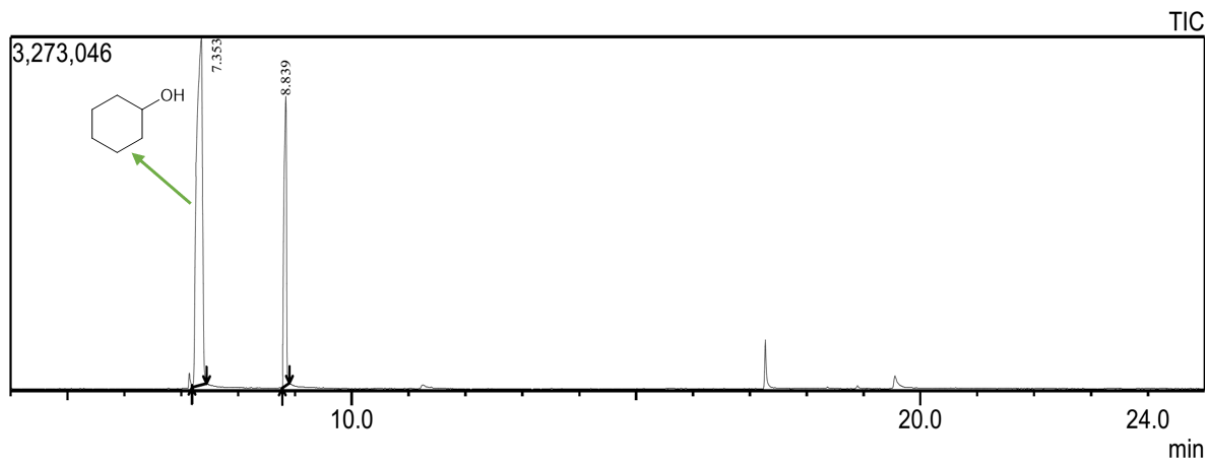
MassPeaks:269

RawMode:Averaged 7.370-7.380(675-677) BasePeak:57(692530)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan



**Entry 3**



Peak Report TIC

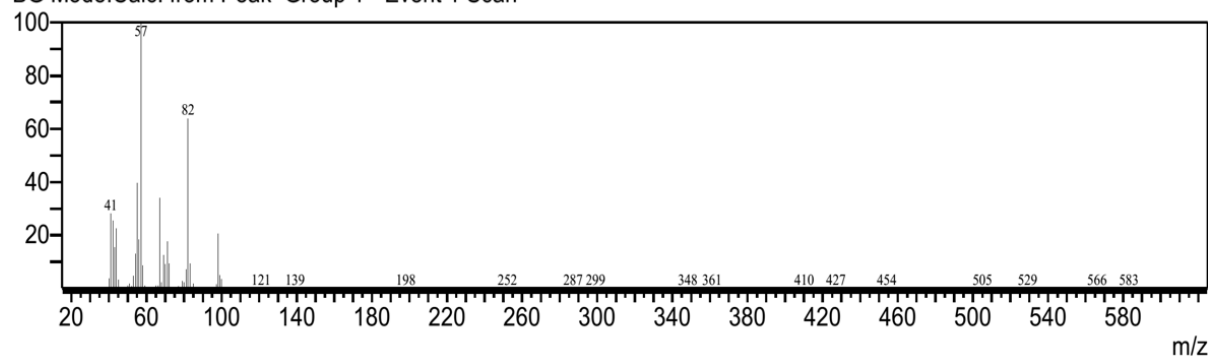
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	7.353	2979637	74.06	3215528	54.60	7.15	Cyclohexanol
2	8.839	8047814	25.94	2674194	45.40	3.01	Decane
		1027451	100.00	5889722	100.00		

Line#:1 R.Time:7.355(Scan#:672)

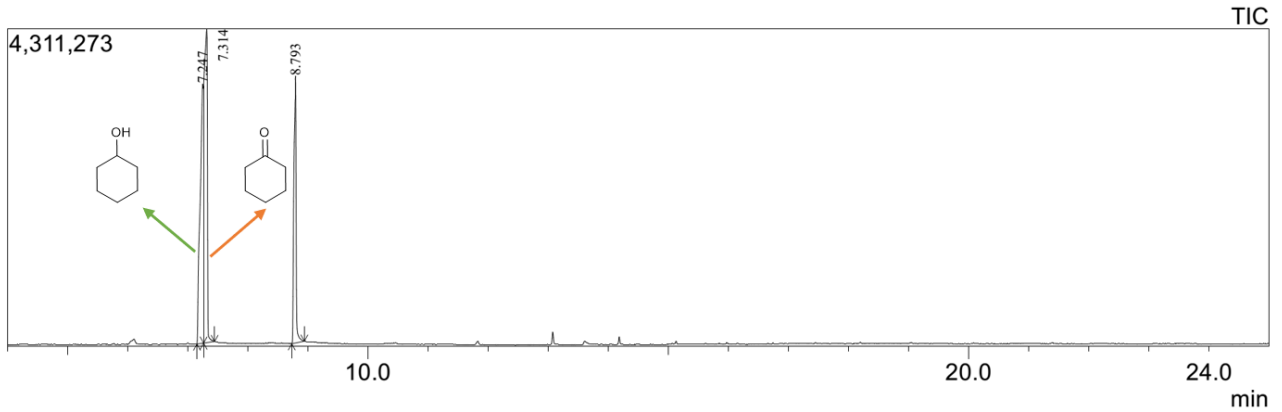
MassPeaks:308

RawMode:Averaged 7.350-7.360(671-673) BasePeak:57(636311)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan



Entry 4



Peak Report TIC

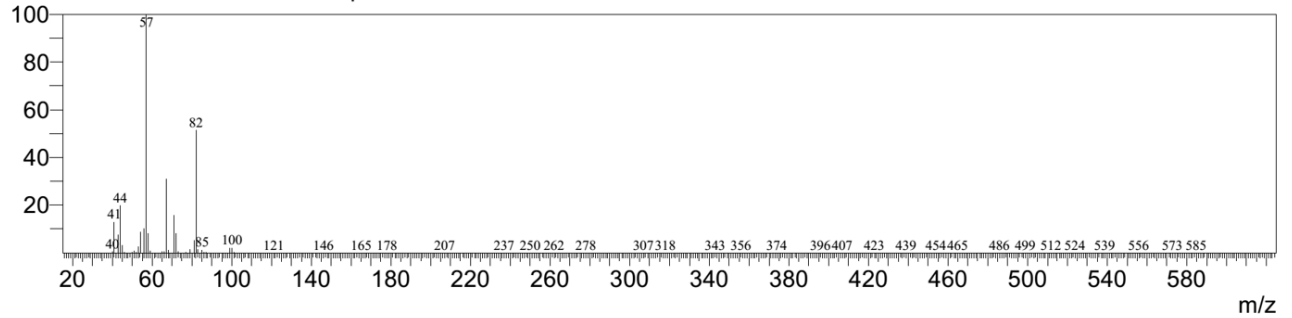
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	7.247	3275239	34.12	3523144	30.88	3.77	Cyclohexanol
2	7.314	5797500	40.60	4259877	37.34	3.71	Cyclohexanone
3	8.793	9835061	25.28	3625197	31.78	2.71	Decane
		8907800	100.00	11408218	100.00		

Line#:1 R.Time:7.245(Scan#:650)

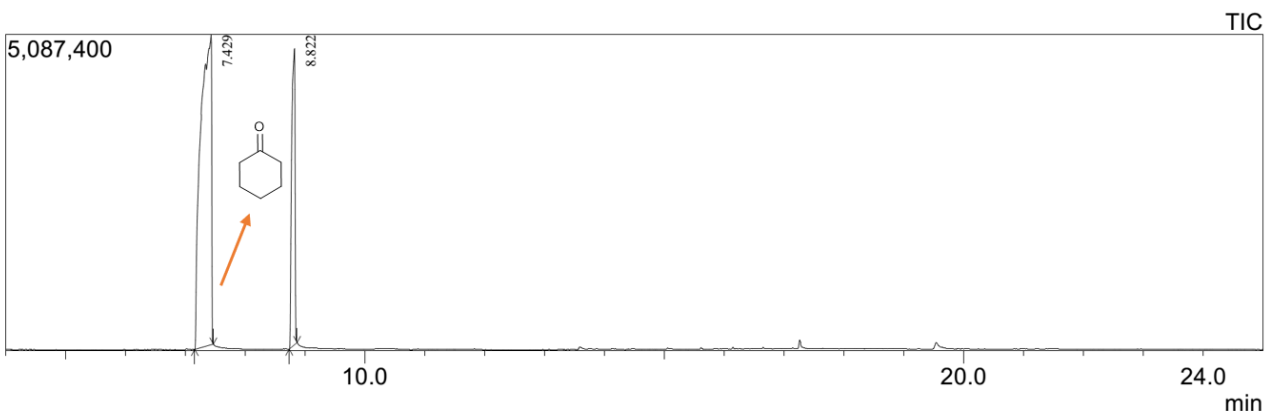
MassPeaks:303

RawMode:Averaged 7.240-7.250(649-651) BasePeak:57(186067)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan



Entry 5



Peak Report TIC

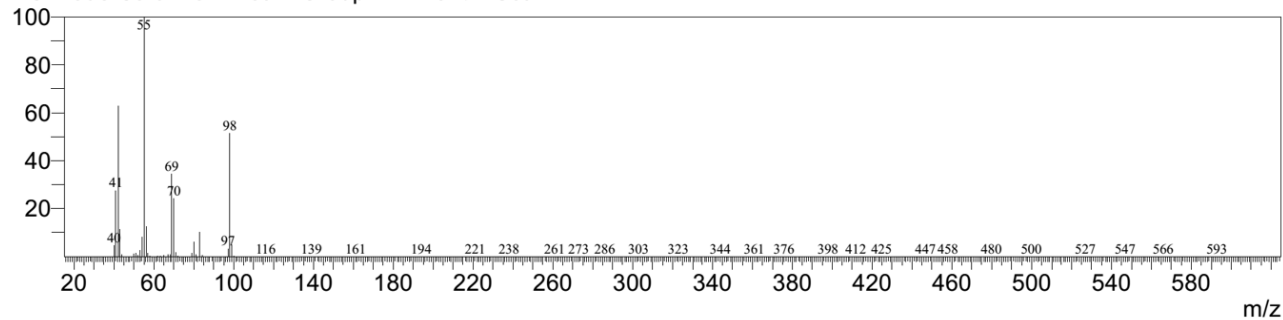
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	7.429	2185999	76.64	4987768	51.14	12.47	Cyclohexanone
2	8.822	8949212	23.36	4765961	48.86	3.98	Decane
		31135211	100.00	9753729	100.00		

Line#:1 R.Time:7.430(Scan#:687)

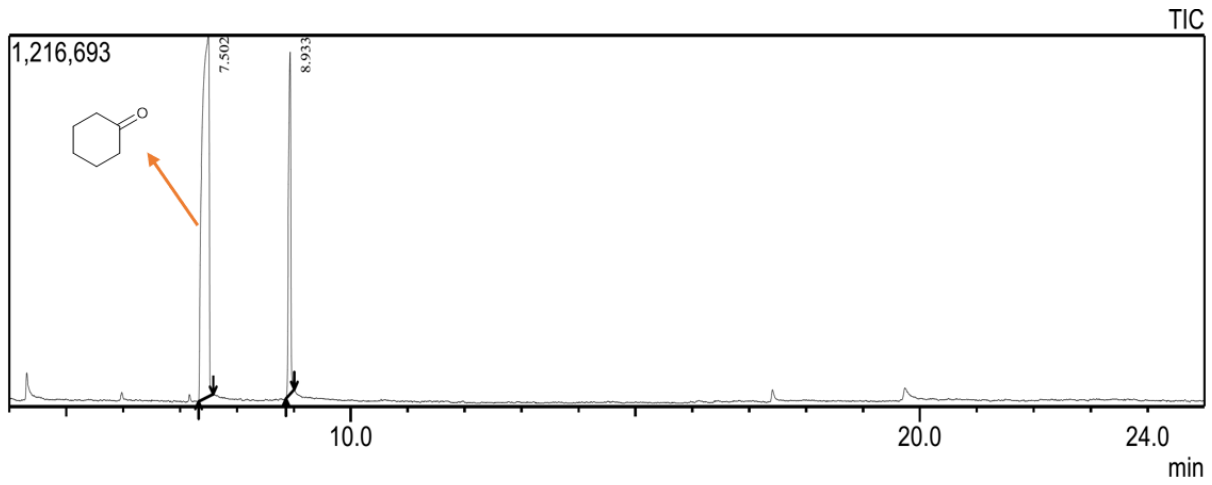
MassPeaks:340

RawMode:Averaged 7.425-7.435(686-688) BasePeak:55(1299627)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan



Entry 6



Peak Report TIC

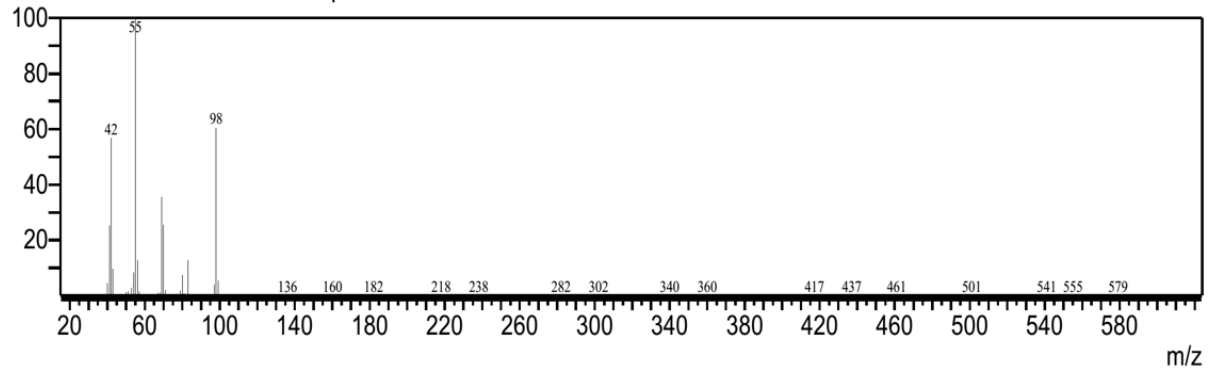
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	7.502	0383725	76.79	1181925	51.33	8.79	Cyclohexanone
2	8.933	3138476	23.21	1120800	48.67	2.80	Decane
		3522201	100.00	2302725	100.00		

Line#:1 R.Time:7.500(Scan#:701)

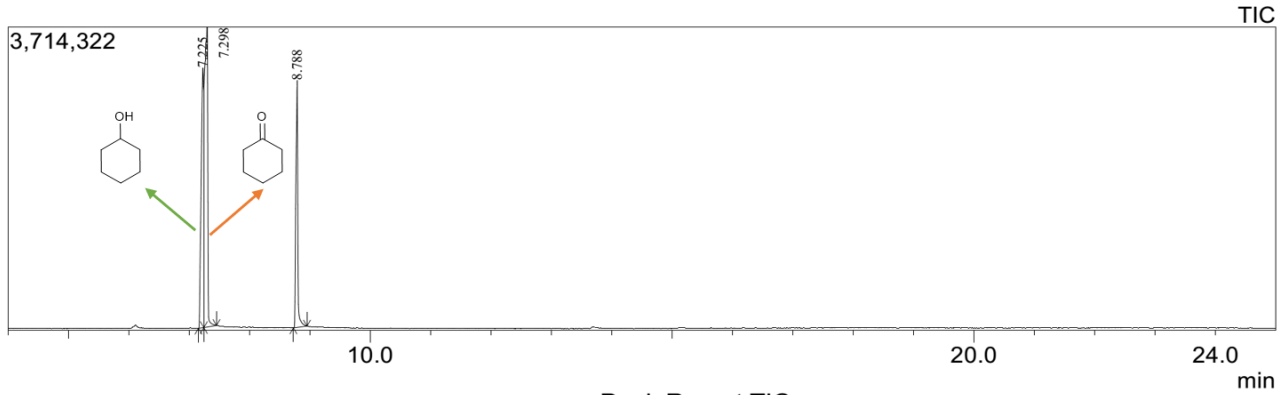
MassPeaks:313

RawMode:Averaged 7.495-7.505(700-702) BasePeak:55(306355)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan



Entry 7



Peak Report TIC

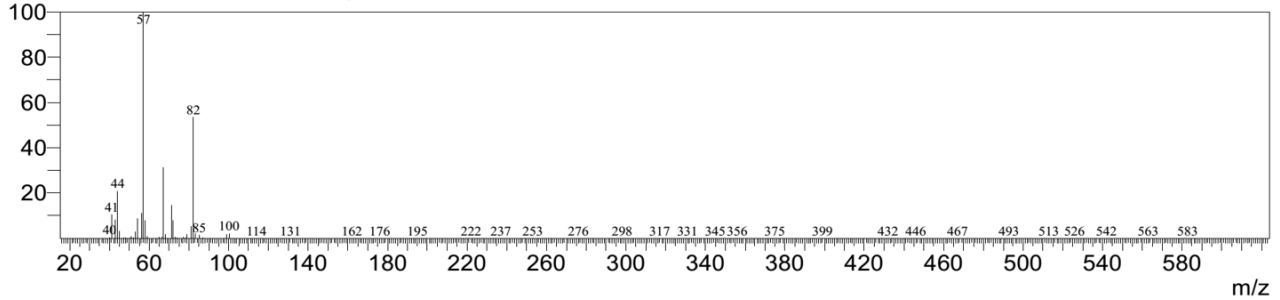
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	7.225	9080785	29.99	3184531	32.23	2.85	Cyclohexanol
2	7.298	3947798	46.07	3671895	37.16	3.80	Cyclohexanone
3	8.788	7249812	23.94	3024663	30.61	2.40	Decane
		10278395	100.00	9881089	100.00		

Line#:1 R.Time:7.225(Scan#:646)

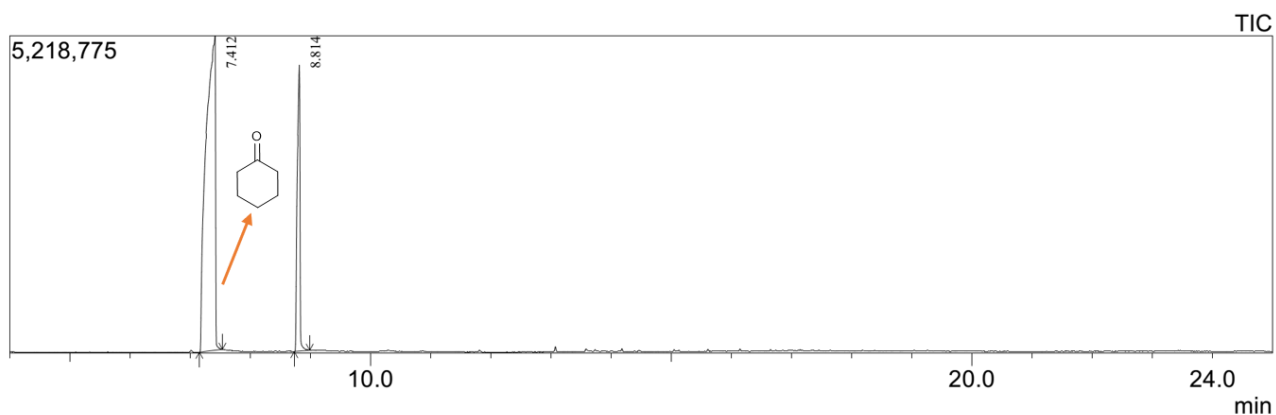
MassPeaks:308

RawMode:Averaged 7.220-7.230(645-647) BasePeak:57(284578)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan



Entry 8



Peak Report TIC

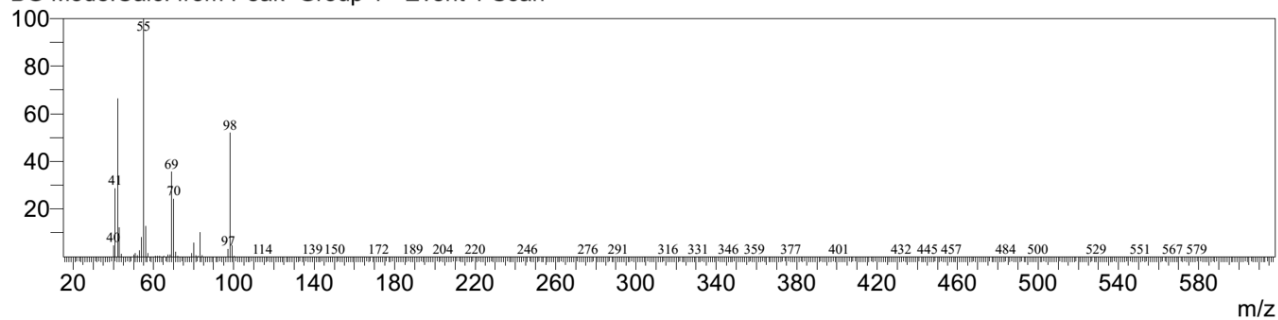
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	7.412	56135544	78.87	5170914	52.34	10.86	Cyclohexanone
2	8.814	5036215	21.13	4708701	47.66	3.19	Decane
		71171759	100.00	9879615	100.00		

Line#:1 R.Time:7.410(Scan#:683)

MassPeaks:326

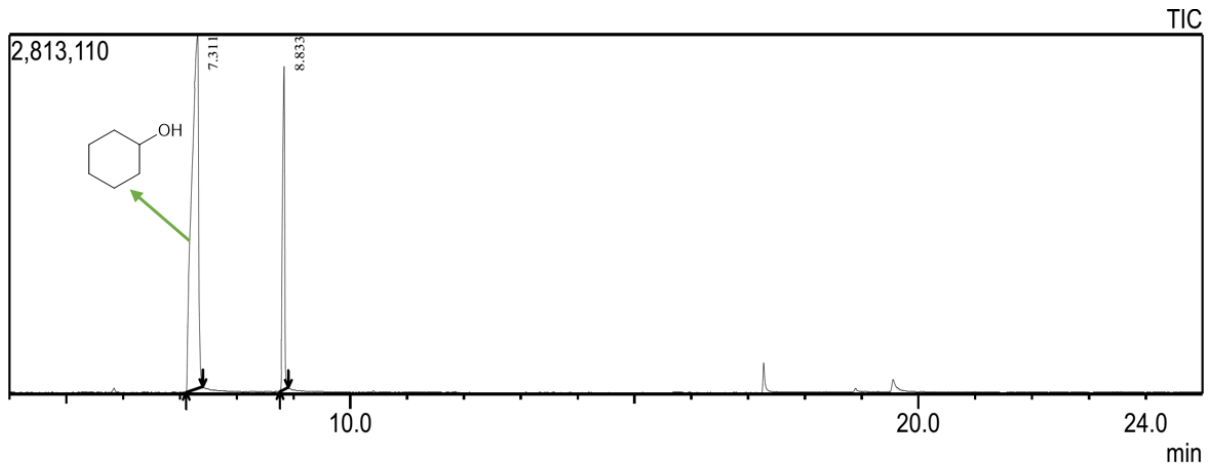
RawMode:Averaged 7.405-7.415(682-684) BasePeak:55(1329410)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan





Entry 9



Peak Report TIC

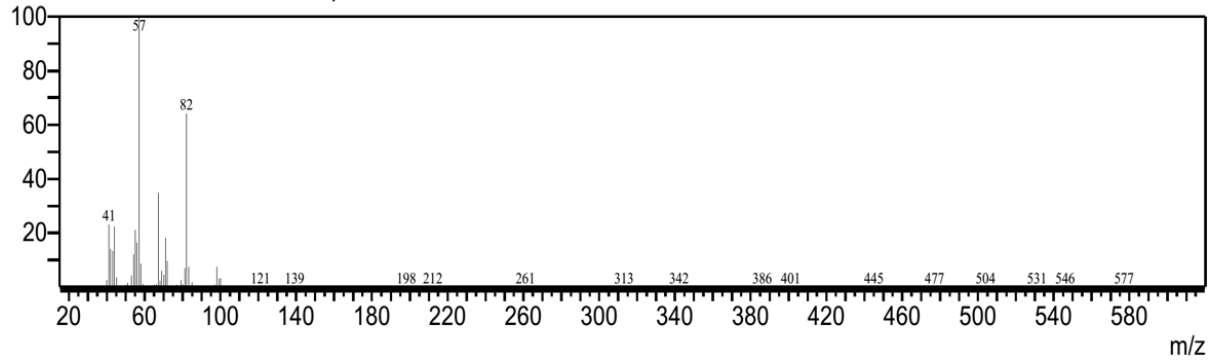
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	7.311	3044057	77.80	2767081	52.25	8.33	Cyclohexanol
2	8.833	6573768	22.20	2529125	47.75	2.60	Decane
		9617825	100.00	5296206	100.00		

Line#:1 R.Time:7.310(Scan#:663)

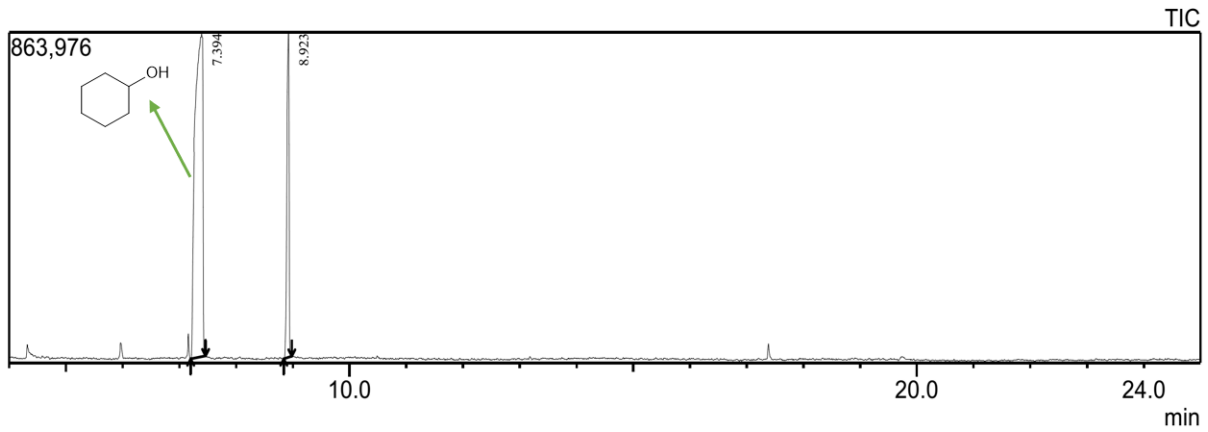
MassPeaks:328

RawMode:Averaged 7.305-7.315(662-664) BasePeak:57(651933)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan



Entry 10



Peak Report TIC

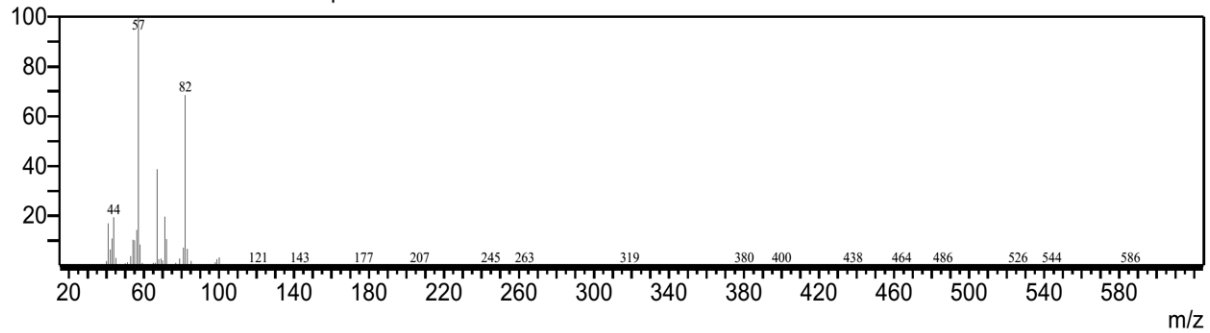
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	7.394	8053202	77.36	843490	49.85	9.55	Cyclohexanol
2	8.923	2356662	22.64	848631	50.15	2.78	Decane
		0409864	100.00	1692121	100.00		

Line#:1 R.Time:7.395(Scan#:680)

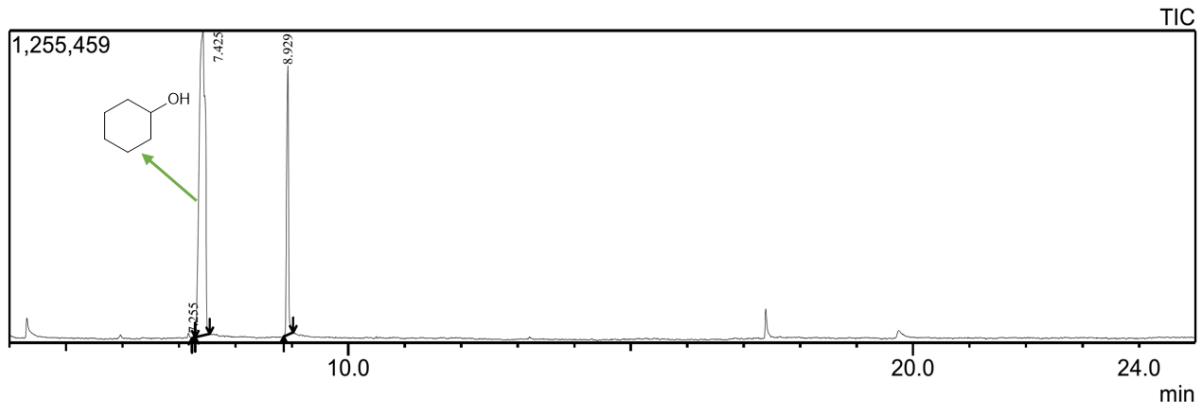
MassPeaks:322

RawMode:Averaged 7.390-7.400(679-681) BasePeak:57(218836)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan



Entry 11



Peak Report TIC

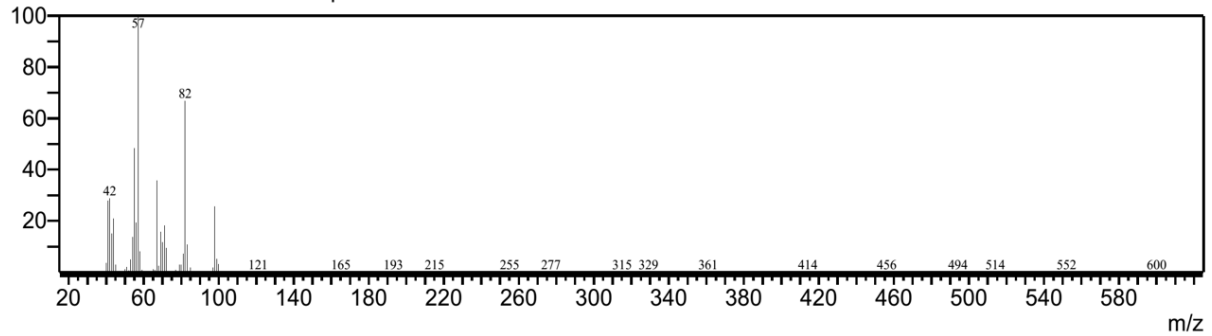
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	7.255	35735	0.30	15223	0.66	2.35	Cyclohexanol
2	7.425	9189175	77.32	1225224	52.74	7.50	Cyclohexanol
3	8.929	2659211	22.38	1082482	46.60	2.46	Decane
		11884121	100.00	2322929	100.00		

Line#:2 R.Time:7.425(Scan#:686)

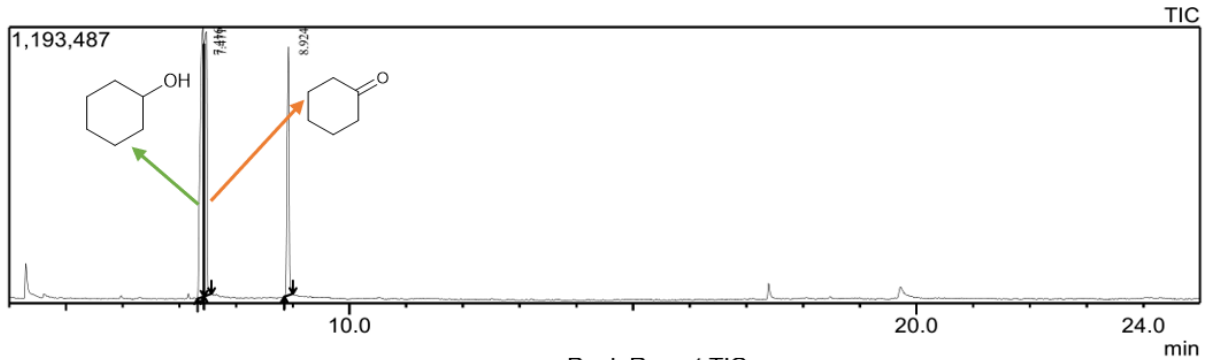
MassPeaks:292

RawMode:Averaged 7.420-7.430(685-687) BasePeak:57(231127)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan



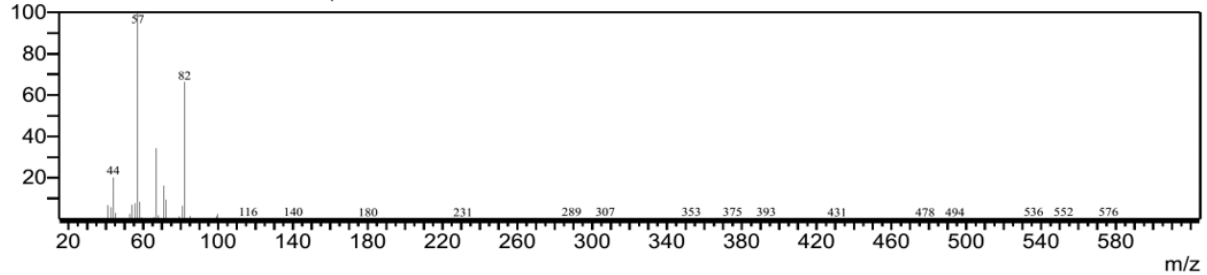
Entry 12



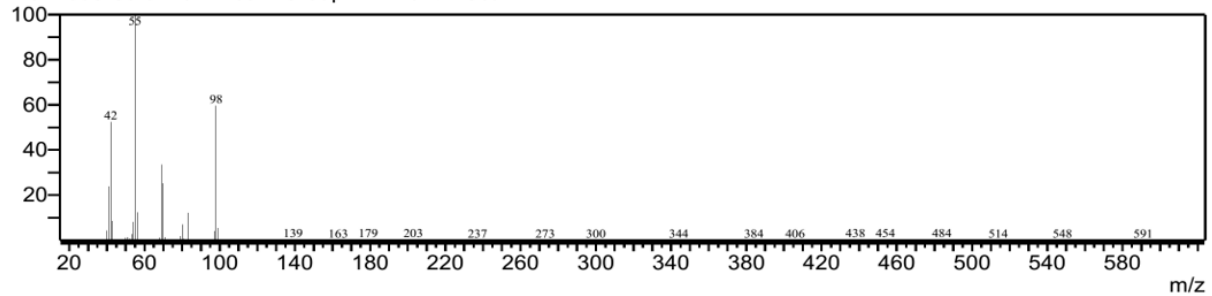
Peak Report TIC

Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	7.416	5344151	44.62	1164728	34.48	4.59	Cyclohexanol
2	7.471	3911335	32.65	1140143	33.75	3.43	Cyclohexanone
3	8.924	2722808	22.73	1073348	31.77	2.54	Decane
		11978294	100.00	3378219	100.00		

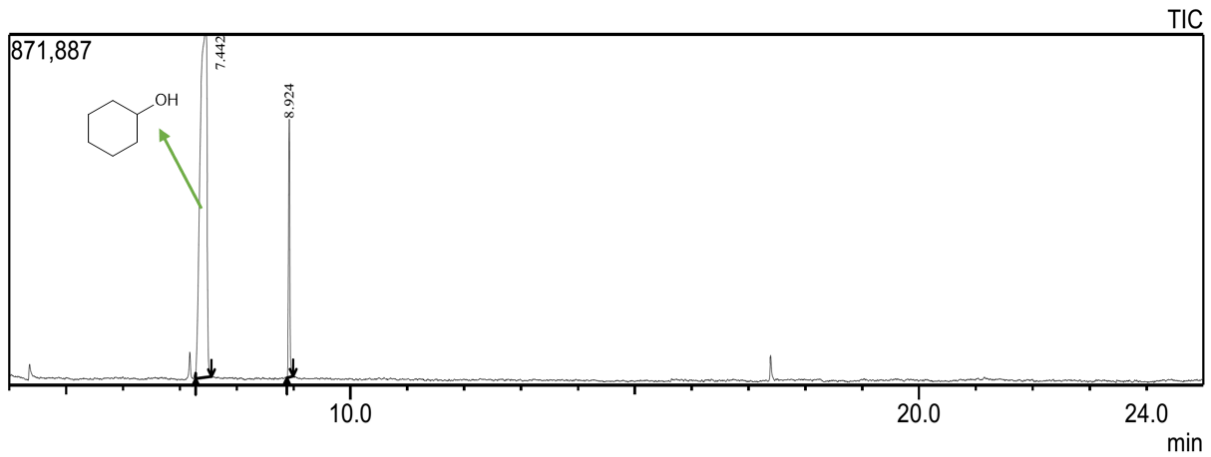
Line#:1 R.Time:7.415(Scan#:684)  
 MassPeaks:302  
 RawMode:Averaged 7.410-7.420(683-685) BasePeak:57(133829)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Scan



Line#:2 R.Time:7.470(Scan#:695)  
 MassPeaks:279  
 RawMode:Averaged 7.465-7.475(694-696) BasePeak:55(92949)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Scan



Entry 13



Peak Report TIC

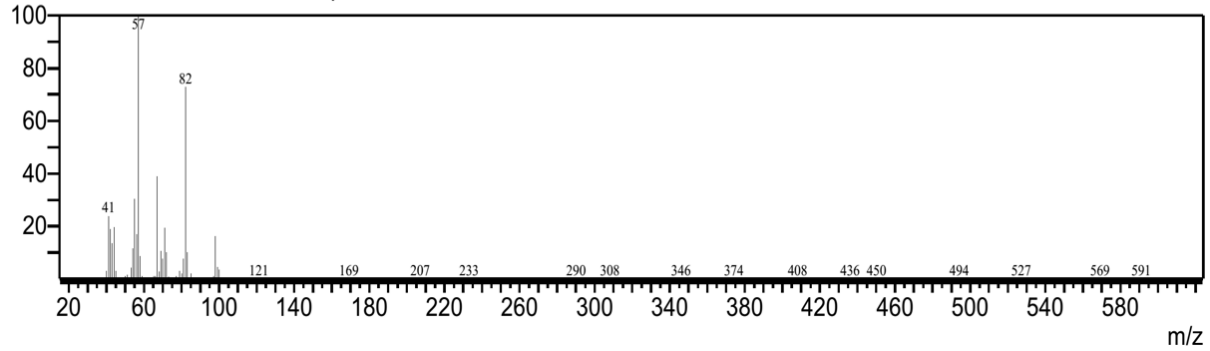
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	7.442	7299980	87.71	852053	57.04	8.57	Cyclohexanol
2	8.924	1022719	12.29	641635	42.96	1.59	Decane
		8322699	100.00	1493688	100.00		

Line#:1 R.Time:7.440(Scan#:689)

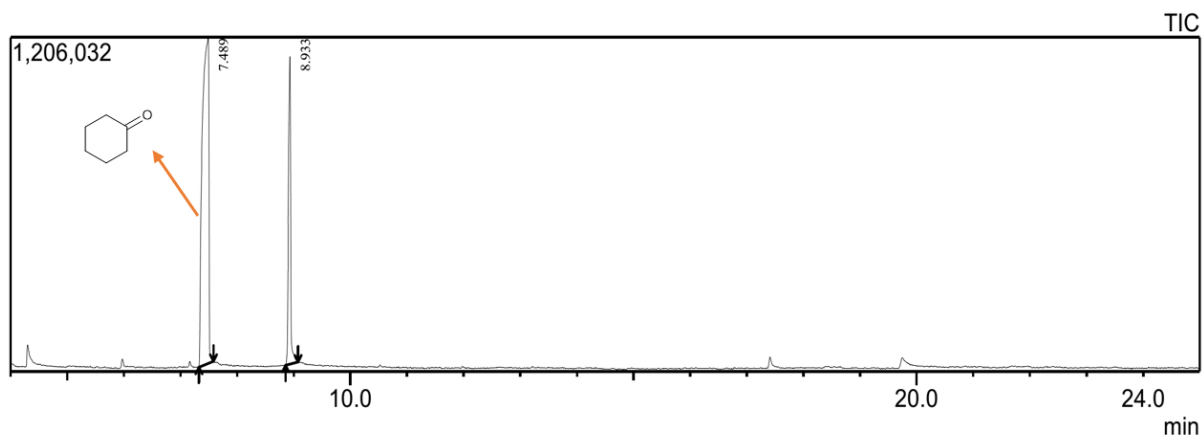
MassPeaks:308

RawMode:Averaged 7.435-7.445(688-690) BasePeak:57(177692)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan



Entry 14



Peak Report TIC

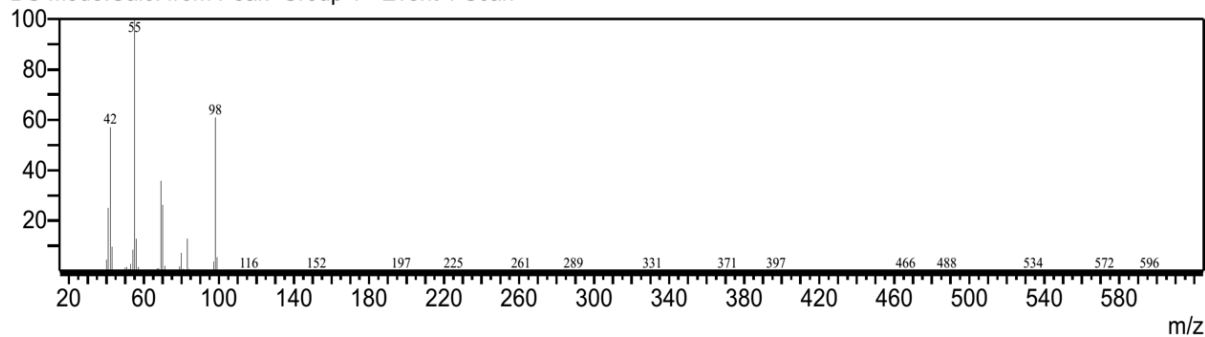
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	7.489	9579193	75.77	1175706	51.43	8.15	Cyclohexanone
2	8.933	3063428	24.23	1110205	48.57	2.76	Decane
		2642621	100.00	2285911	100.00		

Line#:1 R.Time:7.490(Scan#:699)

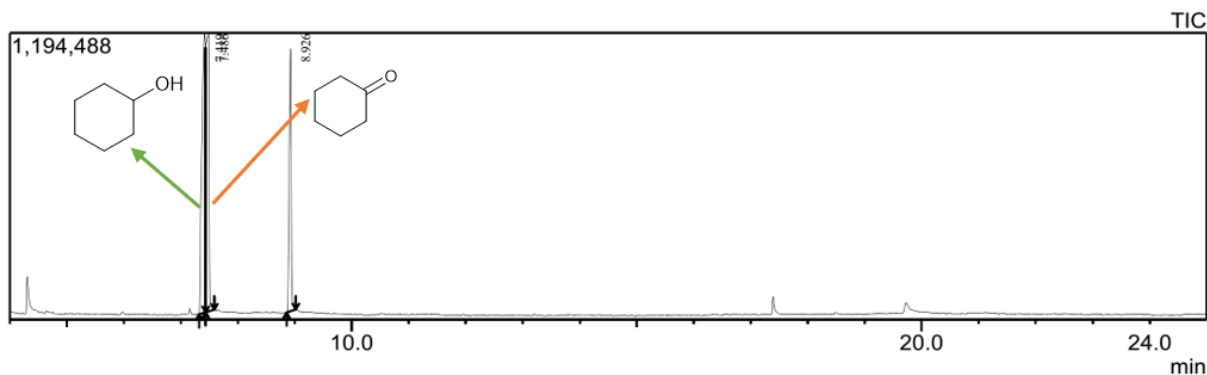
MassPeaks:247

RawMode:Averaged 7.485-7.495(698-700) BasePeak:55(303422)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan



Entry 15



Peak Report TIC

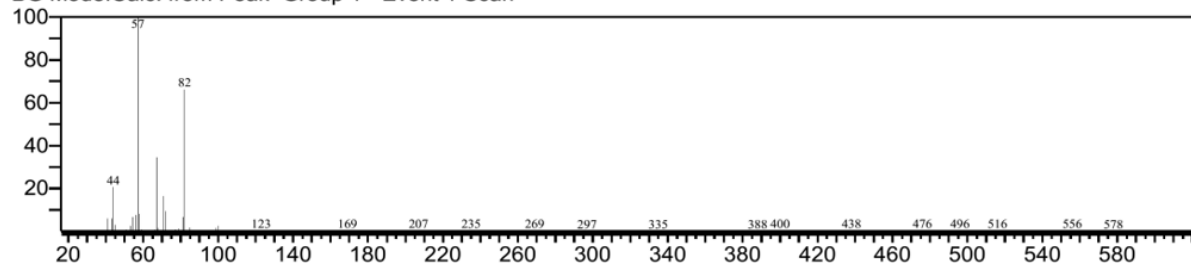
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	7.419	5196937	41.90	1164726	34.11	4.46	Cyclohexanol
2	7.486	4404088	35.50	1156344	33.86	3.81	Cyclohexanone
3	8.926	2803401	22.60	1093583	32.03	2.56	Decane
		2404426	100.00	3414653	100.00		

Line#:1 R.Time:7.420(Scan#:685)

MassPeaks:300

RawMode:Averaged 7.415-7.425(684-686) BasePeak:57(103066)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan

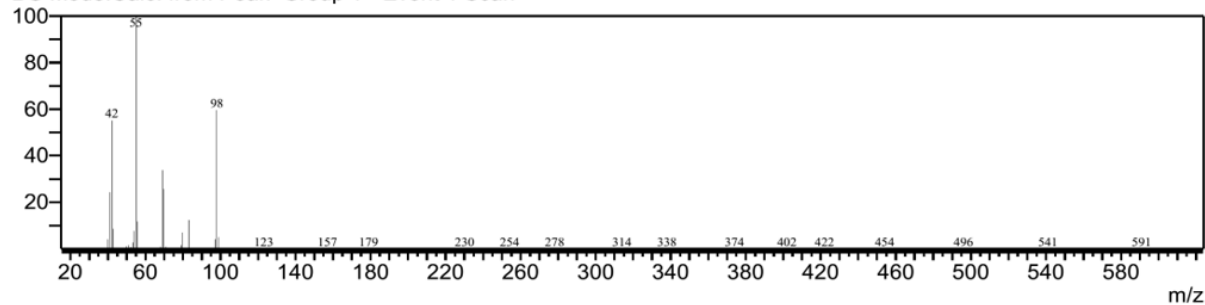


Line#:2 R.Time:7.485(Scan#:698)

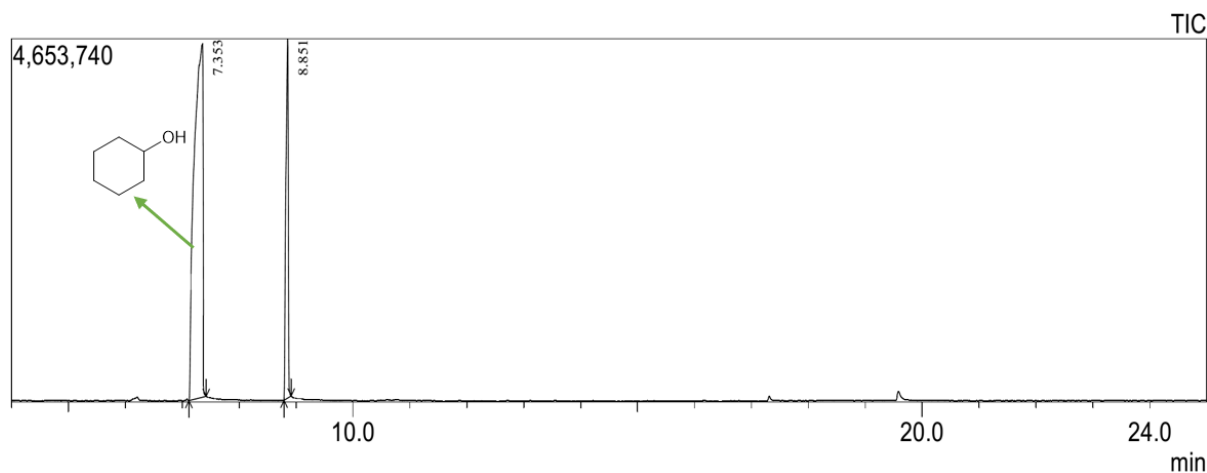
MassPeaks:219

RawMode:Averaged 7.480-7.490(697-699) BasePeak:55(113212)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan



Entry 16



Peak Report TIC

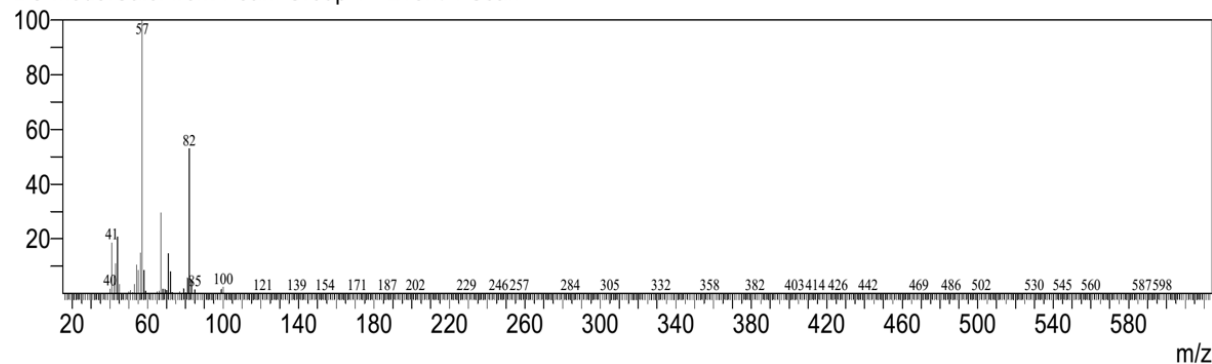
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	7.353	7947032	78.87	4531444	49.62	10.58	Cyclohexanol
2	8.851	2848439	21.13	4600731	50.38	2.79	Decane
		10795471	100.00	9132175	100.00		

Line#:1 R.Time:7.355(Scan#:672)

MassPeaks:332

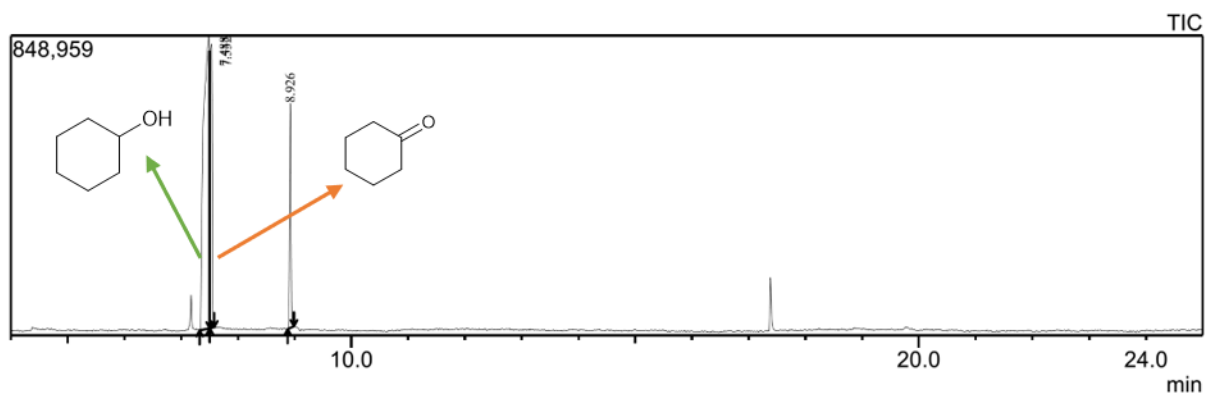
RawMode:Averaged 7.350-7.360(671-673) BasePeak:57(1297951)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan





Entry 17



Peak Report TIC

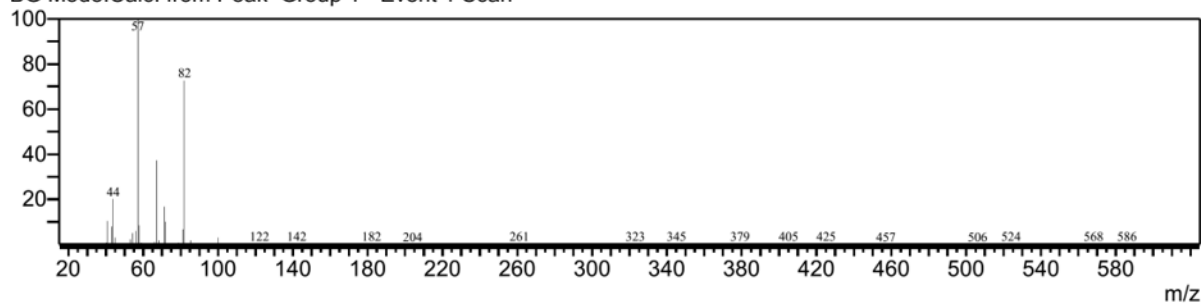
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	7.488	6230132	67.23	828492	36.53	7.52	Cyclohexanol
2	7.532	1984510	21.41	803799	35.44	2.47	Cyclohexanone
3	8.926	1052664	11.36	635461	28.02	1.66	Decane
		9267306	100.00	2267752	100.00		

Line#:1 R.Time:7.490(Scan#:699)

MassPeaks:298

RawMode:Averaged 7.485-7.495(698-700) BasePeak:57(80476)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan

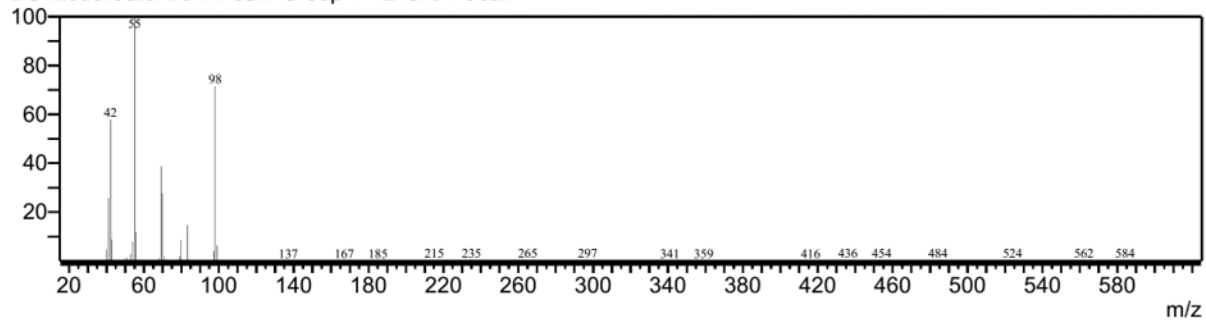


Line#:2 R.Time:7.530(Scan#:707)

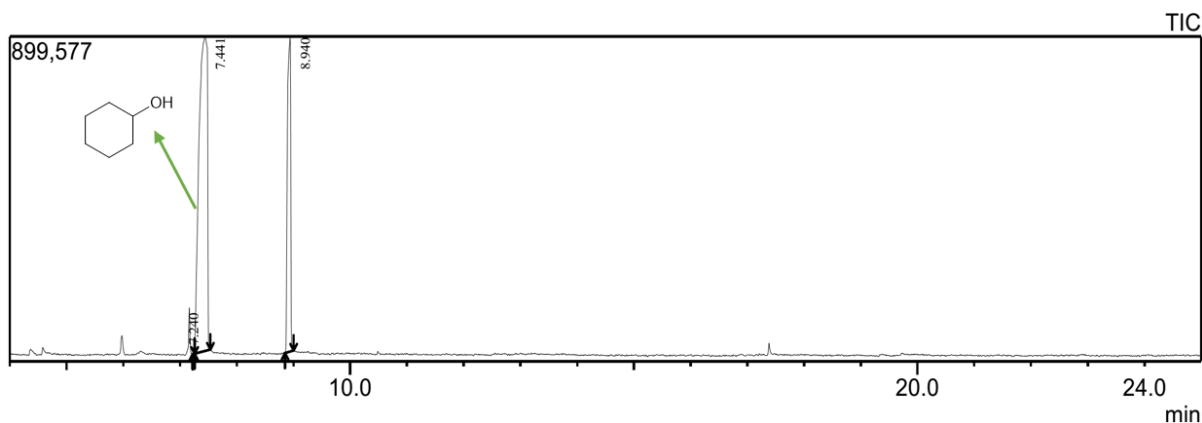
MassPeaks:257

RawMode:Averaged 7.525-7.535(706-708) BasePeak:55(69094)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan



Entry 18



Peak Report TIC

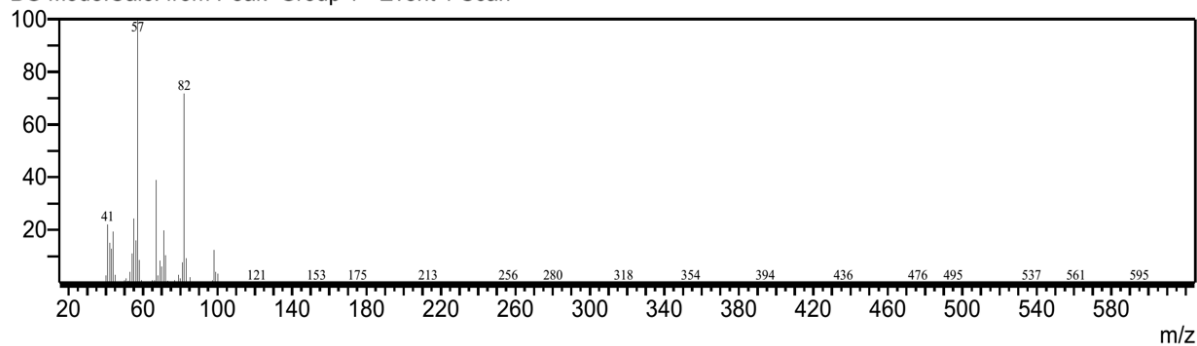
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	7.240	33878	0.27	23138	1.31	1.46	Cyclohexanol
2	7.441	9016110	71.64	870276	49.39	10.36	Cyclohexanol
3	8.940	3534631	28.09	868676	49.30	4.07	Decane
		2584619	100.00	1762090	100.00		

Line#:2 R.Time:7.440(Scan#:689)

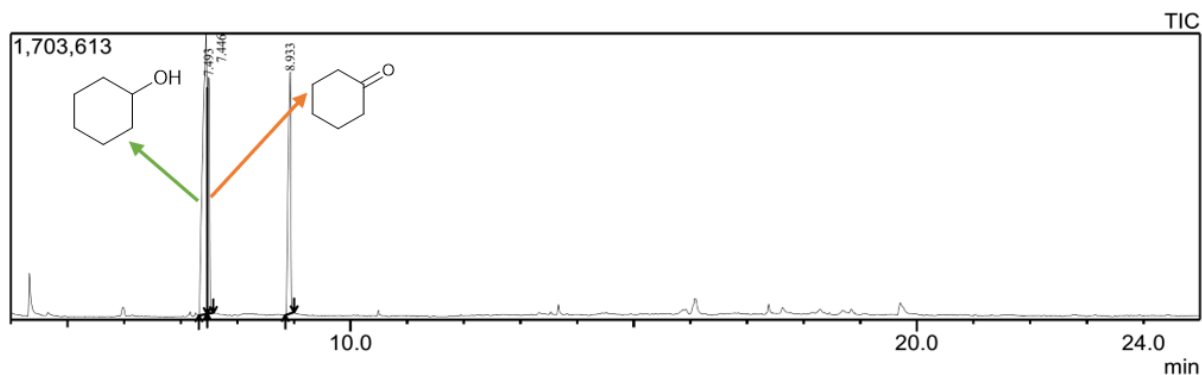
MassPeaks:313

RawMode:Averaged 7.435-7.445(688-690) BasePeak:57(190995)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan



Entry 19



Peak Report TIC

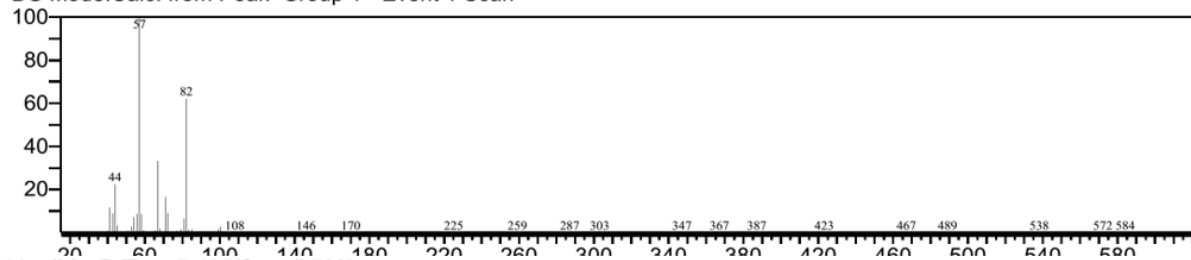
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	7.446	8503554	50.36	1668665	36.97	5.10	Cyclohexanol
2	7.493	3721159	22.04	1407515	31.18	2.64	Cyclohexanone
3	8.933	4661482	27.61	1437306	31.84	3.24	Decane
		6886195	100.00	4513486	100.00		

Line#:1 R.Time:7.445(Scan#:690)

MassPeaks:314

RawMode:Averaged 7.440-7.450(689-691) BasePeak:57(217608)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan

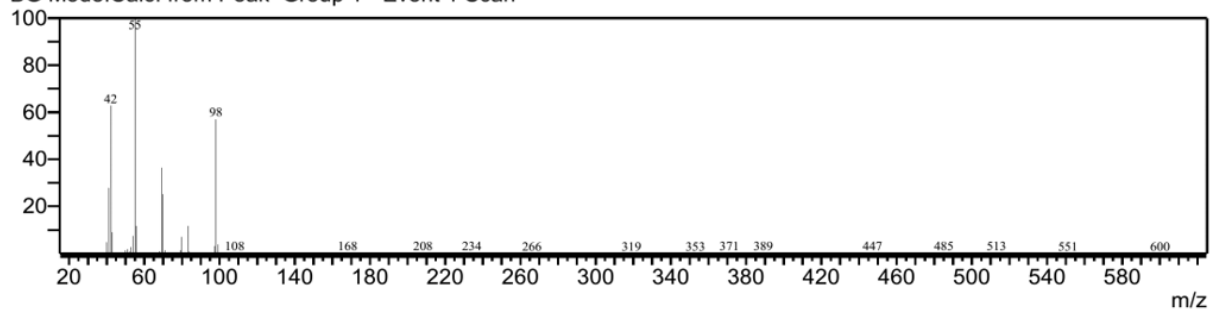


Line#:2 R.Time:7.495(Scan#:700)

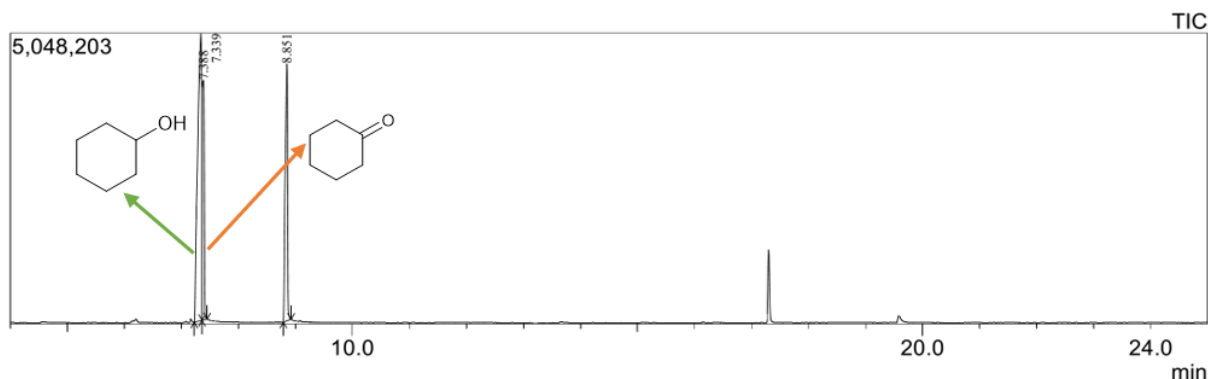
MassPeaks:292

RawMode:Averaged 7.490-7.500(699-701) BasePeak:55(112736)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan

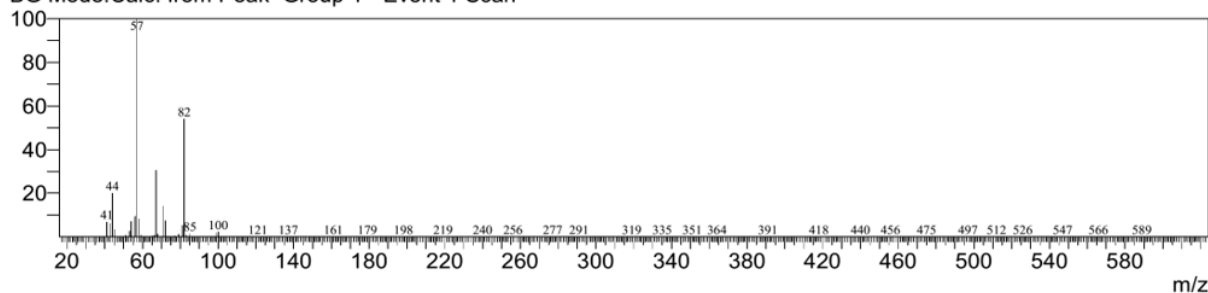


Entry 20

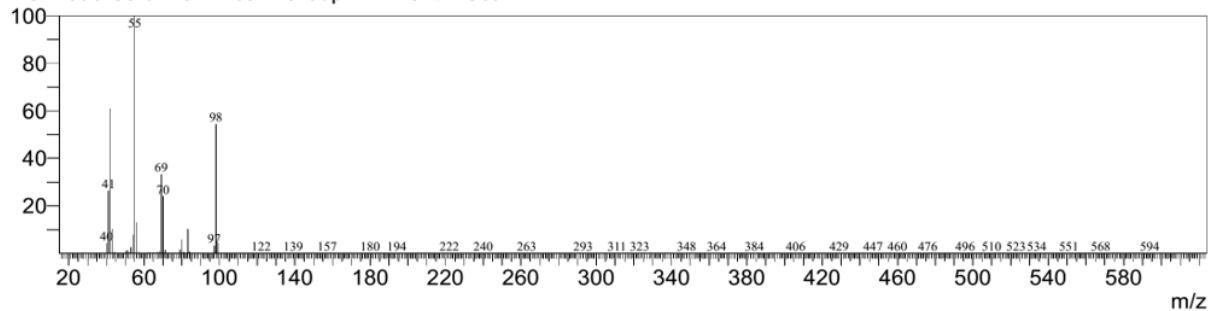


Peak Report TIC						
Peak#	R.Time	Area	Area%	Height	Height%	A/H Name
1	7.339	4624296	52.39	4988924	36.65	4.94 Cyclohexanol
2	7.388	0352401	22.03	4161455	30.57	2.49 Cyclohexanone
3	8.851	2022078	25.58	4461248	32.78	2.69 Decane
		6998775	100.00	13611627	100.00	

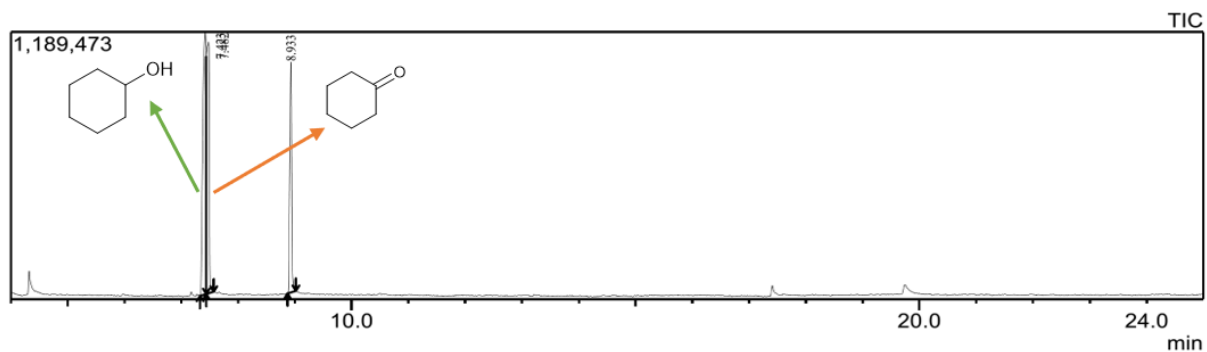
Line#:1 R.Time:7.340(Scan#:669)  
 MassPeaks:280  
 RawMode:Averaged 7.335-7.345(668-670) BasePeak:57(720889)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Scan



Line#:2 R.Time:7.390(Scan#:679)  
 MassPeaks:327  
 RawMode:Averaged 7.385-7.395(678-680) BasePeak:55(389672)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Scan



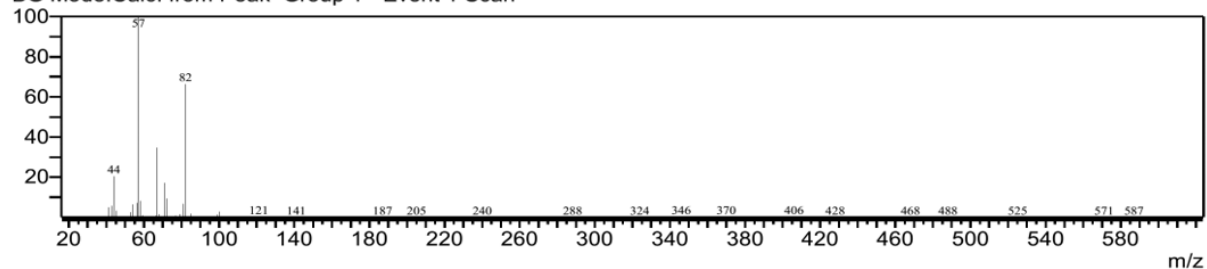
Entry 21



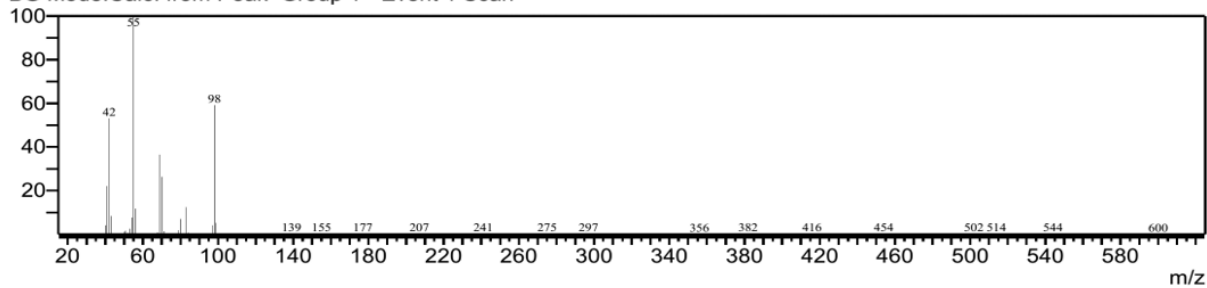
Peak Report TIC

Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	7.423	4826553	43.95	1166136	35.25	4.14	Cyclohexanol
2	7.482	3776462	34.39	1117549	33.78	3.38	Cyclohexanone
3	8.933	2377737	21.65	1024180	30.96	2.32	Decane
		0980752	100.00	3307865	100.00		

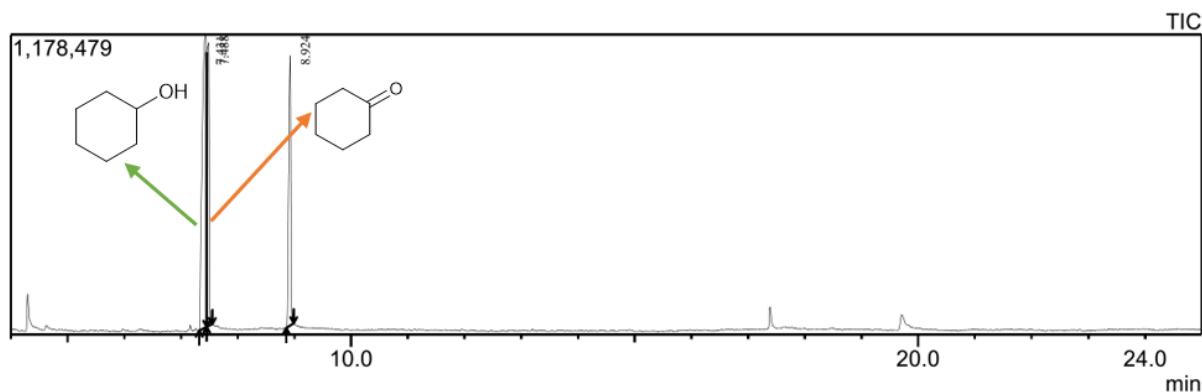
Line#:1 R.Time:7.425(Scan#:686)  
 MassPeaks:250  
 RawMode:Averaged 7.420-7.430(685-687) BasePeak:57(133058)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Scan



Line#:2 R.Time:7.480(Scan#:697)  
 MassPeaks:295  
 RawMode:Averaged 7.475-7.485(696-698) BasePeak:55(105319)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Scan



Entry 22



Peak Report TIC

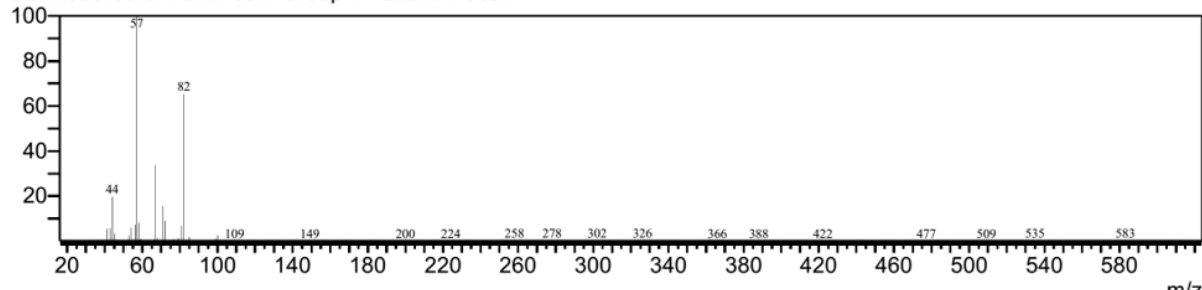
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	7.431	6057901	49.61	1150046	34.62	5.27	Cyclohexanol
2	7.488	3345944	27.40	1112144	33.48	3.01	Cyclohexanone
3	8.924	2807734	22.99	1060080	31.91	2.65	Decane
		12211579	100.00	3322270	100.00		

Line#:1 R.Time:7.430(Scan#:687)

MassPeaks:290

RawMode:Averaged 7.425-7.435(686-688) BasePeak:57(141562)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan

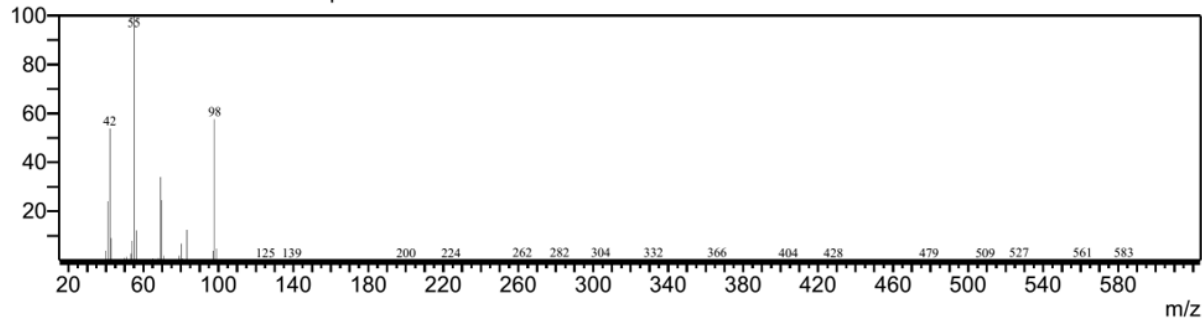


Line#:2 R.Time:7.490(Scan#:699)

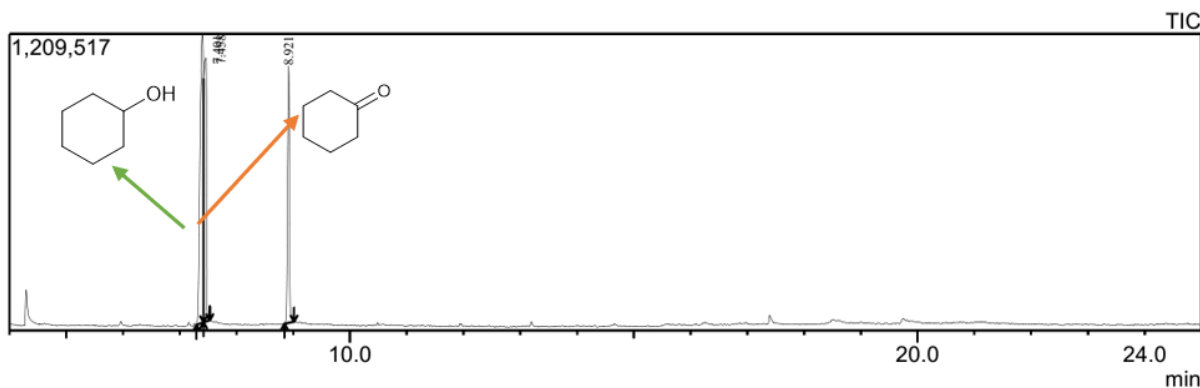
MassPeaks:287

RawMode:Averaged 7.485-7.495(698-700) BasePeak:55(120908)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan



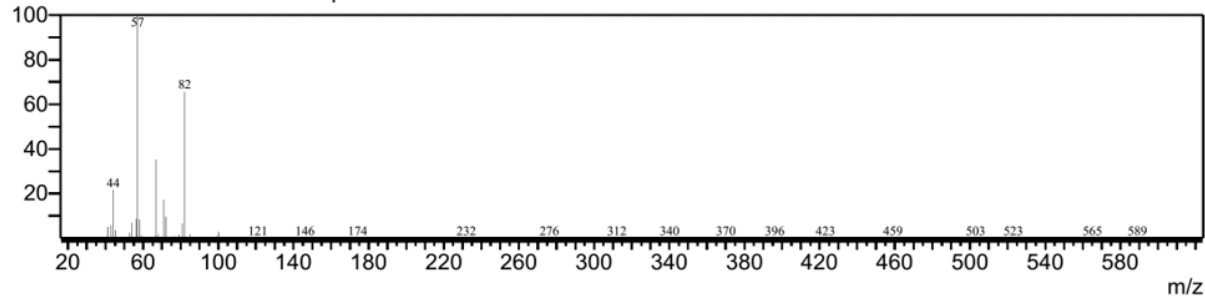
Entry 23



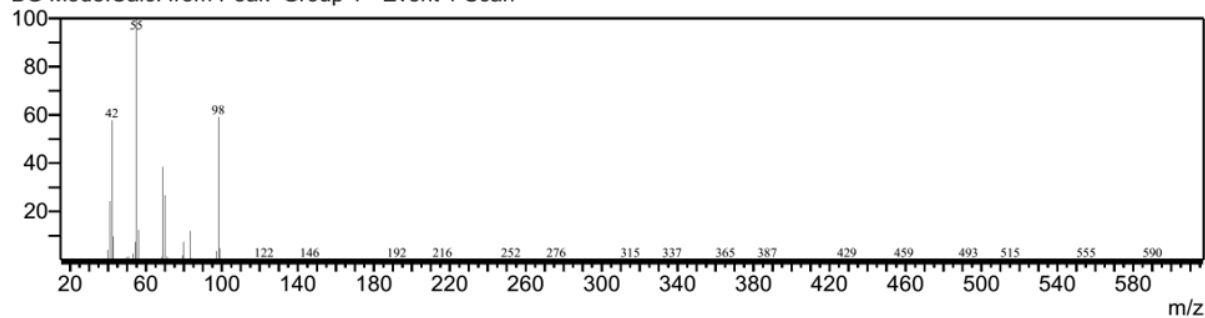
Peak Report TIC

Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	7.401	5010601	46.68	1177350	35.68	4.26	Cyclohexanol
2	7.458	3350205	31.21	1075561	32.59	3.11	Cyclohexanone
3	8.921	2373023	22.11	1046915	31.73	2.27	Decane
		0733829	100.00	3299826	100.00		

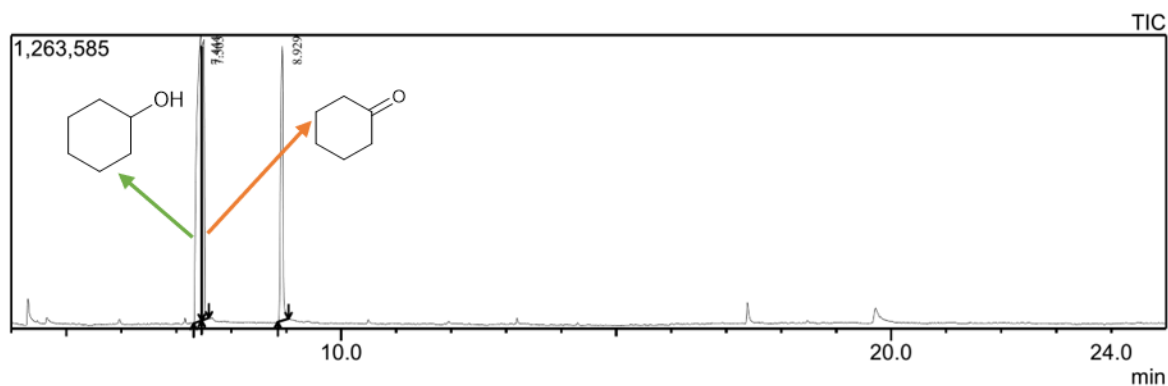
Line#:1 R.Time:7.400(Scan#:681)  
 MassPeaks:251  
 RawMode:Averaged 7.395-7.405(680-682) BasePeak:57(184757)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Scan



Line#:2 R.Time:7.460(Scan#:693)  
 MassPeaks:252  
 RawMode:Averaged 7.455-7.465(692-694) BasePeak:55(115652)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Scan



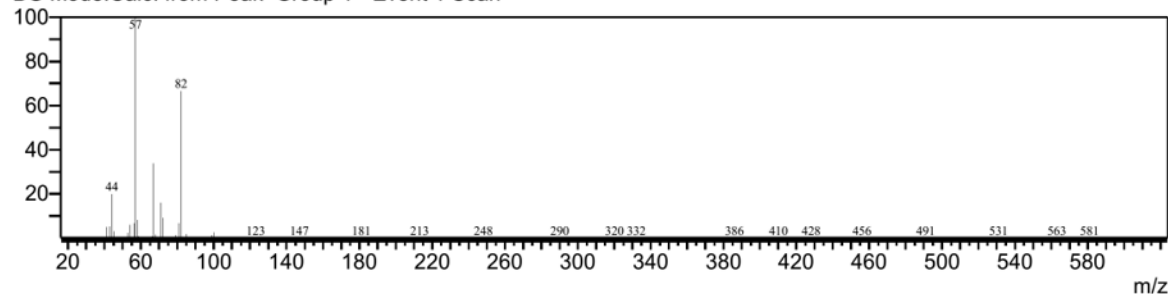
Entry 24



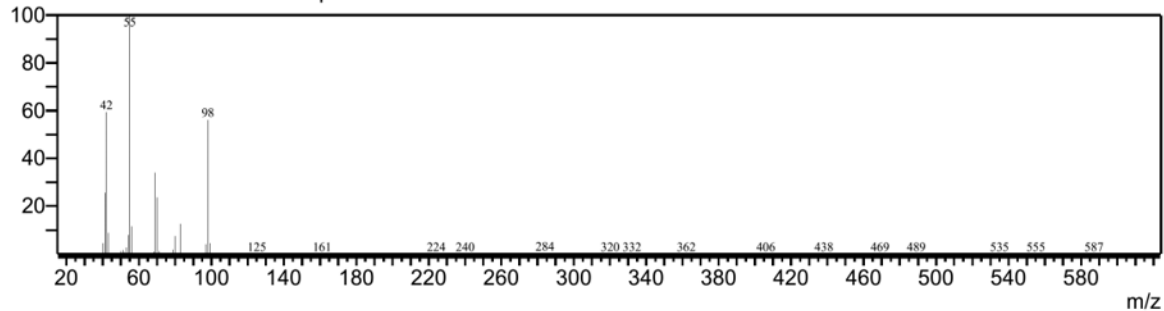
Peak Report TIC

Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	7.444	7398364	49.03	1229007	33.99	6.02	Cyclohexanol
2	7.503	3994531	26.47	1205346	33.34	3.31	Cyclohexanone
3	8.929	3697045	24.50	1181153	32.67	3.13	Decane
		5089940	100.00	3615506	100.00		

Line#:1 R.Time:7.445(Scan#:690)  
 MassPeaks:318  
 RawMode:Averaged 7.440-7.450(689-691) BasePeak:57(103029)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Scan

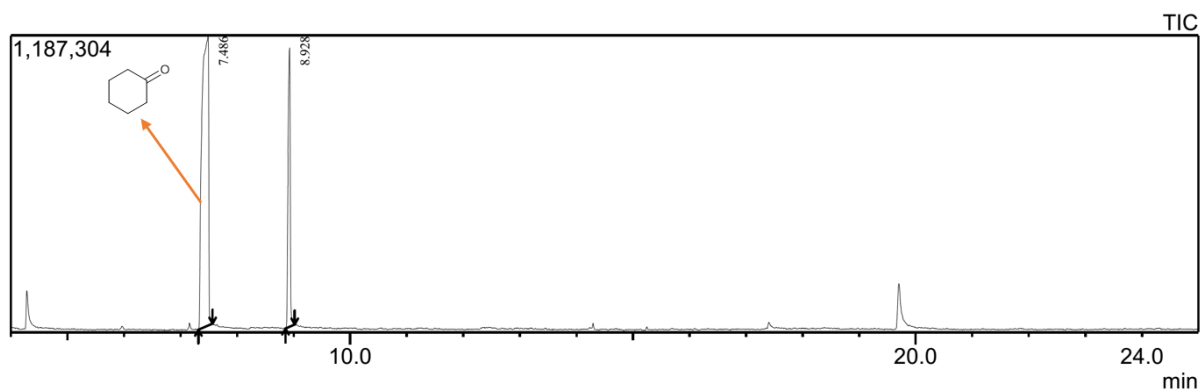


Line#:2 R.Time:7.505(Scan#:702)  
 MassPeaks:302  
 RawMode:Averaged 7.500-7.510(701-703) BasePeak:55(108465)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Scan





Entry 25



Peak Report TIC

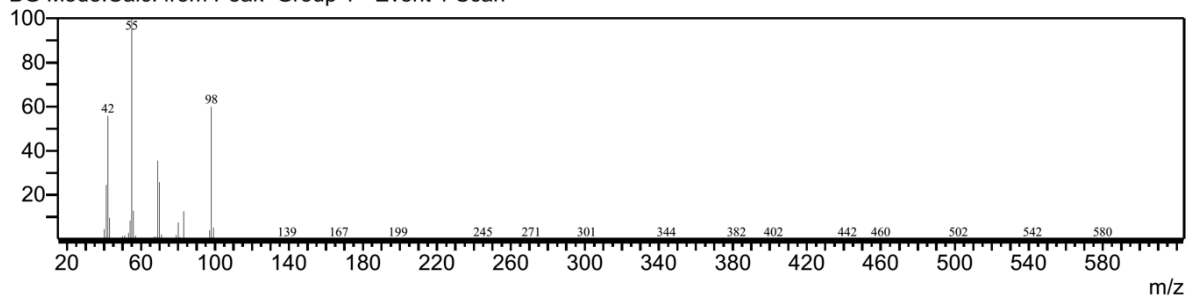
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	7.486	9654031	75.70	1158761	50.95	8.33	Cyclohexanone
2	8.928	3098741	24.30	1115372	49.05	2.78	Decane
		2752772	100.00	2274133	100.00		

Line#:1 R.Time:7.485(Scan#:698)

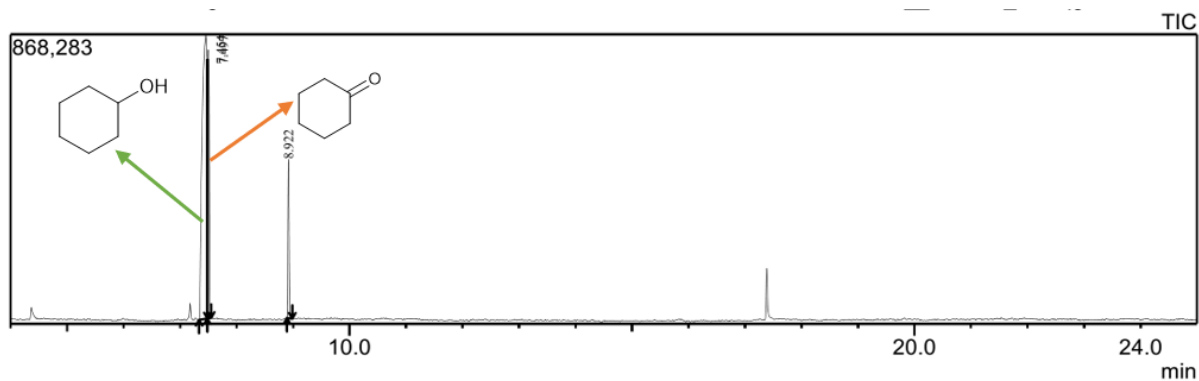
MassPeaks:308

RawMode:Averaged 7.480-7.490(697-699) BasePeak:55(302063)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan



Entry 26



Peak Report TIC

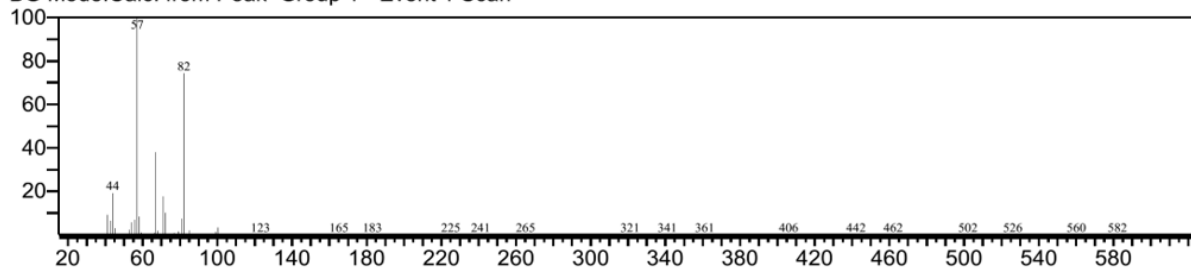
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	7.454	5041525	67.35	852405	39.93	5.91	Cyclohexanol
2	7.497	1767669	23.61	805195	37.72	2.20	Cyclohexanone
3	8.922	676541	9.04	476973	22.35	1.42	Decane
		7485735	100.00	2134573	100.00		

Line#:1 R.Time:7.455(Scan#:692)

MassPeaks:303

RawMode:Averaged 7.450-7.460(691-693) BasePeak:57(112419)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan

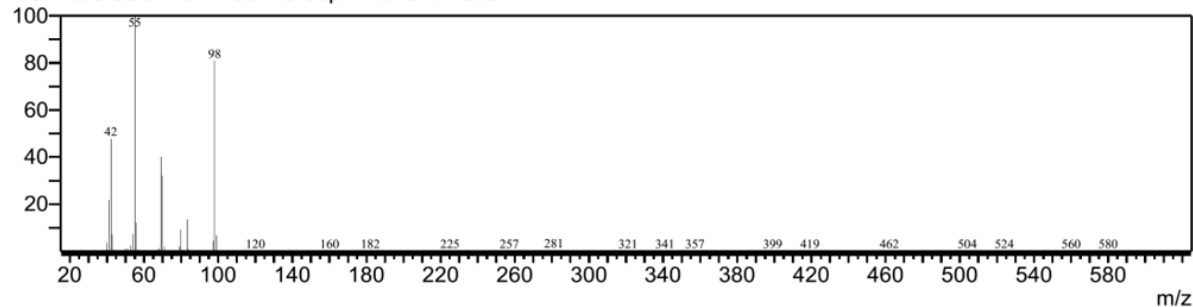


Line#:2 R.Time:7.495(Scan#:700)

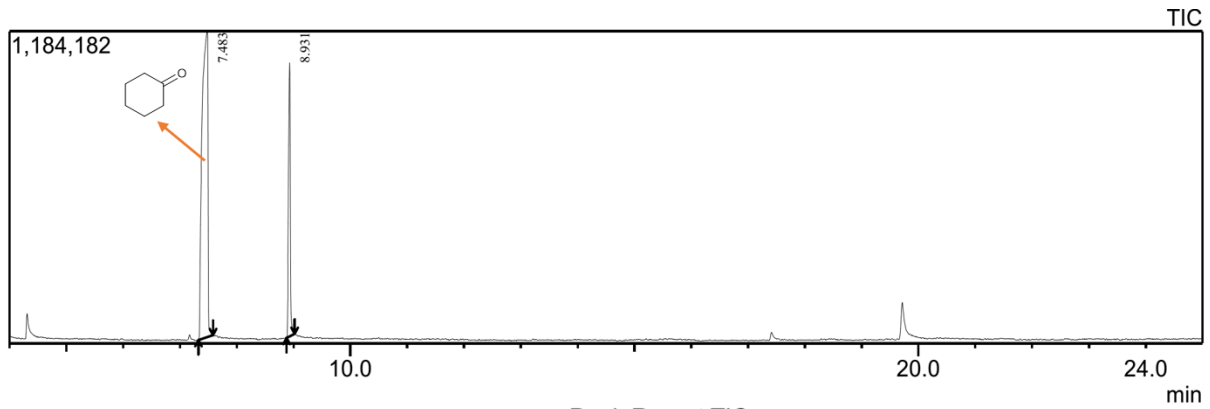
MassPeaks:325

RawMode:Averaged 7.490-7.500(699-701) BasePeak:55(47001)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan



Entry 27



Peak Report TIC

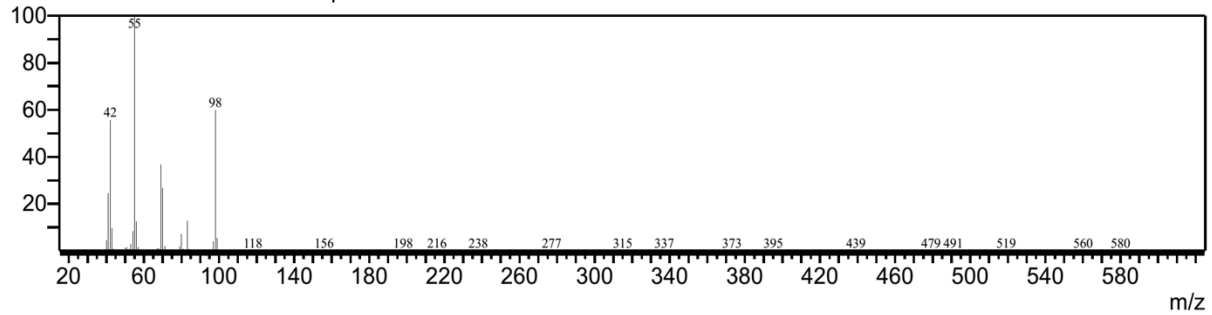
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	7.483	8473977	78.43	1159066	52.77	7.31	Cyclohexanone
2	8.931	2330950	21.57	1037212	47.23	2.25	Decane
		0804927	100.00	2196278	100.00		

Line#:1 R.Time:7.485(Scan#:698)

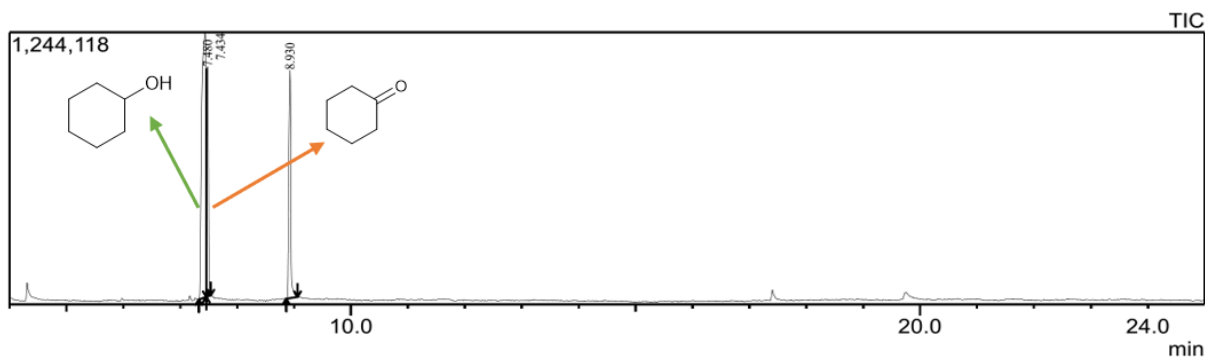
MassPeaks:278

RawMode:Averaged 7.480-7.490(697-699) BasePeak:55(298033)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan



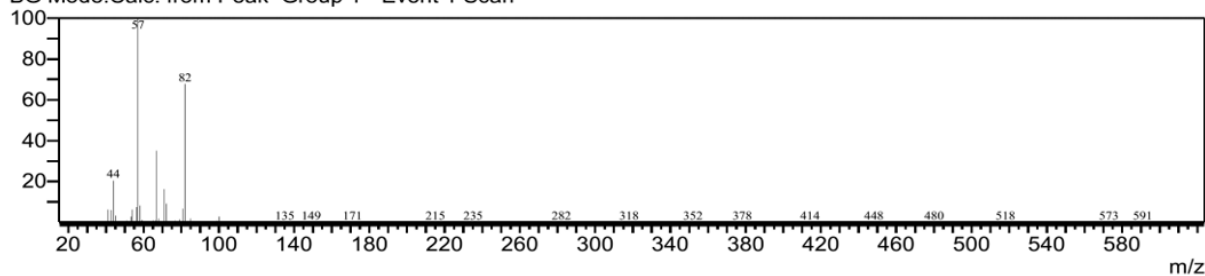
Entry 28



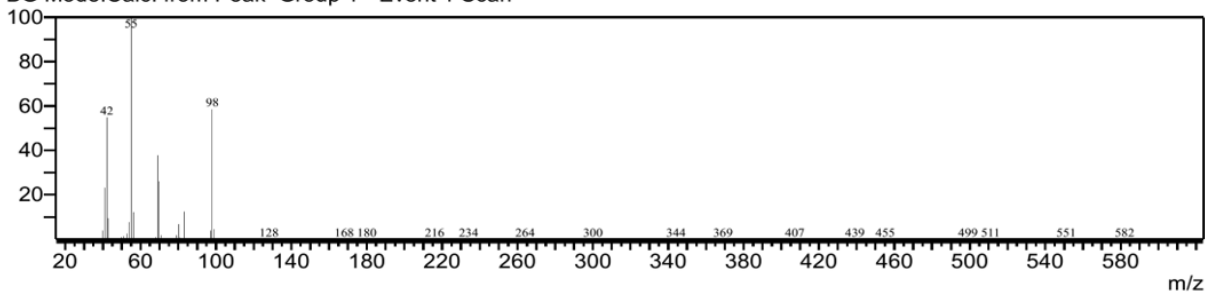
Peak Report TIC

Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	7.434	6361110	55.89	1210916	36.69	5.25	Cyclohexanol
2	7.480	2495533	21.92	1047638	31.74	2.38	Cyclohexanone
3	8.930	2525705	22.19	1041975	31.57	2.42	Decane
		11382348	100.00	3300529	100.00		

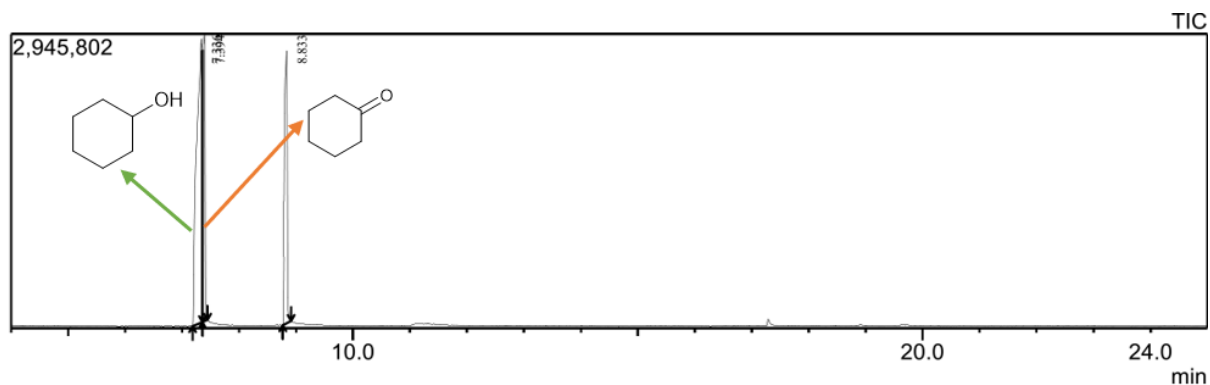
Line#:1 R.Time:7.435(Scan#:688)  
 MassPeaks:301  
 RawMode:Averaged 7.430-7.440(687-689) BasePeak:57(190229)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Scan



Line#:2 R.Time:7.480(Scan#:697)  
 MassPeaks:307  
 RawMode:Averaged 7.475-7.485(696-698) BasePeak:55(87304)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Scan



Entry 29



Peak Report TIC

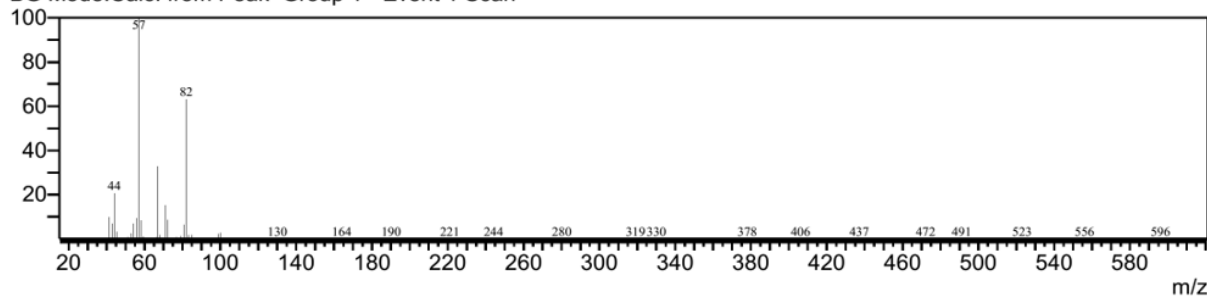
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	7.336	19136611	52.21	2840628	33.66	6.74	Cyclohexanol
2	7.394	8589342	23.43	2872603	34.04	2.99	Cyclohexanone
3	8.833	8928761	24.36	2725460	32.30	3.28	Decane
		6654714	100.00	8438691	100.00		

Line#:1 R.Time:7.335(Scan#:668)

MassPeaks:310

RawMode:Averaged 7.330-7.340(667-669) BasePeak:57(169727)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan

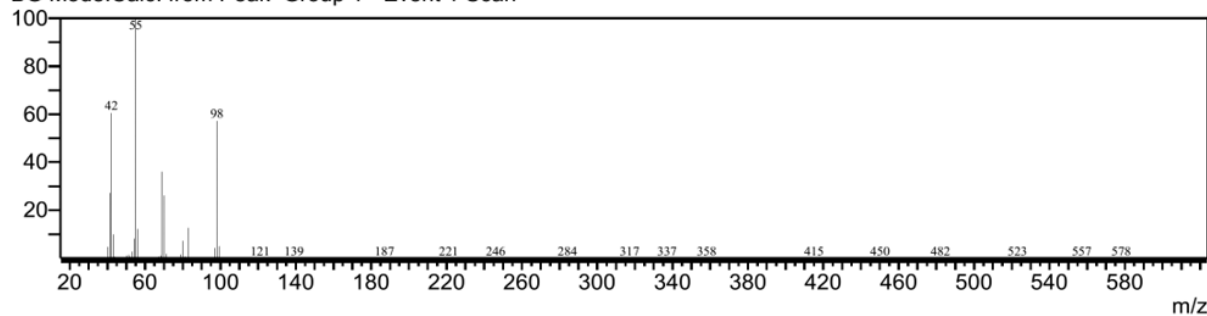


Line#:2 R.Time:7.395(Scan#:680)

MassPeaks:351

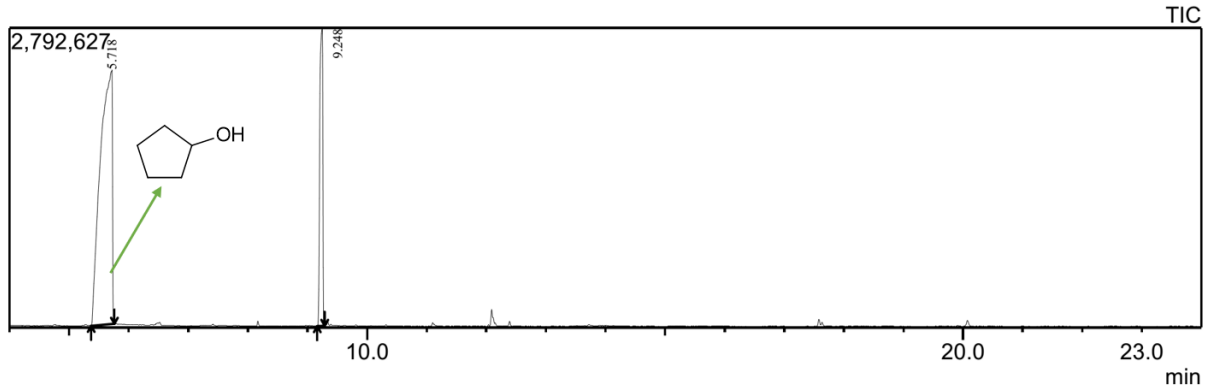
RawMode:Averaged 7.390-7.400(679-681) BasePeak:55(344037)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan



## GCMS of substrates (Table-3)

### GCMS of 10a:



Peak Report TIC

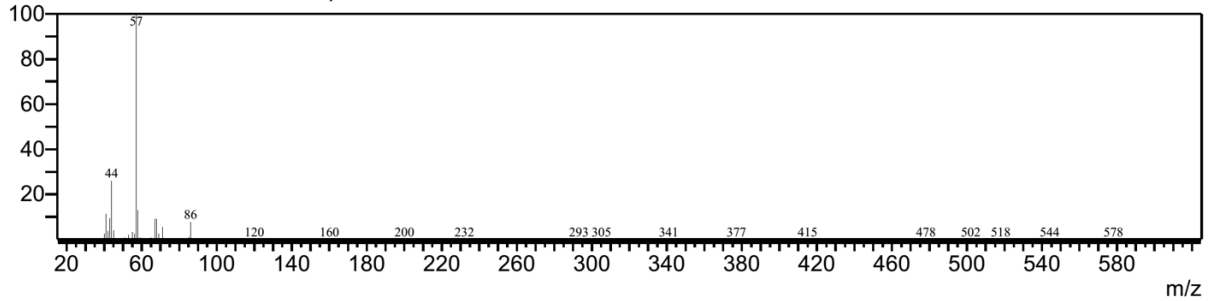
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	5.718	2826642	77.18	2366969	46.04	13.87	Cyclopentanol
2	9.248	9705917	22.82	2774558	53.96	3.50	Decane
		2532559	100.00	5141527	100.00		

Line#:1 R.Time:5.720(Scan#:345)

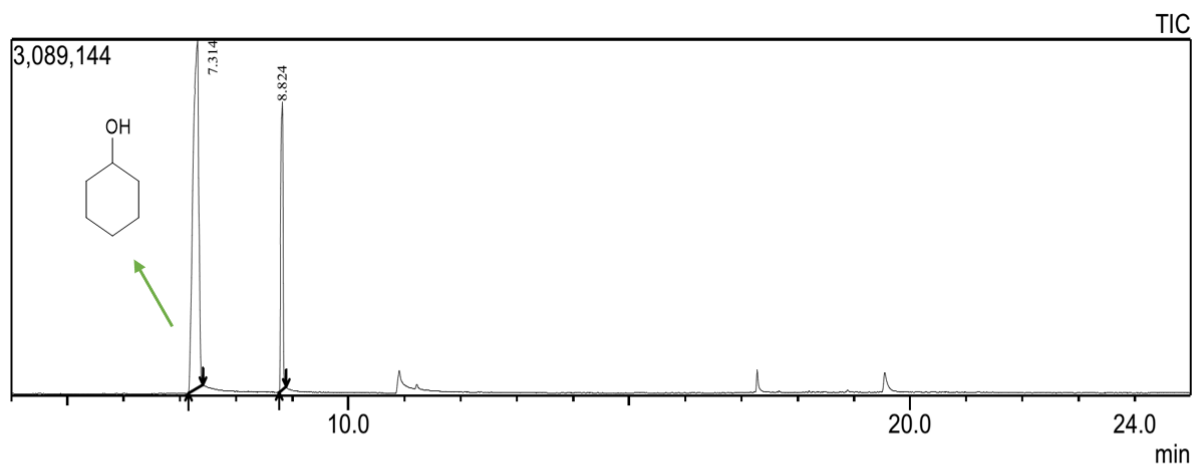
MassPeaks:323

RawMode:Averaged 5.715-5.725(344-346) BasePeak:57(1047490)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan



GCMS of 10b:



Peak Report TIC

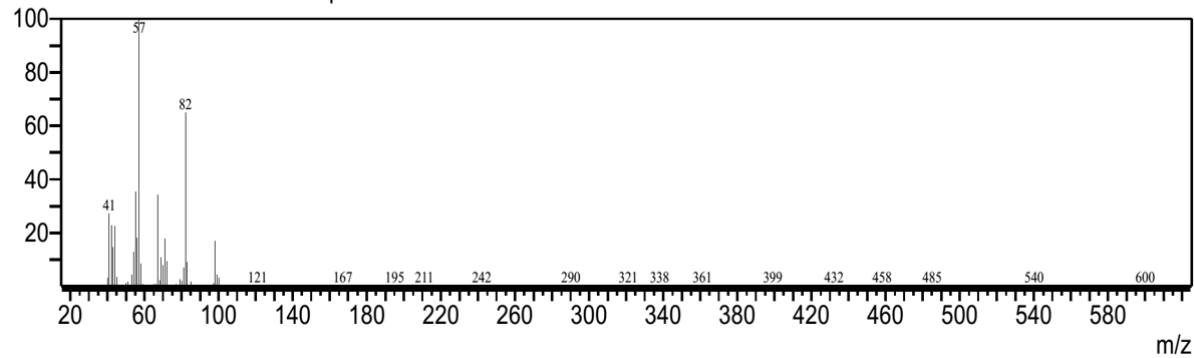
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	7.314	21444886	74.91	3020184	54.77	7.10	Cyclohexanol
2	8.824	7184447	25.09	2493927	45.23	2.88	Decane
		28629333	100.00	5514111	100.00		

Line#:1 R.Time:7.315(Scan#:664)

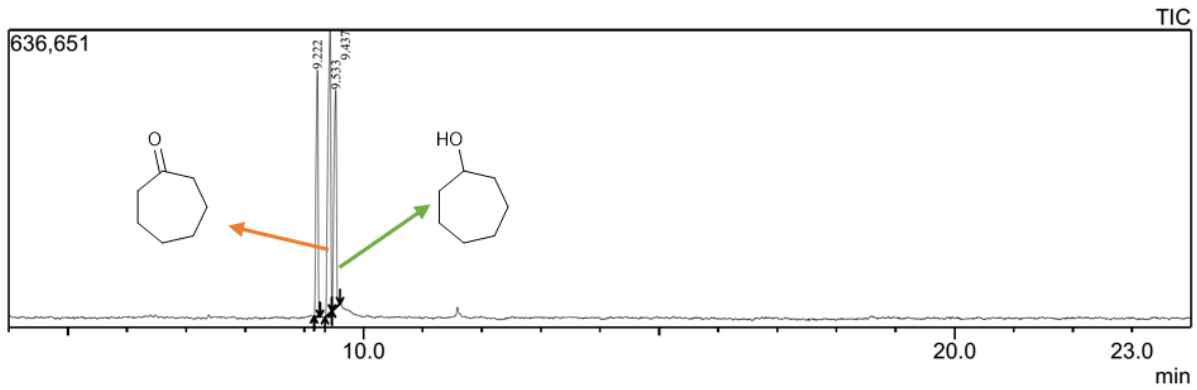
MassPeaks:313

RawMode:Averaged 7.310-7.320(663-665) BasePeak:57(620877)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan



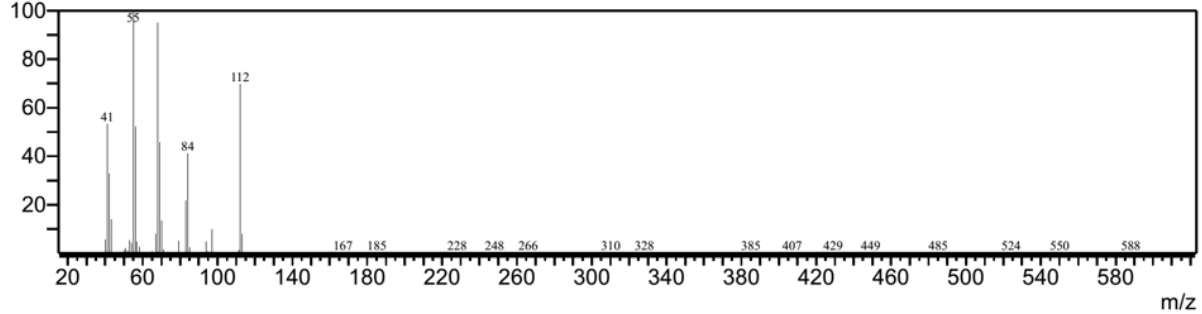
GCMS of 10c:



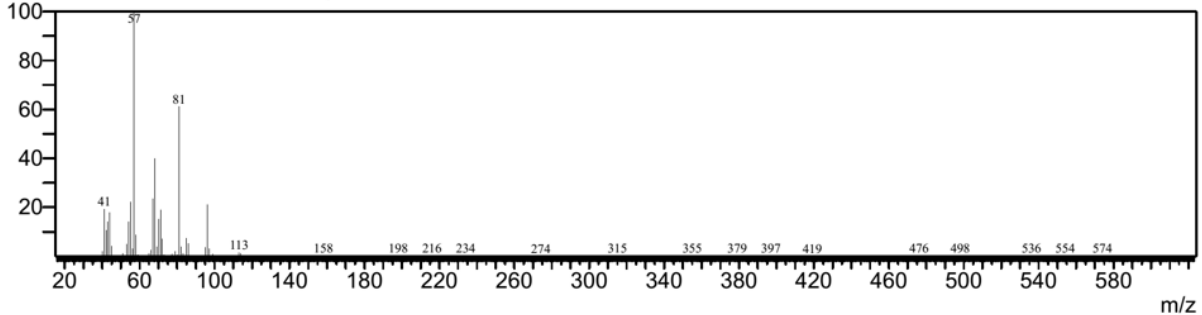
Peak Report TIC

Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	9.222	1270086	26.69	527551	33.00	2.41	Decane
2	9.437	2060325	43.29	605440	37.87	3.40	Cycloheptanone
3	9.533	1429113	30.03	465580	29.12	3.07	Cycloheptanol
		4759524	100.00	1598571	100.00		

Line#:2 R.Time:9.435(Scan#:1088)  
 MassPeaks:315  
 RawMode:Averaged 9.430-9.440(1087-1089) BasePeak:55(93742)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Scan

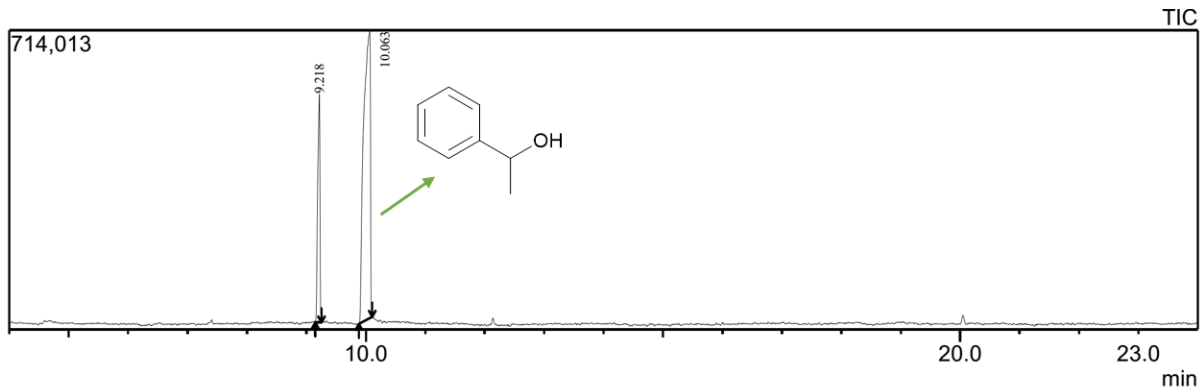


Line#:3 R.Time:9.530(Scan#:1107)  
 MassPeaks:323  
 RawMode:Averaged 9.525-9.535(1106-1108) BasePeak:57(98009)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Scan





GCMS of 10d:



Peak Report TIC

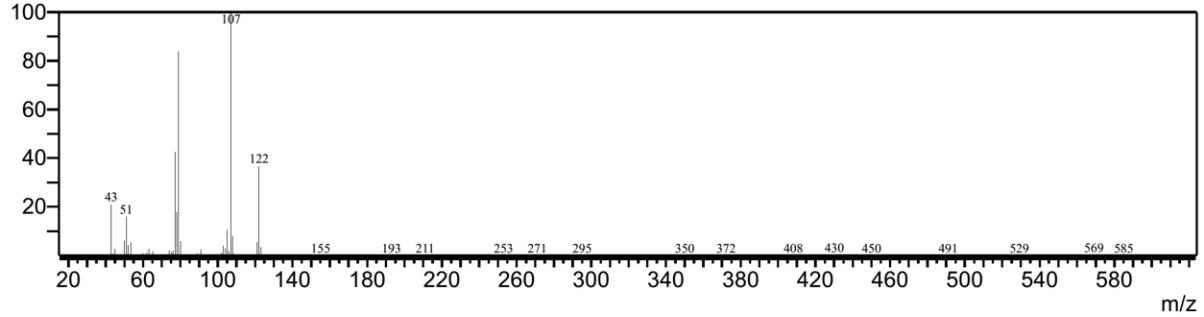
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	9.218	1409954	20.87	544940	44.25	2.59	Decane
2	10.063	5345252	79.13	686495	55.75	7.79	Benzenemethanol, .alpha.-methyl-
		6755206	100.00	1231435	100.00		

Line#:2 R.Time:10.065(Scan#:1214)

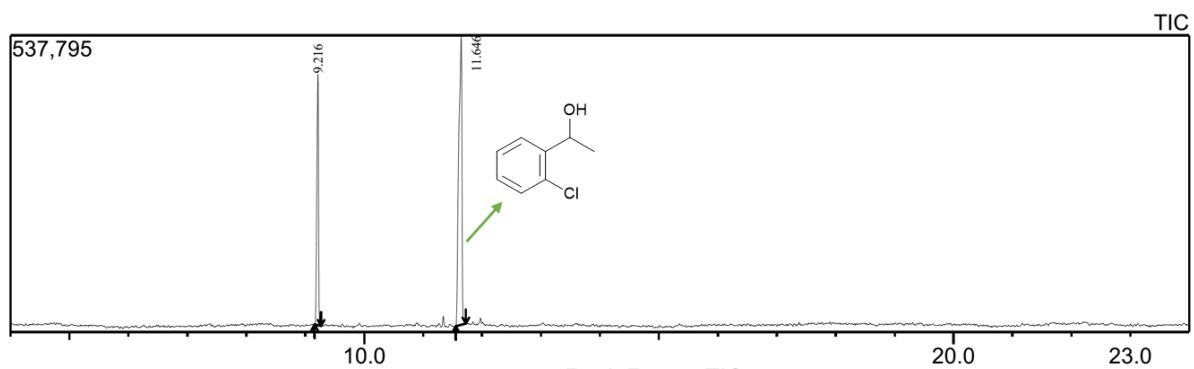
MassPeaks:326

RawMode:Averaged 10.060-10.070(1213-1215) BasePeak:107(167773)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan



GCMS of 10e:



Peak Report TIC

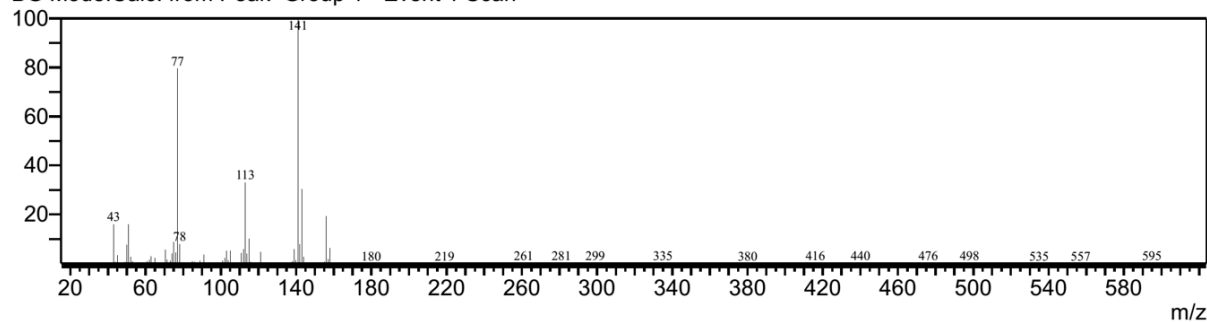
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	9.216	902696	31.56	454971	46.47	1.98	Decane
2	11.646	1957577	68.44	524116	53.53	3.74	Benzenemethanol, 2-chloro-.alpha.-methyl-
		2860273	100.00	979087	100.00		

Line#:2 R.Time:11.645(Scan#:1530)

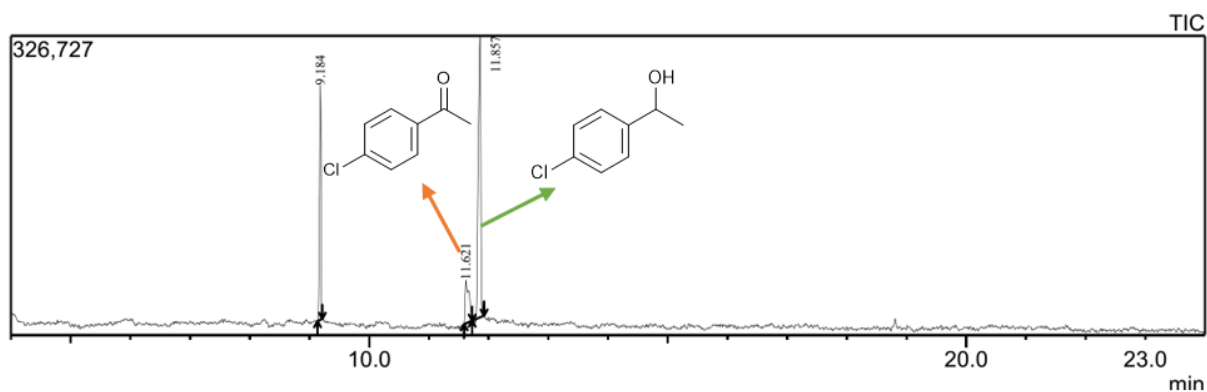
MassPeaks:323

RawMode:Averaged 11.640-11.650(1529-1531) BasePeak:141(115805)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan



GCMS of 10f:



Peak Report TIC

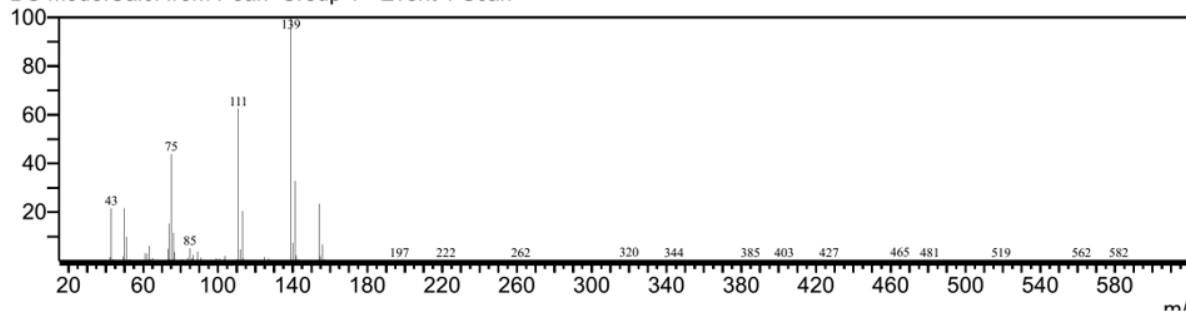
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	9.184	450176	28.74	255757	41.95	1.76	Decane
2	11.621	202067	12.90	46927	7.70	4.31	Ethanone, 1-(4-chlorophenyl)-
3	11.857	914333	58.37	307002	50.35	2.98	Benzenemethanol, 4-chloro-.alpha.-methyl-
		1566576	100.00	609686	100.00		

Line#:2 R.Time:11.620(Scan#:1525)

MassPeaks:302

RawMode:Averaged 11.615-11.625(1524-1526) BasePeak:139(10336)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan

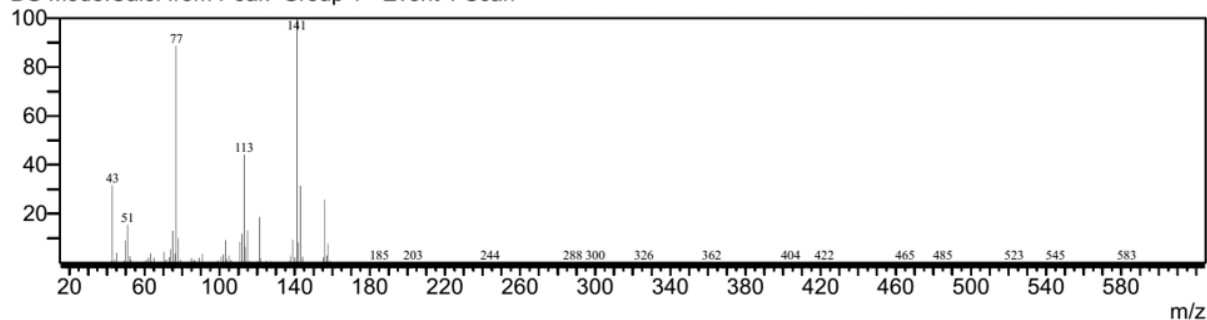


Line#:3 R.Time:11.855(Scan#:1572)

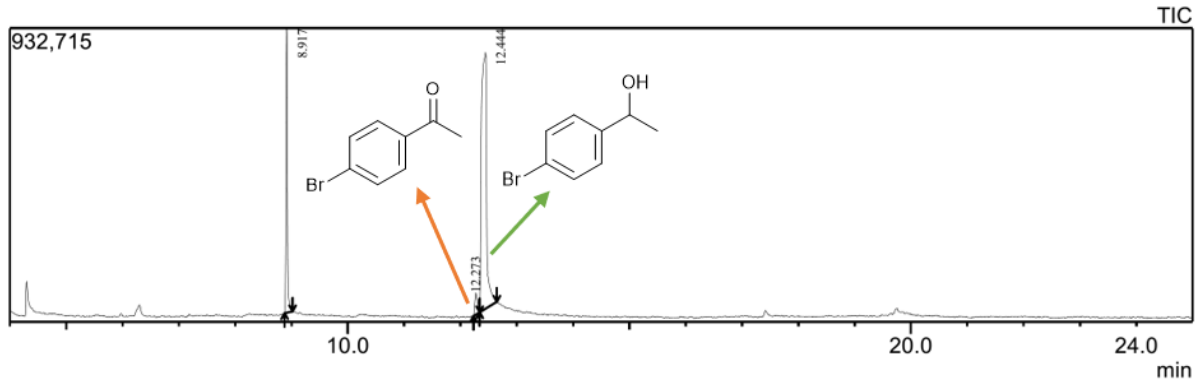
MassPeaks:356

RawMode:Averaged 11.850-11.860(1571-1573) BasePeak:141(55131)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan



GCMS of 10g:



Peak Report TIC

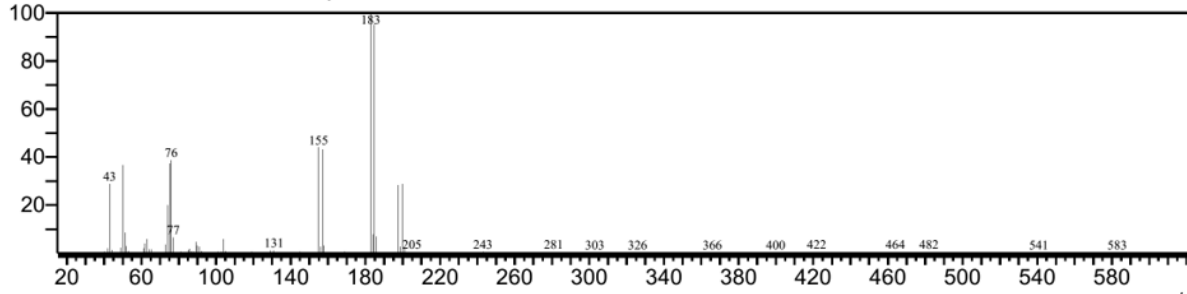
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	8.917	1645828	23.08	902964	50.56	1.82	Decane
2	12.273	236289	3.31	68410	3.83	3.45	Ethanone, 1-(4-bromophenyl)-
3	12.444	5248181	73.60	814464	45.61	6.44	Benzenemethanol, 4-bromo-.alpha.-methyl-
		7130298	100.00	1785838	100.00		

Line#:2 R.Time:12.275(Scan#:1656)

MassPeaks:314

RawMode:Averaged 12.270-12.280(1655-1657) BasePeak:183(10806)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan

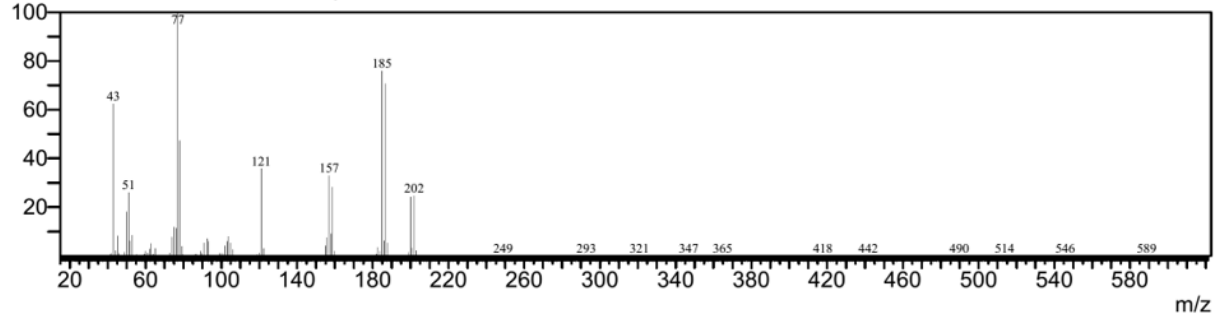


Line#:3 R.Time:12.445(Scan#:1690)

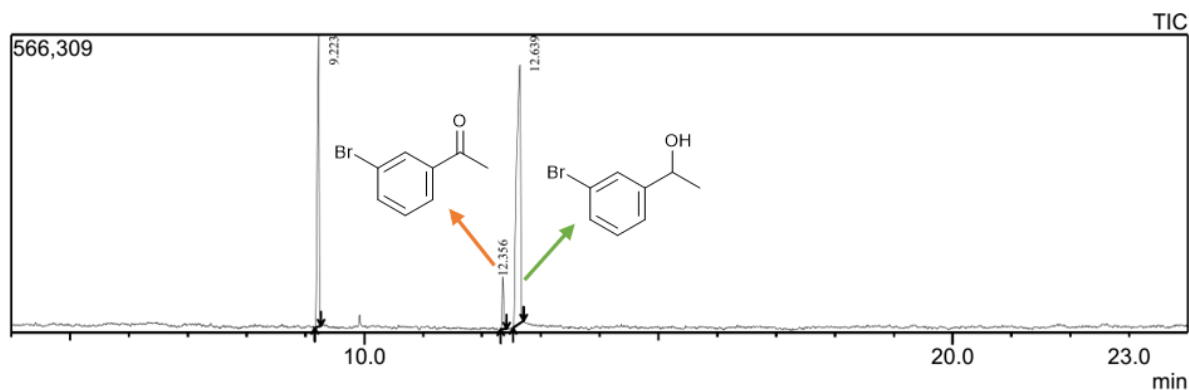
MassPeaks:339

RawMode:Averaged 12.440-12.450(1689-1691) BasePeak:77(108737)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan



GCMS of 10h:



Peak Report TIC

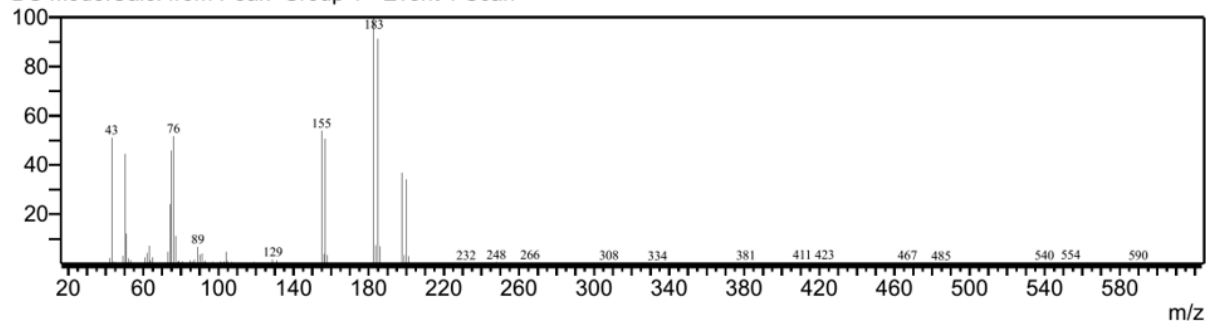
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	9.223	1271397	34.14	554543	48.40	2.29	Decane
2	12.356	180550	4.85	99268	8.66	1.82	Ethanone, 1-(3-bromophenyl)-
3	12.639	2271655	61.01	491986	42.94	4.62	Benzenemethanol, 3-bromo-.alpha.-methyl-
		3723602	100.00	1145797	100.00		

Line#:2 R.Time:12.355(Scan#:1672)

MassPeaks:276

RawMode:Averaged 12.350-12.360(1671-1673) BasePeak:183(12986)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan

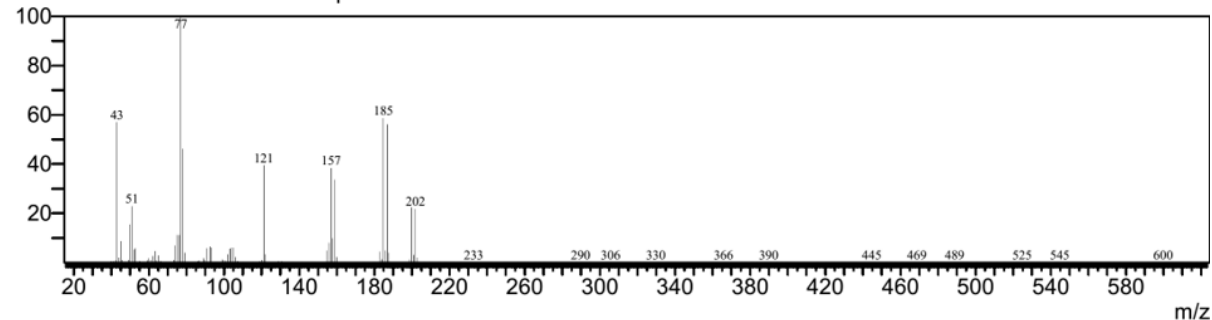


Line#:3 R.Time:12.640(Scan#:1729)

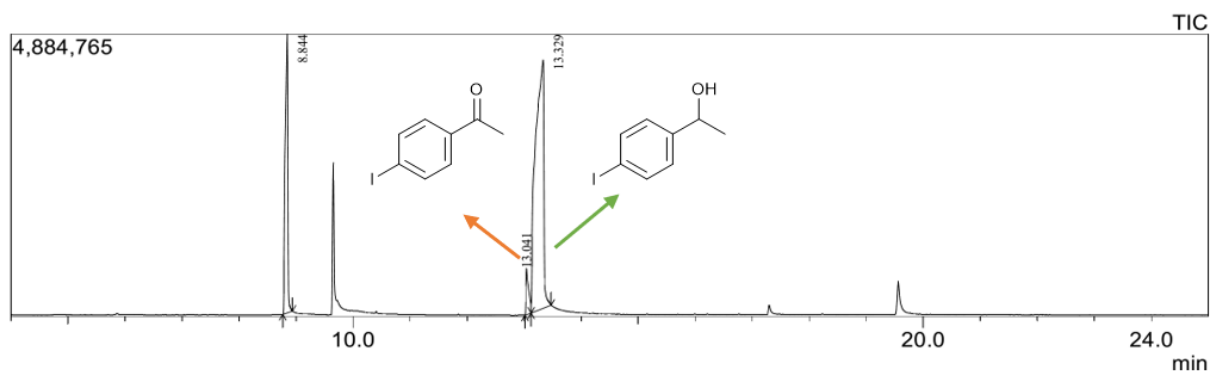
MassPeaks:318

RawMode:Averaged 12.635-12.645(1728-1730) BasePeak:77(69835)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan



GCMS of 10i:



Peak Report TIC

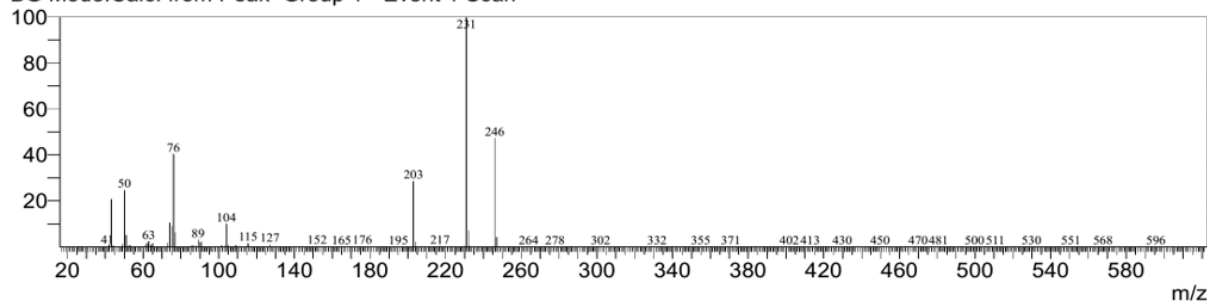
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	8.844	4818297	24.45	4822120	48.61	3.07	Decane
2	13.041	2670156	4.41	798074	8.05	3.35	4-Iodoacetophenone
3	13.329	3105978	71.14	4298928	43.34	10.03	1-(4-Iodophenyl)ethanol
		50594431	100.00	9919122	100.00		

Line#:2 R.Time:13.040(Scan#:1809)

MassPeaks:262

RawMode:Averaged 13.035-13.045(1808-1810) BasePeak:231(210935)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan

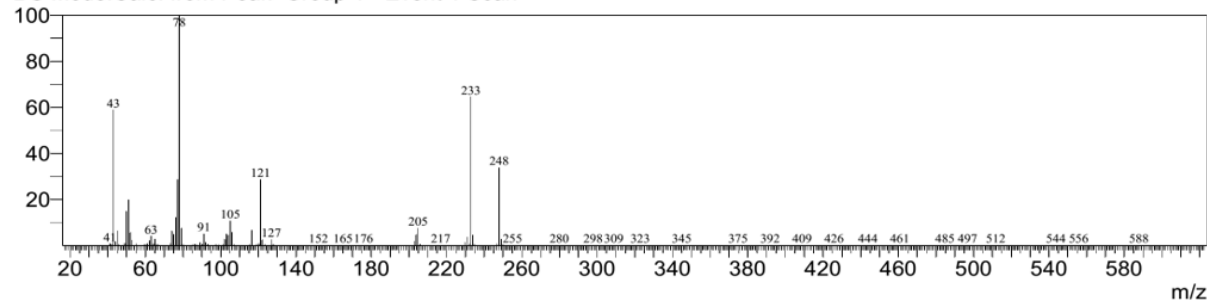


Line#:3 R.Time:13.330(Scan#:1867)

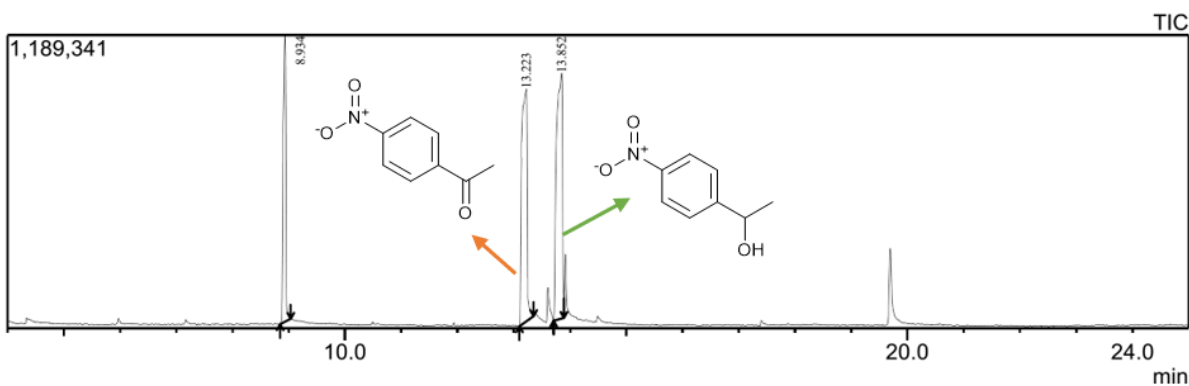
MassPeaks:333

RawMode:Averaged 13.325-13.335(1866-1868) BasePeak:78(853471)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan



GCMS of 10j:



Peak Report TIC

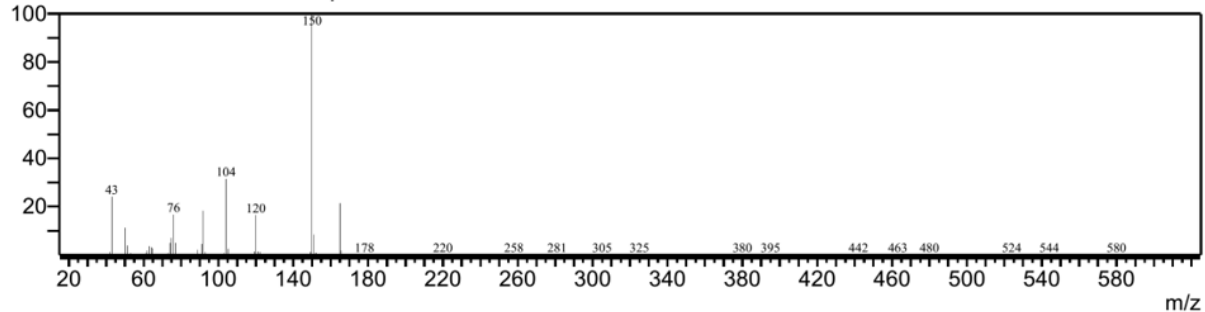
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	8.934	3725900	21.66	1161557	37.47	3.21	Decane
2	13.223	6277301	36.49	942090	30.39	6.66	Acetophenone, 4'-nitro-
3	13.852	7198799	41.85	996058	32.13	7.23	Benzenemethanol, .alpha.-methyl-4-nitro-
		7202000	100.00	3099705	100.00		

Line#:2 R.Time:13.225(Scan#:1846)

MassPeaks:368

RawMode:Averaged 13.220-13.230(1845-1847) BasePeak:150(301801)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan

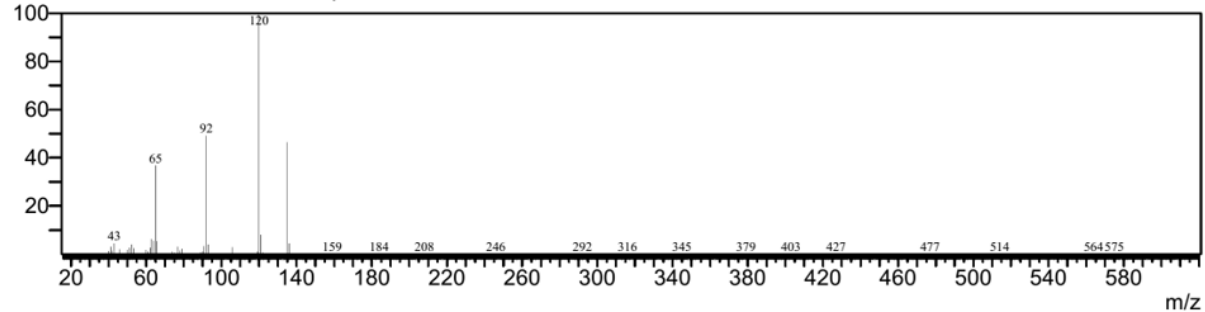


Line#:3 R.Time:13.605(Scan#:1922)

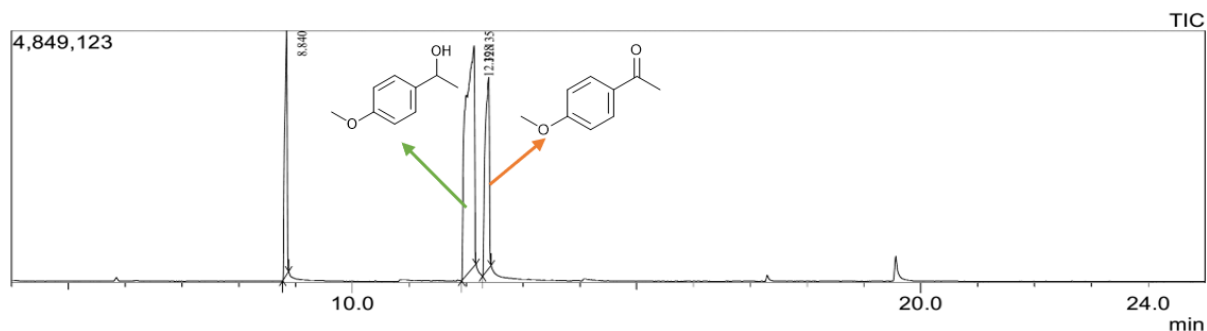
MassPeaks:311

RawMode:Averaged 13.600-13.610(1921-1923) BasePeak:120(42322)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan



GCMS of 10k:



Peak Report TIC

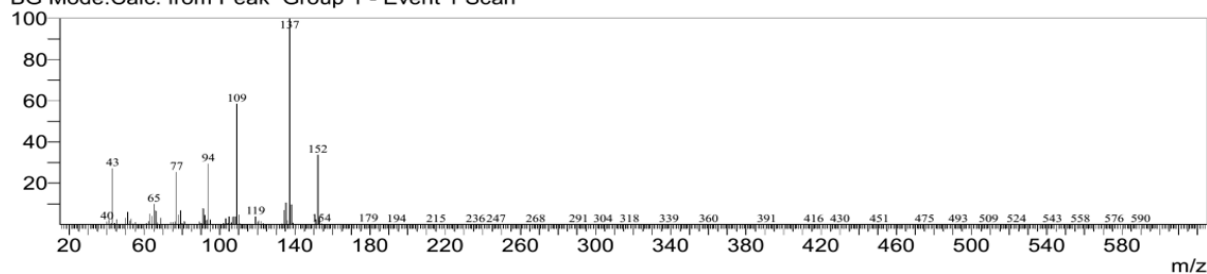
Peak#	R. Time	Area	Area%	Height	Height%	A/H	Name
1	8.840	3683924	17.47	4688638	37.16	2.92	Decane
2	12.135	15605711	58.22	4250072	33.69	10.73	4-Methoxyphenyl methyl carbinol
3	12.398	9045646	24.31	3677603	29.15	5.18	4-Acetylanisole
		8335281	100.00	12616313	100.00		

Line#:2 R. Time:12.135(Scan#:1628)

MassPeaks:328

RawMode:Averaged 12.130-12.140(1627-1629) BasePeak:137(983441)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan

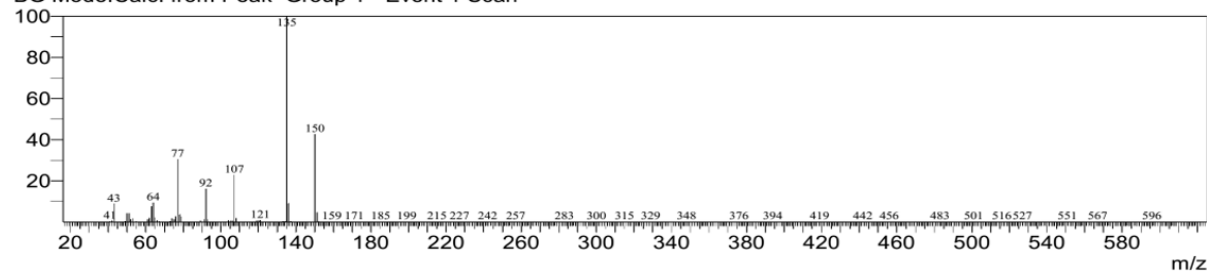


Line#:3 R. Time:12.400(Scan#:1681)

MassPeaks:368

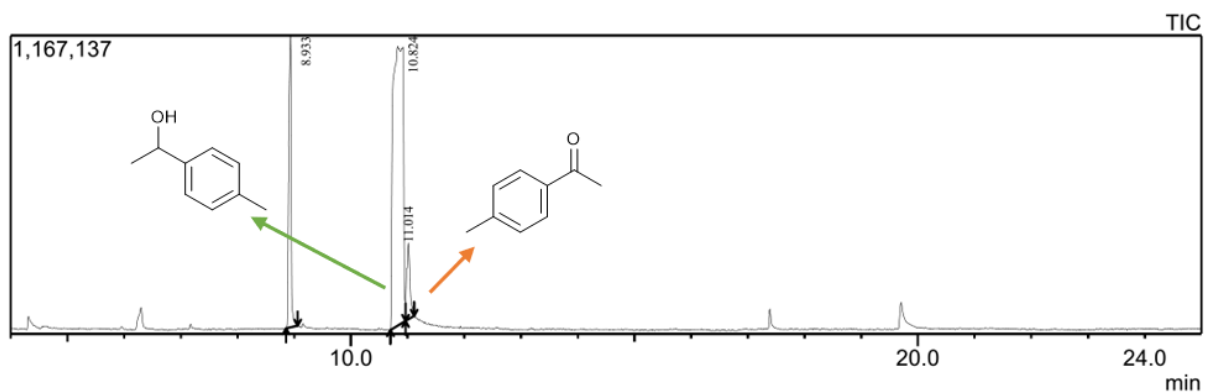
RawMode:Averaged 12.395-12.405(1680-1682) BasePeak:135(1235981)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan





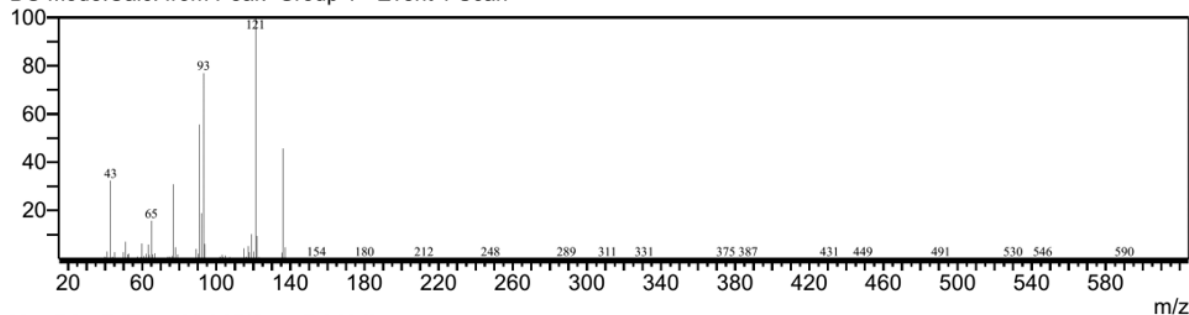
GCMS of 10I:



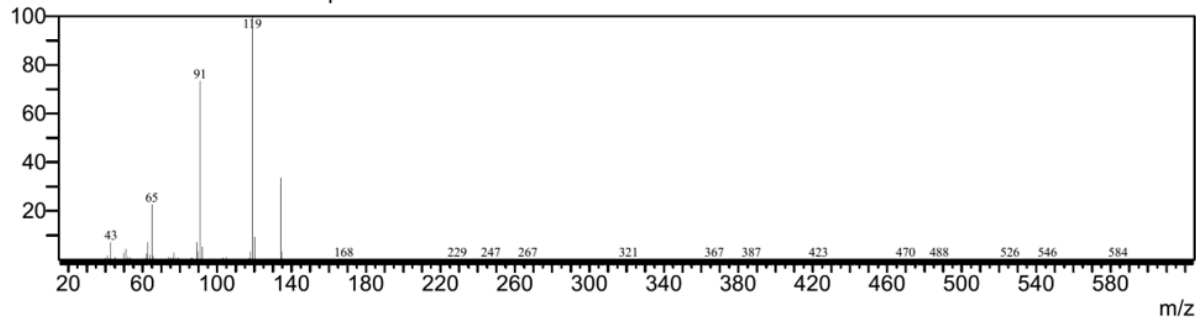
Peak Report TIC

Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	8.933	3524894	19.32	1140626	45.07	3.09	Decane
2	10.824	3578554	74.42	1092911	43.18	12.42	Benzenemethanol, .alpha.,4-dimethyl-
3	11.014	1143115	6.26	297514	11.75	3.84	Ethanone, 1-(4-methylphenyl)-
		8246563	100.00	2531051	100.00		

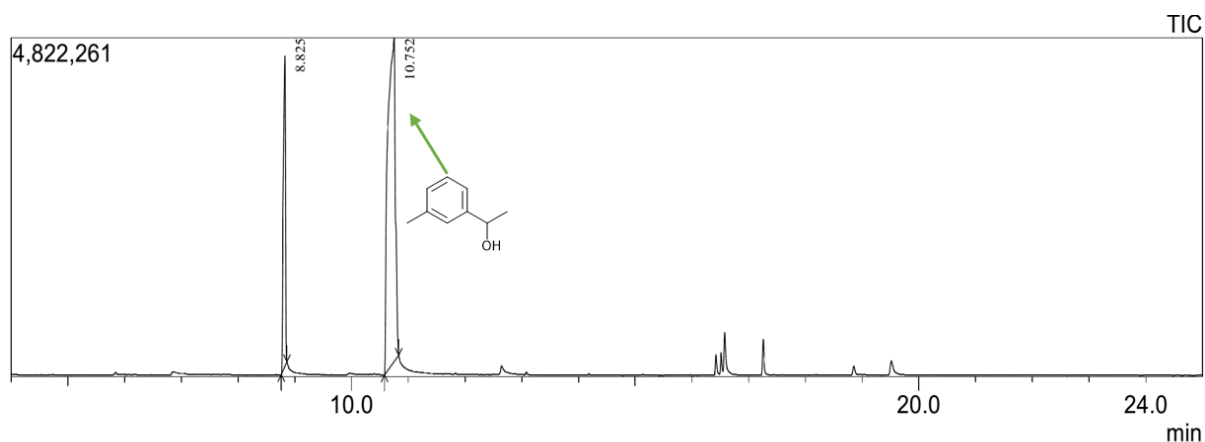
Line#:2 R.Time:10.825(Scan#:1366)  
 MassPeaks:333  
 RawMode:Averaged 10.820-10.830(1365-1367) BasePeak:121(213147)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Scan



Line#:3 R.Time:11.015(Scan#:1404)  
 MassPeaks:292  
 RawMode:Averaged 11.010-11.020(1403-1405) BasePeak:119(80645)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Scan



GCMS of 10m:



Peak Report TIC

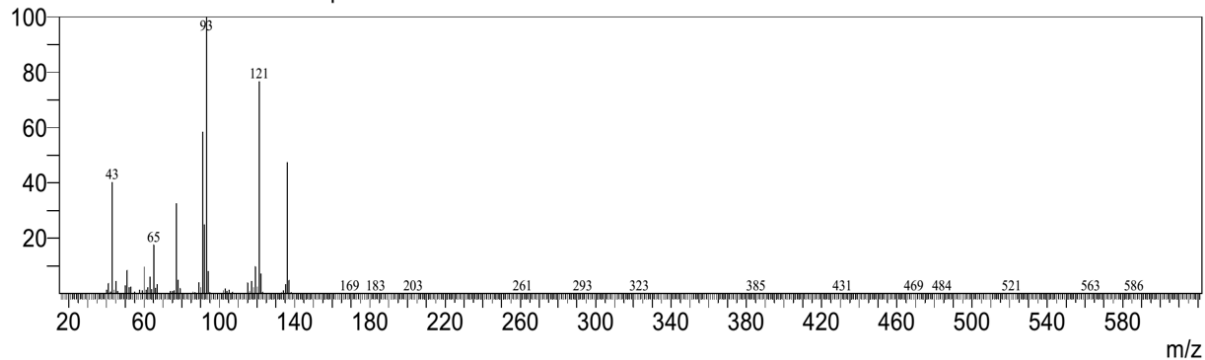
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	8.825	11842112	21.60	4412839	48.95	2.68	Decane
2	10.752	2990866	78.40	4602288	51.05	9.34	Methyl m-tolyl carbinol
		4832978	100.00	9015127	100.00		

Line#:2 R.Time:10.750(Scan#:1351)

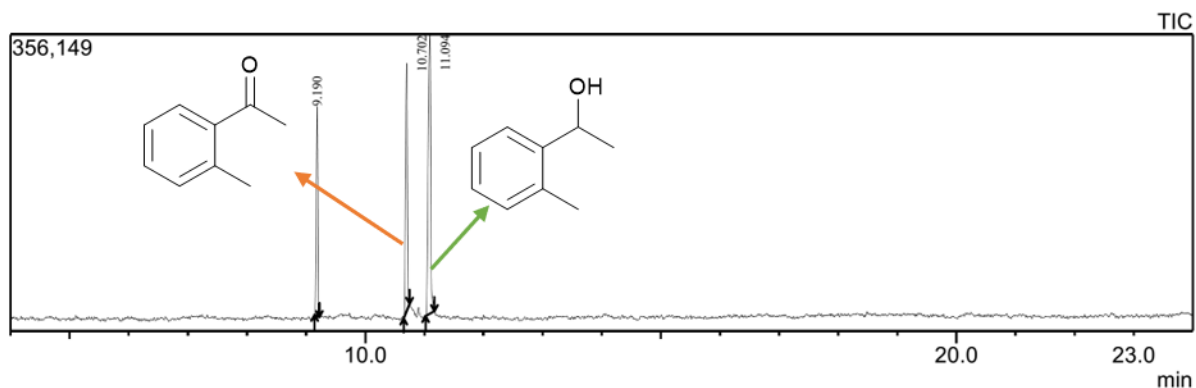
MassPeaks:308

RawMode:Averaged 10.745-10.755(1350-1352) BasePeak:93(867682)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan



GCMS of 10n:



Peak Report TIC

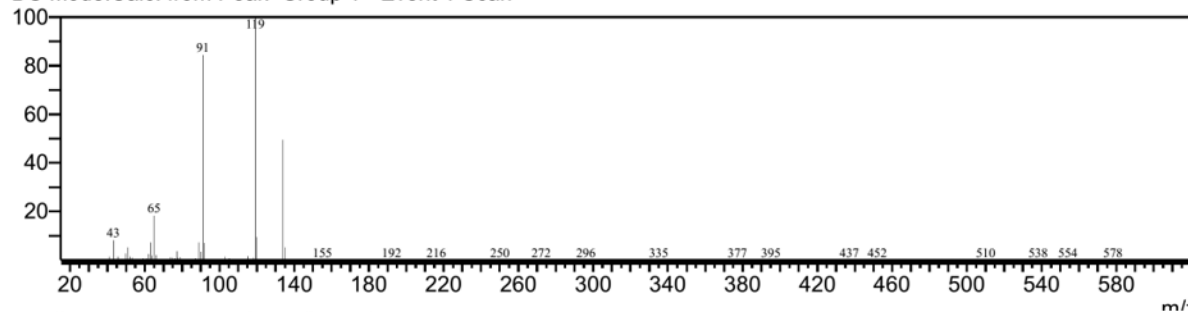
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	9.190	433946	21.11	251494	28.47	1.73	Decane
2	10.702	638430	31.06	296795	33.60	2.15	Ethanone, 1-(2-methylphenyl)-
3	11.094	983100	47.83	335002	37.93	2.93	1-(2-Methylphenyl)ethanol
		2055476	100.00	883291	100.00		

Line#:2 R.Time:10.700(Scan#:1341)

MassPeaks:327

RawMode:Averaged 10.695-10.705(1340-1342) BasePeak:119(84883)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan

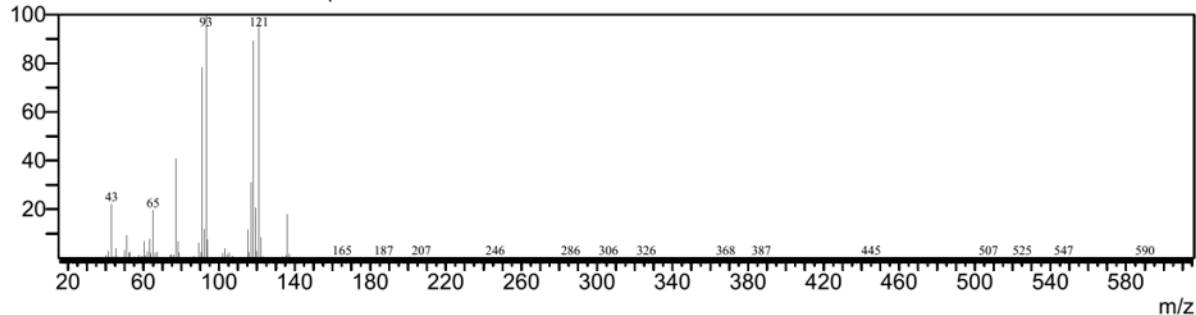


Line#:3 R.Time:11.095(Scan#:1420)

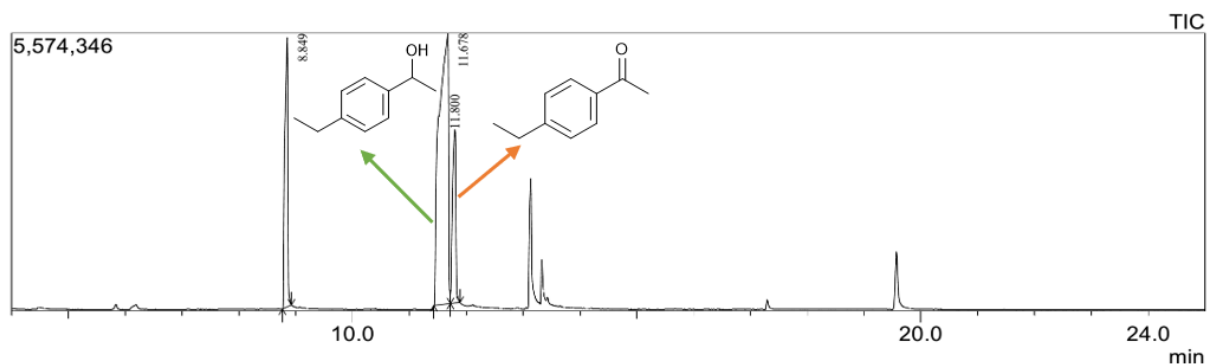
MassPeaks:322

RawMode:Averaged 11.090-11.100(1419-1421) BasePeak:93(49715)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan



GCMS of 10o:



Peak Report TIC

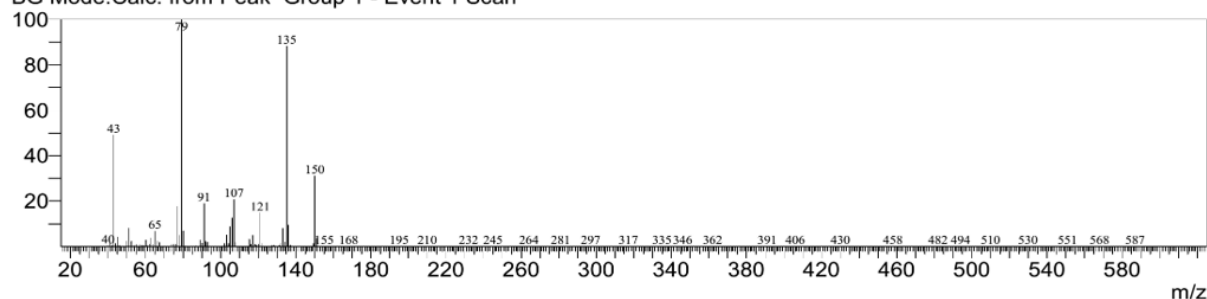
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	8.849	8565526	19.83	5400161	37.74	3.44	Decane
2	11.678	1433914	65.61	5427417	37.94	11.32	1-(4-Ethylphenyl)ethanol
3	11.800	3638239	14.56	3479529	24.32	3.92	Ethanone, 1-(4-ethylphenyl)-
		3637679	100.00	14307107	100.00		

Line#:2 R.Time:11.675(Scan#:1536)

MassPeaks:315

RawMode:Averaged 11.670-11.680(1535-1537) BasePeak:79(1091526)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan

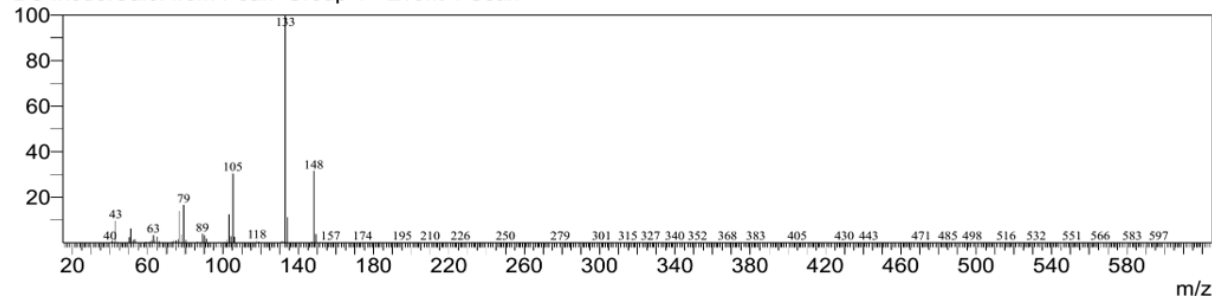


Line#:3 R.Time:11.800(Scan#:1561)

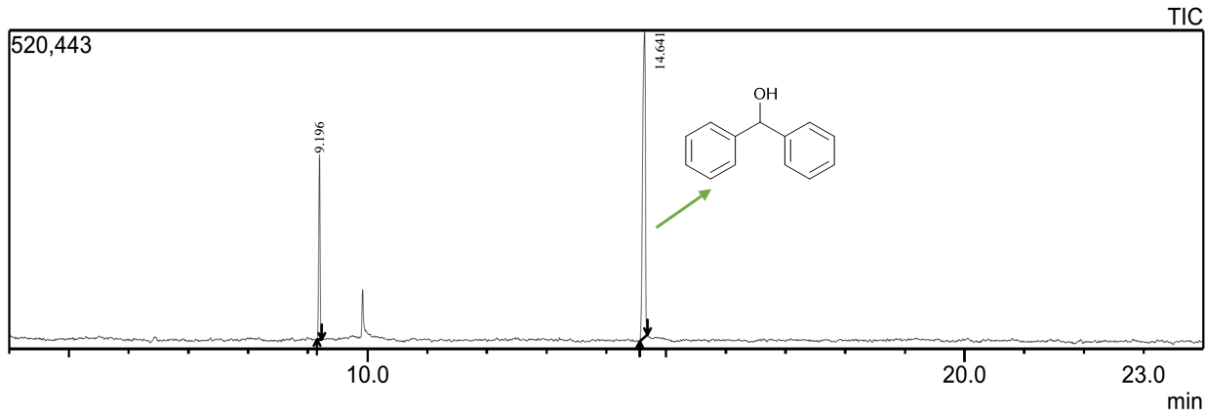
MassPeaks:301

RawMode:Averaged 11.795-11.805(1560-1562) BasePeak:133(1225060)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan



GCMS of 10p:



Peak Report TIC

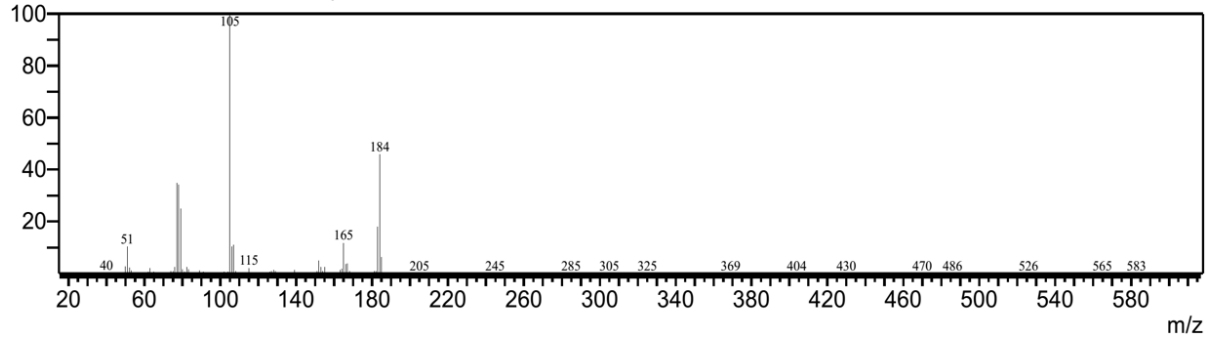
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	9.196	484710	23.26	302391	37.64	1.60	Decane
2	14.641	1598936	76.74	500968	62.36	3.19	Benzenemethanol, .alpha.-phenyl-
		2083646	100.00	803359	100.00		

Line#:2 R.Time:14.640(Scan#:2129)

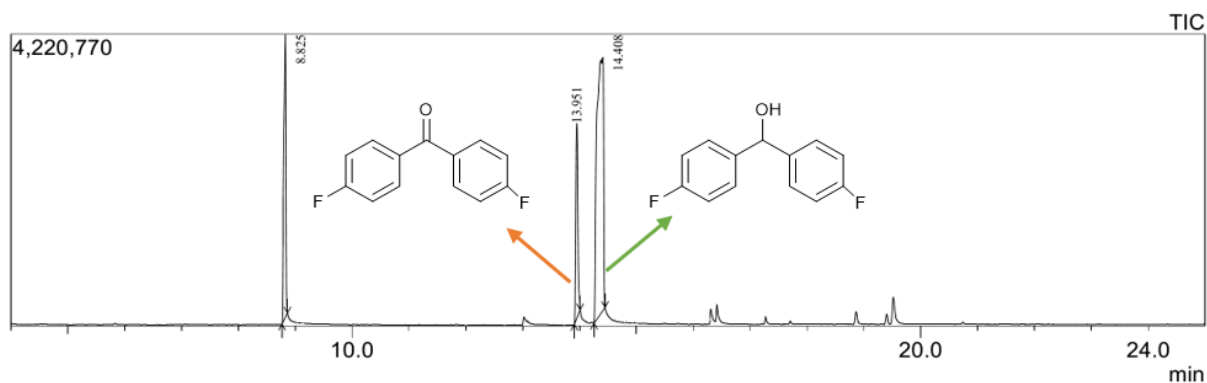
MassPeaks:321

RawMode:Averaged 14.635-14.645(2128-2130) BasePeak:105(132155)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan



GCMS of 10q:



Peak Report TIC

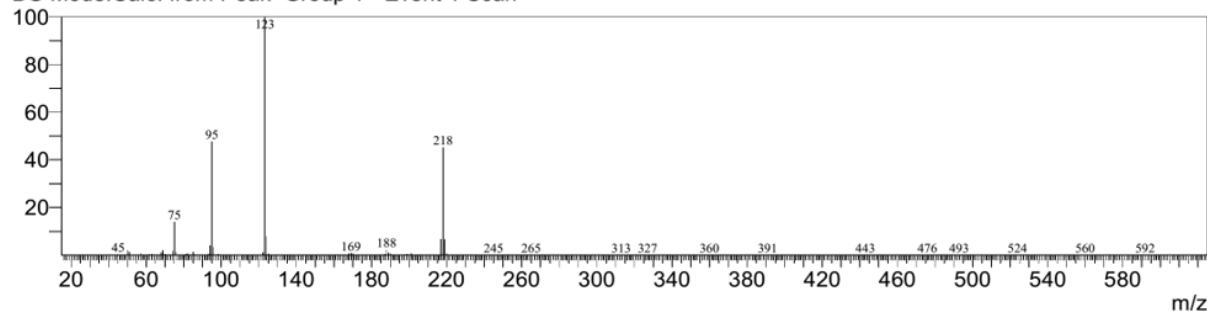
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	8.825	0224904	21.72	4090041	38.67	2.50	Decane
2	13.951	6964676	14.79	2817559	26.64	2.47	4,4'-Difluorobenzophenone
3	14.408	9890593	63.49	3668330	34.69	8.15	4,4'-Difluorobenzhydrol
		7080173	100.00	10575930	100.00		

Line#:2 R.Time:13.950(Scan#:1991)

MassPeaks:333

RawMode:Averaged 13.945-13.955(1990-1992) BasePeak:123(1049401)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan

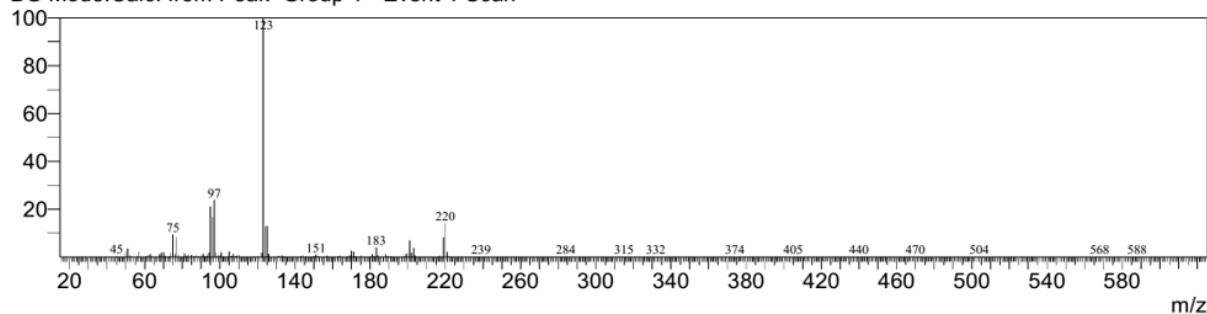


Line#:3 R.Time:14.410(Scan#:2083)

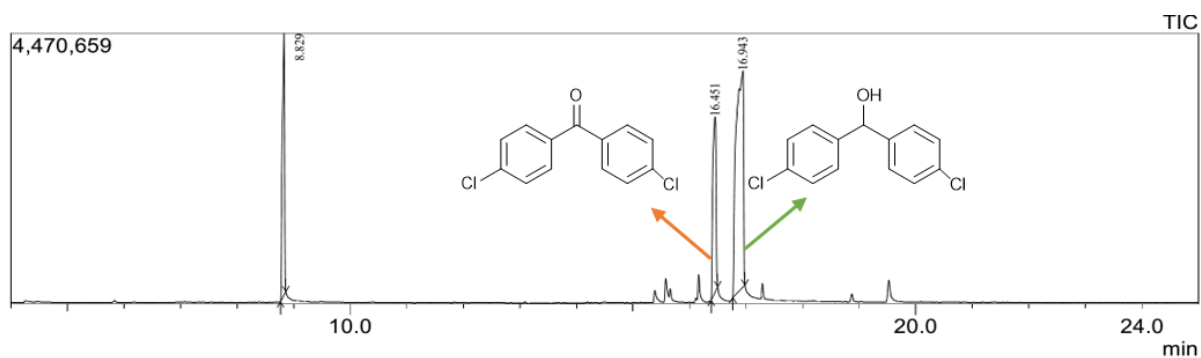
MassPeaks:365

RawMode:Averaged 14.405-14.415(2082-2084) BasePeak:123(1184735)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan



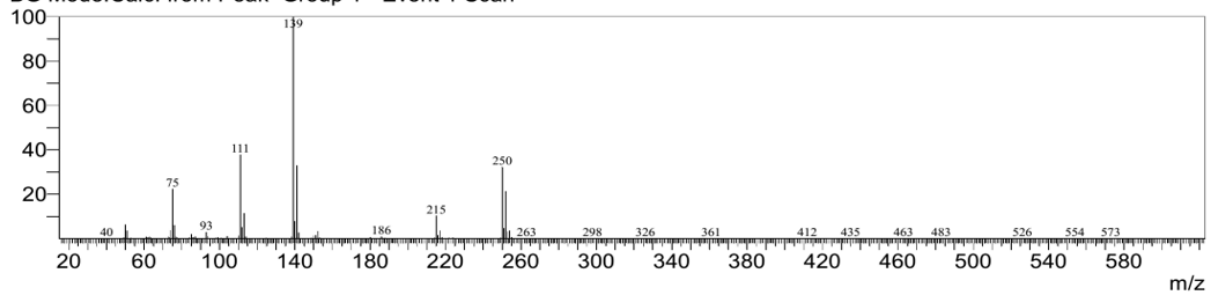
GCMS of 10r:



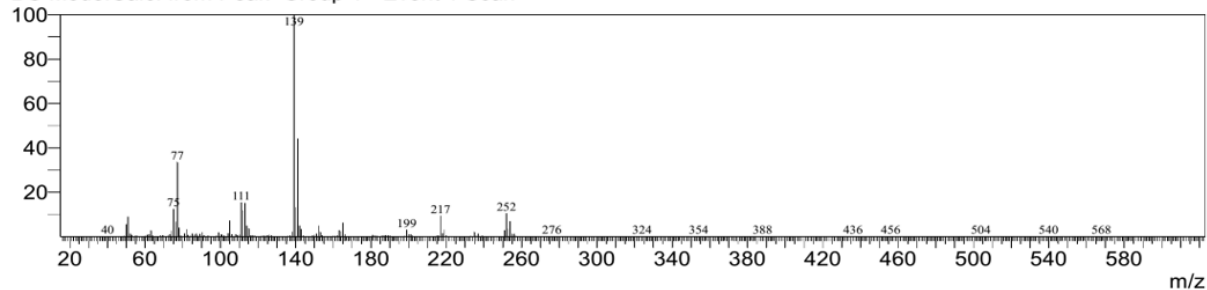
Peak Report TIC

Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	8.829	11896835	21.03	4320982	40.08	2.75	Decane
2	16.451	11495818	20.32	2888627	26.79	3.98	4,4'-Dichlorobenzophenone
3	16.943	33178386	58.65	3571120	33.13	9.29	4,4'-Dichlorobenzhydrol
		56571039	100.00	10780729	100.00		

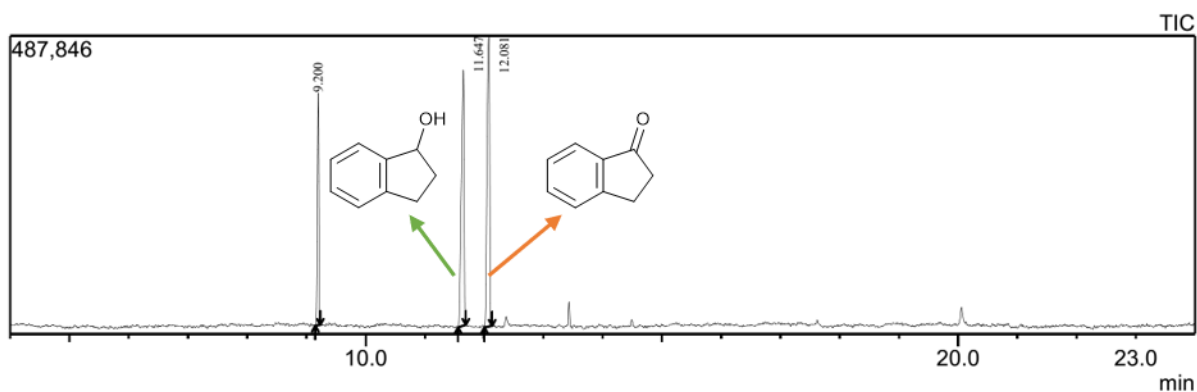
Line#:2 R.Time:16.450(Scan#:2491)  
 MassPeaks:325  
 RawMode:Averaged 16.445-16.455(2490-2492) BasePeak:139(819090)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Scan



Line#:3 R.Time:16.945(Scan#:2590)  
 MassPeaks:338  
 RawMode:Averaged 16.940-16.950(2589-2591) BasePeak:139(869259)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Scan



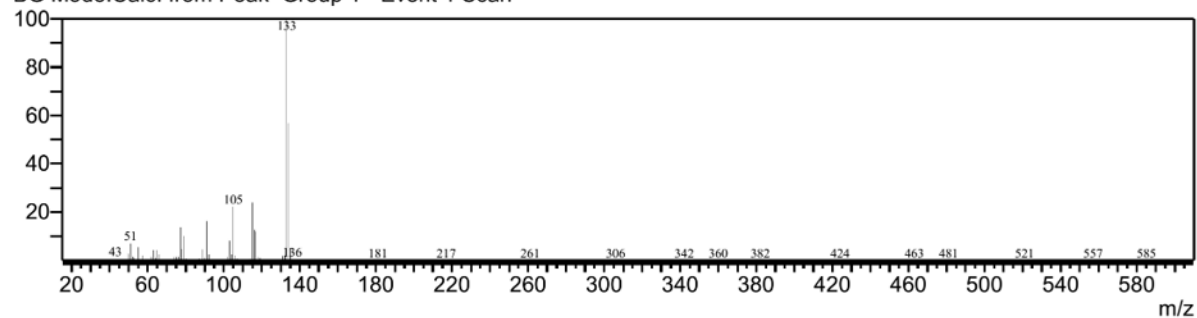
GCMS of 10s:



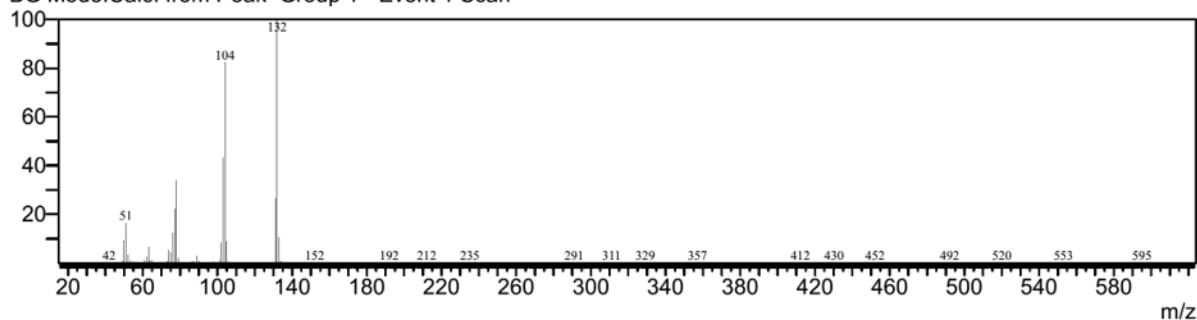
Peak Report TIC

Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	9.200	658630	19.11	380097	29.85	1.73	Decane
2	11.647	1309310	37.98	418378	32.85	3.13	1H-Inden-1-ol, 2,3-dihydro-
3	12.081	1479430	42.91	475043	37.30	3.11	1H-Inden-1-one, 2,3-dihydro-
		3447370	100.00	1273518	100.00		

Line#:2 R.Time:11.645(Scan#:1530)  
 MassPeaks:312  
 RawMode:Averaged 11.640-11.650(1529-1531) BasePeak:133(116651)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Scan

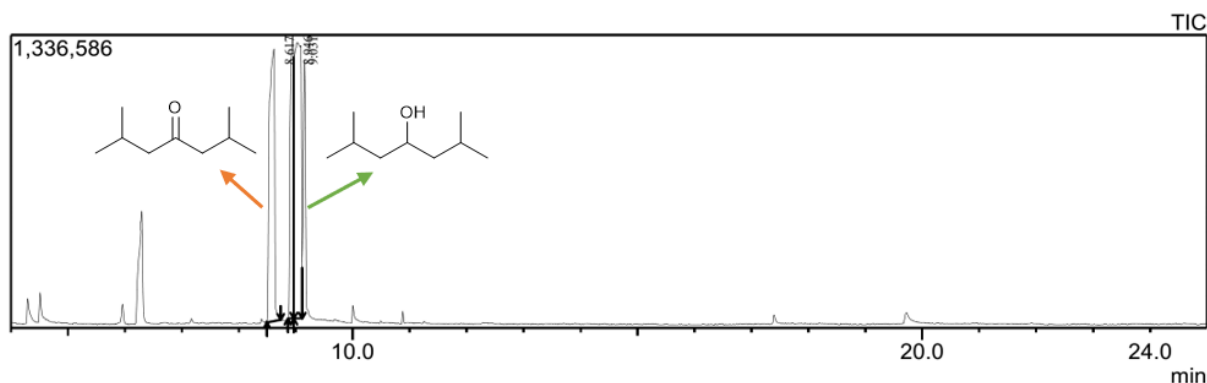


Line#:3 R.Time:12.080(Scan#:1617)  
 MassPeaks:311  
 RawMode:Averaged 12.075-12.085(1616-1618) BasePeak:132(112641)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Scan





GCMS of 10t:



Peak Report TIC

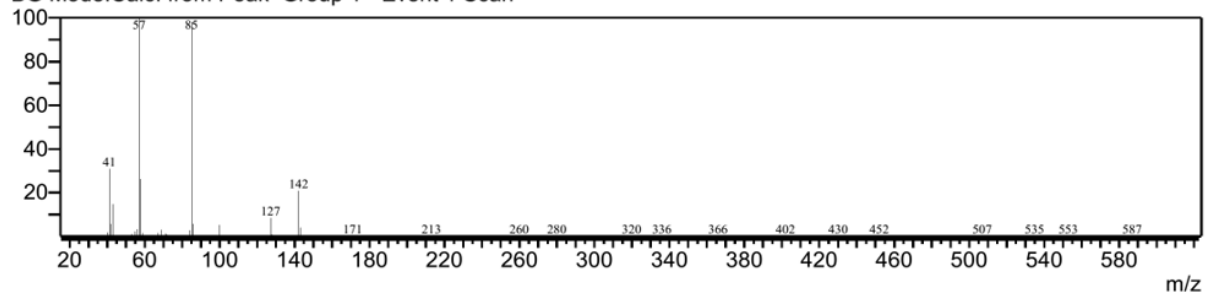
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	8.617	7854953	33.88	1241242	32.72	6.33	4-Heptanone, 2,6-dimethyl-
2	8.946	5300755	22.86	1293425	34.10	4.10	Decane
3	9.031	0028247	43.26	1258771	33.18	7.97	4-Heptanol, 2,6-dimethyl-
		3183955	100.00	3793438	100.00		

Line#:1 R.Time:8.615(Scan#:924)

MassPeaks:255

RawMode:Averaged 8.610-8.620(923-925) BasePeak:57(359050)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan

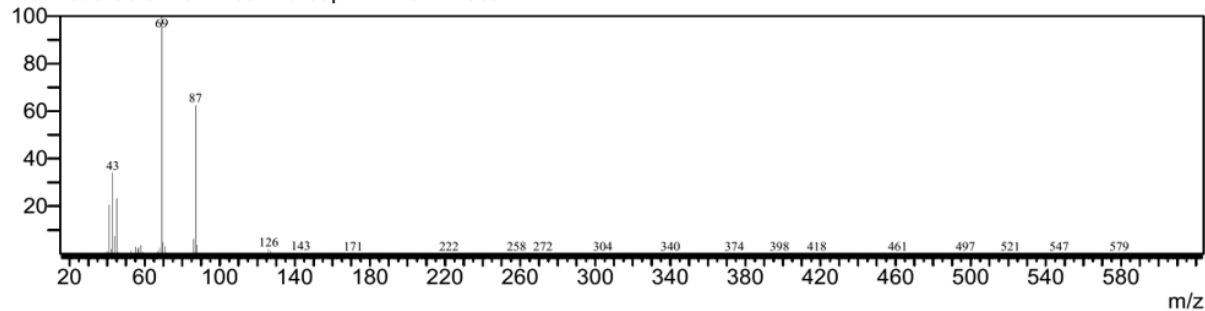


Line#:3 R.Time:9.030(Scan#:1007)

MassPeaks:313

RawMode:Averaged 9.025-9.035(1006-1008) BasePeak:69(176254)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan



GCMS of 10u:



Peak Report TIC

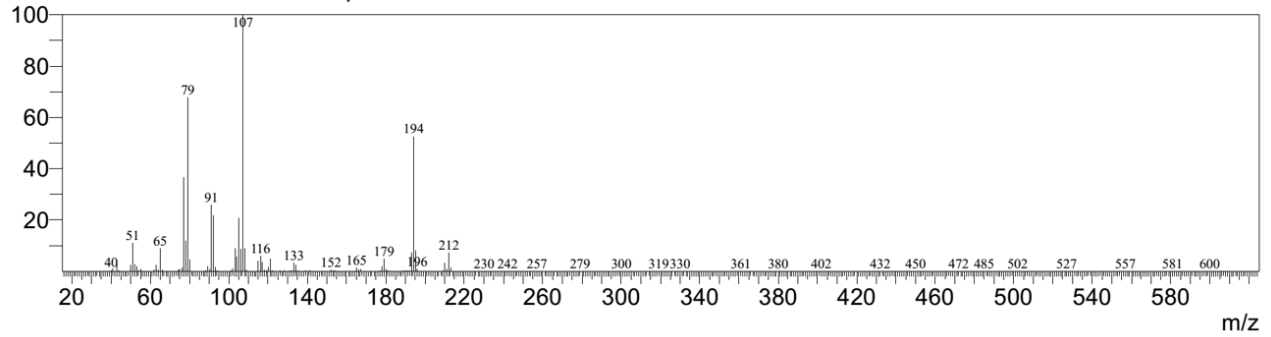
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	8.787	8434009	19.17	3313490	43.93	2.55	Decane
2	15.680	35568871	80.83	4228742	56.07	8.41	1,3 Diphenylpropan-1-ol
		4002880	100.00	7542232	100.00		

Line#:2 R.Time:15.680(Scan#:2337)

MassPeaks:308

RawMode:Averaged 15.675-15.685(2336-2338) BasePeak:107(860431)

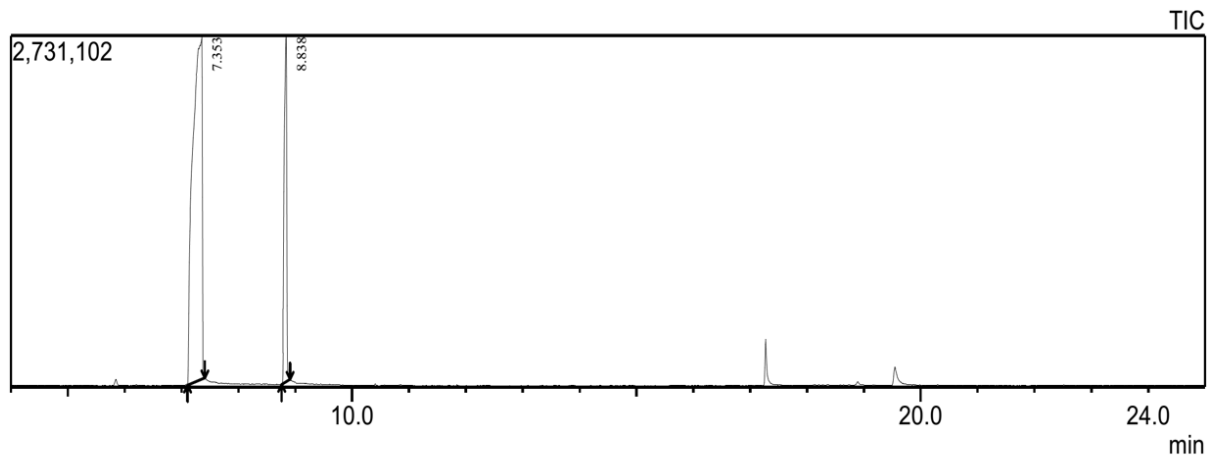
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



## GCMS of Control experiments

Transfer hydrogenation of cyclohexanone with 1 using CuI

Entry 1



Peak Report TIC

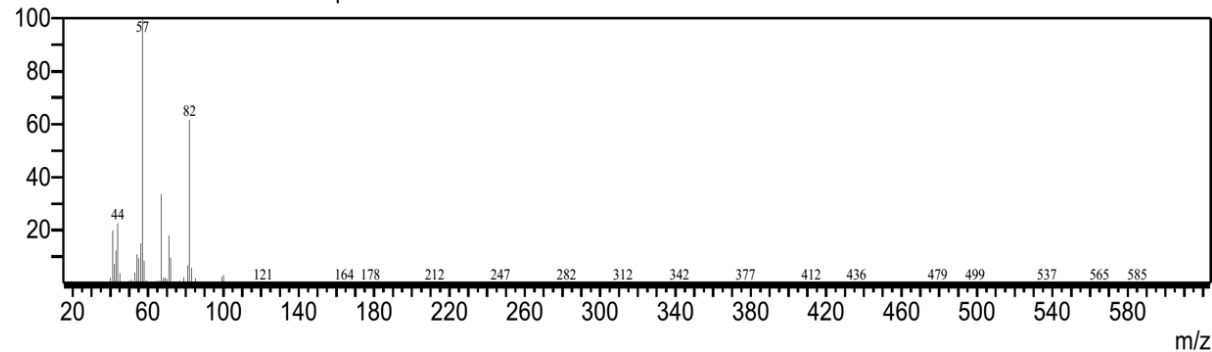
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	7.353	10404150	79.00	2657481	49.72	11.44	Cyclohexanol
2	8.838	8081406	21.00	2687791	50.28	3.01	Decane
		8485556	100.00	5345272	100.00		

Line#:1 R.Time:7.355(Scan#:672)

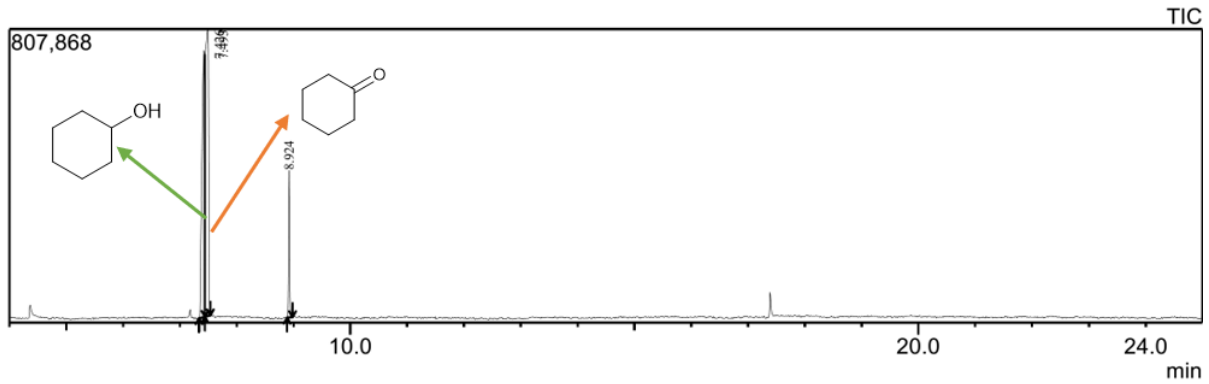
MassPeaks:307

RawMode:Averaged 7.350-7.360(671-673) BasePeak:57(683424)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan



Entry 2



Peak Report TIC

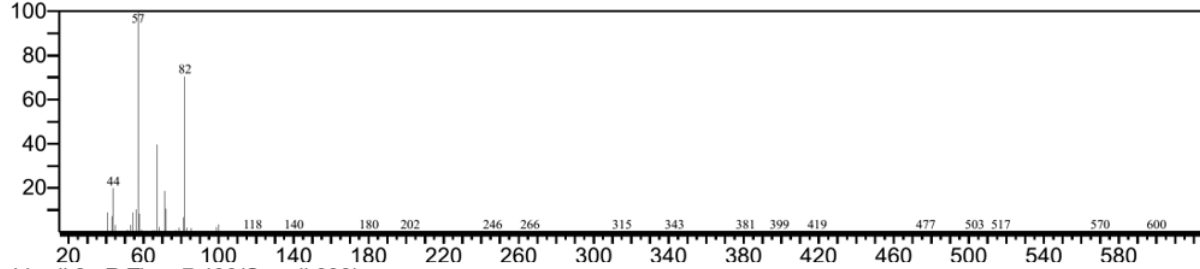
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	7.426	2696109	42.26	733657	38.08	3.67	Cyclohexanol
2	7.493	3173703	49.74	789131	40.95	4.02	Cyclohexanone
3	8.924	510658	8.00	404077	20.97	1.26	Decane
		6380470	100.00	1926865	100.00		

Line#:1 R.Time:7.425(Scan#:686)

MassPeaks:321

RawMode:Averaged 7.420-7.430(685-687) BasePeak:57(40843)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan

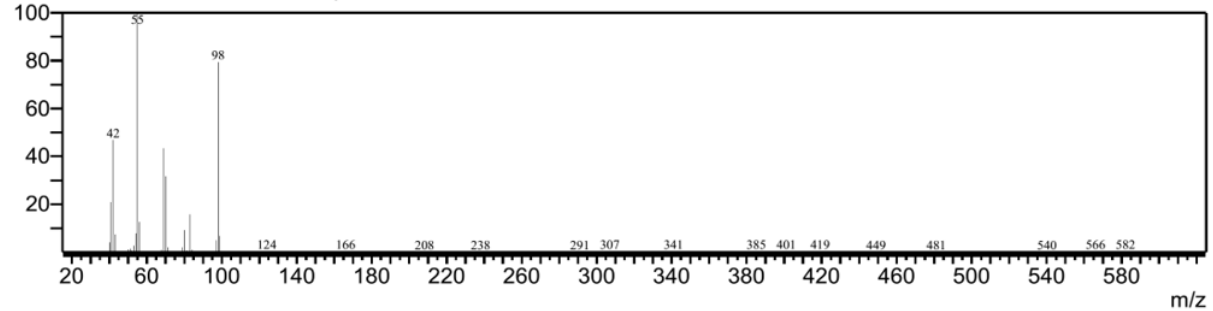


Line#:2 R.Time:7.490(Scan#:699)

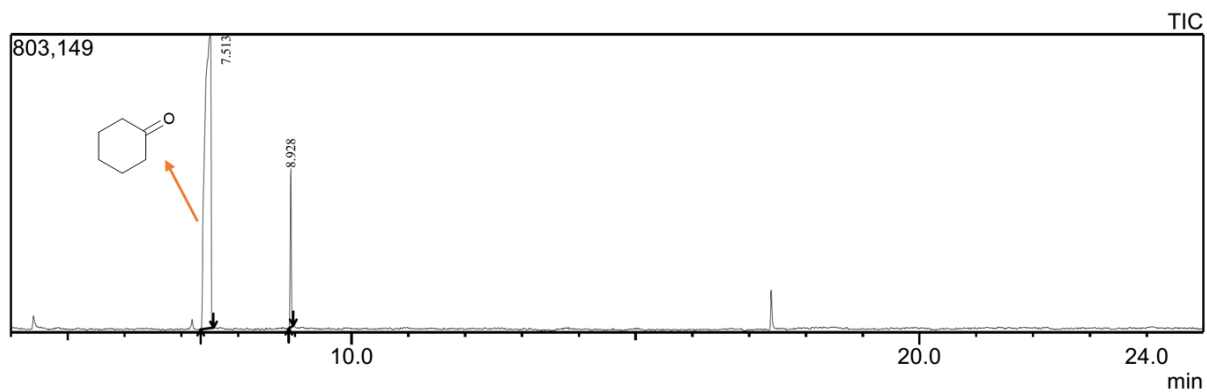
MassPeaks:309

RawMode:Averaged 7.485-7.495(698-700) BasePeak:55(110480)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan



Entry 3



Peak Report TIC

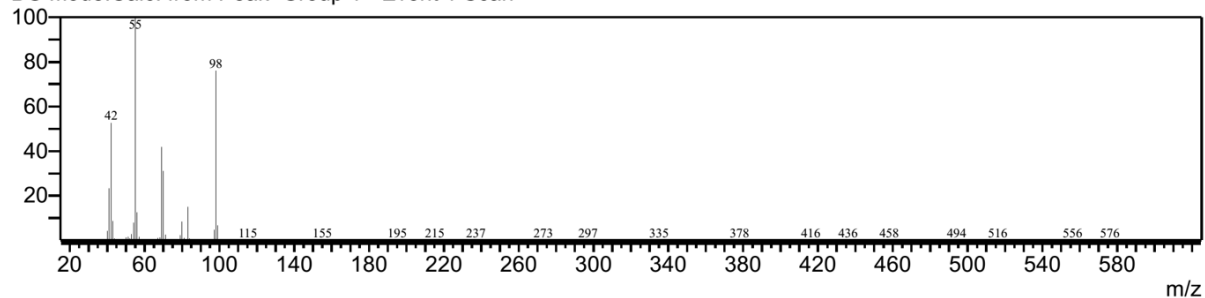
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	7.513	5951827	91.44	790827	64.92	7.53	Cyclohexanone
2	8.928	557014	8.56	427362	35.08	1.30	Decane
		6508841	100.00	1218189	100.00		

Line#:1 R.Time:7.510(Scan#:703)

MassPeaks:293

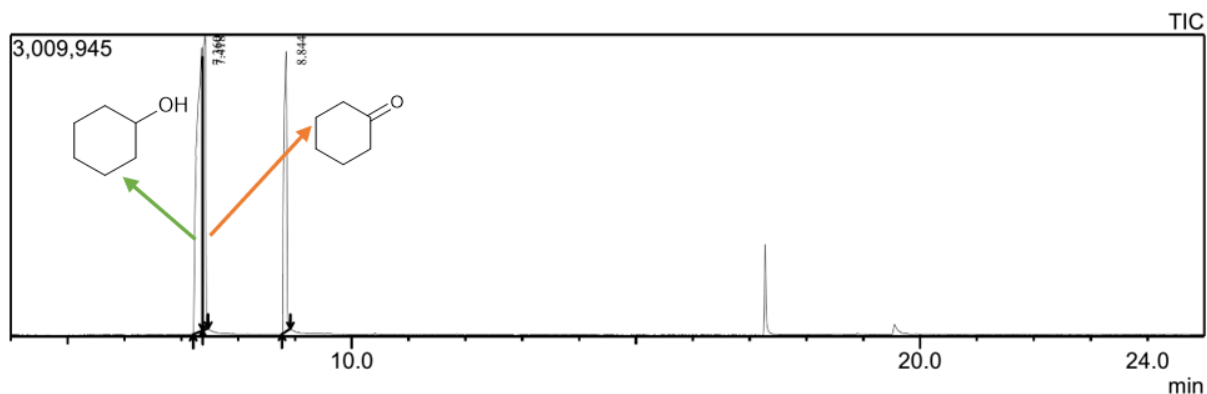
RawMode:Averaged 7.505-7.515(702-704) BasePeak:55(190499)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan



# Transfer hydrogenation of cyclohexanone with 5 using CuI

## Entry 1



Peak Report TIC

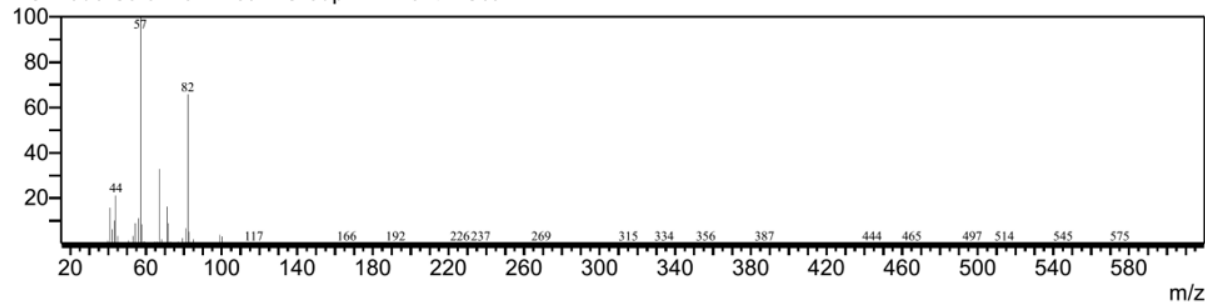
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	7.360	20588976	53.23	2826617	33.03	7.28	Cyclohexanol
2	7.418	8652175	22.37	2939617	34.35	2.94	Cyclohexanone
3	8.844	9439260	24.40	2791801	32.62	3.38	Decane
		38680411	100.00	8558035	100.00		

Line#:1 R.Time:7.360(Scan#:673)

MassPeaks:257

RawMode:Averaged 7.355-7.365(672-674) BasePeak:57(121520)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan

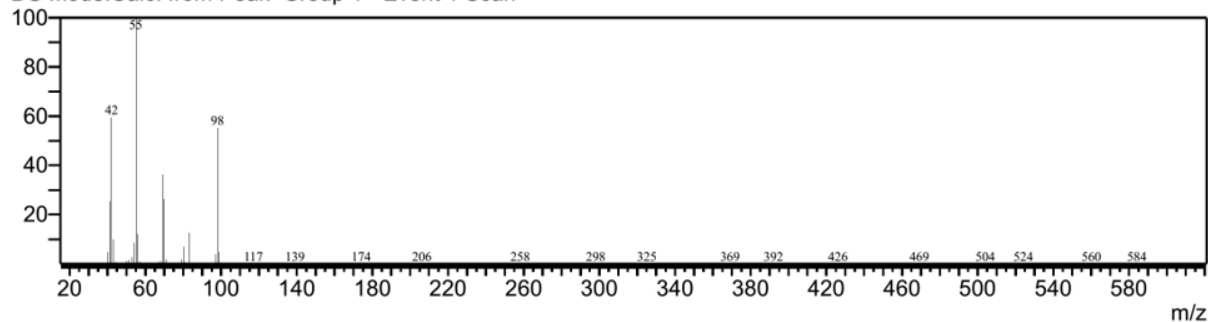


Line#:2 R.Time:7.420(Scan#:685)

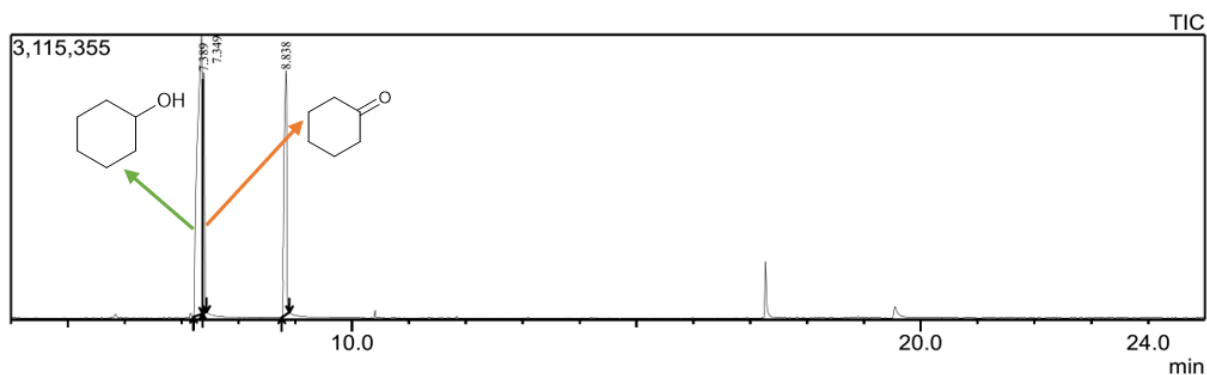
MassPeaks:249

RawMode:Averaged 7.415-7.425(684-686) BasePeak:55(361522)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan



Entry 2



Peak Report TIC

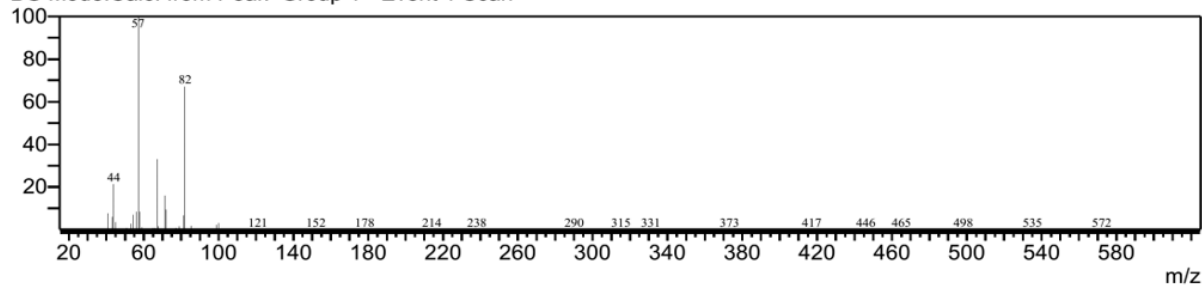
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	7.349	8958326	57.27	3049478	36.52	6.22	Cyclohexanol
2	7.389	5723272	17.29	2632254	31.52	2.17	Cyclohexanone
3	8.838	8419937	25.44	2669031	31.96	3.15	Decane
		3101535	100.00	8350763	100.00		

Line#:1 R.Time:7.350(Scan#:671)

MassPeaks:292

RawMode:Averaged 7.345-7.355(670-672) BasePeak:57(364689)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan

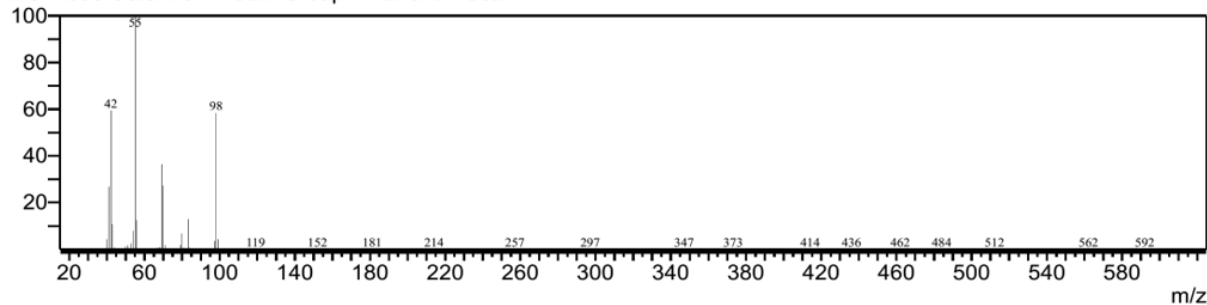


Line#:2 R.Time:7.390(Scan#:679)

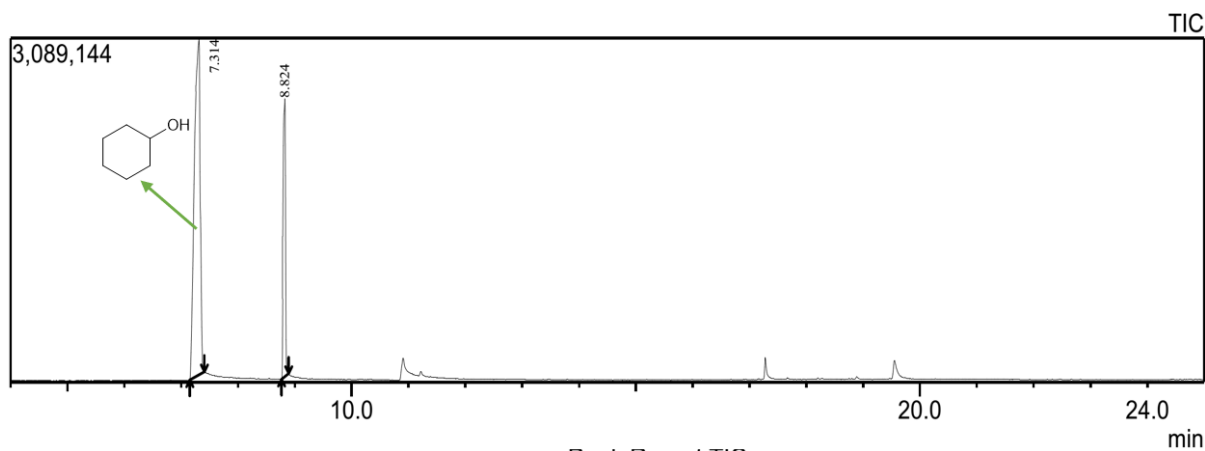
MassPeaks:264

RawMode:Averaged 7.385-7.395(678-680) BasePeak:55(206791)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan



Entry 3



Peak Report TIC

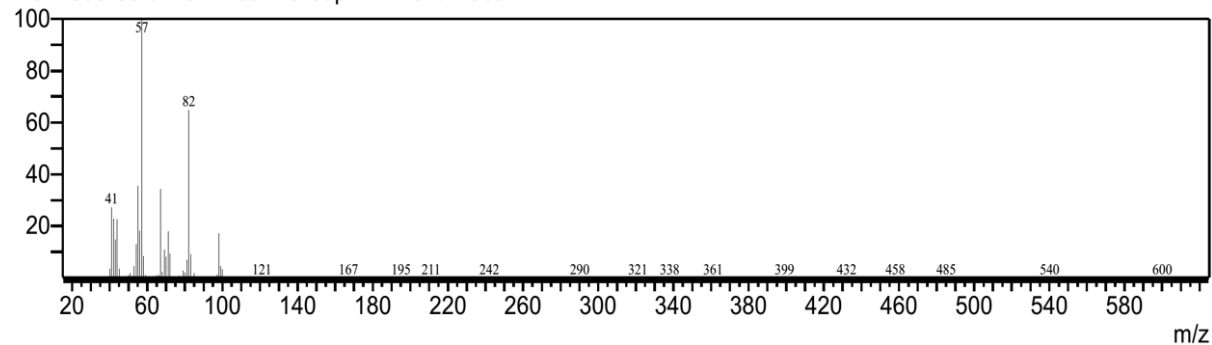
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Name
1	7.314	21444886	74.91	3020184	54.77	7.10	Cyclohexanol
2	8.824	7184447	25.09	2493927	45.23	2.88	Decane
		28629333	100.00	5514111	100.00		

Line#:1 R.Time:7.315(Scan#:664)

MassPeaks:313

RawMode:Averaged 7.310-7.320(663-665) BasePeak:57(620877)

BG Mode:Calc. from Peak Group 1 - Event 1 Scan





**Table S2.** Energies of all optimized structures.

Carbene type	Species	BP86/BS1		BP86/BS1(SMD)	PBE0/BS2
		G <sup>BS1</sup>	(G-E <sub>el</sub> ) <sup>BS1</sup>	E <sub>el</sub> <sup>Sol</sup>	E <sub>el</sub> <sup>BS2</sup>
[[Ru]NHC <sup>H</sup> ]	1(H)-PPh <sub>3</sub>	-3554.665974	0.72826116	-3555.490115	-3555.0342
	1a(H)-PPh <sub>3</sub>	-2519.130707	0.47681831	-2519.697892	-2519.3316
	A(H)-PPh <sub>3</sub>	-2252.477094	0.56292526	-2253.134026	-2252.8313
	TS-I(H)-PPh <sub>3</sub>	-2252.478357	0.56142809	-2253.132118	-2252.8307
	B(H)-PPh <sub>3</sub>	-2252.486952	0.56086789	-2253.136838	-2252.8358
	2(H)-PPh <sub>3</sub>	-3095.09395	0.73514464	-3095.921101	-3095.5142
	2a(H)-PPh <sub>3</sub>	-2059.548415	0.48372371	-2060.118049	-2059.7998
	1(H)-PH <sub>3</sub>	-2169.762269	0.27211656	-2170.118086	-2169.7598
	1a(H)-PH <sub>3</sub>	-1826.667998	0.24897346	-1827.003764	-1826.6859
	A(H)-PH <sub>3</sub>	-1560.020744	0.33514418	-1560.442981	-1560.1897
	TS-I(H)-PH <sub>3</sub>	-1560.021916	0.33377329	-1560.441601	-1560.1892
	B(H)-PH <sub>3</sub>	-1560.031468	0.33377329	-1560.448606	-1560.1959
	2(H)-PH <sub>3</sub>	-1710.187349	0.27994911	-1710.54524	-1710.2346
	2a(H)-PH <sub>3</sub>	-1367.089007	0.25643237	-1367.426353	-1367.1557
	PS-C(H)-PH <sub>3</sub>	-1870.711172	0.49599478	-1871.294938	-1871.0765
	PS-TS-II(H)-PH <sub>3</sub>	-1870.705143	0.49501365	-1871.28905	-1871.0733
	PS-D(H)-PH <sub>3</sub>	-1870.703918	0.49696454	-1871.291232	-1871.0746
	NPS-C(H)-PH <sub>3</sub>	-1676.612993	0.3966251	-1677.095011	-1676.8458
	NPS-TS-II(H)-PH <sub>3</sub>	-1676.604184	0.39659682	-1677.089282	-1676.8401
	NPS-D(H)-PH <sub>3</sub>	-1676.60529	0.39553552	-1677.089517	-1676.8402
	E(H)-PH <sub>3</sub>	-1870.723865	0.49936923	-1871.306919	-1871.0958
TS-III(H)-PH <sub>3</sub>	-1870.723463	0.49672008	-1871.30497	-1871.0909	
F(H)-PH <sub>3</sub>	-1870.721697	0.49867222	-1871.305771	-1871.0915	
[[Ru]NHC <sup>]</sup> ]	1'-PPh <sub>3</sub>	-3554.242555	0.71452201	-3555.017011	-3554.5923
	1a'-PPh <sub>3</sub>	-2518.707899	0.46160879	-2519.222876	-2518.8887
	2'-PPh <sub>3</sub>	-3094.663311	0.72069403	-3095.442088	-3095.0643
	2a'-PPh <sub>3</sub>	-2059.122222	0.46912149	-2059.64158	-2059.3535
	1'-PH <sub>3</sub>	-2169.340508	0.25763632	-2169.640619	-2169.32
	1a'-PH <sub>3</sub>	-1826.250517	0.23436493	-1826.529352	-1826.249
	A'-PH <sub>3</sub>	-1559.605117	0.32153111	-1559.969953	-1559.7553
	TS-I'-PH <sub>3</sub>	-1559.605848	0.31929578	-1559.967279	-1559.7535
	B'-PH <sub>3</sub>	-1559.611853	0.32022854	-1559.973846	-1559.7583
	2'-PH <sub>3</sub>	-1709.764921	0.2653992	-1710.067541	-1709.7933
	2a'-PH <sub>3</sub>	-1366.67066	0.24209486	-1366.951112	-1366.7164
	PS-C'-PH <sub>3</sub>	-1870.292323	0.48154134	-1870.820957	-1870.6388
	PS-TS-II'-PH <sub>3</sub>	-1870.287313	0.48036181	-1870.815092	-1870.6361
	PS-D'-PH <sub>3</sub>	-1870.287164	0.48280388	-1870.818428	-1870.6391
	NPS-C'-PH <sub>3</sub>	-1676.193999	0.38293646	-1676.620366	-1676.4083
	NPS-TS-II'-PH <sub>3</sub>	-1676.188053	0.3818219	-1676.614762	-1676.4041
	NPS-D'-PH <sub>3</sub>	-1676.18706	0.38373081	-1676.616829	-1676.4052
	E'-PH <sub>3</sub>	-1870.309827	0.48539478	-1870.835387	-1870.6626
	TS-III'-PH <sub>3</sub>	-1870.310272	0.48248967	-1870.833121	-1870.6593
	F'-PH <sub>3</sub>	-1870.308699	0.4849824	-1870.834482	-1870.6609
	5(Me)-PPh <sub>3</sub>	-3593.911035	0.75515164	-3594.758213	-3594.3084

[[Ru]NHC <sup>Me</sup> ]	5a(Me)-PPh <sub>3</sub>	-2558.379418	0.50268013	-2558.969542	-2558.6063
	6(Me)-PPh <sub>3</sub>	-3134.346526	0.76096658	-3135.19654	-3134.7918
	6a(Me)-PPh <sub>3</sub>	-2098.799669	0.50911737	-2099.39176	-2099.0771
	5(Me)-PH <sub>3</sub>	-2209.009951	0.29823203	-2209.38915	-2209.0346
	5a(Me)-PH <sub>3</sub>	-1865.91722	0.27361005	-1866.275343	-1865.9599
	A(Me)-PH <sub>3</sub>	-1599.272328	0.36070375	-1599.717807	-1599.4677
	TS-I(Me)-PH <sub>3</sub>	-1599.273384	0.35940482	-1599.716394	-1599.4673
	B(Me)-PH <sub>3</sub>	-1599.284007	0.35894054	-1599.723576	-1599.4746
	6(Me)-PH <sub>3</sub>	-1749.440503	0.30500286	-1749.820395	-1749.5136
	6a(Me)-PH <sub>3</sub>	-1406.341802	0.28164089	-1406.701427	-1406.4345
	PS-C(Me)-PH <sub>3</sub>	-1909.961511	0.52019498	-1910.566973	-1910.3521
	PS-TS-II(Me)-PH <sub>3</sub>	-1909.954831	0.51994067	-1910.561297	-1910.3485
	PS-D(Me)-PH <sub>3</sub>	-1909.954114	0.52246701	-1910.565239	-1910.3509
	NPS-C(Me)-PH <sub>3</sub>	-1715.864498	0.42131953	-1716.36761	-1716.1229
	NPS-TS-II(Me)-PH <sub>3</sub>	-1715.854824	0.42156079	-1716.361641	-1716.1164
	NPS-D(Me)-PH <sub>3</sub>	-1715.853735	0.42317816	-1716.363728	-1716.117
	E(Me)-PH <sub>3</sub>	-1909.969104	0.52588108	-1910.576216	-1910.3701
	TS-III(Me)-PH <sub>3</sub>	-1909.967966	0.5210157	-1910.571892	-1910.362
	F(Me)-PH <sub>3</sub>	-1909.966402	0.52325818	-1910.573572	-1910.3635
	<b>Reagents</b>				
	PPh <sub>3</sub>	-1035.48	0.222005	-1035.418087	-
	PH <sub>3</sub>	-343.06	0.001719	-343.0128892	-
	CyO	-309.513	0.114858	-309.5442496	-
	Me <sub>2</sub> CO	-192.938	0.051783	-192.9595152	-
	KCl	-1060.09	-0.02269	-1059.938999	-
	KO <sup>t</sup> Bu	-832.704	0.085887	-832.6013806	-
	IPA	-194.102	0.076225	-194.1401243	-
	CyOH	-310.681	0.13749	-310.7281758	-
	HO <sup>t</sup> Bu	-233.359	0.101111	-233.4004697	-

### Calculation of final Gibbs free energies

$$G^{\text{Sol}} = E_{\text{el}}^{\text{Sol}} + (G - E_{\text{el}})^{\text{BS1}} \quad (\text{i})$$

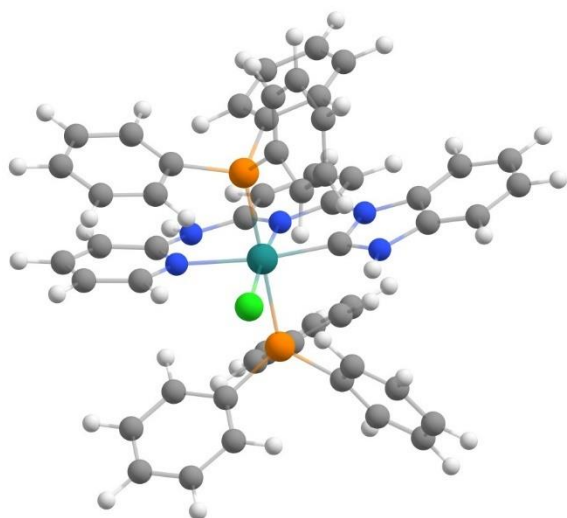
$$\Delta G^{\text{Solv.}} = G^{\text{Sol}} - G^{\text{BS1}} \quad (\text{ii})$$

$$G^{\text{BS2}} = E_{\text{el}}^{\text{BS2}} + (G - E_{\text{el}})^{\text{BS1}} + \Delta G^{\text{Solv.}} + 0.003012 \quad (\text{iii})$$

(Standard state conversion)

## Cartesian Coordinates of all optimized structure

### 1-PPh<sub>3</sub>



Ru	-0.68481351437784	1.99306094577834	-0.28468405141900
Cl	-1.54366721532473	4.24215884540962	0.17365859337535
P	-0.01958243342594	2.65265411285379	-2.47373711705246
P	-1.38939594548868	1.43715137906742	1.91306704841259
N	-1.88808142554340	-0.90764136922639	-1.19272118233655
N	1.90953305458220	3.36796775088380	0.72808331402318
N	-2.56007858110134	1.39667372745676	-1.13572071317317
N	2.04161069066008	1.26495978030799	0.13047263680222
N	0.13754223206123	0.15460122376005	-0.52568868230020
C	0.92247589844467	4.20724893486873	-2.78735142368322
C	-1.07936391249795	-0.34013604259611	2.29190709802855
C	-1.44221718955750	2.89482040194722	-3.61245492851999
C	1.53600662446417	4.39520556838595	-4.04728666406561
C	3.36579617346386	1.66635920969216	0.41840117171609
C	-2.78720949044950	0.11527197900227	-1.50503004088569

C	2.18145162460783	-1.15965199587715	-0.33842283943514
C	1.11937520884693	1.36083478532439	-3.12065576129501
C	-3.16132844246829	1.74534464591287	2.27618857527282
C	-4.71389518455606	2.02591551374217	-2.05184065999693
C	-0.47781471615253	2.34882545061221	3.22978605564612
C	1.68287109642699	6.42078461946688	-2.10821488165526
C	-3.52154006096414	2.32081635035175	-1.39594457460273
C	-3.51491600482211	2.82898608611514	3.10782534355316
C	1.45661649034755	-2.31939967976261	-0.64437047037835
C	1.48902403860830	0.04883182491339	-0.27165157330170
C	-3.97163177809336	-0.26099901051862	-2.18457326518112
C	4.62263235812848	1.04070740289263	0.35657809570053
C	-2.09280708689894	-1.30934760603590	2.41735162630389
C	0.98240294231294	5.23500000273240	-1.82996644291086
C	1.13527079713467	2.33902886418523	0.29251754202777
C	1.67977162755294	-0.92825242920098	-3.78259551079800
C	2.32158421634693	6.59026978593122	-3.34548807005939
C	3.26097895621633	3.02959397856018	0.80932113719192
C	0.58059685078776	4.48512447722850	3.71405428604147
C	5.63225176138004	3.15142527772288	1.11655381422865
C	0.71837388865250	0.05624296224366	-3.49927388632273
C	2.23817546990132	5.57801217395411	-4.31867276116760
C	0.27134809193000	-0.74464689042834	2.38780657392493
C	3.44708947516557	0.64068448542232	-3.25449375945201
C	4.38092983217616	3.78783399979247	1.16301199813107

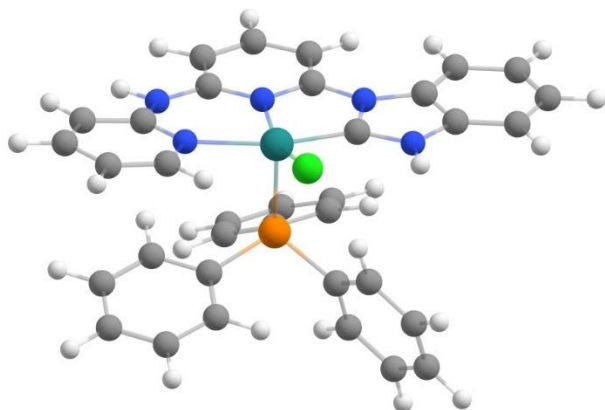
C	-5.53224553597520	1.35002878733552	1.83171102921442
C	5.75165331149894	1.80639480336887	0.71854112177715
C	-3.10171367320114	2.30194962554072	-5.29130754317377
C	-0.10031456754560	3.64099434621001	2.84153112955169
C	2.49349808770484	1.62740199849515	-2.98604076708640
C	0.08849236076257	-2.23289866251990	-0.89362734480871
C	-3.30081622451900	4.40213356868376	-4.09023110964734
C	-2.14165992025643	4.09829444079168	-3.37173154477404
C	-0.42009357860541	-3.05881163706255	2.68502089646193
C	-0.18139311848955	1.90110975116513	4.54028581638496
C	-4.94003445222634	0.70450905714338	-2.46548150089601
C	0.59742658795599	-2.09297260023671	2.58442962763024
C	-4.86382191235921	3.16410495150137	3.30016986047218
C	0.90623822135147	4.04578289023452	5.00106959226518
C	-1.76311989610153	-2.66154566412369	2.60940923106467
C	3.04629564491004	-0.63825539703420	-3.66109080211448
C	-3.79156654266150	3.50063569622238	-5.04672945750199
C	-4.18486354656207	1.01713675965510	1.62841357631458
C	-5.87613364539801	2.42594544556500	2.66681254229293
C	-1.92444583280596	1.99675982949640	-4.58290380348123
C	-0.54297954368886	-0.97002209941343	-0.85519822181035
C	0.52133411216613	2.75607966101838	5.41630734456028
H	1.51220111805559	4.28895342210648	0.90566525574455
H	1.46790581775746	3.61248276820219	-4.81590088211721
H	3.24940524151909	-1.20314869284141	-0.11799241386448

H	-5.44256257805718	2.82443314716361	-2.23391955696135
H	1.71525252596805	7.22255738186064	-1.35657920741033
H	-3.28996062750244	3.33068915356401	-1.03109720285352
H	-2.73249804173332	3.41542082256304	3.60593665298748
H	1.96716152688103	-3.28863111569583	-0.68458252250190
H	-4.11253512083938	-1.30642152491127	-2.49185944505441
H	4.74680481441703	0.00288951786691	0.03142947933021
H	-3.14801897642430	-1.01070859024054	2.39413519127276
H	0.41782954118128	5.12352892706390	-0.89503143289995
H	1.35413212816541	-1.93318892490717	-4.08541008797411
H	2.87084130111659	7.51753640474745	-3.56140434118539
H	0.85730918301385	5.49813512159937	3.38933822362144
H	6.53332790368875	3.71569050187310	1.39110226699005
H	-0.34559367159452	-0.20564784092124	-3.54485821684800
H	2.71822522214630	5.71322399241546	-5.29799413420234
H	1.06989898560268	0.00825085331708	2.33254510075968
H	4.51161990304323	0.87481438478029	-3.14834539952405
H	4.28357577348611	4.83942952757840	1.46080124502164
H	-6.31546331940401	0.76955646143764	1.32463994492904
H	6.74956268980882	1.34336863481673	0.68785653160368
H	-3.47172785327784	1.59960234570429	-6.05119637013914
H	-0.39630870402128	3.99188768132449	1.84384879792052
H	2.82827482882545	2.62173745205103	-2.66271954347870
H	-0.50138022761784	-3.12534748589619	-1.13953898971940
H	-3.82683934102500	5.34763323768726	-3.89709721048159

H	-1.77685845404279	4.79244911043094	-2.60131550067685
H	-0.16471449404224	-4.11643502310744	2.83885749654686
H	-0.48596667519217	0.90009938957466	4.87399802386639
H	-5.85784753378892	0.42570181865619	-3.00064725989577
H	1.65193256290358	-2.39122311640185	2.66105192302288
H	-5.12293677860585	4.01104554831201	3.95071532235703
H	1.45031013831315	4.70676448508855	5.69032935622679
H	-2.56641478945445	-3.40463192724400	2.71691791302179
H	3.79205330900032	-1.41478916152805	-3.87743793407778
H	-4.70553596145616	3.73572566463437	-5.60961266894125
H	-3.94009979101611	0.19331395094842	0.94857643472113
H	-6.93162969593374	2.69074124022051	2.82039864224741
H	-1.38475592575020	1.07039276697546	-4.81037163810965
H	0.76038659553357	2.41071499089449	6.43205512880322
H	-2.26904129697888	-1.82892341377346	-1.40905380476083

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**1a-PPh<sub>3</sub>**



Ru	-0.70288534419027	2.05512550058765	-0.20633360940639
Cl	-1.00739426280666	4.40247443949471	-0.24710512296689
P	-1.21502673500102	1.51451927594128	1.89483078965790
N	-2.15737548226243	-0.65101803041751	-1.34717466191204
N	2.01249576217967	3.17694168420743	0.72534899515586
N	-2.64517396708153	1.68734430798966	-1.05852822122727
N	1.96095286552208	1.07954282916420	0.07025331617272
N	-0.03967612454809	0.17848856735032	-0.63026208047279
C	-0.59304527261257	-0.14591083266195	2.39627966491071
C	3.29663718161652	1.33442015638436	0.44551388902242
C	-3.00861712250947	0.44857531809947	-1.47119087147132
C	1.89330992499865	-1.30546976016560	-0.60087574100543
C	-3.03716306218609	1.59027016891488	2.09672478105246
C	-4.85770106196894	2.50365707060474	-1.61872478999306
C	-0.56268412353643	2.58091523810024	3.24627933573134
C	-3.56615931392839	2.68867988385235	-1.13556959461788
C	-3.60831282935249	2.72371775875703	2.71299233983263
C	1.08044557574729	-2.36047309815392	-1.04508002998782
C	1.30226586087382	-0.05811727043867	-0.39980028652340



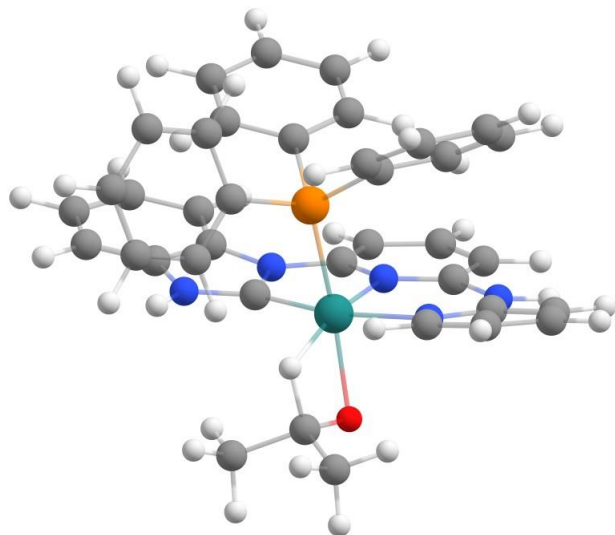
C	-4.29782631417340	0.19016665359780	-1.99960549541943
C	4.46979412898577	0.56664575054975	0.47360847230719
C	-1.38761145927674	-1.30514850944897	2.49313731394032
C	1.16147095709245	2.22640776640275	0.26356287612125
C	3.31608333421757	2.69594376274939	0.86371592530498
C	0.14065845797558	4.75477440748791	4.09289140768440
C	5.65625994102950	2.53816728623546	1.34233348512429
C	0.79873715107448	-0.24589656865469	2.62913531880845
C	4.48663506856182	3.31583168155650	1.31357718671009
C	-5.27527563149699	0.78442061243355	1.54662202024294
C	5.64532270394868	1.19039454462918	0.92978529923322
C	-0.29031269190141	3.94677221280525	3.02813057068937
C	-0.27277956628366	-2.13493018403435	-1.29162538971827
C	0.59074597269954	-2.64143619024007	2.98825089577555
C	-0.41942918294063	2.03752750824941	4.54289887934256
C	-5.22873396424646	1.22335020470978	-2.06872407617855
C	1.38534110642899	-1.48359216857112	2.92135626220088
C	-5.00306204103992	2.88124190475174	2.74472990613770
C	0.30019720330415	4.20887858882657	5.37723491710726
C	-0.79471239580626	-2.54579260123030	2.78422296478299
C	-3.88410606991089	0.62620345663155	1.50485747143918
C	-5.83914021471267	1.91358052123266	2.16565191873480
C	-0.80777498353990	-0.84323892305430	-1.08450140105103
C	0.01409763503464	2.85099893234871	5.60032530053427
H	1.68215089897413	4.12554153586134	0.91648960003592

H	2.95743715502253	-1.46009810805961	-0.40433080543963
H	-5.55649830553285	3.35035542969058	-1.64448642073553
H	-3.20356707632799	3.66590519328299	-0.78033113280075
H	-2.96162625265427	3.48885120087898	3.16526004013835
H	1.51232548676978	-3.35795472190224	-1.20636274381790
H	-4.55340049596914	-0.82355957673512	-2.34341126062829
H	4.49893458252910	-0.48045899450281	0.15210220850549
H	-2.47677651687617	-1.24524322781960	2.37555395194621
H	0.34634865754436	5.82153398746894	3.91608196642458
H	6.59578624746925	2.99045912184065	1.69120747839261
H	1.42462993879778	0.65856191564916	2.61005075512590
H	4.48718682055190	4.36782916141064	1.63141852931598
H	-5.92357044770791	0.02455927791857	1.08535908137873
H	6.57746384417161	0.60805182964303	0.96032925023840
H	-0.44295306429572	4.37588818796112	2.02439386300745
H	-0.92570565310263	-2.94446315314730	-1.64810660210781
H	1.04871352955938	-3.61394376971981	3.22320554002912
H	-0.64784988336943	0.97818901263541	4.72927411055507
H	-6.23478622456116	1.03268172352378	-2.47039459976989
H	2.46832611631109	-1.54103988977380	3.10753710182710
H	-5.43711913926505	3.76920355249034	3.22812722583635
H	0.64166859082469	4.84337515519756	6.20898052402710
H	-1.42784167774501	-3.44185952346053	2.86898321146647
H	-3.45710911765698	-0.24148271914330	0.98650186482941
H	-6.93180574989859	2.03952463031301	2.19359436314306

H	0.12670922479015	2.42003875603116	6.60653219282988
H	-2.60540310233070	-1.51172984510812	-1.66516942555966

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**A (H)-PPh<sub>3</sub>**



Ru	-0.23523537456845	1.72321051134492	-0.60261692568180
H	-0.70639813329166	3.33372579102099	-1.22086037137901
N	-1.21288875377890	-1.31287653643562	-1.39488274348049
N	2.16551537098747	3.31340653901663	0.59358912776942
N	-2.14965967045461	0.88919972719948	-1.14487598077943
N	2.38599387474255	1.13370848064577	0.38152845324908
N	0.63078438309168	-0.12483775853505	-0.42400547784885
C	3.53127244922885	1.57282931103333	1.08746719605603
C	-2.29353111611716	-0.42734587968448	-1.43382587232949
C	2.71011354892811	-1.30721566739797	0.06353060713117
H	3.75753650746491	-1.28170759978600	0.39049363977205
C	-4.55019279773842	1.19284554914584	-1.40484833502793
H	-5.41409322097000	1.87516604647665	-1.35884863225288

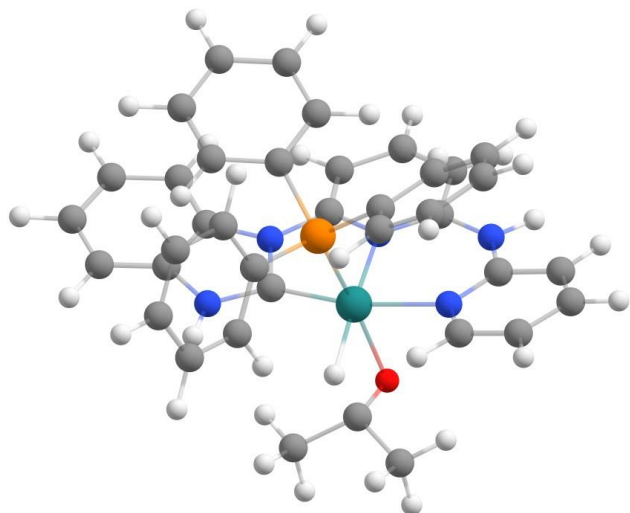
C	-3.27066708776503	1.66574153758293	-1.11434748412104
H	-3.10722809864869	2.72029514397315	-0.83399821058715
C	2.11931388488436	-2.50640260208471	-0.37097198315747
H	2.69821192071211	-3.44537240568759	-0.35523106754040
C	1.93609074523461	-0.13983498804900	0.02495355520634
C	-3.56044153267945	-0.98001315546938	-1.77223282160361
H	-3.64354715964724	-2.05360176444180	-2.01884182680673
C	4.64046721127418	0.92587949605935	1.65662812515881
H	4.78119767180203	-0.16369805435235	1.60909750779978
C	1.51249983324075	2.21286465779272	0.09961343733697
C	3.37726669244061	2.98250119264795	1.21563358691755
C	5.42882424306002	3.12057011138227	2.45333602770184
H	6.18947114593936	3.71146756854700	2.99224557703460
C	4.31459526088170	3.77563951046941	1.89216975436174
H	4.18243168269571	4.86712464772709	1.98567994584428
C	5.58447043296029	1.72185083131207	2.33797203745604
H	6.46363658744072	1.23368763362420	2.79268810000569
C	0.80312802244616	-2.50231686682068	-0.84299582306698
H	0.32957210224890	-3.43251717593102	-1.20223350152762
C	-4.69238490568652	-0.16534013391428	-1.75836648267150
H	-5.68155104842598	-0.58684637046863	-2.00780968141802
C	0.08004080317563	-1.28275328531071	-0.87665451512907
H	-1.46760073215412	-2.24706234408817	-1.73124844768613
O	0.13790298914139	1.90749063426467	-2.65793181688166
C	-0.26185477725922	3.17629049197688	-2.48090783180968

C	0.84713365067949	4.25238351256910	-2.55778277719963
C	-1.52510334704874	3.59036149484201	-3.27052183325579
P	-0.95074935759057	1.90495675102217	1.59713761475394
C	0.22388132301596	1.07340198069569	2.78219473958134
C	-2.65393375449232	1.23989825121225	1.94473670885792
C	-1.05792048150679	3.62417021037676	2.28679877663485
C	0.30447735416826	-0.33816872276238	2.85105480340555
C	1.19217086146683	1.83764097529203	3.47933820349580
C	-3.72321014644010	2.11109974995658	2.26253145780413
C	-2.94097985863618	-0.13173363049915	1.73566559250763
C	-0.94994169647518	4.74440254586900	1.43556953087650
C	-1.29040703585583	3.83015897035773	3.66983974146904
C	1.31222435888620	-0.96489710372112	3.60648585338655
H	-0.41859867778452	-0.97194499756568	2.31397481152031
C	2.20127198122183	1.20827897368968	4.23050870755715
H	1.16779172602510	2.93902203944853	3.44073579037118
C	-5.03609825042731	1.61879221240859	2.38968135971823
H	-3.54003258619779	3.18847126359968	2.40973827090215
C	-4.25059510949946	-0.62181705277111	1.86990447792648
H	-2.14278717089194	-0.83550779361215	1.44657971812091
C	-1.05492967375610	6.05136730725075	1.95184722538868
H	-0.79876482706945	4.58331909941728	0.35150448912310
C	-1.39417093304283	5.13414839844644	4.18468046695305
H	-1.39324688890490	2.96507973691750	4.34943226735828
C	2.26653737846571	-0.19494642200772	4.29730804628147

H	1.34955086563764	-2.06785470134855	3.65210889442443
H	2.94650032094859	1.82633535106371	4.76148561088924
C	-5.30525912263718	0.25232424056105	2.19702400082947
H	-5.85504171366279	2.31539488107580	2.64328553583629
H	-4.44980703239475	-1.69653999478426	1.71104102526737
C	-1.27257615021609	6.24750722049388	3.32811733230721
H	-0.97262484488267	6.91950119186375	1.27367045688391
H	-1.57406796788894	5.28351917934037	5.26420043225516
H	3.05923559514530	-0.68814080317589	4.88705577991466
H	-6.33509142537749	-0.13293868727886	2.30006268644230
H	-1.35431907895356	7.27061838474128	3.73607058419539
H	1.74915631634375	4.24927332830442	0.57797430057008
H	-1.23422422776750	3.70527242335179	-4.33939124404093
H	-1.94240654635189	4.56269911062075	-2.92511887972120
H	-2.31264797143611	2.81201837933540	-3.22441259873919
H	1.10536488874270	4.40799919387907	-3.62986422289095
H	1.76858167285675	3.92397281874865	-2.03618705841186
H	0.51529462874824	5.23424790798926	-2.14922752556471

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TS-I (H)-PPh<sub>3</sub>



Ru	-0.22573223792322	1.60080508076361	-0.56970107383541
H	-1.02762313998827	3.04375713645022	-1.06283878184694
N	-0.61317145042788	-1.58699300327143	-1.31266097003084
N	1.86261669407319	3.62406995346717	0.55229682329855
N	-1.95070129055396	0.40373185836120	-1.06863686758532
N	2.48559795007526	1.52202379262475	0.35734687329425
N	0.99103132365266	-0.06430220576049	-0.39312801084228
C	3.54646445126540	2.18188774226810	1.02263404182158
C	-1.84286683736386	-0.92129319810059	-1.33915352162518
C	3.26819073177943	-0.81571226070204	0.04868197893122
H	4.29950342203868	-0.58747699495116	0.34680986927496
C	-4.37006930594893	0.23176741102573	-1.27805157349984
H	-5.34876164630005	0.73454467210835	-1.21941015281698
C	-3.20118095459471	0.94847906473450	-1.02310618805232
H	-3.23763766786824	2.01883320778197	-0.75960256178263
C	2.90740981189101	-2.11168049175638	-0.36059361314394
H	3.65662581224791	-2.92153745639264	-0.35146038699133

C	2.28203829751214	0.17999081704076	0.02162944258941
C	-2.98563049235499	-1.71276643027006	-1.64377250947613
H	-2.86427479711994	-2.78595173756775	-1.87607848267321
C	4.77409949544540	1.76707769062500	1.56481815967345
H	5.11873137138201	0.72356456008445	1.52590511495095
C	1.41573861800051	2.41302263143374	0.08909047114806
C	3.13194904151197	3.53908105855432	1.13976992266889
C	5.15508673898971	4.08544943453941	2.30919610637159
H	5.80550254929742	4.81925096848348	2.81582024832546
C	3.92084269335013	4.50737552330160	1.77642977620225
H	3.58653004263596	5.55560049088706	1.86053643275611
C	5.56935995789155	2.73940678987058	2.20598642066189
H	6.53795614147877	2.43444730830660	2.63822505123392
C	1.60496689083007	-2.36826435755889	-0.79983259284151
H	1.31201128004547	-3.37709200854556	-1.13897489261013
C	-4.25357143559130	-1.13337327048368	-1.61347246533914
H	-5.14682837186394	-1.74251205301065	-1.83583031552409
C	0.66208942981105	-1.30848022760493	-0.82485113354486
H	-0.69514168952512	-2.55717435622647	-1.63337161686628
O	0.08687586571798	1.78568238222534	-2.65892436680916
C	-0.51650561334223	2.94881595782767	-2.48712451317466
C	0.36515282654973	4.21269285671471	-2.54147532952075
C	-1.87004725158971	3.13652751147131	-3.20159147200411
P	-0.91453039196248	1.68217617601604	1.63666168671524
C	0.42309820435798	1.10890864785851	2.80442514523430

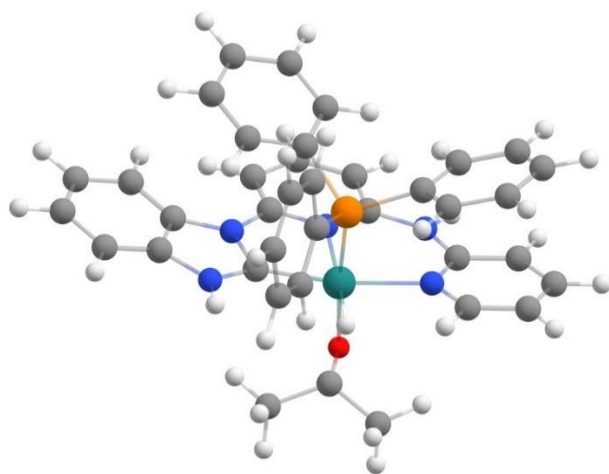


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C	-1.33664766388206	3.35365833017744	2.32260881575937
C	0.77394724920214	-0.25965358514186	2.88939645306025
C	1.24121266141296	2.05619735383930	3.46855898436077
C	-3.65415223021737	1.34105374279261	2.38166975611428
C	-2.45835647869161	-0.70520086845383	1.82996235188030
C	-1.45436131285034	4.47401379710534	1.47311681638731
C	-1.57900131148155	3.51338294522155	3.71032272524226
C	1.89939908219881	-0.66883457977464	3.62747608472997
H	0.17205336300312	-1.02909390347723	2.38084105745204
C	2.36866018353710	1.64479099583884	4.20218823961489
H	1.00413125077961	3.13158608264246	3.41832793302345
C	-4.83809906924827	0.59819607921948	2.55198606538427
H	-3.68396281261196	2.43442546278143	2.52149264620025
C	-3.63914897307609	-1.44508004502109	2.00738355978922
H	-1.54617338787462	-1.23592488164585	1.51068456646019
C	-1.79263765355877	5.73836525515712	1.99517662306775
H	-1.29196673999021	4.34179621314727	0.38670758642827
C	-1.91655115523245	4.77498625392248	4.23049855341063
H	-1.50402447582263	2.64577808144329	4.39043961198876
C	2.70353323703838	0.28136808340455	4.28440719338810
H	2.14820084072505	-1.74335555132022	3.68673627390174
H	2.99227950380892	2.40283045594897	4.70797759156408
C	-4.83541472682715	-0.79585337781713	2.36939877936824
H	-5.77096924484073	1.11978762452576	2.83113035163460

H	-3.62596237792901	-2.53900841954634	1.85521821417796
C	-2.02016856979781	5.89119351474843	3.375273144461655
H	-1.88461138448128	6.60640222235478	1.31803959650297
H	-2.10234866112662	4.88813400377518	5.31340468316897
H	3.58886824119558	-0.04069333962532	4.86051215013169
H	-5.76402375161399	-1.37762675333724	2.50670215775141
H	-2.28494817157643	6.88111174032867	3.78742215948031
H	1.27581655670926	4.46362701566880	0.53907116379559
H	-2.44792027432508	3.99984965883074	-2.80400711854624
H	-2.49041013932850	2.21956565709925	-3.15994913866936
H	-1.65365957430725	3.34140349074969	-4.27549454593877
H	-0.12955947314097	5.09799905953871	-2.08210282666524
H	0.54744152763325	4.45543090868651	-3.61388762491365
H	1.34964236749680	4.04031141372920	-2.06398708625021

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**B (H)-PPh<sub>3</sub>**



Ru	-0.34134514753386	1.66222151145698	-0.49356737227815
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H	-1.31120383635156	2.98343619746298	-0.53795859593835
N	-0.59149838361781	-1.57729103343057	-1.18312746120806
N	1.70097571756975	3.75345259585334	0.57966211180268
N	-1.99922673965324	0.38852275900957	-1.01807174891777
N	2.41449550808643	1.68468333528654	0.33665396010973
N	0.98724091397834	0.01243210479494	-0.35911374120958
C	3.47210175033823	2.39231154056283	0.95596785385711
C	-1.83422963570664	-0.93681439831911	-1.26755157669085
C	3.29481797931872	-0.62590267189014	0.04044339769844
H	4.32485171390211	-0.35624303553980	0.30527068696078
C	-4.39963818416410	0.13534205526673	-1.34710404170084
H	-5.39486047623581	0.60839693472981	-1.34958022634912
C	-3.26883987752910	0.89321183544367	-1.04730134042329
H	-3.34537915203938	1.96743901921703	-0.81308774799894
C	2.97173970019899	-1.94677760857624	-0.32395244566917
H	3.75418465715630	-2.72491060886618	-0.31283507750765
C	2.26597782047500	0.32695904373900	0.01664063250895
C	-2.93896204247396	-1.76843325183441	-1.60977257794897
H	-2.77288082231765	-2.83959083352711	-1.82370907765521
C	4.74499130623370	2.03744184826239	1.43511747265402
H	5.13991800204270	1.01357425244967	1.36963162302030
C	1.28899943937367	2.52869405490982	0.12422708541296
C	2.99844125405147	3.72739750266014	1.10544704822600
C	5.04666389805595	4.36704256231287	2.18113580927176
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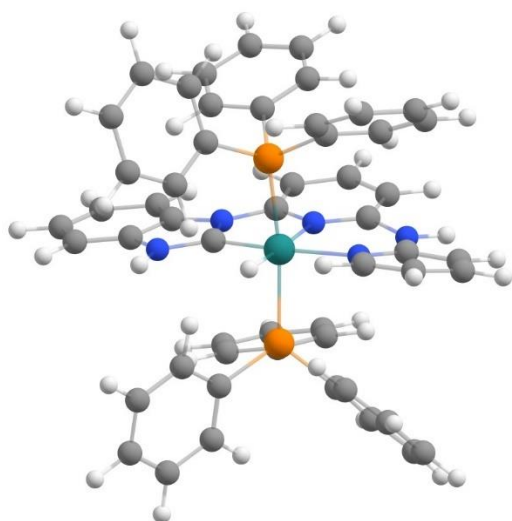
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C	5.52148974559496	3.04407984486150	2.04542394519802
H	6.52417998928600	2.78491246290664	2.42702242804586
C	1.67080764875408	-2.27323527290961	-0.71699752698741
H	1.41219443066540	-3.30346950347577	-1.01769326628803
C	-4.22454055453031	-1.23146152760928	-1.64970321470747
H	-5.08560062673097	-1.87297025790203	-1.90578495231168
C	0.68984995392448	-1.24591421118664	-0.74572180101750
H	-0.65326778350600	-2.55973394872531	-1.46911769760189
O	0.18615346227335	1.47155171433546	-2.61850631739632
C	-0.26979112556824	2.66952683713592	-2.69349108003271
C	0.69556724670603	3.85411373869772	-2.73191629942894
C	-1.63099992762088	2.92998026944181	-3.33709442559534
P	-0.99014424462642	1.69633984823410	1.70977043924214
C	0.36058389214916	1.00420930873374	2.79389534764416
C	-2.56326053846559	0.77187851172151	2.06499755860249
C	-1.32007160736231	3.33811272329410	2.50532301448646
C	0.64025157607876	-0.38232272984947	2.83682697790557
C	1.26673016287862	1.89374653236008	3.42252531540840
C	-3.74694308513941	1.48547859466543	2.37052816498497
C	-2.64769692564428	-0.62927953211074	1.87686556492000
C	-1.43930207641899	4.52062260900745	1.74433653757282
C	-1.49784756794907	3.39911312976023	3.91044932573691
C	1.78421237202042	-0.86481532105972	3.49767631304351

H	-0.02948648665946	-1.10999102995119	2.35333475470357
C	2.41460828605786	1.40973411692289	4.07557850377095
H	1.08423682965439	2.98089474186979	3.40409337629789
C	-4.97546192384917	0.81124083285504	2.50534708104009
H	-3.71879319647542	2.58017146431344	2.50186883528581
C	-3.87367204067102	-1.30036008491254	2.01867343758502
H	-1.75806750885148	-1.21476195909212	1.59463923407463
C	-1.70959613475178	5.75124449835303	2.37535262927529
H	-1.34333681667738	4.45656033025718	0.64365555288295
C	-1.76904920083698	4.62761420430646	4.53716727028338
H	-1.42437991931370	2.48083604753353	4.52038466021141
C	2.67896745502734	0.02871819390204	4.11585157200368
H	1.97665605011586	-1.95200570910597	3.52575386491626
H	3.10784656002320	2.12418404528878	4.55338913907792
C	-5.04357407916964	-0.58261875617812	2.33368161781732
H	-5.88667007401088	1.38621672487503	2.74873715853237
H	-3.91585872272071	-2.39469466924203	1.87551194940244
C	-1.86956623658955	5.80752796781558	3.77224172016183
H	-1.80471517785998	6.66977968513407	1.76893941771923
H	-1.90517740379766	4.66401752259061	5.63262267786572
H	3.57928396754009	-0.35131107851034	4.63023570182723
H	-6.00719634272561	-1.11081523007789	2.44359790777350
H	-2.08157483051107	6.77152093406654	4.26794621021379
H	1.07236637397312	4.56202324805276	0.59672855905857
H	-2.11637683387301	3.84795923858272	-2.94197352747100

H	-2.31596040739725	2.06568593288076	-3.23297276066116
H	-1.46107848048201	3.09212238169253	-4.42950226162775
H	0.28749643233209	4.74716065637051	-2.21038352470600
H	0.84021091512047	4.14544867311348	-3.80087615681285
H	1.68757498655691	3.59005136640833	-2.31460419362167

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## 2-PPh3



Ru	-0.66615693220919	2.01617830058135	-0.35970861685131
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P	-0.02141183431757	2.71272931269577	-2.50772797316628
P	-1.23092249768987	1.63840553571054	1.89299045591055
N	-2.31487210486915	-0.52669734264628	-1.68825411633443
N	2.23619528481702	2.81467514920303	0.47214275136622
N	-2.70207146109587	1.74904761106294	-0.95908237313995
N	1.86187140922743	0.69353198801905	0.02018787316725
N	-0.20517232665191	-0.01121137087604	-0.70821354732935

C	0.86666858382224	4.33427532181858	-2.66139812935857
C	-0.36076200413780	0.13340711234089	2.55664207986288
C	-1.33474143410224	2.92669136335255	-3.79661210802467
C	1.49522933354421	4.67897125182260	-3.88213956661417
C	3.24035857124574	0.79084616228934	0.30696069924992
C	-3.13205352342960	0.60676634959593	-1.55660028877860
C	1.47960498638735	-1.73400288803465	-0.39753974469980
C	1.19904852225044	1.48908326597403	-3.17164853804186
C	-3.04422673666586	1.41413303727411	2.19982785179876
C	-4.94851838665485	2.66978991265881	-1.15282828885100
C	-0.74760063734374	2.91967846834652	3.13923961555550
C	1.51440651640313	6.50346839641807	-1.73556392651023
C	-3.61669973784275	2.74101529543923	-0.74523832715252
C	-3.77927572364398	2.39188785882667	2.91041928791454
C	0.56134043229731	-2.69191935328682	-0.86205655555821
C	1.06409834977433	-0.39511011400303	-0.36179204336647
C	-4.45896358080094	0.48530237472513	-2.05353797889877
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C	-0.92992463077100	-1.15988985944585	2.57236979927821
C	0.87037739896497	5.25831194770801	-1.59512902755345
C	1.22794298388279	1.96339647846352	0.10638031379595
C	1.68640022704595	-0.80043889630099	-3.90425253887044
C	2.15697581632938	6.83263236503762	-2.94345923747573
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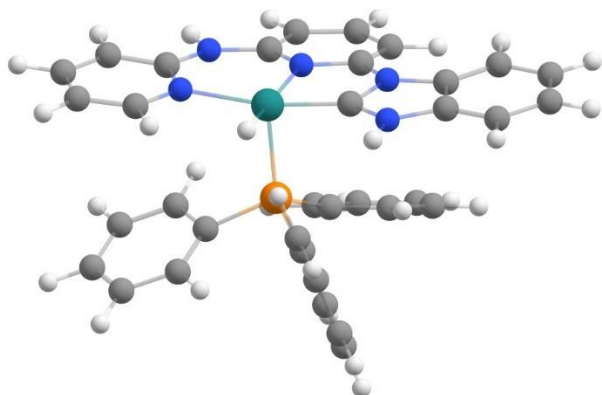
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C	2.14194311897661	5.91957464609376	-4.01768908016981
C	1.00403190334033	0.27876990922094	2.91128822074144
C	3.50998490963403	0.67512686057995	-3.25678646251253
C	4.74396855658905	2.65678173580867	0.92570700910125
C	-5.14773896023534	0.26343380630596	1.68023185988333
C	5.59070259276104	0.36999319403324	0.64443693422739
C	-2.40104072583017	2.51423022856277	-5.95827772702983
C	-0.45208386395610	4.23920818062902	2.73490530257229
C	2.58632313088226	1.70269030220392	-2.98983234738239
C	-0.71360884511370	-2.29780378126137	-1.28575844325785
C	-3.42074665843966	4.06717327031345	-4.38436972939513
C	-2.37231776956355	3.83658853773399	-3.47854574566798
C	1.21123863399872	-2.12932850847732	3.23802613214458
C	-0.70700139373901	2.58887739444360	4.51604179259371
C	-5.37160590502848	1.52095520945299	-1.85087149227856
C	1.78208204985951	-0.84145440065187	3.24962944876094
C	-5.18135739176641	2.30298080121484	3.00509192120117
C	-0.06143581418471	4.87978212397615	5.05664478539073
C	-0.14799622607468	-2.28139357313751	2.90870707666817
C	3.06437411106883	-0.57870321385269	-3.71530339130339
C	-3.44434014961967	3.39700435401140	-5.62348804560559
C	-3.74964760863747	0.35456670006953	1.57571627391214
C	-5.86994609236190	1.24003395252882	2.39312337840821



C	-1.34719028518380	2.28057943503671	-5.05299096268168
C	-1.06499002967087	-0.92695362658519	-1.20253901199946
C	-0.36349038002098	3.56542502449448	5.46716966337246
H	2.07589191579519	3.81897248274743	0.58958340750936
H	1.47921837647659	3.97504695303862	-4.73389965233897
H	2.47785258704385	-2.03375778035850	-0.05687817764437
H	-5.63374436794082	3.50612840101676	-0.94001460463222
H	1.50623851639178	7.22495082845090	-0.89860235088390
H	-3.21889149560758	3.62445271417223	-0.22012632112877
H	-3.25637142565379	3.23492476549114	3.39341096763813
H	0.84791239574808	-3.75680019918602	-0.89528161841076
H	-4.76617963237504	-0.43911253250662	-2.57482489916529
H	4.18402207894335	-1.18494649824664	0.06747286019743
H	-1.99746728541764	-1.30546994923569	2.34310503135432
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H	1.32644050585211	-1.78067406327186	-4.26410199681369
H	2.66298969640970	7.80819316267860	-3.05473084116735
H	0.11592220843554	6.24719937630022	3.36585796374652
H	6.82345229697791	2.08089290536520	1.19868129813424
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H	2.63309933607137	6.17975933208246	-4.97228703884693
H	1.46479926282115	1.28240034851922	2.93754812814833
H	4.58788828356577	0.86016707661221	-3.10351004945244
H	4.90661586286425	3.72488409984718	1.14997470847006
H	-5.67903411149571	-0.57359568369131	1.19321252214536

H	6.44281990461683	-0.33144373853146	0.65851442777420
H	-2.39834676956785	2.00644797441812	-6.93947159979401
H	-0.50882957902521	4.48738220766804	1.65929653339265
H	2.95427375744561	2.67753599526872	-2.62514073920645
H	-1.43728220224338	-3.03875215696191	-1.66805734855040
H	-4.22257767807438	4.78075397114519	-4.12351313833734
H	-2.34356355834688	4.38558283075860	-2.52080522940907
H	1.82174965735271	-3.01079555209044	3.50315082991588
H	-0.94272793166528	1.56178214051978	4.84789711177781
H	-6.40669583565546	1.42801711731372	-2.22279386201186
H	2.84223953839104	-0.70390002250377	3.52752089590421
H	-5.73834980812158	3.07458053142805	3.56607440647771
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H	-0.61288882641397	-3.28338354740625	2.92145217105926
H	3.79049417180142	-1.38304053511084	-3.92879484986141
H	-4.26884268692315	3.57704518679213	-6.33605449189356
H	-3.21062807383991	-0.40446200382956	0.98472059690484
H	-6.96952558190224	1.17149555280866	2.47032161395271
H	-0.52501448297131	1.60595697211613	-5.34516237414421
H	-0.33241824710086	3.29873560248458	6.53866918852863
H	-2.81523962079588	-1.30130657455931	-2.13581098273645

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**2a-PPh3**

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N	2.07719700221014	2.90307367583854	0.85203481311085
N	-2.64596180479742	1.78919143603051	-1.06601933472467
N	1.90765948048778	0.87269993148493	0.01136182999915
N	-0.10198552521513	0.10532082644120	-0.82439580777597
C	-0.36633331961846	0.07779017972005	2.49739485075693
C	3.25267233399946	1.01327754451206	0.42301084302868
C	-3.03821801715557	0.62735381248828	-1.66513597410856
C	1.69405657941354	-1.52173905523744	-0.64798845593213
C	-3.02737643124755	1.47196471143270	2.18521752743180

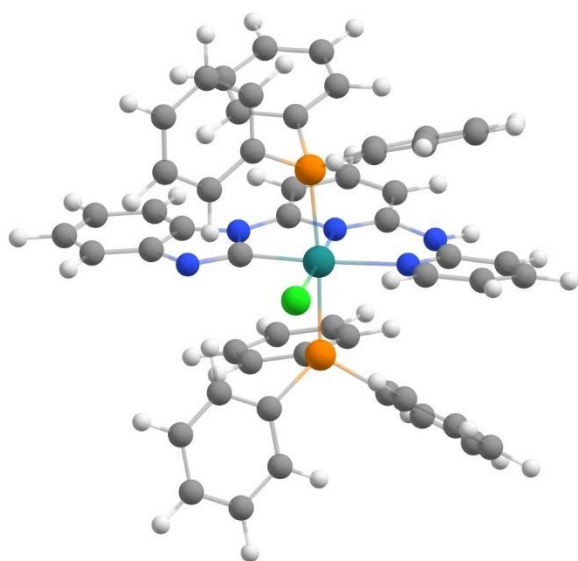
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C	-3.72811714920562	2.44331295286042	2.93795638355866
C	0.83073422598345	-2.50413562307650	-1.17412837257117
C	1.19495103244460	-0.22135263634407	-0.50277559821026
C	-4.33330265596010	0.49316550367637	-2.24144222103909
C	4.38805438120815	0.18503086956882	0.37457419170094
C	-0.96410878145664	-1.19871628027909	2.39357607359519
C	1.16255366328104	2.05703338673954	0.28538211851949
C	3.34733469308447	2.32639288032197	0.97177784194938
C	-0.08964646361452	5.13278313584427	3.89613966786500
C	5.67198852076656	1.98493066386254	1.46486321869459
C	0.99598338326680	0.16332229445157	2.88003613941676
C	4.54556332457748	2.82954749699369	1.49940054704527
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C	5.59252023390177	0.68982643137086	0.90722999879394
C	-0.43899777021631	4.20828365149894	2.89291750193120
C	-0.47659580786457	-2.17317550564797	-1.54063353418162
C	1.14774319695844	-2.26771754946021	2.99699954564524
C	-0.60229168696842	2.44629064177105	4.57725963462334
C	-5.23781818059687	1.55111240041469	-2.16509022270336
C	1.74586663751872	-0.99907187349617	3.12712596902638
C	-5.13354374043772	2.40580676451096	3.01529745063333
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C	-0.21002522694702	-2.36190289170793	2.63999421255415
C	-3.76501705218009	0.46990561197834	1.50651671485079
C	-5.85635138444532	1.40272585683861	2.34466789468394
C	-0.91708469131688	-0.83710426935363	-1.34760098392839
C	-0.25311467757984	3.37329945565813	5.57582428843937
H	1.80898214592326	3.83297541024578	1.18938006341918
H	2.71388525329864	-1.78395272639800	-0.33952678724715
H	-5.52367482324013	3.60411111986008	-1.42399061368765
H	-3.18201838901295	3.71796283725558	-0.48590687098121
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H	1.19125700234484	-3.53975209948408	-1.29625660476155
H	-4.61788306677271	-0.45227816546547	-2.73739524010303
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H	6.63222477898822	2.34522902191299	1.87245279725036
H	1.47803745058544	1.14942898417676	2.99851088352175
H	4.60280812764766	3.84718061856498	1.92202464943901
H	-5.72560092882128	-0.35909702820654	1.06133506399826
H	6.49421485729707	0.05393946110744	0.88000342881299
H	-0.54431858101215	4.52373604557570	1.83768338521962
H	-1.15660854082963	-2.93401804229419	-1.96188687353397
H	1.73581424403318	-3.18212326691833	3.19169423784413
H	-0.80868083253060	1.39735519686624	4.85548721759280
H	-6.24607436190864	1.44938314495102	-2.60310104007868

H	2.80477214342657	-0.91021114648226	3.42837237557793
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H	-0.69529039711600	-3.35107086681079	2.56155857867595
H	-3.24830297257360	-0.28104693674777	0.88695948727478
H	-6.95864265761928	1.37606425685204	2.40742889932654
H	-0.18660859002098	3.04385038800109	6.62800109801979
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### 1'-PPh3



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P	-0.04520915313433	2.72250518981482	-2.55396288453950
P	-1.22702106150670	1.62225048199063	1.88233072326972
N	-2.24310204254095	-0.46507170716730	-1.71121838781219
N	2.10903843052701	3.07960102696432	0.61444851120210
N	-2.76411298381546	1.76603374581440	-0.97751262167249

N	1.88409458041202	0.89291646499668	0.04469883026355
N	-0.16860675501851	0.16386133625999	-0.69265905806843
C	0.82503869337251	4.33092371155385	-2.87390782587879
C	-0.40243130123442	0.05341994319638	2.46431997644732
C	-1.43857682088785	2.84256835065367	-3.77184512274020
C	0.90016395463189	4.81375499178006	-4.20292444522234
C	3.22718282299739	1.03971855337263	0.42197424513845
C	-3.12774352735201	0.61061117746437	-1.58748852618571
C	1.58833890143865	-1.51655250348036	-0.42608541774416
C	1.16843613712671	1.48616375081671	-3.21146466186906
C	-3.05652322223246	1.47678681580280	2.13659246077788
C	-5.05339713012890	2.56165734503161	-1.20996253414421
C	-0.71425601039578	2.74459471935812	3.26605749153476
C	2.14212598378757	6.24112892753967	-2.12635828049554
C	-3.73512126164145	2.70227819370337	-0.77224469613129
C	-3.75895505187022	2.57924861097232	2.68122274897652
C	0.70685856902892	-2.50713413864774	-0.87986178272492
C	1.13147788523794	-0.18800007436417	-0.35960540018465
C	-4.43425061460776	0.41714237739347	-2.11512785123356
C	4.33919761270537	0.18231436518680	0.47878427645575
C	-0.95768635749134	-1.24299532340828	2.38278435924678
C	1.44865545332853	5.05049845967315	-1.83114726635784
C	1.22585601000881	2.19307975628172	0.16959519385154
C	1.71715110224283	-0.79542131801623	-3.92423455403315
C	2.21410464559434	6.72217426363191	-3.44621349214568

C	3.33270797581490	2.42974106612292	0.77736930762375
C	0.51411480042828	4.65825161238588	4.14146253068340
C	5.67766515807833	2.09036406399368	1.27823941170224
C	0.76319444668832	0.19804007141674	-3.63980643931547
C	1.59213527742179	6.00373780807815	-4.48683749101978
C	0.94684219704775	0.18624746226102	2.88151812358385
C	3.50164897468804	0.74437240364601	-3.32209786739525
C	4.56617058482297	2.95331402010084	1.21077723640542
C	-5.20946206050387	0.41100414577443	1.63290332450600
C	5.56673497201321	0.72851541097130	0.91530712656821
C	-2.69071568926318	2.25383272478656	-5.78963963682297
C	0.09720860227624	3.87663240479905	3.04442722293572
C	2.55107475537530	1.74681070095288	-3.05787792146878
C	-0.58567819266104	-2.15181586764198	-1.28282470155278
C	-3.57453543591999	3.93130874831154	-4.26305971891703
C	-2.45072856778180	3.77590209440351	-3.43525963680626
C	1.15859486583537	-2.23406264326472	3.09428933819226
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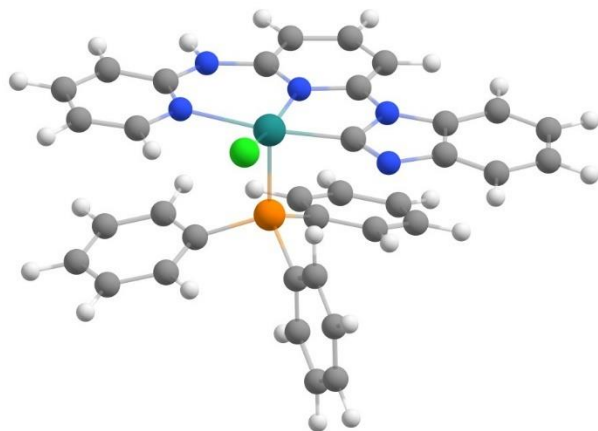


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H	-3.38611646053332	3.61398273602728	-0.25275566342354
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H	6.65378924858377	2.48341218522012	1.61545508582176
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H	1.40288440232067	1.18802618101098	2.96736510319415
H	4.57446782237973	0.96298039444464	-3.17708298032308
H	4.64199451598325	4.02008689543598	1.48406724584590

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H	2.89019236381808	2.73732660723045	-2.70837521537825
H	-1.29354415424403	-2.90897150395170	-1.66345534223914
H	-4.35723680407443	4.66044749173059	-3.98659388672990
H	-2.34083397019666	4.38442800950500	-2.51778666547480
H	1.76572904807656	-3.12534626082276	3.33488992490033
H	-1.71370747941657	1.49945541592112	4.76659384836207
H	-6.42571370518702	1.25871552439917	-2.32336855029762
H	2.77041595455560	-0.81408743227809	3.50255816187291
H	-5.69320917069481	3.45761822426456	3.14471344068176
H	0.45688314956463	4.93989215664782	6.30449423739491
H	-0.64031470083461	-3.37989092747746	2.63327025412435
H	3.83710240296101	-1.31515580760437	-3.96624823991929
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**1a'-PPh3**



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N	-0.09507263145024	0.15587234310707	-0.66399101891108
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C	3.24912022223711	1.10265860372996	0.56848691361634
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C	1.77053609596744	-1.42994692571310	-0.59412491635233
C	-3.02730755553738	1.44818503556625	2.09996991290715
C	-4.96393498348948	2.55137701593979	-1.36400829523058
C	-0.70646604032541	2.69937139503889	3.24515631057037
C	-3.63980290229417	2.71869967378467	-0.95442435136789
C	-3.69185589935180	2.60926834123613	2.56573290194659
C	0.93821439971956	-2.42973297995121	-1.11920634021529
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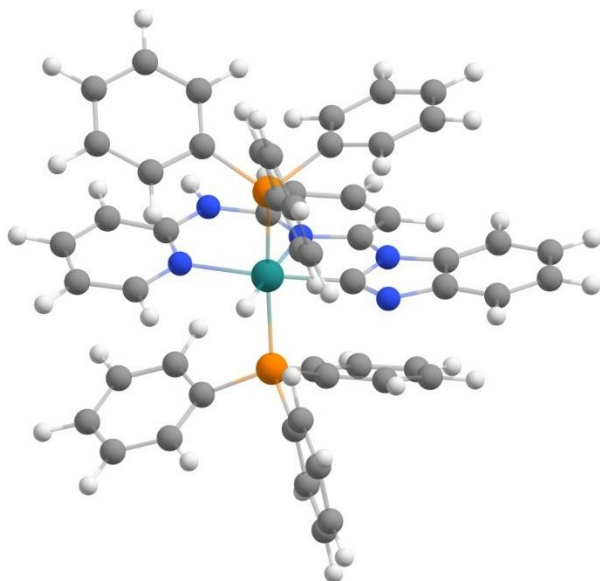
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C	1.21297938443064	2.19832504318138	0.32034406258692
C	3.28140085622998	2.46956401639901	1.01882651444575
C	0.24969002625214	4.76783038812279	4.10121050505084
C	5.59896404225249	2.17084447788288	1.65673022674997
C	0.96647554583881	0.12851939687519	2.94095922374946
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C	-0.99847115040277	2.29252785513754	4.57145928687836
C	-5.35522752774563	1.30173914416106	-1.88634856178964
C	1.76742096216680	-0.99784418573403	3.19485064634672
C	-5.09680589163140	2.66878244331693	2.59241637776778
C	-0.03948959722559	4.36657617340715	5.41727387309424
C	-0.04611671586354	-2.44867910289820	2.47472289152851
C	-3.80839105591692	0.36496688273782	1.63224959435131
C	-5.86334971341821	1.57501170774426	2.14989533069155
C	-0.87793788339433	-0.82027349248269	-1.19268900725590
C	-0.66677705627281	3.12494963521136	5.65254945932760
H	2.81775912110855	-1.64187449121342	-0.34479449082441

H	-5.67312005815617	3.39077324172825	-1.27453688389244
H	-3.26066887668397	3.68246926981762	-0.56561399746413
H	-3.10411095273036	3.48114429388357	2.90060159758346
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H	-4.67940652910458	-0.71689828327136	-2.34770969740820
H	4.38838614372056	-0.77198370376847	0.31456635583287
H	-1.86574918898309	-1.48188173312217	1.82679801378747
H	0.74511299031383	5.73678502654561	3.91137124080185
H	6.53644265463801	2.57040249788283	2.08381403673738
H	1.37853823957889	1.13613538051643	3.12468462593150
H	4.48487547498577	4.05102189716904	1.90776125378113
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H	6.45986907320316	0.19806107132244	1.29202032702182
H	0.15339254090088	4.25594743453842	1.97873245876108
H	-1.06361230565080	-2.89733467672989	-1.85745866707110
H	1.89465512715053	-3.17808708466651	3.15725652614761
H	-1.48579871167009	1.31798641869924	4.75983658354721
H	-6.38910064012514	1.12383136903934	-2.23130633113139
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H	-5.59464174881913	3.58394359430002	2.96038258658048
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H	-6.96689366007372	1.62227174660873	2.17111699369207
H	-0.89604376856582	2.80314765192916	6.68456481070818

H -2.66368745829775 -1.40805964044326 -1.90782458847273

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**2'-PPh3**



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C	3.16723183462400	0.60003304705382	0.27532240952120
C	-3.20169478256414	0.66327232375451	-1.60424727490353
C	1.31483574958412	-1.85393278530005	-0.43286202152939
C	1.41800017770453	1.69238164074415	-3.09241954055482
C	-3.03136467659749	1.51794330108476	2.17920418822481
C	-4.94853748946104	2.78643104505800	-1.20360641380700
C	-0.64437752591830	2.90006235948459	3.08807821697900
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C	-3.61609246674880	2.80942756272718	-0.78890672426696
C	-3.72290747789377	2.55849692586898	2.84292404719035
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C	0.96584260171788	-0.48815111870256	-0.40075556542541
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C	-1.04728447373678	-1.15917452198034	2.59031368374529
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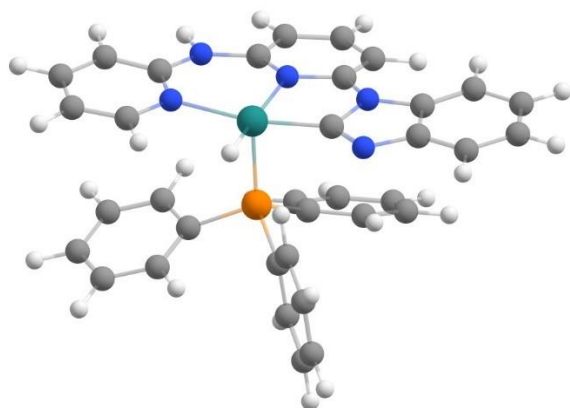
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C	4.69130683295581	2.41441811805216	0.95190653191278
C	-5.19258040013285	0.47551331598640	1.65669444234113
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C	-0.09634198289518	4.12630530504444	2.66023407696672
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C	-0.89589929530084	-2.32541018889045	-1.33390713647226
C	-3.46156384051874	3.63737968798162	-4.47949681139654
C	-2.37065680827054	3.62604054946388	-3.59543734333298
C	1.05770289861209	-2.21429804427270	3.23966680850907
C	-0.74759265786783	2.62341862206621	4.47334095884113
C	-5.40940712610418	1.65588330528697	-1.90815229481056
C	1.68638065144386	-0.95380263528541	3.21780212856725
C	-5.12921887125321	2.55417678693736	2.91575771310830
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C	-0.31228227670416	-2.30972329123575	2.93512800826876
C	3.61239536352197	-0.05074238960026	-3.53086166613517
C	-3.48051979603575	2.77286283840565	-5.59219283287902
C	-3.79011086876847	0.48407366618013	1.57400871394947
C	-5.86954058944037	1.51289762297336	2.32699441982632
C	-1.29278204572798	1.90274699203619	-4.93642600565324



C	-1.18488624725055	-0.94082843388260	-1.24808886725191
C	-0.31509112950583	3.57096134872001	5.41666946474273
H	0.41014999777045	4.55916524889230	-4.79043438733562
H	2.29957791734426	-2.18943724547281	-0.08334234527531
H	-5.60375108993097	3.64697398366506	-0.99112967955423
H	2.09652073102845	6.93737941973876	-0.70035630069473
H	-3.18587063760511	3.67668903794654	-0.26124885023450
H	-3.15675170363701	3.38802604921951	3.30051885426318
H	0.60443406835687	-3.84818773659863	-0.93060964690952
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H	4.06860396110133	-1.39188591529800	-0.00890574029637
H	-2.12216843988924	-1.26239692643211	2.37080503765697
H	1.15153054994790	4.61701783391329	-0.49809306917367
H	2.10634543380762	-1.57966175576959	-3.93869125642838
H	2.20513758857542	8.06715576523444	-2.94834004594339
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H	6.76134901129894	1.79495463111368	1.22734275880812
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H	4.86428715595977	3.47532393056025	1.20382756903144
H	-5.76283488741970	-0.34083905836771	1.17797555812680
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H	-2.38056149785261	1.25374945790767	-6.70759419946273

H	-0.01249372274446	4.31696872353075	1.57612433287176
H	2.93770309541744	3.20892156801154	-2.67845779743166
H	-1.65003809293771	-3.03339996031401	-1.72051956025628
H	-4.30544457714023	4.32698712394878	-4.29742919393858
H	-2.35456116553092	4.31818749847070	-2.73488635319208
H	1.63464239817723	-3.11965778207124	3.50131140872796
H	-1.16568891612910	1.65860512430593	4.81423817052014
H	-6.44483622287290	1.60009961327263	-2.28719747253356
H	2.76017366665621	-0.86003372044807	3.45914033076639
H	-5.64941289758851	3.37784774391133	3.43775861792593
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H	-0.82090547050833	-3.29046313031848	2.96480781147069
H	4.46787000708065	-0.73253824523276	-3.68464274993637
H	-4.34039583612111	2.77766538463404	-6.28615364330975
H	-3.28541178258531	-0.31330544404083	1.00305231625281
H	-6.97294690560960	1.51201130578414	2.38313570395705
H	-0.43572615438609	1.24147930633152	-5.14756087693695
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**2a'-PPh3**

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N	2.05862542107869	2.99546402453975	0.83399128532631
N	-2.66417517656754	1.79055392442916	-1.03686361850004
N	1.91228947819522	0.87787476060809	-0.00463010059469
N	-0.10385758716727	0.12559948079373	-0.81920467917651
C	-0.36324137106829	0.07575919131942	2.49835382480001
C	3.25031512932645	1.03590687158766	0.38150545358490
C	-3.05823867815445	0.62562283804898	-1.63170514288094
C	1.68177711102612	-1.51695662830959	-0.61701728690824
C	-3.02989788500450	1.46608126221062	2.16237414803144
C	-4.88529964777991	2.71621532557693	-1.44867295576657
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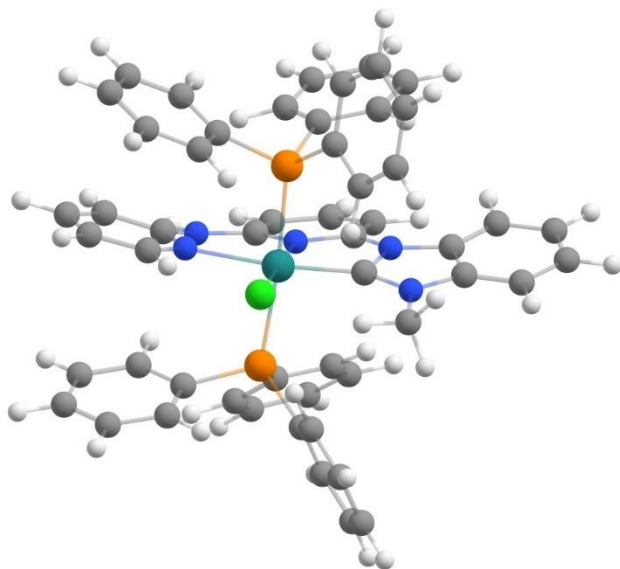
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C	-0.93587080531410	-1.21349019358787	2.41809802830771
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C	3.30621890004015	2.37888926783245	0.89753009668325
C	0.22031444264855	4.95161429984170	3.97635855081596
C	5.66398229121065	2.06625676563419	1.36357097087360
C	1.00003854414958	0.19315230724305	2.86985237527624
C	4.52248383106887	2.89073419451049	1.39242167760142
C	-5.16367183085004	0.41637724586205	1.55464153832407
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C	-0.14760419674788	4.07500252911765	2.93626011361189
C	-0.49739672242273	-2.16904351956190	-1.48618717017054
C	1.19939470113213	-2.23308907468856	3.02347294429868
C	-0.87149868111895	2.43369546216674	4.59896011343334
C	-5.27860805449598	1.52546161866325	-2.09739343227815
C	1.77387063188077	-0.95096648044773	3.12690776022091
C	-5.15737463680052	2.48018182495983	2.84030475951205
C	0.03898897841965	4.57683143386678	5.32026329046278
C	-0.15873657997292	-2.35866912770136	2.67871135989810
C	-3.75911213842728	0.43359170414856	1.52179362266192

C	-5.86996853731920	1.44086725257706	2.21474800816869
C	-0.92211095608336	-0.82587337976523	-1.31582474987448
C	-0.50830930713989	3.31469264477042	5.63180029375815
H	2.69964162946066	-1.77549993133126	-0.29678257733593
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H	-3.21327018587222	3.70500015007477	-0.43896796989516
H	-3.20420945370591	3.32331878280868	3.29817834305500
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H	-4.63794852252007	-0.46895059503705	-2.68665232992094
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H	-2.00075792697588	-1.34086351624445	2.16600471564699
H	0.66214300759654	5.93360457949034	3.72894840005981
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H	1.46514790618873	1.19161167681314	2.94862985164069
H	4.55912380521935	3.91964045599094	1.79072767747965
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### 5-PPh3



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C	2.17040871352906	-1.17714610837166	-0.49503309777374
C	1.05160504279545	1.37295960853919	-3.24612781927217
C	-3.17180732474445	1.62728895135485	2.07066392672806
C	-4.72929934490581	2.22472219966833	-1.80944649682619
C	-0.76377327339797	2.51262146371550	3.46364603738371
C	2.00697583544343	6.35392985430154	-2.30361342755033
C	-3.49617263540509	2.49797542562910	-1.21422406329697
C	-3.79990208373089	2.79352044627907	2.56488992105987
C	1.37907411634694	-2.31716990991987	-0.71191342059263
C	1.52904502110534	0.06520093211509	-0.40453111398758
C	-4.02320258234639	-0.06745634285785	-2.02397607136013
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C	-1.72628939902391	-1.18471206492187	2.91191134019266
C	1.27317010479390	5.20574523609837	-1.94397244212362
C	1.33071061655321	2.36822868609751	0.27288759873237
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C	3.53272943669037	2.84717315604552	0.73778913657880
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C	5.93064485914479	2.79693040452018	0.86689316745589

C	0.52173325222690	0.10856985435682	-3.60182312896923
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C	4.72579300671835	3.48666168958807	1.10807332171334
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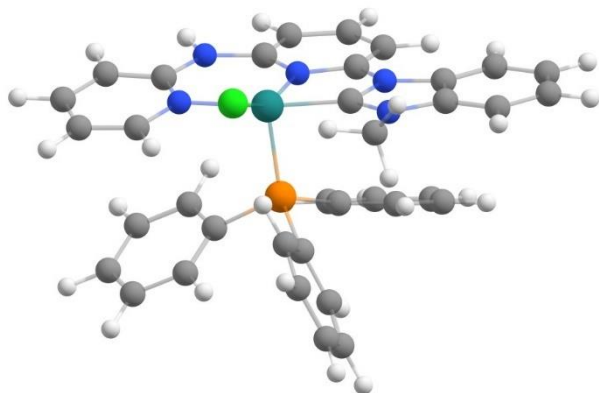


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5a-PPh3



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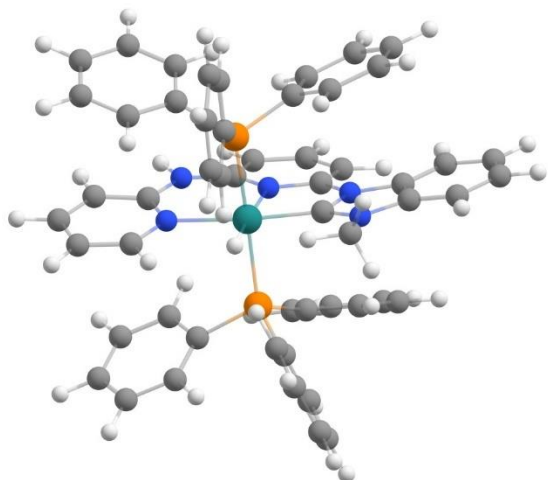
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### 6-PPh3



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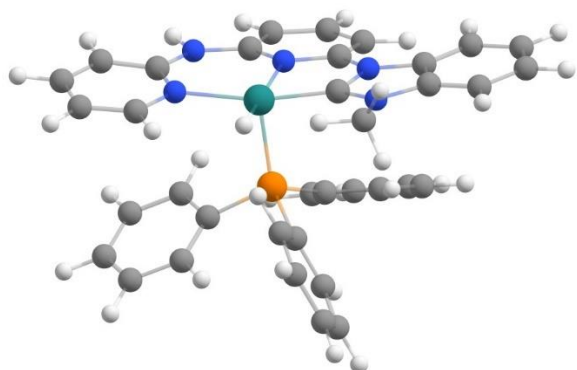
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**6a-PPh3**

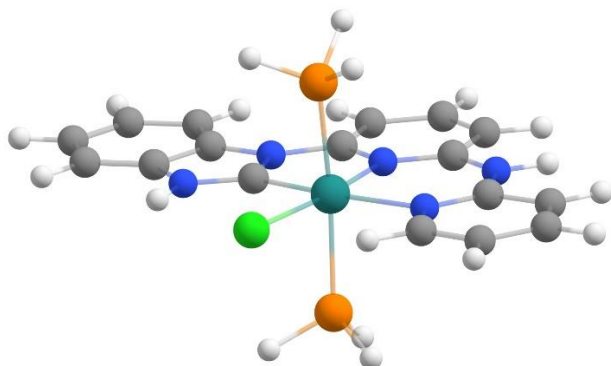
Ru	-0.66856552032607	2.09764747802963	-0.09988526724072
H	-0.96088763374218	3.65058098085107	0.33025026423130
P	-1.17494851547517	1.63669298825870	2.00696522317488
N	-2.22486650853845	-0.35878015430852	-1.71750961817434
N	2.21002484455583	2.92510762545627	0.82224709102698
N	-2.60094738171503	1.91964639255174	-0.97120287935488
N	1.91873161582250	0.85103351776371	0.09864158820763
N	-0.11130322680462	0.16258379720810	-0.75145234264357
C	-0.25639574266241	0.13431711773888	2.60206539736353
C	3.28105408403617	0.94497375402862	0.45247579564415
C	-3.00665239684327	0.80015687236156	-1.63895674059942
C	1.60189447414515	-1.54330983744155	-0.51123215464755
C	-2.98981443638988	1.29925535022433	2.18845101846605
C	-4.76622624405625	2.94558496463677	-1.42418578293411
C	-0.85237436582698	2.86750085734448	3.35355956889975
C	-3.48913742416554	2.96015375464794	-0.86872374074822
C	-3.80859034682848	2.16151158402561	2.95410997911221
C	0.71003031348600	-2.49025726535039	-1.05405701387230

C	1.16163656176075	-0.21827277157675	-0.39823492492411
C	-4.28581269491937	0.73049051407223	-2.26024290655509
C	4.37468910234509	0.06207417080105	0.41011164873771
C	-0.79784960444705	-1.17026231962728	2.56326394012207
C	1.23699784337640	2.08090609337363	0.34251471775356
C	3.45274418207044	2.27753340298238	0.92352415652993
C	-0.74820448422193	5.18574624893204	4.12655185229183
C	5.77715595959496	1.85409737455112	1.35745735012297
C	1.10095437438619	0.29869870224763	2.97593658909577
C	4.69144508256618	2.75124814799785	1.38346929022200
C	-4.99302266563831	0.07126119630127	1.48688564487499
C	5.61954324132156	0.53700670780425	0.87347914372769
C	-0.89684861865009	4.25278051578949	3.08343048778340
C	-0.56718785143355	-2.10175976521751	-1.46762016750143
C	1.36114577867690	-2.11468745110623	3.20556789788045
C	-0.67830215777838	2.42557335624836	4.68803088865896
C	-5.16876591987110	1.80303176705813	-2.14969006376210
C	1.90249241213323	-0.81560054652800	3.27512640801223
C	-5.20488856131579	1.98031858350032	2.98022375625047
C	-0.55545957449773	4.74202744458308	5.44896897153634
C	0.00856487636672	-2.28608492548408	2.85920623196133
C	-3.60077288837968	0.25401413788289	1.45155929221920
C	-5.80154914775680	0.93807549611421	2.24840718335821
C	-0.95068178272019	-0.74488286497509	-1.29781901573285
C	-0.52523491315966	3.36135664389406	5.72703070479749

C	1.99754114529294	4.32789713791980	1.16719841096210
H	2.59632793796098	-1.84971780233516	-0.16347736529102
H	-5.43100889241487	3.81539355880621	-1.29647277895554
H	-3.11221101955614	3.82536164536321	-0.30008632754216
H	-3.36011939504781	2.98558668354497	3.53380301855552
H	1.02371348416983	-3.54357775614045	-1.15176354935020
H	-4.57628620640598	-0.17940229080721	-2.81571468100484
H	4.29788323938252	-0.96378673597202	0.02140733812503
H	-1.86119105794807	-1.32871400068743	2.32342732439242
H	-0.78549433718190	6.26717690216585	3.90409722347285
H	6.76620519673657	2.18949004905833	1.71435294810330
H	1.53713457019621	1.31066162024027	3.04779376906668
H	4.81293191472184	3.78370637078573	1.75154355578703
H	-5.45208930326239	-0.75271614243770	0.91195210912516
H	6.48974737625219	-0.14158179141903	0.85117647823959
H	-1.05793216014392	4.58814416290497	2.04313989063940
H	-1.26887971267084	-2.83319503211233	-1.90498919280953
H	1.99024359277051	-2.99166209543964	3.44036579826071
H	-0.66828172784055	1.34686667955862	4.92286715932722
H	-6.16552361532717	1.75068555131732	-2.62129723367133
H	2.95648067208062	-0.66581329172432	3.56894392384418
H	-5.83002424123139	2.66384557134814	3.58186784976208
H	-0.43443595282528	5.47387014802913	6.26740406507278
H	-0.43222931484621	-3.29842917434232	2.82886381805984
H	-2.98981732402097	-0.42070134949420	0.82977283885947

H	-6.89683631076247	0.79849883236526	2.27155934100490
H	-0.38545068649188	3.00739935901328	6.76395378621205
H	-2.71852218751147	-1.11828877104008	-2.19813436110923
H	0.97015525469304	4.60155741998795	0.85675105734140
H	2.72970833738248	4.96725800318579	0.62596519676711
H	2.11037658536951	4.48856690071096	2.26252912538056

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**1-dft-PH3**

Ru	-0.48978865376733	1.95975073695798	-0.49897093811660
Cl	-1.28647995914165	4.23237318836073	-0.09752871934371
P	-1.16950877223039	1.55246989447320	1.70168873304028
P	-0.05079128985758	2.72041975068100	-2.66710476202874
N	0.45829990822551	0.15695082262693	-0.73633296104574
N	2.26215221560183	1.38209220871594	0.04709281366018
N	-2.39816556520383	1.20347324834105	-1.18955854070635
N	1.96970271354576	3.51409817517133	0.53679558675288
N	-1.47652986903482	-1.00386810083547	-1.54112640215428
C	-0.12864934591980	-0.98271637096253	-1.18845750517035
C	-4.89702016515141	0.25932379207824	-2.08440614241448
C	0.60963178651424	-2.18841055203655	-1.31704544098875
C	5.83509151615614	2.09656371366144	1.12734271478552
C	4.35654454371633	4.05207774773675	1.27658068107469
C	5.62359617827615	3.45864238123677	1.43556116142809
C	3.32027636595532	3.23556281306705	0.80190283234299
C	1.30779137330146	2.42061672296528	0.08104209961279
C	4.79373374243518	1.27438592469745	0.65019398971555

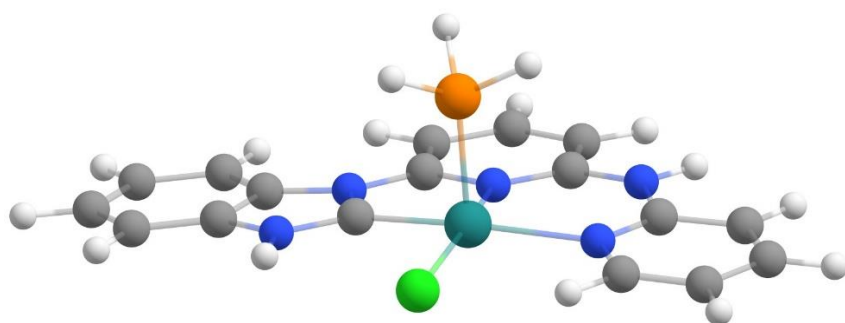
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C	1.80139532500696	0.13313333917127	-0.39943653621445
C	1.96359198963173	-2.20063723950765	-0.97234709128069
C	-3.48601785630882	2.02693959082181	-1.24869940213612
C	-4.74297950621977	1.60312171125611	-1.68502489961631
C	2.58178193850410	-1.02532949225255	-0.50406318087888
C	-2.54154717204109	-0.09214473595210	-1.57258389159853
C	3.52519985276195	1.85806373487875	0.48893522107590
H	-0.78665093206530	0.34980690598403	2.40350966516961
H	-1.18262522432285	2.96040453203290	-3.52095584444662
H	0.60919885482167	3.98680137686787	-2.81185035141548
H	0.75044605989271	1.95669335906873	-3.59462310737942
H	-0.80639428304100	2.50970782956565	2.70844547934937
H	-2.58496077097923	1.49447677384649	1.94910153788456
H	-1.76763022456229	-1.93354420621549	-1.86190372355276
H	-5.87132983412327	-0.12179253908996	-2.43692267193175
H	0.11376395781915	-3.10327278053915	-1.68568365188780
H	6.83936655188619	1.65908187901057	1.26126956261098
H	4.18461527899529	5.11547933020692	1.51489863579982
H	6.46429308790822	4.06961034899252	1.80684442763400
H	4.99827135903429	0.21827949345295	0.42004385530985
H	-3.88368980623999	-1.65041150239464	-2.33537416024035
H	2.54943573931430	-3.13063071279147	-1.06667508112029
H	-3.29418893263169	3.06706318821768	-0.92132013779737
H	-5.58376604781244	2.31596876416893	-1.71025035612898



H	3.64464721421931	-1.02233936929706	-0.22961484470770
H	1.47764528532090	4.41078029770588	0.65062502334647

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**1a-dft-PH3**



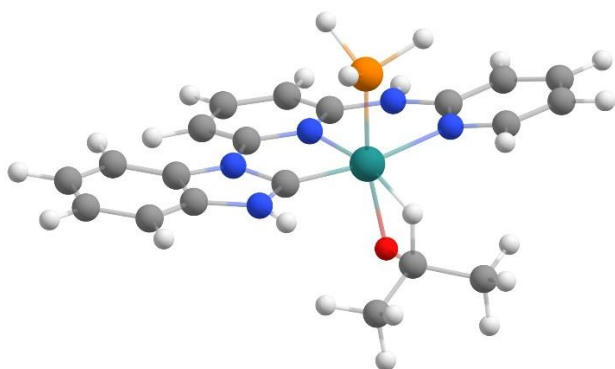
Ru	-0.55520065032469	1.92078206233858	-0.30670271186440
Cl	-1.24671325124187	4.18021541405037	-0.17232770457409
P	-1.08898432568611	1.44808269066567	1.77178192825077
N	0.41280094954628	0.14222294042356	-0.63252316648020
N	2.21921950403568	1.36876451273098	0.14842118996930
N	-2.39838476902402	1.21730497513704	-1.16706808628260
N	1.92241665371170	3.49331398053688	0.66235246278918
N	-1.52136040282497	-1.02397171697316	-1.41852723434868

C	-0.16689853228185	-0.99538451822310	-1.10286977539458
C	-4.85605735767779	0.31667648362577	-2.22214667244902
C	0.58250203208341	-2.18980360179497	-1.27246356009106
C	5.83884502936970	2.14367278477523	1.00274539947403
C	4.33996866646269	4.07386630362690	1.24911792126055
C	5.62363274262986	3.50233905242751	1.32670577181412
C	3.28966489136485	3.23815098816386	0.84127229476376
C	1.25298045764104	2.39183220053002	0.23754921018464
C	4.78495346234878	1.30332455711822	0.59082789012699
C	-3.78026797142971	-0.56026448164665	-2.07778691039716
C	1.76312456115737	0.12357290725497	-0.31539619762695
C	1.93900019914000	-2.19588810509817	-0.94243095932245
C	-3.46225506352423	2.06533857031072	-1.32038359303803
C	-4.69411154523025	1.66427247476896	-1.83642179440937
C	2.55122410263212	-1.02375289607452	-0.45430127345605
C	-2.55169971593305	-0.08249094175330	-1.54397219893555
C	3.49815594325125	1.86437689962945	0.51374273811815
H	-0.38776991164618	0.38450970948588	2.44886313695472
H	-0.95366144471335	2.48709496924758	2.75817044240208
H	-2.44840242773394	1.04229240932107	2.01963390483489
H	-1.81982218440157	-1.95487191541209	-1.72969225815103
H	-5.81311107355044	-0.04591984374536	-2.63617709281173
H	0.09179287527251	-3.09926922800029	-1.66066193358060
H	6.85742903918088	1.72448505349785	1.07113138643306
H	4.16503673195129	5.13466468954703	1.49648063201616

H	6.47588029641836	4.12732820081895	1.64439495497313
H	4.99468061305523	0.25244373467174	0.34226199449937
H	-3.87505625736751	-1.61929130255546	-2.37801700637941
H	2.53420351258777	-3.11644121622506	-1.06618560517449
H	-3.26931504477191	3.10784083725412	-1.00530854591783
H	-5.51189747188772	2.39733428343914	-1.93407550986460
H	3.61682260262342	-1.01772401854238	-0.19051944960400
H	1.43548453478701	4.39448010064640	0.76314598128900

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### A(H)-PH3



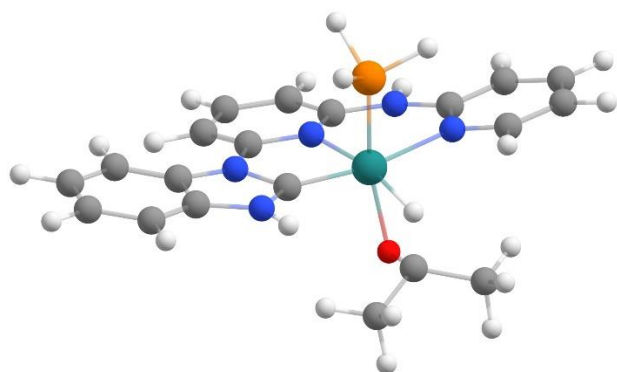
Ru	-0.02569197376287	1.48058595263637	-0.99644105608684
P	-0.89817090547592	1.82691193455946	1.09763756489662
N	-1.75237925136151	-1.19906755823425	-1.85049387767635
N	2.64075267337541	2.36596411949185	0.35581155214579
N	-2.06601304316175	1.18325546161593	-1.68325132142043
N	2.26405616874637	0.20619667548681	0.15829369080380
N	0.29070824551425	-0.54022262841138	-0.77836109004245
C	3.47070156074868	0.32506776762386	0.89375787136719
C	-2.53829922291537	-0.05302490307764	-1.98531806141162
C	1.95059742293105	-2.23282423354532	-0.19624212986668

H	2.94489345189724	-2.49037766483086	0.19118663143266
C	-4.24565101147990	2.13159657256215	-2.21298673755183
H	-4.88278862037036	3.02899668091101	-2.27615323265214
C	-2.92333581135496	2.24106320832522	-1.78174596057441
H	-2.50069830449074	3.21987878997275	-1.49537801329626
C	1.09301323395017	-3.22997966953541	-0.69532663539929
H	1.40413193335399	-4.28811110760684	-0.67052844224716
C	1.51596857276764	-0.90196971497503	-0.25433277543960
C	-3.87141998633854	-0.24415381528635	-2.44897898866520
H	-4.22546650256109	-1.26025036174555	-2.69927134259354
C	4.35757162947112	-0.59323499477670	1.48293463379507
H	4.19974148995684	-1.68130865921057	1.44796207705633
C	1.73688581691753	1.47927673113413	-0.16547021662402
C	3.70785968839707	1.72496556816452	1.00484448001112
C	5.71889274557277	1.31427338551044	2.24693112999608
H	6.61258711808228	1.68171279567131	2.78002491385925
C	4.82764062739766	2.24121998136856	1.67226761511414
H	5.00222400368969	3.32809101731370	1.74805652185708
C	5.48255896235217	-0.07501335806301	2.15699278572425
H	6.19216164039045	-0.77839473325205	2.62559762039788
C	-0.14460090005634	-2.87650988027035	-1.23811689577319
H	-0.82359687076483	-3.64699068449165	-1.64286005713855
C	-4.72502096963910	0.85219566898534	-2.56831998640357
H	-5.76018731683874	0.71219089987830	-2.92511772671711
C	-0.52131503699624	-1.50887519859070	-1.27834793883775

H	-2.23456723184389	-2.03755105155625	-2.19086435350664
C	-0.54056014750588	3.59793291170486	-3.72754500619318
C	0.49364340795557	2.87121932329699	-2.83881361820915
H	0.01148184324972	3.15839407045577	-1.60559634566958
H	-1.50891374304908	3.06021938531338	-3.76196995205856
H	-0.70881619995223	4.65124507258368	-3.41097857749967
H	-0.13685464796378	3.61586642972297	-4.76538080740849
C	1.85563537491338	3.60295128709871	-2.82144415910650
H	2.61452303644758	3.03104171460758	-2.25107040536344
H	2.21849548987261	3.68220931443887	-3.87132816737369
H	1.77768134497739	4.63702411639246	-2.41587416084873
O	0.54674988749886	1.53606707231277	-2.99216885318239
H	-2.28067797863414	2.22351369136110	1.22081212122313
H	-0.33927503061547	2.82701386876889	1.97427068284784
H	-0.93022858058091	0.75593657840896	2.07104585981055
H	2.53070191728611	3.38031216978121	0.26692914049921

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**TS-I-(H)-PH3**



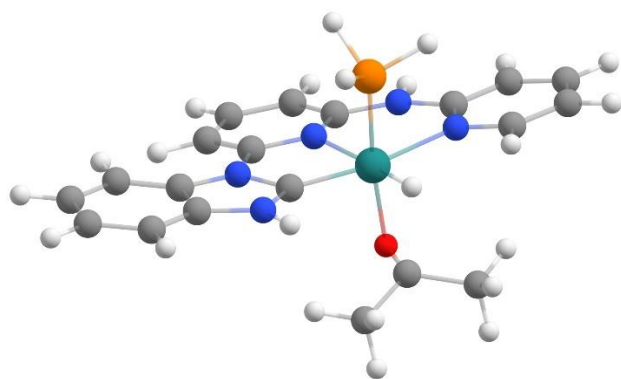
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N	-1.74857203435148	-1.19797608875840	-1.85004284359156
N	2.63431878808374	2.37592221662389	0.36059678490978
N	-2.07036215188916	1.18690265864586	-1.67984418627077
N	2.26720900041895	0.21532750757874	0.14660342614046
N	0.29626808323391	-0.54075474377851	-0.78635461619249
C	3.46900699513085	0.33472601853117	0.88942114472570
C	-2.53944694845232	-0.05343601323589	-1.97402930017285
C	1.96785531941177	-2.22474243428606	-0.22187032249599
H	2.96638332023135	-2.47953020136400	0.15649866849896
C	-4.25971410019821	2.12280482339390	-2.19453457902247
H	-4.90117338335718	3.01724333870799	-2.25639154850182
C	-2.93416988017495	2.24021469823454	-1.77607202737702
H	-2.51210412070400	3.22156870828510	-1.49870223919885
C	1.11155657795344	-3.22366934326018	-0.72055732169580
H	1.42866080290928	-4.28023970239659	-0.70272772506593
C	1.52428914595085	-0.89599003200199	-0.27031475145192
C	-3.87701342179374	-0.25182186854124	-2.42255451425248
H	-4.22916342513142	-1.27063409594275	-2.66446644187620
C	4.35444341641951	-0.58406101470141	1.48013788591500
H	4.19929608297361	-1.67228301301497	1.43867236008238
C	1.73717242087545	1.48981380149946	-0.17339237235125
C	3.70062135985107	1.73478941578090	1.01036113619678
C	5.70480561244373	1.32317369439066	2.26366876506645
H	6.59383501674228	1.69042004037169	2.80465433974600
C	4.81427112564806	2.25048156288789	1.68854222263696

H	4.98452335637263	3.33748395611399	1.77208873439953
C	5.47332200214623	-0.06627554506706	2.16465695419939
H	6.18180018745486	-0.76998216870840	2.63448966950422
C	-0.13189870554337	-2.87560887309840	-1.25394589876029
H	-0.80918105633588	-3.64855061283744	-1.65688478786761
C	-4.73710009328516	0.83952996582678	-2.53848341376401
H	-5.77520774086263	0.69284389837118	-2.88388807090663
C	-0.51366179775553	-1.50889693135925	-1.28572522753205
H	-2.23222577848915	-2.03573931607010	-2.19011190976607
C	-0.53346871415345	3.59702026814536	-3.70611756870715
C	0.50798541638555	2.82706780063170	-2.87058937569290
H	-0.02590144766365	3.15366819789558	-1.50358343926164
H	-1.50764704638390	3.07080537430804	-3.74405515184918
H	-0.68191503980108	4.64007248346808	-3.34996156587838
H	-0.14677771485369	3.64830272772104	-4.75006497594432
C	1.87139540083823	3.54522824024821	-2.81930304227654
H	2.62917019772640	2.94380673404717	-2.27929950140182
H	2.22903095663336	3.66911358669449	-3.86752018876158
H	1.80139251388957	4.56169616059930	-2.37125044248960
O	0.52795271103719	1.50858937342362	-3.02381097955905
H	-2.21575602872932	2.44066640037438	1.18342372123924
H	-0.23189680932201	2.72023278419406	2.01855399215887
H	-1.11894286885750	0.75310713298947	1.98607459115066
H	2.52352724197332	3.38999998574261	0.26943531086878

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**B(H)-PH3**



Ru	-0.14817191339534	1.58626014625776	-0.81310303955784
P	-1.01709423076189	1.84046293581978	1.26157281284729
N	-1.79088859048153	-1.14071688937681	-1.80083966756544
N	2.51358488037155	2.43856381820008	0.54837341431660
N	-2.15967098080115	1.24383238755775	-1.55059468516592
N	2.21980598839432	0.28647145166474	0.17733491512074
N	0.25805434712997	-0.50177360940200	-0.75510490640457
C	3.45069832959072	0.40001756227348	0.87249526510576
C	-2.58791375678892	0.00363928600996	-1.91127501989540
C	1.99799287847157	-2.14264579702317	-0.33355354600762
H	3.01301299510695	-2.38970147357761	0.00308985074015
C	-4.34320988807576	2.15562707015541	-2.13481644177955
H	-4.99842088590002	3.03993038635282	-2.19872719901516
C	-3.04018064278160	2.28460446075708	-1.65512672115746
H	-2.64043952390380	3.26292735337469	-1.33858062631193
C	1.15606179045897	-3.14074253974795	-0.86221721385916
H	1.50886521935404	-4.18528134396420	-0.90939590498430
C	1.50704119403716	-0.82926305673873	-0.29483040502248
C	-3.90261066708736	-0.20151739051696	-2.42290015553285

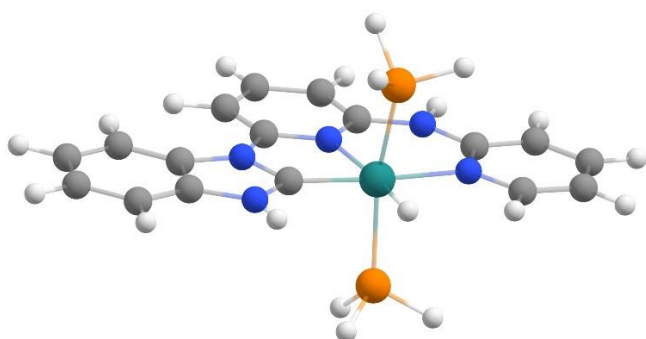


H	-4.22280758121779	-1.21694222963390	-2.71815028965545
C	4.40149190357970	-0.52145932552727	1.34695132064491
H	4.29081787617541	-1.60883581414284	1.22466968995118
C	1.62920049747869	1.56208945172257	-0.01805975948066
C	3.63323703083328	1.79522261854339	1.09607228731882
C	5.71082422255284	1.37529627793428	2.22102306324991
H	6.60935801835961	1.73736846662588	2.74965158009397
C	4.75683704248403	2.30430109107134	1.76314218332270
H	4.88627150121061	3.38791565730968	1.92627761852857
C	5.53049249845346	-0.01078478398264	2.01987363761432
H	6.28839053646467	-0.71789594042076	2.39868761786112
C	-0.11441691312993	-2.81292846851459	-1.34161751344004
H	-0.77511187872847	-3.58804959256948	-1.76735758947837
C	-4.78008399354950	0.87513298366562	-2.53830807823819
H	-5.79891454939835	0.71968799780404	-2.93376774034768
C	-0.53430013069532	-1.45620491231429	-1.28813739181087
H	-2.27019938036983	-1.97017170158005	-2.16651316116249
C	-0.44731152863014	3.44380455679986	-3.60615487182812
C	0.58554211655837	2.56980165364944	-2.89994010606737
H	-0.34182686651073	3.21977942946154	-0.72041963437656
H	-1.44750748266451	2.96907586183909	-3.63068084905229
H	-0.51690581076947	4.46010476854506	-3.16316561561428
H	-0.11259288956415	3.57060285119587	-4.66472203306000
C	1.97968731360718	3.18220215514894	-2.78516140140365
H	2.70051191088083	2.48298408501327	-2.31659324218103

H	2.34163129556168	3.39925952858363	-3.81974030603826
H	1.97328459737281	4.15165047922317	-2.24122329257229
O	0.44349842119299	1.29207955622128	-2.88541050878212
H	-2.36775973106636	2.33017898100017	1.37493192813179
H	-0.38969654037898	2.73877112269130	2.19343316484596
H	-1.14132047121026	0.70505208560058	2.14675139707905
H	2.35555242217975	3.45043635095966	0.53579717007656

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## 2-dft-PH3



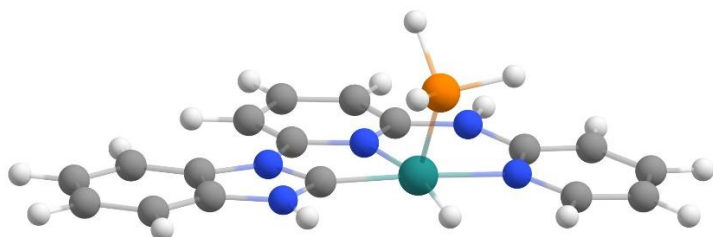
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H	-1.13128883270728	3.48751354755803	-0.25853919834092
P	-1.23243536579700	1.69503790756464	1.67913208545872
P	-0.12986448972874	2.84523425702266	-2.61589711497632
N	0.48165261453888	0.11763549927009	-0.74395022654201
N	2.25986545388506	1.36858424562307	0.03972038486012
N	-2.38461205432629	1.17337775228164	-1.20114096532559
N	1.99742035192742	3.49973785539257	0.53667509822172
N	-1.44979297180145	-1.03930179287621	-1.54169538246949
C	-0.09885201684586	-1.02028671386409	-1.18830174169789
C	-4.87360116326401	0.19613657796118	-2.11256366616565

C	0.63896308196598	-2.22651332791866	-1.30955766012951
C	5.84786201015088	2.04441700263418	1.10309470006651
C	4.39091643935335	4.01203191157050	1.26601909605671
C	5.65338818469677	3.40721998986488	1.41719653533866
C	3.34488982386371	3.20604692834344	0.79450406103101
C	1.30371139701038	2.41792903339099	0.07685585336344
C	4.79515495541681	1.23491041321064	0.62919089300619
C	-3.75907033130313	-0.64057048938793	-2.04305102539660
C	1.81190396640382	0.11119958504085	-0.40196287787134
C	1.99253153255750	-2.22502272047639	-0.95725847684047
C	-3.48706378857488	1.97915975626559	-1.27612607930321
C	-4.73720378628402	1.54362545815453	-1.71904365722450
C	2.60353226265415	-1.04478796187747	-0.49375419718186
C	-2.51370788826973	-0.12820152052741	-1.58034337369208
C	3.52938788948638	1.82916722897934	0.47618925918704
H	-0.89045573222789	0.53983036654995	2.48160431743361
H	-1.27641671910120	3.11005762715155	-3.44735387525539
H	0.50131992582381	4.13200190530058	-2.73640459116654
H	0.66746259766329	2.16994086679688	-3.61795361667516
H	-0.89179536490556	2.69040558718458	2.65981958694571
H	-2.65348906809793	1.66481722189615	1.91481471782611
H	-1.74287739945764	-1.96930735851420	-1.85932986710447
H	-5.84046037713441	-0.19818579517190	-2.47061603130929
H	0.15163478628730	-3.14775836804678	-1.67377524993814
H	6.84796629845501	1.59516819035730	1.22922509834867

H	4.23080918418712	5.07665747629042	1.50790031166560
H	6.50211049333649	4.00866906298537	1.78574502807096
H	4.99236681183410	0.17898161751404	0.39440394636434
H	-3.83644057297450	-1.70047383549061	-2.34550152041464
H	2.58490282686169	-3.15204750035705	-1.04173520058831
H	-3.31746928021389	3.02103366286163	-0.95567522197407
H	-5.58461491419815	2.24797477955882	-1.75400723019363
H	3.66441142590859	-1.04159639199658	-0.21391602122476
H	1.54894021885722	4.41188789060183	0.66503374359763

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### 2a-dft-PH3



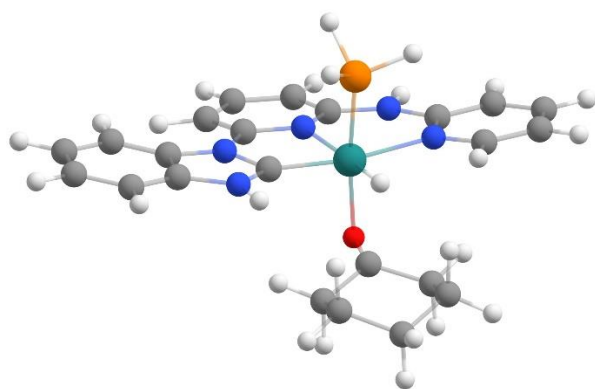
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H	-1.15059884335097	3.37570534546358	-0.15123560189765
P	-1.30346428350950	2.04959954642698	1.79587549831694
N	0.45909725909395	0.05494279110808	-0.69070992156452
N	2.23126757374350	1.31935874057791	0.09326023798003
N	-2.37785355263405	1.10247637874058	-1.11351495998469
N	1.91113941431555	3.38379260767262	0.79758831649151
N	-1.45881968556560	-1.11135200832786	-1.49393299386748
C	-0.10019155587456	-1.07207010658535	-1.19232103004767
C	-4.83006584179994	0.19014735714221	-2.19044850388308

C	0.67173106200419	-2.24318369565926	-1.42085372673954
C	5.85530992055441	2.09029400695504	0.94435472367611
C	4.32526226542876	3.95437976096124	1.39707712106566
C	5.62221825430562	3.40734189080887	1.39776133950571
C	3.28372904351485	3.13721501285690	0.93358528245345
C	1.23226903954621	2.31555389690738	0.28149362688355
C	4.80796807137977	1.27024348456907	0.47693170136662
C	-3.73175327224028	-0.66254685925958	-2.09944980756186
C	1.80983561927448	0.08117526748416	-0.41547426531615
C	2.03583732160571	-2.21038039046404	-1.12509838765149
C	-3.47201246038688	1.92635135058148	-1.21801694529937
C	-4.69844433747845	1.52254301548936	-1.73930500737481
C	2.62995159501268	-1.03620385297274	-0.61645375940542
C	-2.50557272105251	-0.18473657174219	-1.55417370064125
C	3.50702404453885	1.80481080844263	0.47901094504595
H	-0.99453984108312	1.03067119142509	2.77721926017540
H	-0.93436924754497	3.19394845248532	2.59298867157188
H	-2.73280073988704	2.10101581903509	1.99274256314279
H	-1.74778740232082	-2.03201178539612	-1.84237265521516
H	-5.78223548483169	-0.17606639746843	-2.61209088688523
H	0.20248585901850	-3.15507451793009	-1.82917876176838
H	6.88267523773399	1.68733611333612	0.95182902140921
H	4.13576390661404	4.98442850520044	1.74431521357746
H	6.46839258594271	4.01899653727946	1.75511210441829
H	5.03715899205877	0.25407487636813	0.12452450221561

H	-3.80526531203404	-1.70805443737023	-2.44911606353075
H	2.65711260491853	-3.10656884708399	-1.29410885248820
H	-3.30884770965979	2.95482605858896	-0.85529265581017
H	-5.53555078998530	2.23788809376492	-1.79355066122928
H	3.70152359778829	-1.01528446698113	-0.38118521234908
H	1.44708759850225	4.27680697771884	0.99062255554128

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### NPS-C-(H)-PH3



Ru	0.06900795454256	3.06459127407087	-0.83496099922070
P	-0.44562251993177	4.95142251263777	0.30654897970832
N	-2.08810425359807	0.92698601368500	0.54147083871974
N	2.99377813213414	4.07653815502447	-0.52184074152238
N	-2.05554985785384	2.71011817855234	-1.10141990519509
N	2.33347776112933	2.47555252375230	0.83944357584474
N	0.16249544871573	1.68775962065775	0.78452592796756
C	3.65454056019428	2.80628104286935	1.23513072279623
C	-2.71258684490251	1.74023741033820	-0.40950332344993
C	1.68466539397196	0.57626528773020	2.31632556847636
H	2.69071905939639	0.45091097728346	2.73693243633158

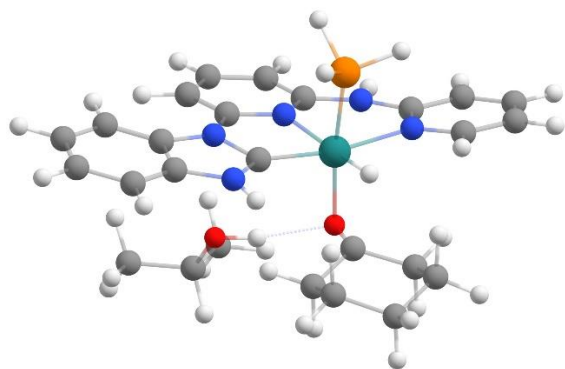
C	-4.13893258902055	3.30792993924176	-2.21697265484177
H	-4.65580762592680	3.95972969067673	-2.94039088155805
C	-2.77624692128061	3.47718947682196	-1.97404645484558
H	-2.19630509694068	4.25598863201728	-2.49784134935770
C	0.63687764174286	-0.28250665667603	2.70230629936956
H	0.82170056567109	-1.06553948639400	3.45759486862511
C	1.40323959729708	1.55546146941927	1.35211725403637
C	-4.10305886141657	1.50168788023155	-0.61475434946472
H	-4.61062402951297	0.70132028188765	-0.04680420009476
C	4.51649015975223	2.36448744561763	2.25489224278522
H	4.22904396191786	1.59633678307381	2.98744296758194
C	1.91715240481189	3.27490248085935	-0.25689611623896
C	4.07267463378127	3.83318623326147	0.34046964822695
C	6.20582859925534	3.95977926749655	1.43186856034962
H	7.21536883077219	4.39591876501022	1.52420509179587
C	5.34397094618109	4.41998147071752	0.41786502745310
H	5.65466602465011	5.21197745988725	-0.28482506527685
C	5.79429108001797	2.95518173460880	2.33496886226002
H	6.48568055889970	2.62091251247709	3.12755233052918
C	-0.62766190280299	-0.15948688888202	2.12202520541158
H	-1.45028743665093	-0.83671780778261	2.41057074616726
C	-4.81665458018244	2.28303679391638	-1.52171920907397
H	-5.89341058269730	2.10111254809296	-1.68311907905120
C	-0.83048473706994	0.84257331812401	1.13494944066466
H	-2.73319058179690	0.22508166668992	0.91919983237467

H	0.11702695412914	4.22058480378426	-2.00596190657687
O	0.33147135766894	1.22990427018359	-1.95972765592822
H	-1.68397601867496	5.61862499809191	-0.00751810589365
H	0.42954218768959	6.09069742129981	0.23293029335440
H	-0.59397028102292	4.92054347262371	1.74370674723280
H	2.99254270540233	4.74605377168651	-1.29762823469151
C	0.62727306171321	2.02067999234461	-2.93174404044115
C	2.08739145024123	2.25140344961700	-3.33178294843282
C	-0.36177898660447	2.24692445833185	-4.07864603070410
C	2.31673203605501	3.56710168714958	-4.10541626492474
H	2.33442381523406	1.39240836281361	-4.00878940314111
H	2.75669708479683	2.14093133106354	-2.45288827192796
C	-0.11908641601764	3.54890914238125	-4.87138586970233
H	-0.20527562084406	1.37065040932028	-4.76071737040356
H	-1.40773346521357	2.15499495033819	-3.71817430152576
C	1.35443709582611	3.69405111927721	-5.30531616820425
H	3.37564878925253	3.62745831589384	-4.44670352856569
H	2.14870915455221	4.43258318321659	-3.41769210456376
H	-0.79023301867234	3.58077431970854	-5.75996287283038
H	-0.39988338247667	4.41934010434055	-4.22984308155139
H	1.50805967640560	4.66983739469726	-5.82060033523720
H	1.60074092730959	2.90685503483988	-6.05935064362468

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**PS-C(H)-PH3**



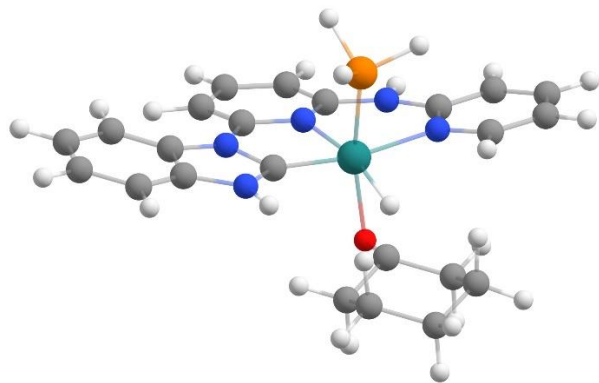


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H	-1.13676589244669	3.33009261921094	-0.47219392440912
P	-1.25106002916287	1.95624838469539	1.56126563384214
N	-1.25254564445145	-1.28152483451908	-1.39778263624993
N	1.94190635198629	3.49126398476761	0.56105201782832
N	-2.30810393069482	0.88659323899137	-1.16138787938084
N	2.17885805740186	1.30437935162804	0.48963938573972
N	0.52195729284835	-0.04504608949080	-0.38344859056539
C	3.37261432358089	1.80754662345367	1.06052346488006
C	-2.35863311506956	-0.43211179043832	-1.49220200730878
C	2.60619821960054	-1.13389316206282	0.21473602530291
H	3.63237492393251	-1.08175689014082	0.59811741687483
C	-4.68970270499322	1.08585004168784	-1.64131743285168
H	-5.58413126212793	1.72949556261736	-1.67306066323128
C	-3.46734823569256	1.60893710198014	-1.22164758918637
H	-3.37322507393587	2.66683992599758	-0.92307947202690
C	2.07835923676936	-2.35294852909064	-0.24714574037990
H	2.69145560405185	-3.26898322450574	-0.19458342279633
C	1.79818323128840	0.00835966371568	0.11547814914350
C	-3.56866190797550	-1.03057024923698	-1.95114653164187

H	-3.57864191683005	-2.09957462384606	-2.23016923943889
C	4.54843921896904	1.22190991992560	1.56282489397269
H	4.71591889343225	0.13542554051273	1.57718886475676
C	1.29502072533354	2.35952864466364	0.15657238141430
C	3.20825478798731	3.22152394236178	1.10053657130861
C	5.37270682009288	3.48235255415475	2.10007050535302
H	6.17398766721341	4.12167284184656	2.50885303304178
C	4.19347963770167	4.07735584647955	1.61272890225618
H	4.05051016926241	5.17127371025929	1.63293490620694
C	5.54128968279878	2.08042805182904	2.07710332940503
H	6.47244778078153	1.63907621842582	2.47228749840381
C	0.78993601655121	-2.40870935607034	-0.78670759619023
H	0.37237072794142	-3.36000653793005	-1.15942087389186
C	-4.73396816135508	-0.27062682691973	-2.03096711098659
H	-5.67297366650730	-0.73100444191236	-2.38434246204122
C	0.02642103015516	-1.21344761137163	-0.84629565990578
H	-1.46981987254489	-2.22457239752483	-1.73655980770401
O	0.09668446172121	1.67724558815031	-2.64486128489131
C	-0.20936786005097	2.94680195978333	-2.59997733368845
C	0.90263374127407	4.00086676022080	-2.61826138375694
C	-1.49833683934678	3.43310779279132	-3.26959311874061
C	0.43797804445480	5.38128918494616	-2.10943117486500
H	1.18710990847589	4.10002779787123	-3.69835572945634
H	1.81611637438128	3.62663070367774	-2.11135372576776
C	-1.95957188098083	4.82601995419945	-2.79288527559059

H	-1.24652161592316	3.48760273090921	-4.36060782802519
H	-2.30089617797749	2.67084001611842	-3.19126471155107
C	-0.82157558989450	5.86628490691922	-2.85858020332127
H	1.26346422562227	6.12241455699993	-2.21294100302778
H	0.19761907642312	5.31256746538564	-1.01855147010793
H	-2.82922215308329	5.16400712949777	-3.40158974898441
H	-2.32300533058908	4.74703445115460	-1.73897641838246
H	-1.16716479957187	6.84083408954096	-2.44386031007113
H	-0.55799992945714	6.06269178258545	-3.92652612405424
C	2.98519585809562	-0.72844158213732	-3.84933236606470
C	3.64941246769946	0.58612619678659	-3.39761655553328
H	3.69861576429585	1.27533828535987	-4.28518840856569
H	1.95249838423152	-0.55000681078173	-4.22788493673307
H	3.56086338169133	-1.21216965789184	-4.67086116156362
H	2.92208847042826	-1.44765766577299	-3.00069092291490
C	5.07890056033984	0.37662600220745	-2.88211099860488
H	5.51611948571001	1.33834967820338	-2.53410329542740
H	5.09082721805964	-0.33631995082579	-2.02532410751995
H	5.73626648947883	-0.03385375281615	-3.68012462183512
O	2.90366994760636	1.21249184088398	-2.34113413392995
H	1.95664524442457	1.30919858804050	-2.62380308829554
H	-0.98989205227360	0.88327445436595	2.49188947512520
H	-2.67653628690751	2.04439252180528	1.74969029339176
H	-0.85580139662016	3.04925139726600	2.40650410326007
H	1.54404560082467	4.42441843100144	0.41401348921807

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**NPS-TS-II(H)-PH3**

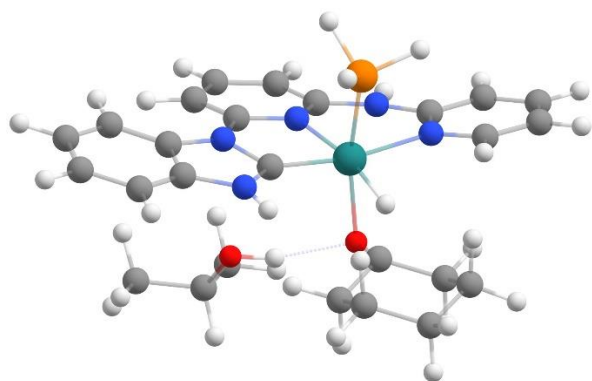
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H	-0.75866906390857	3.30652035020552	-1.35819495056596
P	-1.03439188882392	2.03701278090351	1.35817917974311
N	-1.32622988917067	-1.36549735808632	-1.33834514978646
N	2.15270320451413	3.35924457311952	0.23005374748705
N	-2.24573498475688	0.86104761820706	-1.22605202388023
N	2.33781659263744	1.16573951950814	0.17159785161633
N	0.55731765295343	-0.13326998964018	-0.51484794987192
C	3.53160682676001	1.64199207636913	0.77006730938851
C	-2.39726764630532	-0.47359369421491	-1.42622132401010
C	2.65484962277781	-1.28931316610870	-0.05017656938232
H	3.71374871493163	-1.25203905115913	0.23708040445609
C	-4.64087299478869	1.16755250853685	-1.54871758944615
H	-5.49730883835976	1.86110464203680	-1.57603280937497
C	-3.36078350710796	1.64755734016348	-1.27060014106315
H	-3.19001773434505	2.71903935545548	-1.06854093631670
C	2.05126311230260	-2.50632878037355	-0.41631218952730

H	2.63464301236127	-3.44219997251142	-0.38460099815630
C	1.87622721526505	-0.12532495192426	-0.11255291382721
C	-3.66963695740297	-1.03685404437079	-1.73139037506409
H	-3.76181635460650	-2.12469871411689	-1.90058679986756
C	4.67474257239745	1.02505988825006	1.30811455306471
H	4.80213807696689	-0.06701714305285	1.34211726256515
C	1.46878022180392	2.23605424139237	-0.15360925595392
C	3.40363878301673	3.06037143033664	0.79144178161307
C	5.55310321082897	3.26627083162012	1.83761962727088
H	6.36297598952521	3.88685863020477	2.25820640298558
C	4.40398466519733	3.89140469233816	1.31562385566061
H	4.29421613842164	4.98932121924384	1.32309941917191
C	5.68032428111715	1.85995854431802	1.83771804420465
H	6.58668646158820	1.39650960382094	2.26389653372706
C	0.71921811067902	-2.52606958467244	-0.83723382707718
H	0.23639600919184	-3.47235173537740	-1.13711413202213
C	-4.79291094156554	-0.21331911848401	-1.79881125196698
H	-5.78211531135496	-0.64338790957751	-2.03333849786705
C	-0.00934289014284	-1.30918734395369	-0.88865673778731
H	-1.60047855458191	-2.31973607406379	-1.59448255619944
O	0.03377696974940	1.76970702838843	-2.85251673707990
C	-0.32332237497486	3.04452490412079	-2.73306886053672
C	0.78524091267036	4.11579064607148	-2.86832273090537
C	-1.61409366728710	3.49635643208597	-3.45684813585433
C	0.32225550678830	5.51568204149551	-2.41560580814617

H	1.03893455377842	4.14026284308301	-3.95659507094153
H	1.70961243978643	3.78180662043703	-2.35158331346179
C	-2.08562726695394	4.89923220359924	-3.02192088865702
H	-1.35019155551343	3.50414201436844	-4.54292490137823
H	-2.41108109623097	2.73053991656388	-3.34873589358913
C	-0.96372951102748	5.95252700778903	-3.15099797851090
H	1.13508108618130	6.26033979973970	-2.57782265368173
H	0.12427680172988	5.50405785298109	-1.31218002319296
H	-2.97482747889505	5.20434886236322	-3.61963590461247
H	-2.43072979701067	4.86002353261832	-1.95732827575435
H	-1.31402862807159	6.93777240501973	-2.76672648005861
H	-0.72859885774803	6.10910880024625	-4.23176186786992
H	-0.66352456759550	3.22170227550674	2.09169710598459
H	-2.45514734444244	2.09775210993068	1.60538118042642
H	-0.70948743014657	1.08778251838217	2.40191788293645
H	1.77294977499689	4.30222545240053	0.10223104210065

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**PS-TS-II(H)-PH3**



Ru	-0.34693927946394	1.73895571696764	-0.66708591971357
H	-0.81665522925089	3.31178578485621	-1.14567344531824

P	-1.16458085026980	2.00459641217458	1.44198166731446
N	-1.24928051612344	-1.36425322582802	-1.36871432392613
N	2.06183423302606	3.39125672627631	0.43301822640935
N	-2.24222004766665	0.82929259317694	-1.21604310946366
N	2.22432644895663	1.19839674064551	0.48616254182124
N	0.53310164550322	-0.12266358984707	-0.36023065770071
C	3.41181481030964	1.68968357200228	1.07774298077512
C	-2.34152475404742	-0.50094548571622	-1.47552060986575
C	2.60605048330706	-1.24478700980094	0.25262454637147
H	3.63490937313913	-1.19600723173389	0.63078316872292
C	-4.62967334117134	1.07470364193371	-1.63826340553092
H	-5.50642674451301	1.74188171546716	-1.67605261495449
C	-3.38057619197083	1.58120843254836	-1.27897620497026
H	-3.25478877867706	2.64778617213796	-1.02502382582771
C	2.06345936718147	-2.46267624706880	-0.19327296494724
H	2.66298987853395	-3.38690124999965	-0.13282135422542
C	1.81492565894744	-0.09256917448975	0.14364597784154
C	-3.57902349211198	-1.08804936651451	-1.86802556823378
H	-3.62725142845539	-2.16995164864239	-2.08635779079093
C	4.53871468085788	1.08912817943533	1.66617227876645
H	4.65527817347270	-0.00091873293580	1.75484465180044
C	1.39166953702294	2.25946817058588	0.06370513074391
C	3.29750673000567	3.10812742995199	1.03447380218688
C	5.42748728134678	3.34458781147136	2.11175424767234
H	6.23514763583904	3.97672029530752	2.51918471295434

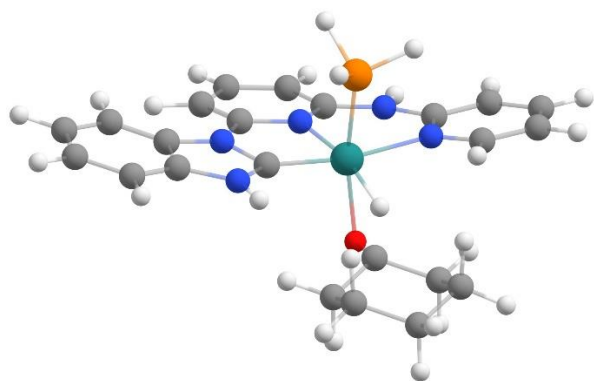
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H	4.19245978379233	5.05231318126203	1.49766257596444
C	5.54215255373704	1.93858345002145	2.17577426125809
H	6.43685303343464	1.48722166982511	2.63811383959246
C	0.77390130129328	-2.50037565748000	-0.73090709679617
H	0.33995192953388	-3.44793944074976	-1.09432107796475
C	-4.72409385270194	-0.29750836214078	-1.95617127681570
H	-5.68626647580075	-0.74686893887377	-2.25748951716247
C	0.02595175669491	-1.29759549399393	-0.80940341143159
H	-1.47930660208310	-2.31379904918091	-1.67967796968582
O	0.08637010845400	1.80419455953199	-2.74465420493182
C	-0.29446909490738	3.07103283812082	-2.58679438608562
C	0.79661422256711	4.16056846396112	-2.65066958326941
C	-1.57575920531475	3.52213405505523	-3.31804410276772
C	0.29882769077659	5.53227765671500	-2.15261868699833
H	1.06413803087884	4.23810878068694	-3.73389391823289
H	1.72233522617784	3.81541207689638	-2.14455997218730
C	-2.08321830440341	4.89869611537901	-2.84143096747533
H	-1.28881109971207	3.57725433285392	-4.39732038428760
H	-2.35983453141978	2.73843339191166	-3.25830348901066
C	-0.97805473412732	5.97592483129981	-2.90029754675246
H	1.10216857546480	6.29563284279621	-2.26740179532186
H	0.07466937385803	5.47345355756772	-1.05597612391081
H	-2.96229993094289	5.21076605845939	-3.45017238438488
H	-2.45358915664378	4.81047637736957	-1.78865774943083



H	-1.35610632860189	6.93800713502201	-2.48511098147133
H	-0.72032413506980	6.18080774507426	-3.96770382178922
C	3.03341818867444	-0.65527815351648	-3.75400263255936
C	3.67203856153934	0.68661948317952	-3.34740087959533
H	3.76690277651915	1.32122463854724	-4.27134798561925
H	2.01725116282003	-0.50376504471477	-4.18507529355298
H	3.64589810636240	-1.17897530590733	-4.52283490920843
H	2.93779823030182	-1.32909350751135	-2.87159077599924
C	5.07251836566886	0.51415785016889	-2.74543413009477
H	5.49629850462483	1.49847685094403	-2.44756607191032
H	5.03498557930230	-0.13057094172436	-1.83672310674566
H	5.76850768188010	0.04373359192209	-3.47461667920490
O	2.87347876766067	1.37177675110333	-2.37056081958695
H	1.94252783741137	1.46267390707464	-2.70645753033177
H	-0.83519224614629	1.06049740181687	2.48791403110187
H	-2.59459073225494	2.00641050886614	1.63584693039684
H	-0.86332185253793	3.20050285724785	2.18679132790891
H	1.70170920815119	4.33055499464725	0.23959090065362

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**NPS-D(H)-PH3**



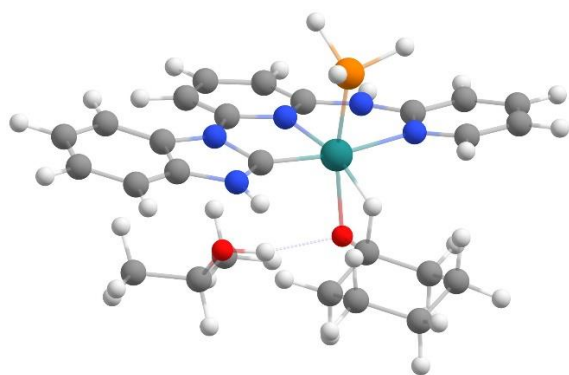
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N	-1.81656249109202	-1.51558733524670	-1.09885459129095
N	2.23191836590749	2.92223505429476	-0.21131512506077
N	-2.46371950033471	0.79874445969736	-1.28888660775839
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N	0.21385756358650	-0.41802271839639	-0.45073466067018
C	3.40386952917024	1.14364843680183	0.56704822772064
C	-2.77562452684143	-0.52246296304630	-1.30826674551831
C	2.16155257209839	-1.74481103233924	0.18086360730595
H	3.22086784773337	-1.79739927038914	0.46394996979097
C	-4.80948480397624	1.34492817998508	-1.65108956891247
H	-5.57782117493241	2.12627118478055	-1.77100728706693
C	-3.47734085746806	1.70074187171380	-1.43800875320226
H	-3.17833505174671	2.76156601374352	-1.37913487946471
C	1.40898604059656	-2.91815968570674	-0.00924095378291
H	1.87412419603904	-3.90439330844048	0.15853057773470
C	1.53011712069011	-0.51492095213759	-0.05044412915158

C	-4.11015280590529	-0.96488449123730	-1.53738581939350
H	-4.33374549750035	-2.04653723634309	-1.56039890208550
C	4.47498297222079	0.47456918493598	1.18490263929252
H	4.47097275987959	-0.60889506105979	1.37484529437293
C	1.41045809091459	1.84777083729663	-0.42862139315799
C	3.44846363636409	2.55552313053740	0.38469402637547
C	5.62771584202789	2.64391571570021	1.38464829615254
H	6.51492405548632	3.21429623888432	1.70933560058830
C	4.55200783720438	3.32409837463430	0.78136367001774
H	4.57556703434927	4.41698586910986	0.63124758497313
C	5.58443345803427	1.24706480597217	1.58625319905354
H	6.43674349971282	0.74151733611152	2.07191923017587
C	0.07875561180439	-2.83390887526630	-0.42786060583003
H	-0.51994556103095	-3.74682980268862	-0.59094054744710
C	-5.12809826296268	-0.02860577212890	-1.71569398575128
H	-6.16478420403606	-0.36407772225688	-1.89239088585925
C	-0.49716248062115	-1.55694388342863	-0.65530241102882
H	-2.20567490353801	-2.45615039691963	-1.22251936378797
O	-0.13134383342489	1.20020373681559	-3.03085321057171
C	-0.33564729637136	2.51614074600451	-3.08405092358454
C	0.89033496016134	3.41618321323532	-3.37194617479009
C	-1.57387022801782	3.00952495425702	-3.87108228619413
C	0.60320300749447	4.91192972984409	-3.12820599759454
H	1.12963130953038	3.25225001852798	-4.45125692157533
H	1.77514756557490	3.05165874570118	-2.80897827213410

C	-1.86967182902400	4.50657978152291	-3.64564928145181
H	-1.32612236900605	2.82798453764749	-4.94564625742905
H	-2.45399952590730	2.36771815724223	-3.65447108580957
C	-0.63258448374808	5.38834448836853	-3.92268132902830
H	1.49579788456054	5.52314471908715	-3.39516469504406
H	0.42190291288471	5.08453345758299	-2.03540941346286
H	-2.72467484600633	4.82580569779786	-4.28443429759483
H	-2.20268748675318	4.66381482294972	-2.58802364238818
H	-0.85767562991613	6.45344722213315	-3.68621696951980
H	-0.39632675070915	5.35786757336578	-5.01403574125562
H	-0.78057147140624	1.34834795761520	2.27453408712710
H	-0.57857674378650	3.40186697489455	1.65101871763586
H	-2.46675743279844	2.37100425492385	1.37305231244964
H	1.96697953540137	3.87680196038356	-0.47276388944314

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### PS-D(H)-PH3



Ru	-0.32503250179572	1.72845903339560	-0.60995391162835
H	-0.76761991281344	3.34273944401542	-1.25752041784704
P	-1.14636694851698	1.91393614722360	1.51518445855974
N	-1.22674986737857	-1.34754694340323	-1.35463194595012

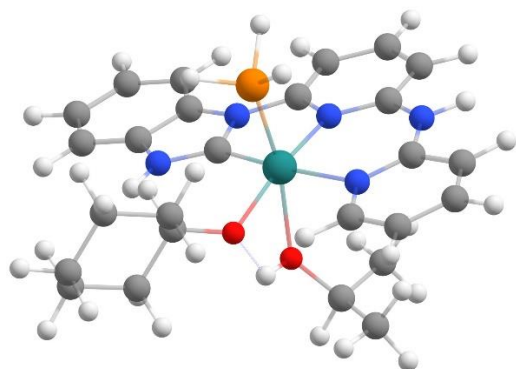
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N	-2.21539912651947	0.84077299537494	-1.18738548029236
N	2.25197393545100	1.20126570362677	0.52417352782299
N	0.55569308432856	-0.10585866599134	-0.33498349822151
C	3.44343426495861	1.69280147134660	1.10803791439945
C	-2.31649334937368	-0.48361780515469	-1.46912156988240
C	2.62699125308687	-1.23990859723329	0.27344683337043
H	3.65416704688729	-1.19476604799892	0.65648882567577
C	-4.59391760564529	1.10599114648101	-1.63839571781364
H	-5.46730588092362	1.77744410693198	-1.67732817604063
C	-3.34753951353648	1.60063407180168	-1.25340700924342
H	-3.22150890284516	2.66232702171231	-0.97783954109384
C	2.08232348173153	-2.45429600728513	-0.17819659892285
H	2.67839116635758	-3.38084805014617	-0.12136271773204
C	1.84094049002271	-0.08453494928465	0.17003624156884
C	-3.55013444534785	-1.05928626315775	-1.88837475484725
H	-3.60052609150091	-2.13716524043622	-2.12512143082481
C	4.58317311509796	1.09286125624664	1.67132497080150
H	4.71116387361176	0.00268977679515	1.74030893961976
C	1.40912541444394	2.26021540361853	0.12433536086593
C	3.31793988496427	3.11075506567510	1.08489831121319
C	5.46032195144032	3.34892880318027	2.13647412082635
H	6.26878169445949	3.98169766130863	2.54130280574773
C	4.31379042118651	3.95774369777007	1.59032849060309
H	4.20473782515647	5.05537205272730	1.56166460866172

C	5.58700805615239	1.94317140860214	2.17877899070410
H	6.49206966096369	1.49257039707047	2.62124326095980
C	0.79341390639243	-2.48335809136821	-0.71724240863124
H	0.35639762753562	-3.42709036270903	-1.08686622128489
C	-4.68971138192845	-0.26066114471835	-1.97939554077277
H	-5.64986711175651	-0.70006829161138	-2.30112097484986
C	0.04659385733264	-1.28013338157156	-0.79197684822783
H	-1.45178686767015	-2.29566670661711	-1.67352316816754
O	0.10242525776455	1.89399471493862	-2.66106395248019
C	-0.31953640367069	3.17171086447943	-2.49371386235233
C	0.76445419873650	4.27435062478953	-2.58976460399036
C	-1.57717977129789	3.58418958134483	-3.29683702144352
C	0.23688369133082	5.65136167318211	-2.13755667702265
H	1.05267609792086	4.31939210711231	-3.66832335613852
H	1.68486671949238	3.96225400830932	-2.05209241037585
C	-2.11846488718817	4.96353667371136	-2.86591436856231
H	-1.25445778564975	3.61493068027227	-4.36584581301810
H	-2.35471888142629	2.79299882844826	-3.24041372885249
C	-1.02894108486301	6.05685777479237	-2.92444550631585
H	1.03147887803410	6.42357689315615	-2.25400294318295
H	-0.00707718840422	5.61864553149254	-1.04366998741476
H	-2.98748842151886	5.24703003208388	-3.50252337897693
H	-2.51500277594796	4.89591275732774	-1.82063830747193
H	-1.43137186511597	7.02258736884470	-2.54175487910143
H	-0.74945887418788	6.23976104327200	-3.99036653858078

C	2.85515498198177	-0.58304110576878	-3.74371709248941
C	3.58031802091681	0.71919066091833	-3.35155157554440
H	3.67465645286601	1.35548323422300	-4.27461383995549
H	1.82921547647269	-0.37406014917702	-4.12420510808459
H	3.40379464203785	-1.12710338654475	-4.54614590633992
H	2.76718076327749	-1.26409351583189	-2.86600217285569
C	4.99178639091164	0.46345390428636	-2.80705617280442
H	5.47754509569125	1.41942525883507	-2.51153148496849
H	4.95404771430702	-0.19339908498370	-1.90696372416916
H	5.63398067401181	-0.03131737831551	-3.56887339916456
O	2.85852238982451	1.43759510176113	-2.34106067557683
H	1.92130051067570	1.58358924337955	-2.64532407377229
H	-0.77328250806778	0.95636282828952	2.53418450875432
H	-2.57434476329622	1.85063965915634	1.71760356872434
H	-0.89575097044719	3.09844454911613	2.29877678184400
H	1.70632902246457	4.33275267289780	0.32320588372736

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### E(H)-PH3



Ru	0.01017041678338	1.33822882230482	-1.08724894150868
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H	0.19192303071863	4.45754645755311	-1.07729181041802
P	-1.17952733163620	2.08321248916723	0.66374538121399
N	-1.27242700963401	-1.67075670309525	-0.67108955926283
N	2.43681323483200	3.11287232129557	-0.28335412436015
N	-1.74462222849641	0.36363528206327	-1.87905139678503
N	2.40556563524902	1.04258249027725	0.46110814999060
N	0.62958409474918	-0.33640630496906	-0.07710846291918
C	3.62245505785164	1.60383169568009	0.92506352335122
C	-2.07329132943324	-0.90584307896127	-1.52886854818621
C	2.39579190046568	-1.29729285528007	1.31016093759839
H	3.35190986687088	-1.18959211601655	1.83786736664325
C	-3.76354819511843	0.51740146902415	-3.21785560410389
H	-4.40188494699530	1.12282272977152	-3.88248643268776
C	-2.57958014129874	1.05429058484063	-2.70856647286230
H	-2.21597825506084	2.07239914337918	-2.94912817554814
C	1.69622093448719	-2.51876203301209	1.33989920166887
H	2.11089976952459	-3.37842683329070	1.89295515971339
C	1.83556171782269	-0.23327385634542	0.59204474986727
C	-3.26009799013460	-1.52123280157138	-2.01584936749499
H	-3.50502958968074	-2.55776828578803	-1.72207687093188
C	4.70287851516474	1.12558872547911	1.68812063555096
H	4.74833530208700	0.10046832350115	2.08388818322107
C	1.67211762121110	1.98465368499212	-0.29672968984941
C	3.62869206937775	2.94271632547082	0.43635665165141
C	5.76378571626540	3.33891399344489	1.45589972012875

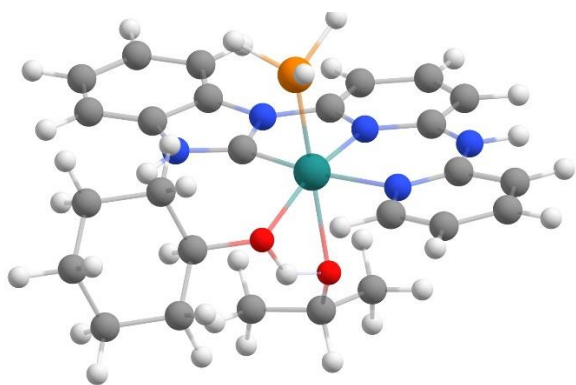


H	6.61680100732967	4.00348260248819	1.67641703654505
C	4.68758918616537	3.82618752661925	0.69005969127435
H	4.67835110152953	4.85938303100974	0.30297703560954
C	5.76814154854427	2.01325321445023	1.94320561092261
H	6.62583078410730	1.65665966735469	2.53918429601149
C	0.47726182337487	-2.63835055269070	0.66793433126794
H	-0.08276474175468	-3.58965244230888	0.68100084758265
C	-4.10860278796081	-0.80366548949804	-2.86187148644221
H	-5.03349062104686	-1.27208536878560	-3.24157026448373
C	-0.04076352923596	-1.51941313595332	-0.03412229299420
H	-1.66822049523731	-2.60354146200643	-0.51347512219822
O	-0.37407153193468	2.91159559169420	-2.38792223353463
C	-0.32091782086121	4.28830240580851	-2.07368389930576
C	0.49311070784254	5.06260259543859	-3.13889268458025
C	-1.73725897397491	4.89862496454983	-1.93602638264271
C	0.54012286001492	6.57989765811329	-2.84948108631095
H	0.02155350417661	4.87626733323550	-4.13508697807370
H	1.52512170712426	4.63809952478393	-3.20288750848999
C	-1.69484883290265	6.41165034201115	-1.63112105649176
H	-2.28272618444819	4.72244359821380	-2.89611234178262
H	-2.30932719620406	4.35207823339045	-1.14792676803373
C	-0.87549790807573	7.17475621537543	-2.69345560079183
H	1.09981233230173	7.10592796125512	-3.65697749529635
H	1.11952212293664	6.76122421483063	-1.90893726582240
H	-2.72972925415767	6.82013139411894	-1.56669786724337

H	-1.23856718474243	6.57592389186754	-0.62266775365672
H	-0.81338500410968	8.25646546926693	-2.43289731086361
H	-1.40580681271367	7.12278806609835	-3.67595701264890
C	0.01093836203098	-0.11695193519261	-4.87683189491230
C	1.27608734007944	-0.00602559538513	-4.01475751633841
H	2.12355071484130	0.32230722296887	-4.66872388660835
H	-0.29361026461303	0.87216320680600	-5.28693931631920
H	0.20230257497963	-0.78739408227004	-5.74452397227420
H	-0.84573932661261	-0.53833165355221	-4.30744103561325
C	1.66951832106711	-1.32424867433345	-3.34388984928545
H	2.55683772655927	-1.19223255009681	-2.68687692259687
H	0.83317599341966	-1.73661157321257	-2.73616758573882
H	1.92818541206930	-2.08291816789021	-4.11483866857202
O	1.16648093039072	1.01916882751882	-2.98146800176285
H	0.74926794755806	1.88349652264302	-3.30751157633278
H	-0.96443757583299	1.51204802641219	1.97427543483024
H	-2.61740642545485	1.97055440225919	0.62818209504869
H	-1.08726286740316	3.47174650006216	1.04584728524830
H	2.14605346486148	3.97078280261614	-0.76614722997929

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**TS-III(H)-PH3**



Ru	-0.77982571243300	-0.52778043129417	0.18886956649333
H	0.51769740813038	2.31479505013940	-1.10304176723228
P	-1.85487000196561	0.18059049435936	2.07459103230589
N	-2.08317528643099	-3.55109633991864	0.37052204702780
N	1.66563974337091	1.16970261684330	1.12298214788575
N	-2.67125513989642	-1.37529058665478	-0.47640217287450
N	1.62597586154379	-0.95885481243270	1.67668874148577
N	-0.17234228997482	-2.26615662812380	1.05422177411579
C	2.79405208318438	-0.42433378395522	2.27571026041401
C	-2.96425723584350	-2.68426356189842	-0.28336107997943
C	1.66501042353791	-3.38168953526628	2.22131166200730
H	2.66028419628848	-3.33509945291574	2.68126227618979
C	-4.81194021440485	-1.06970367240207	-1.58393769128176
H	-5.50938045600133	-0.38685958359135	-2.09654395291227
C	-3.58431015157352	-0.59280087049582	-1.11944472193785
H	-3.26895620410729	0.45483844175004	-1.26869142333909
C	0.97183560718572	-4.60327719141304	2.13001505361376
H	1.41895743744922	-5.52450665246750	2.54016107238540
C	1.06144305722327	-2.23910998936720	1.68236812643794

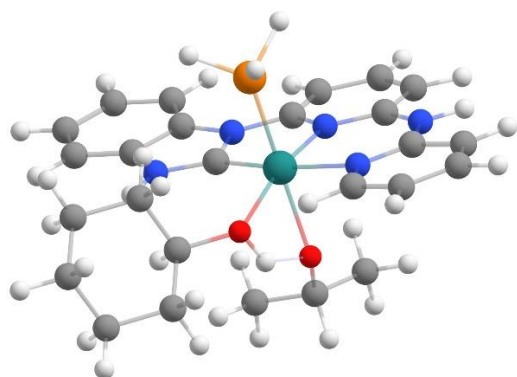
C	-4.19201545834544	-3.24488695928579	-0.73343649355426
H	-4.40395119031158	-4.31604326345623	-0.56488323746614
C	3.80956766706113	-0.94753118694547	3.09568388251912
H	3.82610802236242	-1.99470295406923	3.43155033486165
C	0.91924888104200	0.03558573869190	0.95335154671372
C	2.81205280644433	0.94981326136236	1.90067843020083
C	4.85349924162401	1.28544977671380	3.11591619524785
H	5.67572562026176	1.93923535282774	3.45416095497164
C	3.83327607571168	1.82082963739882	2.30587327911279
H	3.83580051703023	2.88242981060962	2.00515345362204
C	4.83631173372459	-0.07169229493741	3.50521024187848
H	5.64379874535088	-0.46270355251162	4.14787202079818
C	-0.27893239266911	-4.64462769726866	1.51258327334242
H	-0.83617709363258	-5.59411984001789	1.43196007420740
C	-5.12031554892017	-2.43142393970552	-1.38479216634150
H	-6.07685531201396	-2.85581488709583	-1.73646249394862
C	-0.83476164957068	-3.45357364735116	0.97485509073663
H	-2.44875559378962	-4.50828871085618	0.40793933040093
O	-1.20336190531688	1.11076089407437	-1.16613689287885
C	-0.60327872687054	2.41428636733693	-1.18806006383656
C	-0.89199251887871	3.09953990825919	-2.54086438935582
C	-1.11538922591233	3.27178350218249	-0.01678074443801
C	-0.29391806722878	4.52325749842730	-2.58899410260007
H	-1.99929332766165	3.14391181087831	-2.68151906024337
H	-0.49022655794380	2.47433302331752	-3.37239922155444

C	-0.52320990999212	4.69908507383206	-0.05575752786590
H	-2.22977028516481	3.32046279214982	-0.07953055646292
H	-0.87802218037894	2.77512718995442	0.95439437024481
C	-0.79136458383573	5.38709098457889	-1.41105439685342
H	-0.54459056002030	5.00454445818220	-3.56156529304113
H	0.82209111843028	4.45873494821228	-2.55822541966597
H	-0.93626419873332	5.30393561574201	0.78360168474575
H	0.58181073530605	4.65036741105923	0.11903443424084
H	-0.31063572578798	6.39176016569553	-1.43481324034014
H	-1.88910773608825	5.56558295469637	-1.52005324706705
C	1.30948519014033	-2.79857725357731	-2.07475403188334
C	0.98457176414998	-1.34218572046220	-2.44825997250962
H	0.77744317906710	-1.31784400790585	-3.55126481323960
H	0.43022221755425	-3.45564036656966	-2.25462748079826
H	2.15533598132785	-3.18589298634361	-2.68597736644899
H	1.60429094767216	-2.89083909613391	-1.00468684708478
C	2.17219961648214	-0.39709624793450	-2.18256469401536
H	1.91429882196743	0.65911942730960	-2.42354265689723
H	2.50974838822489	-0.44297057267991	-1.12278711792895
H	3.04367306349238	-0.67624320396448	-2.81701106858280
O	-0.23873217337316	-0.92121508289651	-1.83302722684798
H	-0.67418102629333	0.33008798382778	-1.84645989566720
H	-2.18395431575251	-0.75639484599953	3.12888089239226
H	-3.16791050860640	0.75565897022829	1.92076314415358
H	-1.29172963863398	1.19944572914320	2.92654943821080

H 1.41758395201608 2.05897452038106 0.67699869601119

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**F(H)-PH3**



Ru	-0.31962	1.24173	-1.16538
H	0.95588	4.13186	-2.46226
P	-1.40472	1.94398	0.73085
N	-1.61179	-1.78439	-0.99239
N	2.12230	2.94846	-0.24180
N	-2.21554	0.38951	-1.82991
N	2.07750	0.82619	0.33559
N	0.28724	-0.48705	-0.29536
C	3.24491	1.36506	0.93145
C	-2.49554	-0.92373	-1.64947

C	2.11658	-1.59238	0.89510
H	3.10720	-1.54014	1.36431
C	-4.35370	0.67963	-2.94776
H	-5.05626	1.35933	-3.45752
C	-3.13475	1.16600	-2.47036
H	-2.83774	2.21997	-2.60737
C	1.42731	-2.81604	0.80473
H	1.87264	-3.73394	1.22411
C	1.51581	-0.45404	0.34427
C	-3.71258	-1.49571	-2.11484
H	-3.91199	-2.57106	-1.95812
C	4.25767	0.84886	1.75906
H	4.27155	-0.19476	2.10592
C	1.37370	1.81352	-0.40140
C	3.26621	2.73492	0.54157
C	5.30580	3.07978	1.75775
H	6.12856	3.73572	2.09047
C	4.28802	3.60826	0.93984
H	4.29350	4.66655	0.62765
C	5.28546	1.72704	2.16133
H	6.09107	1.34124	2.80946
C	0.18237	-2.86313	0.17633
H	-0.37207	-3.81420	0.09535
C	-4.64614	-0.68796	-2.76531
H	-5.59444	-1.12076	-3.12880

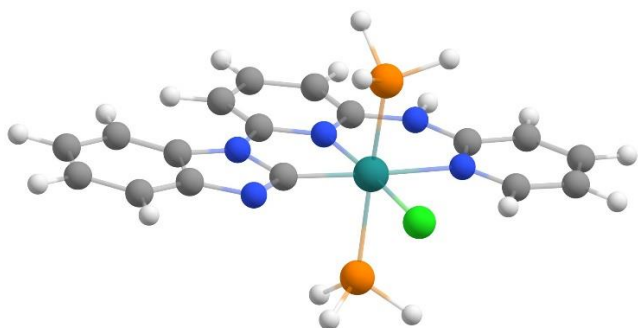
C	-0.37134	-1.67709	-0.37415
H	-1.96859	-2.74505	-0.96066
O	-0.75792	2.91628	-2.51409
C	-0.16358	4.23229	-2.53867
C	-0.47256	4.92178	-3.88296
C	-0.67992	5.06437	-1.35388
C	0.10210	6.35585	-3.92008
H	-1.58125	4.95032	-4.01584
H	-0.06506	4.31175	-4.72293
C	-0.11129	6.50155	-1.38375
H	-1.79531	5.09583	-1.40735
H	-0.42575	4.56124	-0.39075
C	-0.40155	7.19880	-2.72971
H	-0.16416	6.84166	-4.88606
H	1.21910	6.30984	-3.89846
H	-0.52845	7.08970	-0.53483
H	0.99537	6.46908	-1.21738
H	0.06241	8.21133	-2.74641
H	-1.50282	7.36029	-2.82905
C	1.61240	-1.18034	-3.41091
C	1.41466	0.31317	-3.73679
H	1.24448	0.38642	-4.84498
H	0.68241	-1.75348	-3.62098
H	2.42867	-1.61812	-4.02897
H	1.88907	-1.33673	-2.34342



C	2.67894	1.13859	-3.41979
H	2.51810	2.22095	-3.62650
H	2.99283	1.02683	-2.35728
H	3.53516	0.80533	-4.04922
O	0.22218	0.82756	-3.15075
H	-0.27431	2.23804	-3.19198
H	-1.71614	1.00538	1.78935
H	-2.72739	2.50063	0.58738
H	-0.85575	2.97207	1.58195
H	1.87770	3.83503	-0.69366

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**1'-dft-PH3**



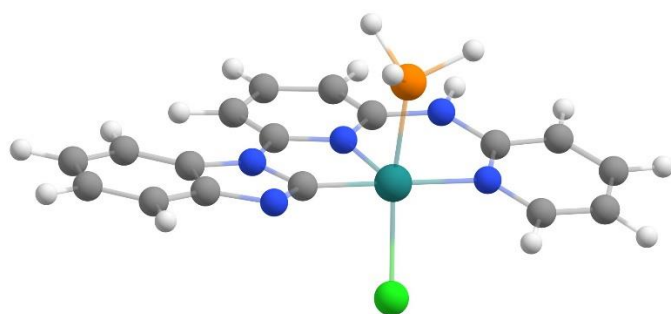
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Cl	-1.48352752528255	4.18630605257842	-0.16502164891201
P	-1.06708147746372	1.65884468447964	1.71891763972036
P	0.01777123699796	2.79388719060672	-2.60397939619916
N	0.43886922378435	0.16365400436645	-0.74378892015220
N	2.25247318428565	1.35970985546648	0.03451435556549
N	-2.43304685166825	1.17494185760933	-1.20178654613469
N	1.94627888995497	3.56503240388160	0.53415931608535

N	-1.48802964915736	-1.01469760661376	-1.55454349527645
C	-0.13708873920962	-0.97924612976972	-1.19605826948190
C	-4.92416483045750	0.18772872844637	-2.10645864432294
C	0.59217872637228	-2.18849674266986	-1.32987575310408
C	5.81580689839675	2.05416455742752	1.13038201311534
C	4.32886557407637	4.00543607610609	1.26056773524882
C	5.59729492141217	3.41762971677712	1.43196606312285
C	3.27376066924132	3.20588941539944	0.78014535505338
C	1.31487292129129	2.49467068743924	0.09211638286846
C	4.77309854307028	1.23297271022724	0.64747740742453
C	-3.80408093814129	-0.64412885641997	-2.04785261875973
C	1.78843922910571	0.14040890865313	-0.40536852377735
C	1.94904875031120	-2.20388976259900	-0.98556976215040
C	-3.53712261716371	1.97465324940525	-1.26457480953926
C	-4.78827611618856	1.53203926133799	-1.70415546024929
C	2.56318843180579	-1.03253074621008	-0.51758576463958
C	-2.56166865875818	-0.12190697957602	-1.58739641508908
C	3.50699636019965	1.81908551928652	0.47640964176333
H	-0.65063674274364	0.49499957122040	2.47547724387577
H	-1.04079674057892	3.06892443126578	-3.54580385281218
H	0.67372646825717	4.07100712672154	-2.64193591339480
H	0.89181705221734	2.09505628137945	-3.52457828219136
H	-0.60544741169218	2.66305425841154	2.63604042233952
H	-2.45598475934091	1.63315048552024	2.10947096884796
H	-1.76281931682222	-1.94789844116616	-1.87562839299072

H	-5.89143631714302	-0.20925373501544	-2.46210631377634
H	0.08856799854021	-3.09854209941080	-1.70076568628905
H	6.81977154719703	1.61599610093923	1.27308321814429
H	4.14442831878228	5.06878988451891	1.49231980724829
H	6.43661837206805	4.03008994013761	1.80807301339667
H	4.98058097614680	0.17409874851417	0.42289178092717
H	-3.87293601862446	-1.70370291127840	-2.35526911712791
H	2.53443697710122	-3.13460037576245	-1.08217839434416
H	-3.35441732291883	3.01798000184887	-0.93482931217403
H	-5.63838822974241	2.23440184086786	-1.72915085224715
H	3.62628250369936	-1.02441235824526	-0.24346555073787

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### 1a'-dft-PH3



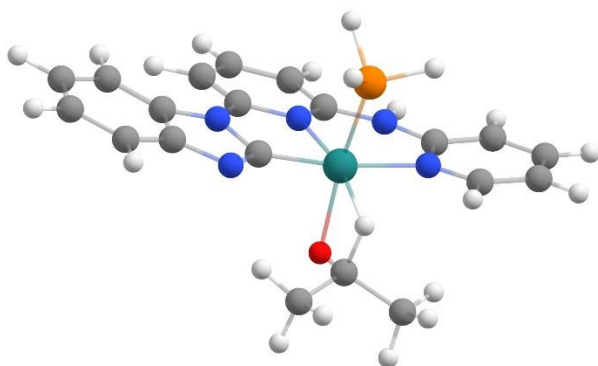
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Cl	-0.21530888261026	3.02195322565589	-2.53598388381690
P	-1.01032553215629	1.40705757593344	1.66210634461074
N	0.43189954279410	0.16516908149844	-0.66645322852955
N	2.27527358835794	1.38356566891131	0.00077192261364
N	-2.36989315973425	1.19279261175657	-1.24254413886232
N	1.89316699539935	3.53255712898423	0.66164528607386
N	-1.56648780722385	-1.06097920704067	-1.21005919618827

C	-0.17732795202001	-0.99329888898267	-1.04897839789994
C	-4.89334656513368	0.27837333528592	-2.09089133753807
C	0.56320406087737	-2.18306702977417	-1.25199361666170
C	5.82470383978333	2.12070131431197	1.10111808501566
C	4.27331942415971	4.00537290843743	1.39301431762589
C	5.56296852669706	3.44941336965063	1.50583309566419
C	3.23923792561833	3.20775352641770	0.86727924328456
C	1.30672803699408	2.47467405252388	0.14128614051672
C	4.80422780069850	1.30199750487943	0.56936609910585
C	-3.85356148911126	-0.62484166522414	-1.84980540924604
C	1.81058354202563	0.16570704820926	-0.43142600885104
C	1.94746207956206	-2.17463160528681	-1.03684419104208
C	-3.37878799915565	2.06422248999067	-1.51899149013595
C	-4.65126527074003	1.65943302716257	-1.93278275924512
C	2.58424601837396	-0.99589255679922	-0.62171539364294
C	-2.58678342668950	-0.13170471443920	-1.43310388151392
C	3.51810721092082	1.85601349511151	0.45981038193057
H	-0.38855700769490	0.27788999877959	2.33046761257969
H	-0.73615268840533	2.38553522462623	2.68803683107006
H	-2.37281728039796	1.10247145252932	2.05109624430555
H	-1.87445701789293	-2.02150635115772	-1.39075306413323
H	-5.88210913689073	-0.09106311221729	-2.41471745615507
H	0.04431547005402	-3.09923512647285	-1.58360680252312
H	6.84571210937691	1.71033551678916	1.19734373085943
H	4.05979092193395	5.04308881420954	1.70258749717156

H	6.38644019312441	4.06210313168909	1.91504826206561
H	5.04096043956608	0.27170842137257	0.25654772477902
H	-4.00500821367938	-1.71030484198770	-1.99180050352201
H	2.53705280614956	-3.09324589641344	-1.19909631496172
H	-3.12539340328267	3.13277622079206	-1.39594717838563
H	-5.43271657841968	2.41150378402443	-2.13136079798212
H	3.66894078863736	-0.96696725318046	-0.45078565891750

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### A'-PH3



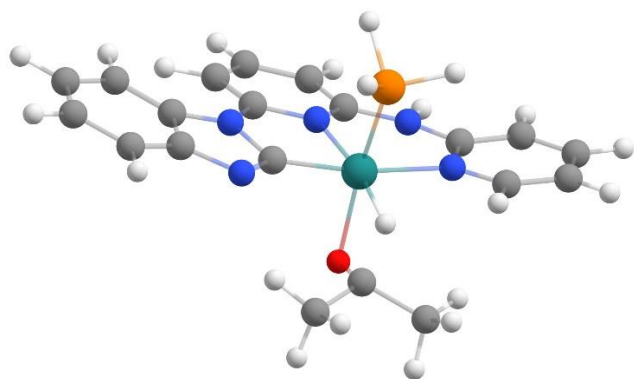
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P	-0.88880778728351	1.79568308792937	1.06533526006369
N	-1.76909070210828	-1.21315489390226	-1.86579841652480
N	2.60097075760710	2.39536106134736	0.32928034913942
N	-2.05252568290764	1.17344727541798	-1.76167530492232
N	2.23921666798734	0.15230758963205	0.18155973109495
N	0.27610536951694	-0.56106597631674	-0.78950377303544
C	3.45852776595959	0.28751852388986	0.86994249903375
C	-2.55379745676268	-0.06803850669466	-2.00458858968968
C	1.89898369187883	-2.27659490084689	-0.15460005450440
H	2.87900089332894	-2.53921029112808	0.26601204912206

C	-4.24825332090294	2.12241171820682	-2.24856066602006
H	-4.87528129081839	3.02647978533853	-2.32276651738658
C	-2.90723792910663	2.23255419373541	-1.87349021600026
H	-2.46392766907213	3.21633871269767	-1.63959113404725
C	1.03998410440999	-3.26525782893709	-0.65789106271557
H	1.33447995322029	-4.32807052773831	-0.61336835320645
C	1.49538814661713	-0.92885673391516	-0.23485338828715
C	-3.90608041897347	-0.26232958841736	-2.40630583849538
H	-4.27686880843072	-1.28514785561176	-2.60137552283399
C	4.37380439567346	-0.61149349638837	1.44290840793476
H	4.23152787406487	-1.70438223755098	1.42335313158126
C	1.74703767608967	1.49386261759539	-0.13134014617743
C	3.65560536550197	1.71061700401254	0.93826468484715
C	5.72343748163625	1.32678707799502	2.14091110167385
H	6.62680708413346	1.71571168580413	2.64464048642009
C	4.79988437788364	2.22808299294915	1.57598383116074
H	4.95149298714268	3.32042819139660	1.62566056757937
C	5.51253447204838	-0.06950730256625	2.07900128781734
H	6.24815890256832	-0.75517578687748	2.53608216126224
C	-0.18580556386940	-2.90109460939718	-1.22791775323333
H	-0.87308051404864	-3.66362103234049	-1.63455622346166
C	-4.75748931740533	0.83759174420278	-2.53508194478327
H	-5.80764019118110	0.69492755160986	-2.84414244606705
C	-0.53790142215326	-1.52843763951488	-1.28354585978973
H	-2.26252364676090	-2.05557780895597	-2.17584681437154

C	-0.45503509974255	3.55438190651720	-3.74627266768350
C	0.56541444939320	2.91712530983374	-2.76658388563793
H	0.01116648807821	3.15362075530496	-1.60457391164489
H	-1.35643149336753	2.91955192678329	-3.86691964937775
H	-0.76118963437000	4.58065082220919	-3.43969919505339
H	0.03412467350615	3.63129941686453	-4.74445183971142
C	1.85431377859072	3.76401379391755	-2.65374209072326
H	2.49849863520912	3.42408669824548	-1.81755082090639
H	2.41348781460947	3.66676215539844	-3.61239559966400
H	1.61819175045461	4.84138284283436	-2.49771751057028
O	0.73652906067411	1.58806580217795	-2.94156774928778
H	-2.27281128647246	2.20142567822887	1.23084398005555
H	-0.30854218296855	2.80605668868628	1.91779642513287
H	-0.92125723263425	0.74812101621228	2.07228564795316

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### TS-I'-PH3



Ru	-0.03033913648943	1.48459487393283	-1.02804513193211
P	-0.85772648906258	1.89110857791717	1.03275376736119
N	-1.75396173255164	-1.20380063339808	-1.89257779707044
N	2.61910257709409	2.40471028259383	0.32018787712082

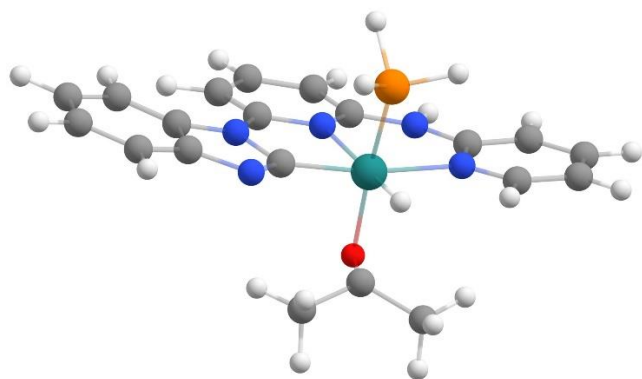
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N	2.23517425147867	0.16445643746003	0.17442893106760
N	0.28021991100893	-0.56098927097227	-0.80233911969525
C	3.44826810814357	0.29008671684219	0.87430327118326
C	-2.54576102595087	-0.05968458164158	-2.00851890306377
C	1.91604436497695	-2.26509037482960	-0.18743385315835
H	2.89973683792807	-2.52614238265620	0.22532251558829
C	-4.26444671226666	2.11625500676838	-2.21667629877083
H	-4.90060785420931	3.01505227770281	-2.27657781344379
C	-2.92012042765921	2.23695030719370	-1.85799472052487
H	-2.48083483177858	3.22224674635838	-1.62565801563928
C	1.06435608534621	-3.25389916422173	-0.70296911924706
H	1.36888040144435	-4.31453606851832	-0.67107700457687
C	1.49847724794461	-0.91931518919955	-0.25196578428692
C	-3.90159870846413	-0.26261889211155	-2.39509345607480
H	-4.26531913940559	-1.28767487760553	-2.59192874965156
C	4.34687098570245	-0.61557830938711	1.46413751589339
H	4.19158417881951	-1.70676236279427	1.45196274188267
C	1.75617573920386	1.51447405698512	-0.14729191509313
C	3.65974459152175	1.71085961685894	0.94093510319003
C	5.70924880557998	1.31130559585025	2.16947506375599
H	6.61058736178415	1.69287507725417	2.68241936006216
C	4.80171079039348	2.21952989438013	1.59003011089004
H	4.96307494683024	3.31056801145889	1.63765487346542
C	5.48345440595799	-0.08281248497565	2.11157094563123



H	6.20520949637421	-0.77434518391993	2.58183281650527
C	-0.16499129579443	-2.89624637025888	-1.27029978396433
H	-0.84472661583493	-3.66080211290475	-1.68567406379558
C	-4.76540697511609	0.82899647724446	-2.50605189318503
H	-5.81789765103444	0.67796188510366	-2.80306654781182
C	-0.52391623766287	-1.52424474733826	-1.30969518623265
H	-2.24656328153220	-2.04282218187510	-2.21297379499693
C	-0.47707898397304	3.49606568963609	-3.71290995138646
C	0.59541159920059	2.83163998440930	-2.82000895305271
H	-0.05472790314371	3.14526220229368	-1.39581819686325
H	-1.35159807090436	2.83217401493935	-3.86440564420562
H	-0.81465527916530	4.48252830303103	-3.32366931729539
H	-0.01460892148611	3.67179725305989	-4.71282864939180
C	1.84898668862660	3.70853727845621	-2.65148785371252
H	2.51215384984035	3.34683599892966	-1.84070352470848
H	2.40559428824965	3.68699556684324	-3.61803921039930
H	1.57675933017428	4.76580300507187	-2.43509236632536
O	0.75893338968509	1.53274295788075	-2.99443964374656
H	-2.22949622747313	2.33759034441424	1.18769597724980
H	-0.24202627153395	2.90342501029427	1.85423112346398
H	-0.91595152807767	0.86568716738265	2.06058395330100

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**B'-PH3**



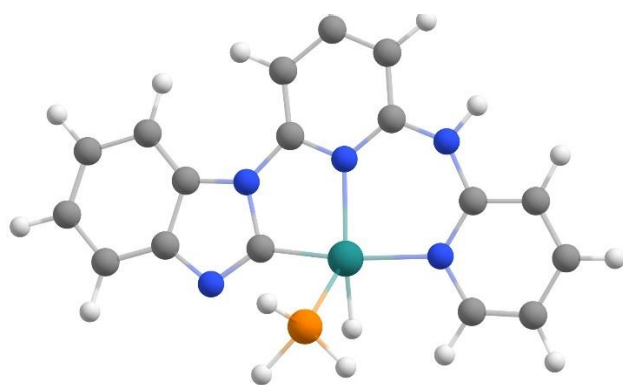
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N	-1.79928146198285	-1.16812558082032	-1.85526006960267
N	2.44649275588781	2.49414916407901	0.51690601420432
N	-2.18300355315262	1.21005821153533	-1.61649401758968
N	2.20440204766376	0.25645682066728	0.13269287358333
N	0.24585420439333	-0.51610908462858	-0.80413062860850
C	3.41925777571766	0.38936451794527	0.82927978796689
C	-2.61447536177610	-0.03815609705364	-1.94835027202830
C	1.97183411915540	-2.16710508356980	-0.34373854441243
H	2.98168233408882	-2.41103595817676	0.01198367086255
C	-4.40204592617611	2.08936877538125	-2.12482750083439
H	-5.06689118321480	2.96786685114777	-2.17245321745032
C	-3.08053422036262	2.23597293091922	-1.69932919260299
H	-2.67706845677815	3.22103511777949	-1.40780965990881
C	1.13153930981361	-3.16476545368465	-0.86255676783005
H	1.47774932357500	-4.21294084226183	-0.88933997812733
C	1.49858364615345	-0.83665923820636	-0.32667877438728
C	-3.94651157298595	-0.26409505797261	-2.40642991002441

H	-4.26429772896707	-1.28778610850881	-2.67672053759530
C	4.39090035209274	-0.50918992648541	1.30333439466386
H	4.31451365868249	-1.60037849244518	1.16867944547380
C	1.63818841204346	1.60715536250503	-0.04523431331543
C	3.53829207663557	1.80663523608000	1.04751269101298
C	5.63427241001256	1.41839455883754	2.20052727818957
H	6.51808420732589	1.80338943229938	2.74077882751103
C	4.65644249875003	2.31886716186500	1.73502286554077
H	4.74509118160664	3.40702824152615	1.89866861847860
C	5.50191665879958	0.02690078454337	1.99131090165218
H	6.27874687027121	-0.66038831750563	2.37145616572639
C	-0.13620129663615	-2.83745711945687	-1.36009625386083
H	-0.80164269546402	-3.61227043892166	-1.77965487448976
C	-4.84195915203227	0.80098603289885	-2.49976198033629
H	-5.87353979639463	0.62999410269347	-2.85429225305535
C	-0.54126276852107	-1.47696043777132	-1.32664391115512
H	-2.27268295753441	-2.00550998290717	-2.20734084811071
C	-0.34590733813765	3.51931185615641	-3.50647086395433
C	0.63196313810353	2.56305587786399	-2.80933992972985
H	-0.40113758658758	3.19244087539862	-0.77566405347678
H	-1.37877487817107	3.11784208088065	-3.52545189555771
H	-0.34527563028374	4.52904291599785	-3.04163355627300
H	-0.01478731781798	3.63980289711351	-4.56782953047162
C	2.05330756459358	3.11357328533481	-2.67735495125851
H	2.76128338303159	2.31787780607756	-2.37178546152805

H	2.37387760801662	3.50607315838899	-3.67430657355109
H	2.11985824570701	3.94524838692497	-1.94431152090456
O	0.44993237681498	1.28359564049655	-2.93672893808249
H	-2.23160420655806	2.49151744925450	1.40476117566502
H	-0.17218285316150	2.86196290995655	2.03337290258635
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### 2a'-dft-PH3



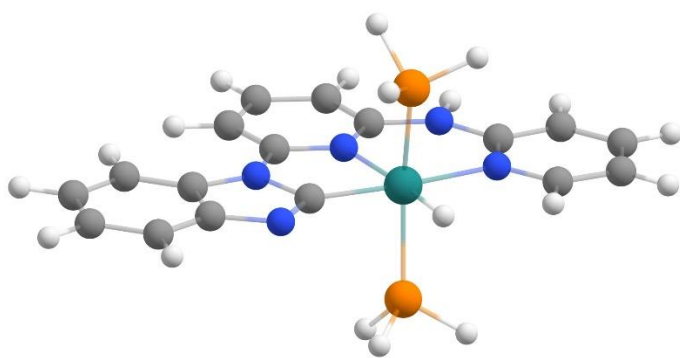
Ru	-0.58127154078616	1.74150973165960	-0.18142155257048
H	-0.96910463219134	3.27951918042380	-0.47111714080246
P	-1.34246217427088	2.63983528545586	1.65194647689886
N	0.48658172813690	-0.00775773199635	-0.73193662733743
N	2.25884602118855	1.22784624427241	0.07907733947239
N	-2.37485896137459	0.98637557507423	-1.02569261659033
N	1.84559967844691	3.28155734210817	0.99485596666746
N	-1.42493654213967	-1.18146282183910	-1.54428839850608
C	-0.05609605887036	-1.11198435375886	-1.29581593416262
C	-4.86540483155171	0.03875460036897	-2.02961066116188
C	0.73357495693461	-2.24042628764402	-1.64299352876728
C	5.84521055081082	2.02272790444513	1.02604649449388

C	4.24026679859042	3.78279563067607	1.62343188134154
C	5.55747932934376	3.28485526909561	1.59182665360723
C	3.20549685150514	2.99562550165268	1.07964723259244
C	1.24115550032928	2.26186337443333	0.39584183391476
C	4.82390726405905	1.21602549506606	0.47473022986842
C	-3.73647981553124	-0.78045340273682	-2.01933093339078
C	1.85413295105934	0.05022282421311	-0.49873294206762
C	2.11041166196390	-2.18188630850711	-1.39669743604564
C	-3.49738152953389	1.78033440968085	-1.07069648549905
C	-4.73784756710190	1.36025771994634	-1.54273377879166
C	2.69166001094999	-1.03774944677530	-0.82460910274453
C	-2.50032270876972	-0.28669964668683	-1.51448688136640
C	3.50905300560796	1.70889690308979	0.51082556357254
H	-1.16676070101168	1.93438381966962	2.90913758447555
H	-0.86350625281964	3.92332705975946	2.10378246014268
H	-2.76714973599415	2.89133663575170	1.81262675601409
H	-1.69602678288565	-2.08976105996257	-1.93345988277858
H	-5.82699008303908	-0.33962916746735	-2.41735692622060
H	0.27213656952516	-3.13205689881378	-2.10213153038360
H	6.88621055273281	1.65354897536062	1.01000178373122
H	4.00300698588869	4.76902671459592	2.05887474546677
H	6.38042658466089	3.89006649236617	2.01326690792018
H	5.08821721760824	0.23959206247748	0.03727367278218
H	-3.79258792261827	-1.81662962436035	-2.40078473626958
H	2.74976942513454	-3.04303615748954	-1.65994875206608

H	-3.34677019216289	2.80671615201544	-0.69701382562656
H	-5.59046022499867	2.05992012553037	-1.53626760941636
H	3.77150461317446	-0.99638812115087	-0.63124630039656

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### 2'-dft-PH3



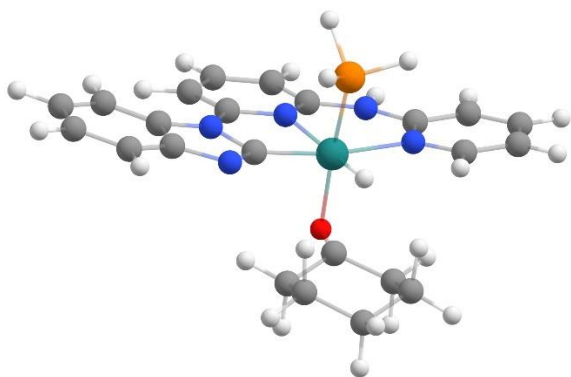
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P	-1.12341378993589	1.79029276551706	1.68712035546259
P	-0.04754772214823	2.90817054597740	-2.54480667798395
N	0.46130223918429	0.09543606189504	-0.75617671227302
N	2.24738146981385	1.32754400823804	0.02187798945942
N	-2.40585515602139	1.13704362146932	-1.21516890674945
N	1.93729992724204	3.53546002225016	0.52476096057705
N	-1.46729645101789	-1.06850380698060	-1.55528653151822
C	-0.11055089393651	-1.04342613826851	-1.20056295554057
C	-4.89990435673959	0.14524227645348	-2.12521865386487
C	0.61955947676262	-2.25234564921693	-1.32904247119228

C	5.81236984237869	2.03571712443454	1.10749839070366
C	4.32009286775365	3.98102165431429	1.24480507504366
C	5.59124641664152	3.39803172660449	1.41166199996839
C	3.26491141230029	3.17917416712752	0.76704759000952
C	1.30056075778896	2.46413048271335	0.08088459135352
C	4.76976255351020	1.21258214054251	0.62746985598516
C	-3.77896755571916	-0.68530830125086	-2.05562478822489
C	1.79967655019018	0.09610571781325	-0.41343453863521
C	1.97738502662509	-2.25019987787775	-0.97920540515678
C	-3.51451354095375	1.93277922735765	-1.29080845449913
C	-4.76582194113970	1.49277587844931	-1.73194349167735
C	2.58589650907784	-1.07355949073606	-0.51587259381227
C	-2.53468892994066	-0.16672420257384	-1.59450360971080
C	3.49983320873429	1.79281308153228	0.46113585965597
H	-0.73161740370047	0.70033378167127	2.56599396247777
H	-1.11363364848907	3.24703469873139	-3.46342779501573
H	0.59451013939721	4.19542476725556	-2.52188412740496
H	0.82226174190223	2.31645830673383	-3.54850471264222
H	-0.68921922002184	2.85262926137452	2.55462325048737
H	-2.51843950951834	1.79110006953825	2.07316417742770
H	-1.75205358622544	-2.00023146601949	-1.87208123548827
H	-5.86551586379933	-0.25398498789200	-2.48197440301878
H	0.12674479788710	-3.17020785404710	-1.69542654351736
H	6.81810532307468	1.59990308908537	1.24541366596398
H	4.13383592009782	5.04393691052706	1.47799317941613

H	6.42996161374240	4.01294499267972	1.78539780493611
H	4.98103674358374	0.15526880265689	0.39989168230014
H	-3.84903623252133	-1.74666907112070	-2.35673271488847
H	2.57047418884905	-3.17712531200355	-1.06820764045695
H	-3.34398596743056	2.97479144839429	-0.97004278913058
H	-5.61488956107831	2.19574485260880	-1.76504671942227
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### NPS-C'-PH3



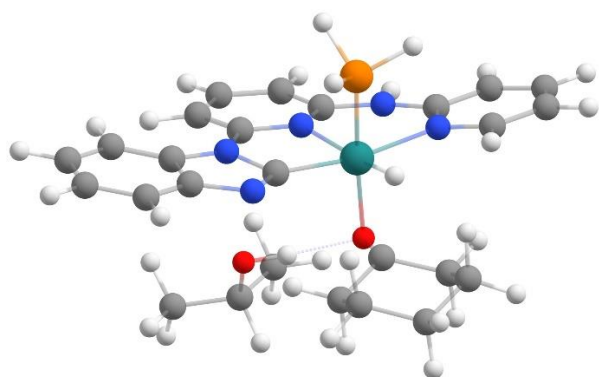
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N	-2.10650456308636	0.86920505918209	0.52592407578288
N	2.93745811914916	4.08236163059195	-0.61639552201026
N	-2.09082816154742	2.63485110559137	-1.12934295002007
N	2.30950461411689	2.42610900192228	0.82265355490145
N	0.14307908542792	1.64353878744122	0.75794457631068
C	3.61674783342784	2.77984631204979	1.20332672934755
C	-2.74849988486214	1.68621778961519	-0.40690408749941
C	1.65308294026520	0.57365779866000	2.33666119559616
H	2.65642449199383	0.47061670883374	2.77098797475744



C	-4.20464379996509	3.27614961120159	-2.16784156631414
H	-4.72997025005596	3.93683299801780	-2.87742971156326
C	-2.82824801781081	3.41075528144784	-1.97763436188412
H	-2.24817143394517	4.17119551252279	-2.52843109363861
C	0.60796732669073	-0.27484692855066	2.73461158031469
H	0.78752113842666	-1.03616300960456	3.51397219602497
C	1.38996731909274	1.53387707984465	1.33519949293718
C	-4.15159822392411	1.47877050234090	-0.55861653124048
H	-4.65432360394114	0.69375255837464	0.03549738784484
C	4.49928795559567	2.36271169124718	2.21480940642358
H	4.24053050265288	1.58564533614439	2.95203771848892
C	1.93259982008905	3.26604622678997	-0.32900152203865
C	3.97768663360907	3.81756375134922	0.27459311285541
C	6.13346312841426	3.99848445375311	1.36610138139073
H	7.13285930122071	4.46324961126458	1.44587338240046
C	5.24621298720638	4.42486953087577	0.35882312831463
H	5.51962414417307	5.21894636539372	-0.35767397013657
C	5.76463061903307	2.98668821413754	2.28145186320087
H	6.47518664081475	2.67397695442834	3.06734308660240
C	-0.65541954057470	-0.17268292703057	2.13903477573582
H	-1.48185579975898	-0.84180816394758	2.43639951857608
C	-4.88226754410200	2.27115571765308	-1.44371736206365
H	-5.96835634493458	2.11327084945667	-1.56421323755674
C	-0.84509635866668	0.80467144456824	1.12669261543484
H	-2.74561819472855	0.17366747634317	0.92226643674667

H	0.06656328362098	4.15841602512564	-2.03812366125946
O	0.32474142239772	1.15778614856960	-1.99281398795359
H	-1.52806939973393	5.69434713388600	-0.12829456859353
H	0.63049192735564	5.99739881215526	0.00585160696741
H	-0.44276362939358	5.01156963968108	1.61353054650470
C	0.64372034788404	2.03339993676729	-2.89731073604324
C	2.11311328377667	2.23080208735614	-3.29153919887573
C	-0.31681188675286	2.29422982495870	-4.07263307522915
C	2.37861577179486	3.57065573319013	-4.00621809666725
H	2.34025611471904	1.38518242117360	-3.99431367848157
H	2.77612396848944	2.09680154701808	-2.41307843694645
C	-0.05134981728842	3.62486440534434	-4.80624309349512
H	-0.14523409441218	1.44591465300730	-4.78629242447907
H	-1.37318876166340	2.19773727847861	-3.74317946292726
C	1.43189642291324	3.77272044329297	-5.20856689406891
H	3.44078472650794	3.61236219254724	-4.34315855916188
H	2.25653345038645	4.39271659695455	-3.26343288966214
H	-0.70992399492360	3.70581957717215	-5.70346327196868
H	-0.32811321806389	4.46740657549893	-4.12669957321733
H	1.60335366724017	4.77238243018018	-5.67313413959213
H	1.67117239061168	3.02017493618881	-6.00175738724733

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**PS-C'-PH3**

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N	-1.11934790323448	-1.29787075519192	-1.41863512734599
N	1.81560734423743	3.61236006251612	0.66919248005794
N	-2.23436766631231	0.84057973875648	-1.23779402171017
N	2.20654227196563	1.36923630511809	0.53794470233748
N	0.59916089345395	-0.00636994718025	-0.37095642030760
C	3.32346031050207	1.90686645771691	1.20042956515445
C	-2.25121065472493	-0.48918805606371	-1.53072023292693
C	2.70655101477940	-1.04305117687051	0.25745244010516
H	3.72946984918975	-0.95366952005307	0.64518150602921
C	-4.62391509749052	0.95557578158304	-1.72044428462702
H	-5.53423539592636	1.57566395934521	-1.77233588387709
C	-3.41367790999374	1.52441979862972	-1.32081487218504

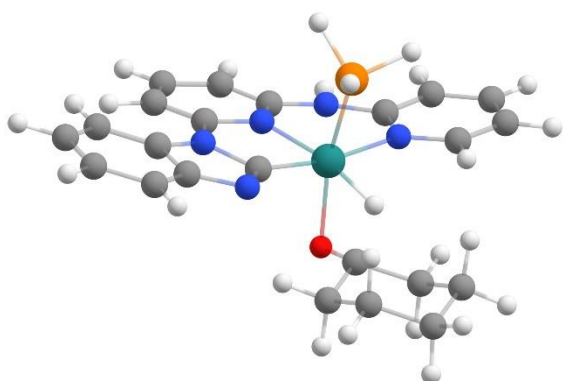
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H	2.85438885178196	-3.17334294689258	-0.13833241129505
C	1.87088002920974	0.09010418261536	0.15272440346548
C	-3.44557883340807	-1.13652890734472	-1.96637899484344
H	-3.42362306241164	-2.21422328792968	-2.21106978454509
C	4.49344800786582	1.36748752993201	1.76207024514289
H	4.72436710846790	0.29029505788311	1.74501204448669
C	1.30065113530858	2.48177632170515	0.21002507909368
C	3.04320578585000	3.31544265649556	1.26505030538716
C	5.13511214350089	3.64710518024204	2.43981994180026
H	5.86564588592715	4.31596637166280	2.92974079471267
C	3.95799414133079	4.18743919124662	1.88662532437735
H	3.73882861807662	5.26848542896152	1.93107630273649
C	5.39645747160559	2.25933773405965	2.38113355524250
H	6.32429148392193	1.85793238944582	2.82649366295662
C	0.93336171635446	-2.36787622437416	-0.75556654908807
H	0.54157323102516	-3.33025453644129	-1.12843552025821
C	-4.63350470450777	-0.41333913490522	-2.06753003084858
H	-5.55990035831472	-0.91076511572310	-2.40427341572401
C	0.14918501459761	-1.18933550349676	-0.83588909022942
H	-1.30034948245722	-2.25171142809730	-1.74528828880740
O	0.21978092990436	1.69931711390587	-2.65023132399799
C	-0.09410169630861	2.97314139867946	-2.53709377210880
C	1.02159289380408	4.02325991362273	-2.52583595219751

C	-1.36048041448737	3.47625153762956	-3.24953907774592
C	0.54981297380104	5.39188317300375	-1.99793993747368
H	1.33688748104216	4.12781888802870	-3.59837793878485
H	1.90891866773469	3.65165084518853	-1.97577782009230
C	-1.83716637553372	4.85469812380153	-2.74836381556126
H	-1.07723310992921	3.56156148948679	-4.33132471266601
H	-2.16620115856742	2.71303862337629	-3.21111688535065
C	-0.69645644974151	5.89546946647791	-2.75711104630428
H	1.37851581093216	6.13255181467682	-2.08399339971744
H	0.33650641154824	5.29035460309738	-0.90890371148300
H	-2.69547955017416	5.20954442951717	-3.36670566775727
H	-2.21977715659656	4.74395826061649	-1.70413340024549
H	-1.05479924818653	6.85761436614866	-2.32085589444176
H	-0.41941395352849	6.12288511741719	-3.81726188588204
C	2.58522438780914	-0.85737331180676	-4.00453011518191
C	3.41726340158275	0.39529998973904	-3.65469771448484
H	3.35494625157673	1.10115275001608	-4.53187141660766
H	1.51305724358920	-0.59400652990279	-4.15215189147371
H	2.94746655958327	-1.33836618810449	-4.94306523413735
H	2.64436560595774	-1.60800683781267	-3.18282082871734
C	4.89900887818655	0.05994257529610	-3.42768183796509
H	5.46866022380604	0.97763453315216	-3.16138027353595
H	5.00963293990449	-0.66336485478481	-2.58672238783756
H	5.35869920200653	-0.38804586186419	-4.33740452331073
O	2.94301102649137	1.03575496171284	-2.47334654477040

H	1.97658900289287	1.25543558264558	-2.59275053929605
H	-0.91586703613734	1.10895647002343	2.52680516345912
H	-2.62029651113201	2.18418175829526	1.73523555464956
H	-0.78791378195839	3.26007130979043	2.24906638177919

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**NPS-TS-II'-PH3**



Ru	-0.31059721826492	1.72219893328925	-0.83856125405066
H	-0.76250408600915	3.30150857735193	-1.28575593619339
P	-0.99250474000449	2.09822938521928	1.28093828845733
N	-1.33563758082763	-1.37773766502022	-1.37793116573535
N	2.10352547901501	3.39794584000320	0.17043235371336
N	-2.24885755235402	0.85245751324446	-1.30505850495556
N	2.32351507313727	1.12920907919467	0.16857676985248
N	0.54523971477557	-0.14953896280298	-0.54571100894301
C	3.51055211186143	1.61939842023965	0.74161371609502
C	-2.41058752529746	-0.49088389011193	-1.45444255873539
C	2.61966998836941	-1.32291132050364	-0.01518506407538
H	3.66980167049810	-1.28836965780147	0.30475422459452
C	-4.65974557181738	1.14152241373848	-1.56092848122571

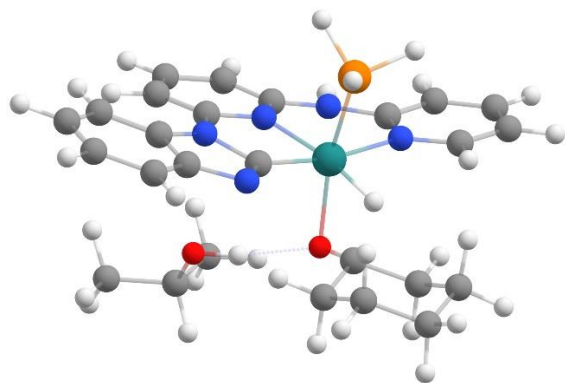
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H	-3.19170799897987	2.70923515121127	-1.18924385181496
C	2.01496822230195	-2.53587037892032	-0.37867777682080
H	2.58834507607396	-3.47729297158684	-0.31857078298453
C	1.86038875152337	-0.13814277399224	-0.11169782092695
C	-3.69226444093880	-1.06523136771622	-1.69439696701675
H	-3.78559138903504	-2.15965755369097	-1.81816511896961
C	4.66382632502861	1.02618259820769	1.28298745585831
H	4.80688140732389	-0.06549826889277	1.33553996576906
C	1.47736138155915	2.27994937507471	-0.17130661568595
C	3.33773161275300	3.04737968856930	0.72016506611494
C	5.51157165869538	3.28829791268904	1.76303600116407
H	6.31567393871418	3.92882919053769	2.16836240313946
C	4.35029096822408	3.88270094676151	1.23176993355693
H	4.21646815967422	4.97834136642728	1.21229702123471
C	5.66433547394872	1.88339948695651	1.79224890582181
H	6.58076468152833	1.44118118912625	2.22222844726885
C	0.68953534505670	-2.55171930555262	-0.83097213982570
H	0.19990824937413	-3.49615076467373	-1.12668691875614
C	-4.82174661730730	-0.24694625689221	-1.75507143806570
H	-5.81756480311621	-0.68633493738017	-1.93987720956120
C	-0.01876592942669	-1.32531033292761	-0.90963778069279
H	-1.61374857162576	-2.33591365509715	-1.60996513069528
O	0.14523406775864	1.79248937359659	-2.90693228398949

C	-0.23787090316255	3.04665597218912	-2.74088288083418
C	0.83711376967159	4.15473458372794	-2.79043619346989
C	-1.53065640340099	3.49045923231828	-3.47280270088445
C	0.31237343622152	5.52195132275676	-2.31171539595363
H	1.14345757319330	4.21614905269286	-3.86556622558670
H	1.73129423474565	3.85226569952853	-2.20969774319348
C	-2.05865344350571	4.85932027874127	-2.99855989128766
H	-1.24879138363959	3.55133877409117	-4.55369603804292
H	-2.30302043588427	2.69437434013283	-3.40781671024667
C	-0.96590596045890	5.94882182611214	-3.06429964660636
H	1.10769654511668	6.29427352710819	-2.42837130024116
H	0.11172815273392	5.45549225484951	-1.21492941712810
H	-2.94907209908665	5.15864895207514	-3.60043203264672
H	-2.41510647139681	4.76862216770274	-1.94122972630065
H	-1.35781634286076	6.91015458180768	-2.65597371912227
H	-0.71551443804369	6.14805547856862	-4.13613356967826
H	-0.58359876395315	3.30982295092560	1.94666373552223
H	-2.40929764626293	2.19047664529576	1.57881446974019
H	-0.66679219585960	1.19839233898293	2.37444784974993

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**PS-TS-II'-PH3**



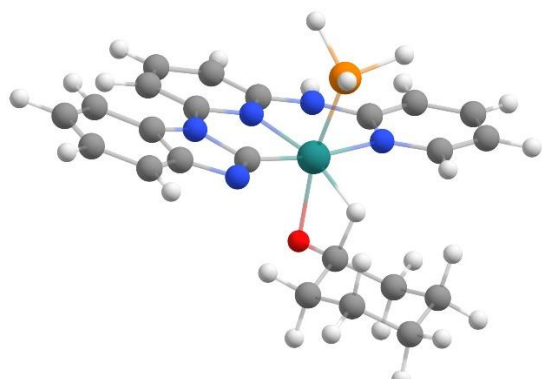


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H	-0.77470670731036	3.34469437355545	-1.06675188244856
P	-1.10904319742202	2.04772051202889	1.37902106467848
N	-1.02906721314292	-1.35820261538596	-1.41795394012183
N	1.96861647538232	3.55819844834917	0.54941616964061
N	-2.09498660703621	0.80278841989402	-1.33792137151735
N	2.29140045489359	1.30352599558862	0.56641282483693
N	0.67647049677096	-0.05502820390582	-0.35525231832257
C	3.39799887539282	1.84382795999281	1.24323722792023
C	-2.14868278620946	-0.53927585798793	-1.56150689230959
C	2.75916792803658	-1.11635446100244	0.34066787710781
H	3.77422497566407	-1.02764378846709	0.74992162609619
C	-4.48789548744233	0.94736393748851	-1.80104639162785
H	-5.38471651281153	1.58511041844020	-1.87094931875059
C	-3.26036076440671	1.50693005546647	-1.44013363897905
H	-3.17367068390964	2.58379661646062	-1.21491248251697
C	2.26680428629065	-2.35005091784402	-0.10559245167592
H	2.89006114893031	-3.25675439571772	-0.01549221663604
C	1.94161880978611	0.02436923256394	0.20002874200814

C	-3.35998513268838	-1.18076387238969	-1.95289538596970
H	-3.36462722835135	-2.27026614417913	-2.13884052577759
C	4.52090595694930	1.30018417947753	1.88976799496239
H	4.70947620453126	0.21601639505129	1.95032725968976
C	1.43620367909685	2.41422458240954	0.14411723393536
C	3.16163706250458	3.26163329159074	1.21318219374401
C	5.21109152526188	3.59502780617249	2.45979945765682
H	5.94215057362818	4.26844052852445	2.94269298563396
C	4.07856626197741	4.13937282564183	1.82328565411960
H	3.89553392508714	5.22770284477003	1.79619010502611
C	5.42653685582334	2.19851244843988	2.49581606613228
H	6.31863643384834	1.79560486625890	3.00782932083023
C	0.99326761749164	-2.43259883817247	-0.68504932616255
H	0.59407642940128	-3.39470029927729	-1.05076124112599
C	-4.53279329009559	-0.43543802492036	-2.08129999143932
H	-5.47401880100201	-0.92726079885116	-2.38314420447308
C	0.22495314876646	-1.24772946370125	-0.80564711473173
H	-1.21664230756045	-2.31972904098840	-1.71710412875947
O	0.34377583562236	1.93887327293221	-2.73641580021898
C	-0.12027159672297	3.16962467943323	-2.51878407766251
C	0.89863559612394	4.32315929018555	-2.45461647689175
C	-1.37986164607344	3.57284141474274	-3.31912578076528
C	0.27392377598452	5.64011819496292	-1.95658386573659
H	1.26721692197979	4.44702452266852	-3.50468422499334
H	1.77015549320896	4.03955770339229	-1.83144026448710

C	-2.00953997704215	4.89262165583108	-2.82994777419804
H	-1.03205742857772	3.69198261944499	-4.37580621557076
H	-2.112051391222103	2.73781772018431	-3.33639179033472
C	-0.97247459910632	6.03613748617639	-2.77657046808593
H	1.03513184718560	6.45347243759742	-1.98903685295849
H	0.00721429183818	5.51642901412421	-0.87927990525327
H	-2.87063924765759	5.17159003538056	-3.48171123551729
H	-2.43240362980713	4.73847629261679	-1.80510210348961
H	-1.43979393750929	6.95803978782487	-2.35722945978642
H	-0.66272187580638	6.29388462814351	-3.81996272033034
C	2.37684960500854	-0.76371829779339	-3.92009933879139
C	3.39135253892448	0.36234529045284	-3.62218929180826
H	3.44773848994780	1.01820778761584	-4.53830682679460
H	1.35814370814859	-0.34657075762085	-4.08659127492805
H	2.66297725798051	-1.33870291931886	-4.83192537028941
H	2.32272628746297	-1.47606590360950	-3.06490365532422
C	4.80059719447639	-0.18859701438825	-3.35520455483733
H	5.50542016971041	0.64118616115372	-3.12634860372416
H	4.78909027205096	-0.87642132436915	-2.47804073732510
H	5.19121404631429	-0.74963471562448	-4.23416450415652
O	3.01666662301649	1.13443259483514	-2.48562515611946
H	2.09820843811420	1.49505216512450	-2.63428389098098
H	-0.78566431663093	1.13775222550918	2.46265142175426
H	-2.54482463807579	2.02950323867215	1.57995290309351
H	-0.82835824628609	3.26633542771058	2.09348121411660

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**NPS-D'-PH3**

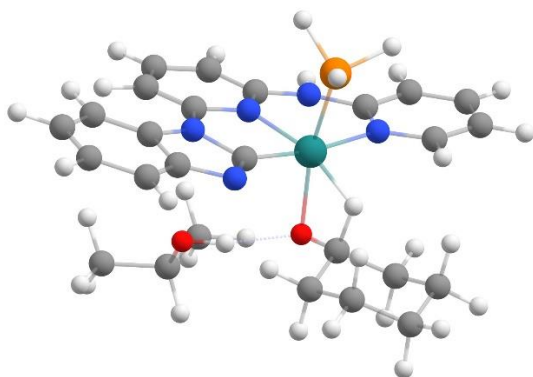
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P	-1.02943935286675	2.11929334427342	1.09078992287139
N	-1.83219391292537	-1.53414871928167	-1.10636533621355
N	2.19676656878406	2.93285461213954	-0.23482067240163
N	-2.45358519403636	0.77717418669233	-1.35203394663543
N	2.14559665661724	0.67717192478055	0.07835358758566
N	0.20429603454507	-0.44373322373200	-0.45443651529411
C	3.40135047648867	1.09142949085670	0.55798457607790
C	-2.78853816484058	-0.54093041020030	-1.31793252292424
C	2.11974463692885	-1.79275102181936	0.24523399904858
H	3.16898423750397	-1.84699175067262	0.56527297761364
C	-4.80733563297769	1.33778100477248	-1.67283939064913
H	-5.56595704577158	2.12736946842065	-1.80306047339476
C	-3.46319520245208	1.68196903381577	-1.51084374516918
H	-3.14864291347882	2.74019878442961	-1.49942977281749
C	1.36015755847848	-2.95701619560240	0.05527494086691
H	1.80762965591492	-3.94686825428758	0.25094000640393

C	1.51992488199496	-0.54558253052960	-0.02167253960232
C	-4.13440939773543	-0.97366936734117	-1.49134719648591
H	-4.36936351203691	-2.05344716079887	-1.46615251327834
C	4.49422014787208	0.43969061856638	1.15397052709750
H	4.50908729007761	-0.64449776980368	1.35238495758767
C	1.43449625537267	1.86203761280188	-0.40457580420884
C	3.39885899508642	2.51318426362462	0.33921045705556
C	5.62116449146993	2.62484874155288	1.29801422771950
H	6.50968671664426	3.21101507949754	1.59473147529426
C	4.52102582975885	3.27946538004303	0.71029956139309
H	4.51879806353815	4.37013777890491	0.53959241877420
C	5.60712004566272	1.22888615071728	1.51975290152333
H	6.47955051123611	0.74015756615835	1.98902909230383
C	0.03772656714603	-2.86245110333512	-0.39526757284299
H	-0.57435637895317	-3.76708641279654	-0.55686816797765
C	-5.14874473674895	-0.03162710233822	-1.67646757873299
H	-6.19432144100173	-0.35958443470150	-1.81064550325646
C	-0.51174915121789	-1.57997712838839	-0.64870971467103
H	-2.22854941394729	-2.47397099421155	-1.20076787722706
O	0.03041351799965	1.26977864297122	-3.02248161340345
C	-0.25264030593433	2.58538416145001	-3.03181016557030
C	0.93193313987868	3.55969107441728	-3.26450469272588
C	-1.47390876304835	2.99851023555994	-3.90210598734011
C	0.52780322240760	5.03558529109052	-3.07262923344257
H	1.26824670635535	3.38265037721416	-4.31607750183783

H	1.77511729249475	3.29912417719339	-2.59270368506402
C	-1.87979885043869	4.47338988241915	-3.70716910844321
H	-1.15750554421537	2.82926066000790	-4.96060889568799
H	-2.32369816763569	2.30377333687639	-3.72628343740639
C	-0.68786457298114	5.42738966054844	-3.93899336827275
H	1.39541128612090	5.69868093949334	-3.29730994099467
H	0.29306450613512	5.20159679903517	-1.99225028204047
H	-2.72912898043001	4.73268544029836	-4.38247057270868
H	-2.26145653781714	4.61813764386020	-2.66411573485424
H	-0.99169345629730	6.48108897950578	-3.73401545657300
H	-0.39968332238543	5.39291610404982	-5.01914410212061
H	-0.75647710041421	1.32929748456344	2.27950071529412
H	-0.50539010189558	3.35958092837627	1.60997776490397
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### PS-D'-PH3



Ru	-0.24443665141447	1.73420141291758	-0.59488215097564
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P	-1.10699168660981	1.88963956334389	1.49065285655439
N	-1.04226594539319	-1.36168754838697	-1.35203057897306

N	1.97592095572336	3.52215516620004	0.63947636878468
N	-2.07529194023895	0.80846884886528	-1.29256126859221
N	2.31773032522311	1.27180569890652	0.62230725048737
N	0.68231411046385	-0.06201702711035	-0.30153327980248
C	3.44115014943598	1.81265160989378	1.27056419612077
C	-2.14673193379954	-0.53008236138115	-1.52454554975341
C	2.76807201031311	-1.14668994103799	0.36404951411667
H	3.78594026293646	-1.06610260802993	0.76810619531739
C	-4.45030642256807	1.00114419761169	-1.81813579986140
H	-5.33341205886765	1.65513643307161	-1.90865266252672
C	-3.22225707919994	1.53655550719278	-1.42280918416500
H	-3.12370113587188	2.61070565957116	-1.18656654568222
C	2.26490959466084	-2.37432429884483	-0.08685926247345
H	2.88279626963027	-3.28579243827809	-0.01180712263591
C	1.95854504359701	0.00014515032018	0.24355977066947
C	-3.35832174960764	-1.14892189569787	-1.94830118662645
H	-3.37829404151115	-2.23726343521339	-2.13967023057787
C	4.59044409738431	1.27048822416647	1.86954040915693
H	4.79119335157412	0.18741813319363	1.90658691078145
C	1.44563376228753	2.37645853385907	0.23963185070965
C	3.19218017371270	3.22875431474031	1.26406180725172
C	5.28049615558982	3.56444650862869	2.44305000924118
H	6.02265622542037	4.23838106260461	2.90791280529975
C	4.12231865412795	4.10697808144770	1.85270388965373
H	3.93073085656379	5.19411502262111	1.84389716318013

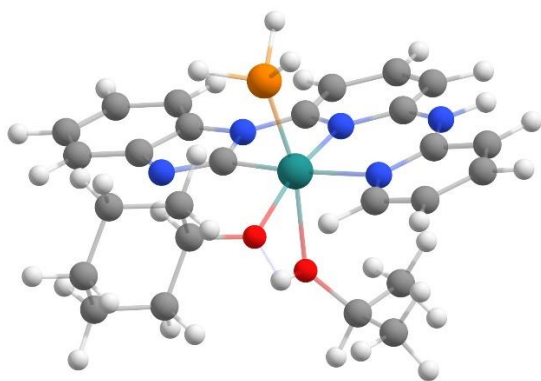
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H	6.42282486790488	1.76871234285914	2.92840110208586
C	0.98432264777542	-2.44110553539106	-0.65102869835481
H	0.57425128153618	-3.39637733212821	-1.02253906380748
C	-4.51337125306786	-0.38009787349331	-2.10287398342747
H	-5.45593775524706	-0.85304622508864	-2.42953326036326
C	0.21852527762582	-1.25349141904537	-0.75487283753479
H	-1.23459776108487	-2.32333410007722	-1.64772897781690
O	0.36127753959009	2.04472368611103	-2.59307859737496
C	-0.15738169197859	3.28791225609645	-2.39346465368579
C	0.85433997908757	4.45855371231458	-2.34711859329212
C	-1.35533756705915	3.63631469825034	-3.31723433905941
C	0.18078570879562	5.79142102639265	-1.96298520890672
H	1.29589494329158	4.52586078946416	-3.37199757084235
H	1.67680752771492	4.22410179010729	-1.64028790935354
C	-2.03212313703538	4.96869499879451	-2.93586803128734
H	-0.93178501965429	3.70510822160852	-4.34899887945628
H	-2.07931318056120	2.79325622783649	-3.34212834143769
C	-1.01444455153816	6.12889450410868	-2.87917770075055
H	0.93259124492714	6.61398735211838	-1.98514368068950
H	-0.16088009421505	5.72423846331340	-0.90062937880805
H	-2.85444683045205	5.20015681573491	-3.65306517006748
H	-2.52119585537948	4.86302633175758	-1.93373069314147
H	-1.51593960726345	7.06544426195952	-2.53920490688314
H	-0.64143502363314	6.33506990516784	-3.91315834774640



C	2.24315372945330	-0.64807678285728	-3.87256820490260
C	3.29761319430540	0.45006464802120	-3.60888249409666
H	3.32093829537950	1.11960896653239	-4.51667797425724
H	1.22549291123537	-0.20534873822861	-3.95898583768221
H	2.45813542873983	-1.20091899617381	-4.81721842477960
H	2.23114992023849	-1.38577114839668	-3.03722716549557
C	4.70538346608249	-0.13785588489118	-3.42531641496228
H	5.44188048333562	0.67185650927569	-3.22598881537852
H	4.72320465284877	-0.83467477282317	-2.55519467691308
H	5.03437851958187	-0.69862452879856	-4.32939925148482
O	3.00079596730904	1.21053851207413	-2.44296359516474
H	2.08938887402372	1.60865995895444	-2.54804845058064
H	-0.73734213615059	0.95491260316908	2.53876663446248
H	-2.53979804422449	1.79479422323364	1.69829578088874
H	-0.89083417289331	3.08746914923739	2.26559396065305

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**E'-PH3**



Ru	-0.01899406576275	1.29962617358325	-1.09278878125461
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P	-1.14238662558451	2.04092608163996	0.67734671500033

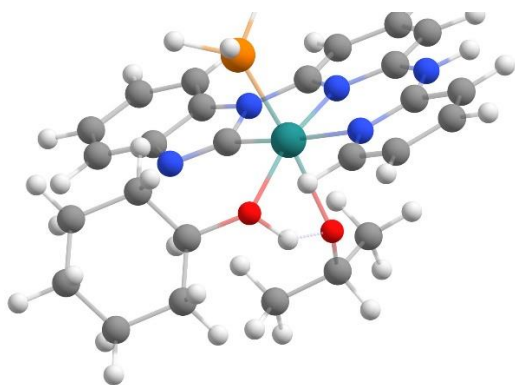
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N	2.37648102016798	1.03521515803180	0.48192133615964
N	0.64706073959005	-0.36644295546900	-0.11930891070067
C	3.50908105891246	1.65413742806383	1.03968841230691
C	-2.08429812750142	-0.96611022711294	-1.51844272130261
C	2.48719809223018	-1.34502465551467	1.16369541205765
H	3.46142328161630	-1.23005226013322	1.65746263358703
C	-3.89550763867600	0.49319808874382	-3.04204163677226
H	-4.58139447737668	1.11477714053498	-3.64196831560943
C	-2.67429209937313	1.01893221685348	-2.61092583471716
H	-2.32153427766549	2.04139851784392	-2.85665994588168
C	1.83909350564991	-2.59092743052654	1.13188735334273
H	2.30476553564032	-3.46810827363958	1.61339844828013
C	1.86920831021650	-0.24633988950244	0.53531731788835
C	-3.30612124199701	-1.57183847153042	-1.92808095640071
H	-3.52935010239508	-2.61388594715086	-1.63471571015051
C	4.58647305165208	1.22213065816806	1.83230495522467
H	4.70043752488168	0.18027366384698	2.17374733711181
C	1.62259993787573	2.05484844838438	-0.25745676858763
C	3.39100857581005	3.02560071282824	0.61969159103331
C	5.45100356118917	3.52877943029587	1.79027289192919
H	6.22943338399495	4.25078663308063	2.09655253379580
C	4.37016100160293	3.96397764774140	0.99853536420728

H	4.27571914677851	5.01425403420786	0.67207851983052
C	5.55612112285376	2.18062733713916	2.20114584305193
H	6.41207355191559	1.86384867392126	2.82356152706152
C	0.60393473740283	-2.71810257650071	0.48483269624391
H	0.07848716787822	-3.68868205200759	0.44752304644981
C	-4.21604279828170	-0.83632789933099	-2.69285244729118
H	-5.16850040020174	-1.29594097154118	-3.01102968657512
C	0.03001713114415	-1.57657065946865	-0.13041185344565
H	-1.57488526061673	-2.69571768732759	-0.61261921729287
O	-0.42074897467249	2.83685555210010	-2.45561887761758
C	-0.19686537167683	4.21729641971189	-2.19687562037478
C	0.39545689260927	4.90091430648806	-3.45113875941703
C	-1.50921916872519	4.92621540601109	-1.78220139271662
C	0.61131217247764	6.41547613961522	-3.23476439484379
H	-0.29862759786336	4.73191675605136	-4.31348934534915
H	1.36098365520172	4.40695613108594	-3.71327325343735
C	-1.29386571582751	6.43611407895281	-1.53959123677757
H	-2.26975138695613	4.77922584771445	-2.59067250414915
H	-1.92768530201002	4.44050428187914	-0.86843072434470
C	-0.68672405971235	7.11945543075884	-2.78383367292317
H	1.00608410588614	6.88682644801009	-4.16598850590939
H	1.39879400765631	6.56327123707815	-2.45536214482199
H	-2.25396944895146	6.92803748939609	-1.25379305736304
H	-0.60358908543603	6.57294081649791	-0.67066916782884
H	-0.49345851698914	8.19944226456329	-2.58015311368325

H	-1.43175668830333	7.08846888562604	-3.61795992609250
C	-0.04264830217112	0.02675673156647	-4.87595921130465
C	1.25094716909989	0.06949297399568	-4.04493856310470
H	2.08535132268440	0.39996364850233	-4.71813958874219
H	-0.33249014644500	1.04176694723922	-5.22885652431996
H	0.10294055221992	-0.61355754285380	-5.77583427917061
H	-0.89254741404284	-0.39154861328676	-4.29439391962723
C	1.62725995923061	-1.29670497141822	-3.45956758243235
H	2.53326021995427	-1.21866451342405	-2.81966106263295
H	0.79890235392272	-1.71390835719970	-2.84433469828787
H	1.84290350465938	-2.02346042240518	-4.27478400831372
O	1.20463147617599	1.03425327055040	-2.96924501634303
H	0.71355242826388	1.91317616307314	-3.20776118026927
H	-1.00162254654571	1.36880954415507	1.95640118014500
H	-2.59081205396762	2.07980237158004	0.66162969613752
H	-0.91760834928802	3.38145483157207	1.16592814511760

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### TS-III'-PH3



Ru	-0.84707563421844	-0.57994316738353	0.17031947296131
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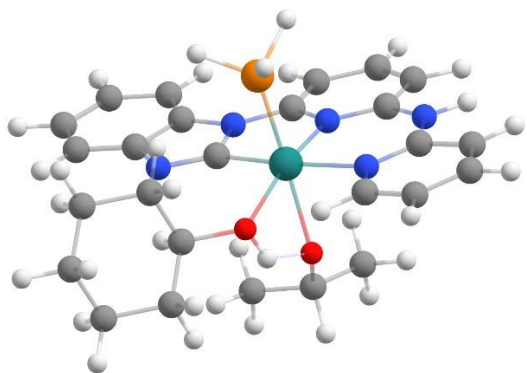
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N	-2.17959658277888	-3.57821113535992	0.41225021907215
N	1.59673965078387	1.15910288303374	0.99356053590136
N	-2.72452350282230	-1.43115659871534	-0.52213762779519
N	1.56177345581131	-1.01365388555241	1.67477616471804
N	-0.25150734014574	-2.30083756725297	1.06711591534930
C	2.74165821976120	-0.47250920549934	2.21646306282998
C	-3.04244704757705	-2.72720103492110	-0.28026962204744
C	1.54811042886182	-3.40812172726583	2.30568713277639
H	2.53234950340743	-3.35371438931011	2.78958392449836
C	-4.85270559465863	-1.13251089646115	-1.65810337067928
H	-5.53344486386626	-0.45716451410830	-2.20290407082929
C	-3.61658467523801	-0.66088594804171	-1.20571328646679
H	-3.27134933244007	0.37385362047427	-1.38929052301337
C	0.84112273143526	-4.61972219909391	2.24107731379054
H	1.26624658360551	-5.53319424985787	2.69151217005633
C	0.98110878868339	-2.26405404519902	1.71377438743721
C	-4.28020978852879	-3.28249256477248	-0.71408790745698
H	-4.51260725104786	-4.34220744798316	-0.50231058259619
C	3.77760064417869	-0.96976476311809	3.02544844333126
H	3.80148410910305	-2.00666388586424	3.39826755364665
C	0.88413654938584	0.04264679185587	0.91295657017828
C	2.73048500624867	0.89314546376132	1.76464588218221
C	4.82463085660104	1.25754604421689	2.92665112215017
H	5.65821512857602	1.92260507195705	3.21620249458257

C	3.78215671094785	1.75867309034834	2.12237343225318
H	3.77205854211627	2.80543568911317	1.77193140781392
C	4.82125150524383	-0.08338689907082	3.37289173347458
H	5.64751142267799	-0.45137452960818	4.00700136299415
C	-0.40108386768995	-4.66564639459924	1.59931074857312
H	-0.97425724172867	-5.60747270653128	1.53796938392403
C	-5.19029928199525	-2.47833640086568	-1.40383295079885
H	-6.15406111677044	-2.89842842194515	-1.74188426460757
C	-0.92552758412505	-3.48039260128470	1.02138021254851
H	-2.55817602425711	-4.52717073709721	0.48582323937758
O	-1.24932922486278	1.04860776301655	-1.18759412031794
C	-0.58831736472747	2.32619559569989	-1.14940766182679
C	-0.81939102225148	3.05548734881738	-2.49066293125214
C	-1.09587222182609	3.17245740249110	0.02999437257145
C	-0.16049451091256	4.45259834637151	-2.49245399429733
H	-1.92058846135892	3.15252622923021	-2.66117975235922
H	-0.42362601568162	2.43565964484221	-3.33025350924589
C	-0.44200309835471	4.57156335509249	0.03666003284747
H	-2.20923593687820	3.26481144906306	-0.03751471160185
H	-0.85372132641129	2.64543229127095	0.97966686952005
C	-0.64923996789194	5.30777149268056	-1.30394639929235
H	-0.36166847383385	4.97188563736395	-3.45896268653571
H	0.94951447963717	4.33536352984883	-2.42847632605341
H	-0.84323252894224	5.17841337458984	0.88213876261543
H	0.65151075302875	4.45155815524407	0.23166239500041

H	-0.12576739777473	6.29295521529156	-1.29303872235001
H	-1.73668319355013	5.53437172596854	-1.43742801626813
C	1.67847386000631	-2.48732754615121	-1.80074019971825
C	1.03134994655251	-1.25959355456151	-2.46526518599500
H	0.81743842884350	-1.53591354406994	-3.53436279576155
H	0.95437138791868	-3.32950691605332	-1.73114267446100
H	2.55484857068398	-2.83778979190381	-2.39255641157287
H	2.04332563910953	-2.24828840739643	-0.77737476045468
C	1.98476889385542	-0.04823390556036	-2.48065212848269
H	1.53400792452810	0.81284594385863	-3.02439760750379
H	2.23612629321909	0.28899277908258	-1.45098425689747
H	2.93547894589892	-0.30440265076044	-3.00305486305392
O	-0.24253585131544	-0.96781201775349	-1.87910749978371
H	-0.67893458408212	0.22370297789706	-1.86292156315472
H	-2.18704741101649	-0.75186747873566	3.12006159775929
H	-3.12891749435524	0.80533274995180	1.95356934960374
H	-1.20194363952487	1.15378347503541	2.89224960173064

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**F'-PH3**



Ru	-0.39582314527483	1.21991397948292	-1.18619856165204
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P	-1.41056155075141	1.92671993303609	0.71092112295566
N	-1.66884242325277	-1.79476947989151	-0.92540945607149
N	1.98830270438754	3.02916784517265	-0.35678493563858
N	-2.25578968305338	0.33013511649884	-1.88140006422376
N	2.03758582847875	0.84586900233868	0.28663301096655
N	0.24445333501051	-0.47875029123518	-0.30243335309043
C	3.21147750150864	1.41549938731230	0.81217926719528
C	-2.54417851172528	-0.97151628813010	-1.63508253283073
C	2.08602955338606	-1.55071001673055	0.90607072270719
H	3.07665450340118	-1.47676759636477	1.37414145916718
C	-4.37748251840089	0.56722798599069	-3.04479689750344
H	-5.06778530895272	1.22153043696950	-3.60301836437222
C	-3.15804999571101	1.07141344221763	-2.58180866751306
H	-2.84707046789305	2.11504746032539	-2.76932015749930
C	1.40006593511715	-2.77494519838897	0.85583450454103
H	1.85021651996241	-3.68007413466517	1.29866593578599
C	1.48761818072862	-0.41684774734997	0.32537562566851
C	-3.76267870726681	-1.56089629742404	-2.07861332214891
H	-3.96974327437084	-2.62522410099304	-1.86364686087970
C	4.28215368218377	0.93633484740994	1.58582964086160
H	4.34901387704760	-0.10700372901283	1.93470425197805
C	1.31427903663054	1.88987854971170	-0.44608531746757
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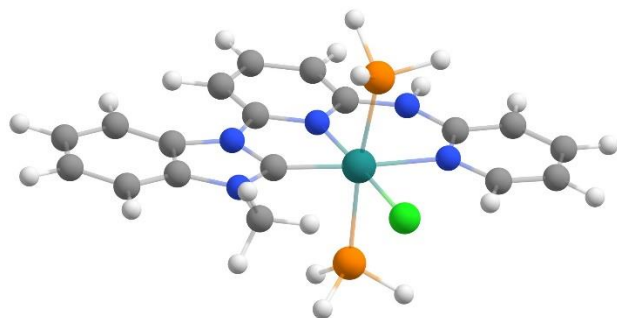


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C	4.17862924406484	3.67944150565137	0.73484467741249
H	4.12889108974694	4.73144671603512	0.40391226626671
C	5.30588906818852	1.84883848766937	1.92508568768057
H	6.15942856319183	1.49545490111628	2.53067699815178
C	0.14698585648982	-2.84410376032621	0.23795781341081
H	-0.40889571875605	-3.79667951825007	0.18597662555397
C	-4.68493032929928	-0.78454605985604	-2.78378301909327
H	-5.63383494897047	-1.23079689688142	-3.13007322554149
C	-0.40891483036968	-1.67079324383270	-0.33430011011915
H	-2.02793620382033	-2.75035313689064	-0.84121598126290
O	-0.81596733509785	2.91858842556118	-2.52911575918752
C	-0.15819353925043	4.21109791540783	-2.43837265743043
C	-0.24810125132864	4.93052235310048	-3.79801397775459
C	-0.80963343642120	5.03763516279971	-1.32201247494109
C	0.38692460717850	6.33734454776351	-3.72154660644838
H	-1.32313552484889	5.01193143706077	-4.09604613194305
H	0.25549842734218	4.31931894945968	-4.58455439124668
C	-0.17876831189412	6.44471589366480	-1.23894229319968
H	-1.90894271436734	5.11638337691118	-1.51494739936111
H	-0.67454045079988	4.50755498516170	-0.35269301999588
C	-0.24474348989140	7.18138548303271	-2.59383667758887
H	0.28681764283170	6.85593979671286	-4.70367311191253
H	1.48414226556048	6.23571152211127	-3.53442001633790
H	-0.68268260005340	7.04225061556224	-0.44366633068723

H	0.88703806688689	6.33978081964935	-0.92114531365542
H	0.26048398439256	8.17330093194652	-2.52275062527927
H	-1.31331063635405	7.39362351761896	-2.84807454445286
C	1.59731519745126	-1.18462305340817	-3.41729478559725
C	1.41424199434070	0.31684845726405	-3.73279905131177
H	1.28354873259468	0.39637897287937	-4.84909743021482
H	0.67050784379802	-1.75046897072040	-3.66217425140898
H	2.43453474865648	-1.62226369379980	-4.00921703033743
H	1.83139456797433	-1.34906487451009	-2.34120485451491
C	2.68206359244846	1.12403847921395	-3.37531926065764
H	2.52643241499427	2.21234576285020	-3.54602220081949
H	2.97272777741865	0.98978856182842	-2.31017099075854
H	3.54587951537943	0.80017347750008	-4.00167063294292
O	0.21732858707719	0.82613170408800	-3.17432191498482
H	-0.29220421509013	2.27285342620449	-3.18553116812658
H	-1.69533578596616	0.99859652258536	1.79456776355189
H	-2.74100957828328	2.49366206679995	0.64264324728970
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### 5-dft-PH3

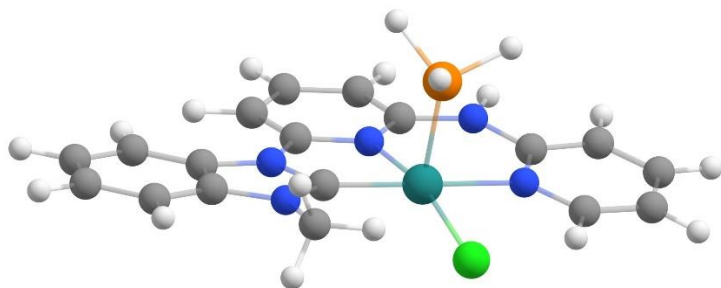


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P	-0.08731637670866	2.76638300884416	-2.65442385663272
N	0.43046805535957	0.19313171922982	-0.72931042550354
N	2.22980808120179	1.42192509153092	0.04859069801153
N	-2.44507839184218	1.17446322987392	-1.21585729438676
N	2.00102870121322	3.55892048359849	0.57033058007355
N	-1.47945615258517	-1.01563101234411	-1.53186821010966
C	-0.13813117836757	-0.96096757390416	-1.17343608186373
C	-4.91409025937234	0.14601905033984	-2.14563276127037
C	0.60944907494922	-2.16214519079638	-1.28973258390784
C	5.84136561963945	2.02930024242369	1.06948025254880
C	4.40850904443383	4.00951961867757	1.27363595575615
C	5.66572454113133	3.39005561783387	1.40289559548997
C	3.34789756945166	3.21863256655645	0.80505107793544
C	1.29046165182115	2.48663587979175	0.10447414770174
C	4.77429794593356	1.23705956291763	0.59965271811070
C	-3.78573057966557	-0.66970462261195	-2.05956357728978
C	1.76919210626451	0.17583291719982	-0.38958232319247
C	1.95928496479466	-2.16449214302011	-0.93682431061512
C	-3.56097149238787	1.95878228589987	-1.30738472540920
C	-4.79839446367577	1.49618650746593	-1.75926998266086
C	2.55939481174060	-0.97935632134055	-0.47632789246904
C	-2.55742562096733	-0.12748486696603	-1.58851094595584
C	3.51289147551645	1.84854014233646	0.47188094038017

H	-0.76316921643673	0.42278860263183	2.43186922487128
H	-1.20500758943063	2.95490677058200	-3.53992999178798
H	0.52012546067500	4.06054840673132	-2.78958341415332
H	0.77167782874030	2.03827851745392	-3.55846880347501
H	-0.93006693822251	2.57965420090089	2.69165294391732
H	-2.62892996058548	1.43459937778711	1.94041367845032
H	-1.74829016377512	-1.95519904924888	-1.84244618087838
H	-5.87124281522128	-0.26624603420155	-2.50982727270019
H	0.11875625245881	-3.08133809134386	-1.65438259895495
H	6.83808447321702	1.56759950509669	1.17616065427435
H	4.26699636704599	5.07253041253114	1.52960815246895
H	6.52538819995298	3.97788629948262	1.76804819948126
H	4.96320882990058	0.18397870979164	0.34792073788330
H	-3.83745249300659	-1.73330130812081	-2.35445040817502
H	2.55374002305484	-3.09024787284354	-1.01720483299403
H	-3.41450051322404	3.00811886636402	-0.99100447728430
H	-5.65474180779948	2.18929626682121	-1.80510949787410
H	3.61727114687869	-0.96818571168371	-0.18971141479862
C	1.49810523656496	4.91320635796881	0.81579892467813
H	0.41875775729478	4.95317222157529	0.56523901826149
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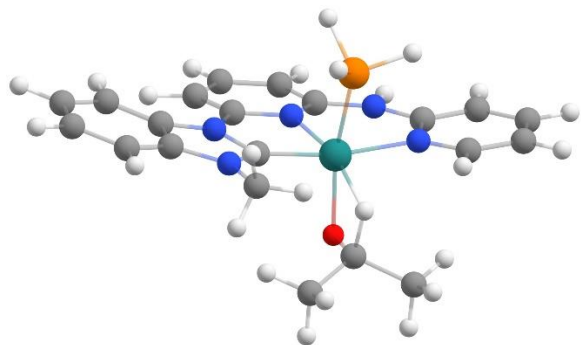
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**5a-dft-PH3**

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N	0.40511951129352	0.18235273441428	-0.68471279756815
N	2.22275005420462	1.43879292956853	0.01032494444212
N	-2.42635141149060	1.18453332102793	-1.24894213466990
N	1.95321365807970	3.52974261441235	0.68202470781143
N	-1.53590216742397	-1.05925884622318	-1.33331966465613
C	-0.17019516136198	-0.98238836025983	-1.09495456151901
C	-4.91951697353385	0.15148372603260	-2.10989179347911
C	0.59185488908549	-2.16683057122882	-1.27314940916094
C	5.83699407983744	2.06698376995018	1.00157893988415
C	4.36286703054009	3.99305582389652	1.36920537430639
C	5.63586445594760	3.39736249189442	1.43198203016556
C	3.31133903181024	3.20884663439524	0.86863563640606
C	1.26487976528394	2.47755525295662	0.14397523592182
C	4.78066801107772	1.28228690479882	0.49744444163513
C	-3.82340899931828	-0.69037420174152	-1.92497820986284
C	1.76544409869288	0.19070685050715	-0.43049046271927

C	1.96293590116845	-2.13953217593649	-1.01863335052639
C	-3.51413282216993	1.99432482288920	-1.44110280474356
C	-4.75905104867632	1.53092806116720	-1.86508125596780
C	2.57050971490469	-0.94393991538584	-0.59108653950627
C	-2.58156317990499	-0.14546703168165	-1.49476758662246
C	3.50235099306038	1.86848330064663	0.43867972944478
H	-0.40141915095304	0.69584751073808	2.43807283221312
H	-1.15661411452150	2.75445907745536	2.53582862867583
H	-2.48476635360407	1.12751965951091	1.87180216491270
H	-1.82772230779775	-2.01437909881779	-1.56745536086543
H	-5.88703856423887	-0.26173675650471	-2.44442993559860
H	0.09765558244661	-3.09290933844498	-1.61458299558459
H	6.84697132913852	1.62542103240771	1.05586659268304
H	4.20246722101403	5.03343844245700	1.69688237344369
H	6.48939977024726	3.98022507668314	1.81873861274000
H	4.99005044452459	0.25557580184333	0.16528245838925
H	-3.90992713348954	-1.77549069659724	-2.11393056954302
H	2.57189937130613	-3.04902447169602	-1.15610596360927
H	-3.33364462260675	3.06530784388721	-1.23777274223123
H	-5.58918975299526	2.24426609230933	-1.99840747308429
H	3.64800657182100	-0.91073021968230	-0.39158988641312
C	1.41286536866165	4.84216895836120	1.04795017770199
H	0.33081348326051	4.87144826500521	0.81478122111399
H	1.92137600669829	5.63658533672611	0.45849073565723
H	1.58679718368443	5.02904692550435	2.13094391602632

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**A(Me)-PH3**

Ru	-0.03516080407981	1.49634252933634	-0.99124699648668
P	-0.91427103715389	1.87749810295521	1.09001816842247
N	-1.77556359435378	-1.18995463048474	-1.80562341360608
N	2.60213426565993	2.39614921190910	0.43827251277933
N	-2.07200977573082	1.19611228907274	-1.67795540218908
N	2.27593399399246	0.22814926723733	0.12664234851308
N	0.28928560257038	-0.52315671800788	-0.77952663136492
C	3.46973477594937	0.33186004716443	0.88015368931377
C	-2.55895686370959	-0.04321454384501	-1.94240499633801
C	1.99953241459051	-2.20010600090289	-0.31014028857262
H	3.01376603872485	-2.44781921947412	0.02906759408526
C	-4.25558619737683	2.14779481534329	-2.18777466060610
H	-4.88674934224741	3.04855260881771	-2.26196733432226
C	-2.92371463497766	2.25789773044315	-1.78761557631514
H	-2.48823934458207	3.24049432029573	-1.53509861311941
C	1.14349583079275	-3.19831494232142	-0.80936502670605
H	1.47545556789520	-4.25018500972830	-0.83055872789544
C	1.53720645775219	-0.87705160014767	-0.30778238575301

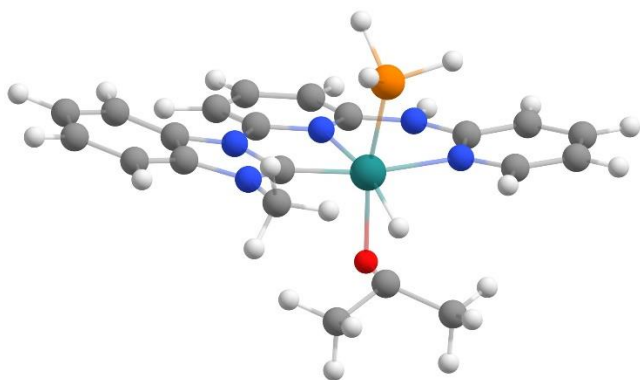
C	-3.90445083151602	-0.23609406197217	-2.36863501323265
H	-4.27114802599462	-1.25560121703321	-2.58451726043533
C	4.36586893086258	-0.59650548894898	1.43800086673068
H	4.22995674698336	-1.68440269777105	1.34845424569143
C	1.73004519285471	1.50670662142842	-0.14307573752015
C	3.67259925214995	1.72793327636753	1.06190435566323
C	5.67524075042668	1.29809919699816	2.31475661830233
H	6.55350546033323	1.65761553590071	2.87811443750209
C	4.77198026638991	2.23349582143799	1.77251034884405
H	4.92579433971948	3.31742969663150	1.90565417701123
C	5.47034018502693	-0.08944167944306	2.15387454999327
H	6.18807567782377	-0.80023844997783	2.59832478965140
C	-0.11849410259135	-2.85239793444014	-1.29768262965651
H	-0.79618646404647	-3.62260171765941	-1.70513024670959
C	-4.75302054101724	0.86302886646210	-2.49647367516289
H	-5.79736350763419	0.72173103604336	-2.82484222210960
C	-0.51996800851310	-1.49120719954156	-1.28518092628878
H	-2.26605716345629	-2.03134776957790	-2.12625913849163
C	-0.54114678478443	3.49553990545188	-3.81971303903113
C	0.49542266790769	2.80779606977958	-2.90291738330931
H	0.02024237389271	3.15261603988178	-1.68173976067976
H	-1.51232604512032	2.96183775635873	-3.82124398031513
H	-0.70208820944594	4.56364987381002	-3.55294946192344
H	-0.14461542435260	3.46194863965034	-4.85995836872777
C	1.86424330044506	3.52260593820945	-2.93705664141839



H	2.61250797551277	2.99476706298566	-2.31204937972545
H	2.23088301275038	3.50115095332434	-3.98844102935645
H	1.79782078469638	4.58891496546675	-2.62731222451909
O	0.54073729450175	1.46724349858435	-2.98584441104503
H	-2.30798716615755	2.23913393670407	1.20200729425443
H	-0.38970617139218	2.91066353102622	1.95015529410308
H	-0.91950447011722	0.83050274634130	2.08921259533506
C	2.42348371700324	3.84472030328360	0.47972774564949
H	1.46250836128465	4.09745294098790	-0.01105499895520
H	3.25255406407850	4.36289243308721	-0.05091943759058
H	2.39795920778002	4.19933331249933	1.53448538763302

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### TS-I(Me)-PH3



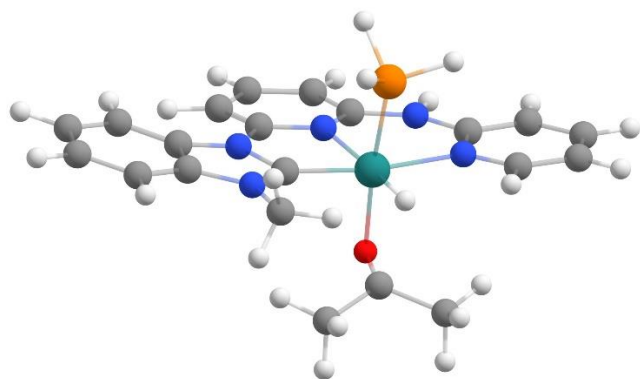
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N	-1.77378595347890	-1.18994036278717	-1.80343680825572
N	2.60100179343435	2.39984837839161	0.44380545762179
N	-2.07198827637740	1.19978220545640	-1.68213390793481
N	2.27541145460860	0.23290815629748	0.12259610036132
N	0.29027021837043	-0.52558391185718	-0.78099944531973

C	3.46803106376232	0.33407870830693	0.87834734918502
C	-2.55793813488869	-0.04272110891997	-1.93761172782058
C	2.00550535253212	-2.19639376509975	-0.31813770281059
H	3.02140870284400	-2.44312305641865	0.01656925180159
C	-4.26237352281931	2.14256710189900	-2.18387980426534
H	-4.89617675137397	3.04144840387457	-2.25874248526680
C	-2.92847468757156	2.25839367241884	-1.79250710315062
H	-2.49318211798498	3.24269450951043	-1.54803691645456
C	1.14952026246520	-3.19622625215200	-0.81504507169062
H	1.48421936303805	-4.24727669008582	-0.83723986155997
C	1.53855725743322	-0.87453247235182	-0.31288416384964
C	-3.90593346467747	-0.24052224521533	-2.35432566362139
H	-4.27129499105976	-1.26216507852147	-2.56235029388461
C	4.36397616630571	-0.59618449825248	1.43367959307834
H	4.22883733436411	-1.68378906827514	1.34031584643574
C	1.72959286476551	1.51342341309018	-0.14348441456453
C	3.67080027820770	1.72916093328069	1.06633197590859
C	5.67220584487090	1.29518144664738	2.31938336699591
H	6.54989394590129	1.65254596191096	2.88500339582914
C	4.76912750869879	2.23242452046514	1.77998084509783
H	4.92257643536539	3.31581622251490	1.91774166701632
C	5.46751018105032	-0.09166636774215	2.15278956985222
H	6.18472376521425	-0.80422660502805	2.59528701142112
C	-0.11508095796549	-2.85439133143547	-1.29963881960785
H	-0.79202907833357	-3.62660644634030	-1.70451487881873

C	-4.75863726905560	0.85514003816104	-2.48267730261118
H	-5.80466484379907	0.70911269485736	-2.80354677520269
C	-0.51741650491896	-1.49318193430275	-1.28536815139288
H	-2.26698785565511	-2.03079815497004	-2.12131372485711
C	-0.53101003432257	3.49926272358211	-3.78848381085299
C	0.51613112696553	2.77942064490885	-2.91596316929353
H	-0.02086836337309	3.15240461702333	-1.56718956582761
H	-1.49537613522988	2.95462895744115	-3.81345964359693
H	-0.69994512949846	4.55242807689995	-3.47354701447266
H	-0.13634300367405	3.51848448231124	-4.83054885703363
C	1.87500880647618	3.50460043020448	-2.90148117667708
H	2.62290640309261	2.95891460555730	-2.29245489127748
H	2.24971977972679	3.52727194623456	-3.95081684271478
H	1.79580030855378	4.55778052441212	-2.55427419101777
O	0.55029507742214	1.45655906210022	-3.00554751845923
H	-2.30460699784385	2.28462491682578	1.17534641882715
H	-0.37931252730945	2.93320076210274	1.93056461055026
H	-0.94021629340901	0.85999991321596	2.07655172211492
C	2.42457403230979	3.84850259847222	0.49279843531602
H	1.46787810450957	4.10606055514475	-0.00360207451709
H	3.25919179859453	4.36758777711001	-0.02847383667765
H	2.39310514790282	4.19643793528297	1.54968619794223

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**B(Me)-PH3**



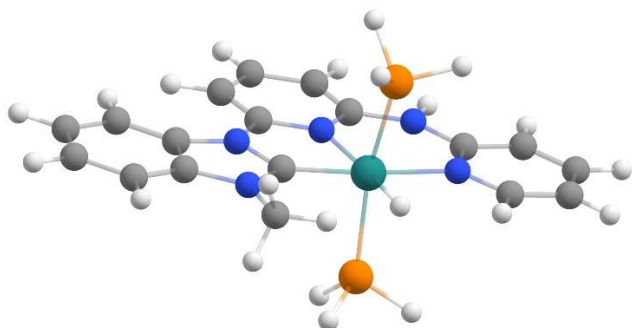
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N	-1.79777975958429	-1.13410550377869	-1.78222973358305
N	2.50545661130969	2.45499781660697	0.60140810205875
N	-2.16144814667005	1.25101331244576	-1.54132978504840
N	2.22008312709437	0.29843539449934	0.17864339238470
N	0.25510469578415	-0.49067434258277	-0.74633173851674
C	3.44546515129876	0.39528050103158	0.88113816744641
C	-2.59411655762666	0.00977284831188	-1.89407928080665
C	2.01626805756351	-2.12095977759853	-0.37576622994638
H	3.03956444163504	-2.36217271818224	-0.06108552596668
C	-4.34543365035453	2.16357470626599	-2.12561369712369
H	-4.99860851313772	3.04909557413045	-2.19343746127149
C	-3.04063104954084	2.29311353533691	-1.65107507630141
H	-2.63737722579603	3.27230996033085	-1.34226875496666
C	1.17717631989530	-3.11949079735696	-0.90738228566329
H	1.54001496487226	-4.15936124778029	-0.97655774230116
C	1.51213434139930	-0.81330514538283	-0.30706487025174
C	-3.91140083510553	-0.19614745561249	-2.39877662836015

H	-4.23431618639873	-1.21300594998273	-2.68601917730040
C	4.39506020862703	-0.53441326313883	1.34151423936950
H	4.28792248861577	-1.61927904096331	1.19660284454637
C	1.62814901360131	1.57906060115173	0.01118877887521
C	3.62063459023831	1.78397092554588	1.13587449086414
C	5.69355894937861	1.34596951307549	2.26509842148221
H	6.58774485072290	1.69895769743724	2.80713210852095
C	4.73908139700962	2.28204839018931	1.82149726932023
H	4.86767445641703	3.36087233545138	2.01089174828470
C	5.51854934356144	-0.03557779726546	2.03287378334374
H	6.27569017486675	-0.74902093243512	2.40130855493587
C	-0.10277622787016	-2.79672128926476	-1.36411100610820
H	-0.76176025431487	-3.57106050314364	-1.79389764824518
C	-4.78729988559968	0.88132175573100	-2.51795551520192
H	-5.80814485023741	0.72533759964760	-2.90794401334099
C	-0.53322248983705	-1.44462284194643	-1.28626983493184
H	-2.27781492112729	-1.96495399119380	-2.14365067960722
C	-0.45695998037981	3.39563693462828	-3.65249994765288
C	0.59100888537400	2.55265142423493	-2.93247566016153
H	-0.38212468975775	3.22618825817061	-0.72924329748586
H	-1.44289154829240	2.89228139938150	-3.68478774619025
H	-0.55897041380573	4.41081464592936	-3.21320497023808
H	-0.11401864205730	3.53064130043639	-4.70742831823391
C	1.97428995044123	3.18655326935499	-2.82468332818150
H	2.68589768346626	2.53879016899481	-2.27508493306835

H	2.36551610888600	3.31417985390432	-3.86367660235874
H	1.94245375836338	4.19960820201944	-2.37055242628557
O	0.46236724731891	1.27936940648601	-2.86868226630037
H	-2.40513327940721	2.23777794738623	1.39898789743272
H	-0.45213389505310	2.77695361160578	2.19688742313291
H	-1.07256552684505	0.70101183270803	2.17983389386655
C	2.31585286454596	3.90088196291923	0.68393097313175
H	1.34961164991398	4.15149233253159	0.20101999467848
H	3.14142431088144	4.43417929360935	0.16218088314409
H	2.29701589175202	4.22986467327332	1.74713726938948

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### 6-dft-PH3



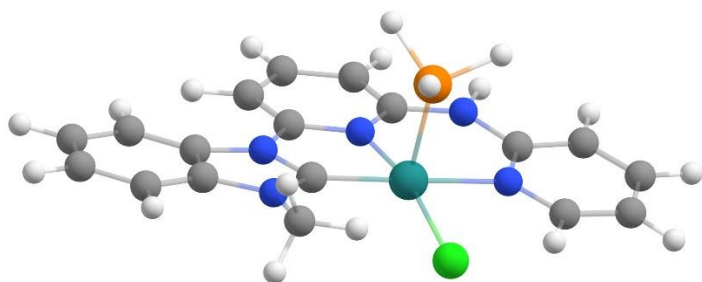
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P	-1.20621752405084	1.69950853954117	1.68405304930574
P	-0.11219747756954	2.84425690264063	-2.61623506227638
N	0.48642682985172	0.12701612851368	-0.74004560137240
N	2.26887268739825	1.37203121175229	0.04173365996365
N	-2.37763812282683	1.18526797966527	-1.19570379716079
N	2.02037102879405	3.51805369235944	0.53892102314701
N	-1.44677436964357	-1.02728497632413	-1.53924832695102

C	-0.09584258640476	-1.00967287434751	-1.18587798084183
C	-4.86979536571101	0.21075552576892	-2.10514573578957
C	0.63896093831526	-2.21722431965569	-1.30993785167542
C	5.86046826949774	2.01437934954943	1.10821720968079
C	4.41845249287165	3.99311845753328	1.26581367197527
C	5.67629667473154	3.37880157167823	1.41999376146004
C	3.36593386263190	3.19460289501768	0.79321267741858
C	1.32296629681884	2.43294218822807	0.07977526985413
C	4.80160189859355	1.21297278914791	0.63352705536405
C	-3.75584510225714	-0.62666076314196	-2.03795902512555
C	1.81651620349912	0.11732527888719	-0.39967438904572
C	1.99280478772417	-2.21888951176768	-0.95928413005784
C	-3.48041375164232	1.99137825099547	-1.26817105388220
C	-4.73148266055484	1.55750578474778	-1.70977372099680
C	2.60583973015862	-1.04052312858308	-0.49463222172533
C	-2.50942672925530	-0.11580013071104	-1.57604552442958
C	3.54137433548425	1.81791802518383	0.47750972736703
H	-0.79861177783475	0.57583274570900	2.50004070745612
H	-1.24989188353878	3.08022730674969	-3.46903714477247
H	0.49447127102805	4.14271701905206	-2.73895782303440
H	0.71501553290193	2.17901464292906	-3.60036655137575
H	-0.91571127787498	2.72317433934687	2.65189796291692
H	-2.62283262197372	1.59712525476394	1.92934335934369
H	-1.74029396780136	-1.95676804666879	-1.85792076478504
H	-5.83746468142449	-0.18213700429231	-2.46257421379269

H	0.14892815608855	-3.13640260728692	-1.67565950225382
H	6.85652481552557	1.55685099289283	1.23684844723993
H	4.26991377035251	5.05889287387250	1.50739210550692
H	6.52911194746493	3.97397752515049	1.78936628401700
H	4.99147557681478	0.15510460319753	0.40182809348111
H	-3.83419562651477	-1.68617185437989	-2.34152257597948
H	2.58371478753790	-3.14660388029512	-1.04640119950598
H	-3.31014367397580	3.03269364951043	-0.94677239309436
H	-5.57828558725066	2.26268210147496	-1.74242241268641
H	3.66716158109821	-1.03978566728673	-0.21740387424539
C	1.44740442310498	4.84720632518897	0.74176533812537
H	0.37501172284148	4.80209685029855	0.46084474576546
H	1.96950509635052	5.59719683662531	0.10629190412059
H	1.54230202597655	5.15323568733942	1.80769051150972

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### 6a-dft-PH3



Ru	-0.56223753335435	1.97921376423829	-0.44706606182644
Cl	-1.38236514056928	4.18426305295600	-0.65294169410527
P	-1.15415708977950	1.62956560555941	1.63561250028849
N	0.40511951129352	0.18235273441428	-0.68471279756815
N	2.22275005420462	1.43879292956853	0.01032494444212

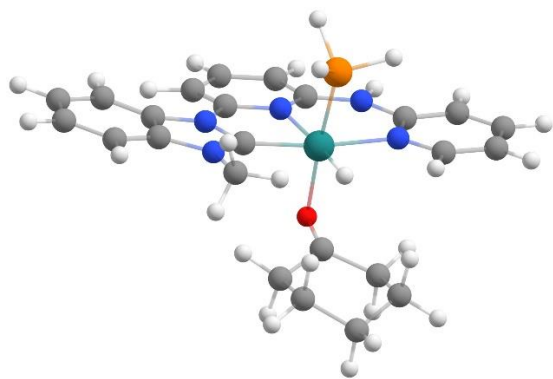


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N	-1.53590216742397	-1.05925884622318	-1.33331966465613
C	-0.17019516136198	-0.98238836025983	-1.09495456151901
C	-4.91951697353385	0.15148372603260	-2.10989179347911
C	0.59185488908549	-2.16683057122882	-1.27314940916094
C	5.83699407983744	2.06698376995018	1.00157893988415
C	4.36286703054009	3.99305582389652	1.36920537430639
C	5.63586445594760	3.39736249189442	1.43198203016556
C	3.31133903181024	3.20884663439524	0.86863563640606
C	1.26487976528394	2.47755525295662	0.14397523592182
C	4.78066801107772	1.28228690479882	0.49744444163513
C	-3.82340899931828	-0.69037420174152	-1.92497820986284
C	1.76544409869288	0.19070685050715	-0.43049046271927
C	1.96293590116845	-2.13953217593649	-1.01863335052639
C	-3.51413282216993	1.99432482288920	-1.44110280474356
C	-4.75905104867632	1.53092806116720	-1.86508125596780
C	2.57050971490469	-0.94393991538584	-0.59108653950627
C	-2.58156317990499	-0.14546703168165	-1.49476758662246
C	3.50235099306038	1.86848330064663	0.43867972944478
H	-0.40141915095304	0.69584751073808	2.43807283221312
H	-1.15661411452150	2.75445907745536	2.53582862867583
H	-2.48476635360407	1.12751965951091	1.87180216491270
H	-1.82772230779775	-2.01437909881779	-1.56745536086543
H	-5.88703856423887	-0.26173675650471	-2.44442993559860

H	0.09765558244661	-3.09290933844498	-1.61458299558459
H	6.84697132913852	1.62542103240771	1.05586659268304
H	4.20246722101403	5.03343844245700	1.69688237344369
H	6.48939977024726	3.98022507668314	1.81873861274000
H	4.99005044452459	0.25557580184333	0.16528245838925
H	-3.90992713348954	-1.77549069659724	-2.11393056954302
H	2.57189937130613	-3.04902447169602	-1.15610596360927
H	-3.33364462260675	3.06530784388721	-1.23777274223123
H	-5.58918975299526	2.24426609230933	-1.99840747308429
H	3.64800657182100	-0.91073021968230	-0.39158988641312
C	1.41286536866165	4.84216895836120	1.04795017770199
H	0.33081348326051	4.87144826500521	0.81478122111399
H	1.92137600669829	5.63658533672611	0.45849073565723
H	1.58679718368443	5.02904692550435	2.13094391602632

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**NPS-C(Me)-PH3**



Ru	0.12300074328788	3.17308053395906	-0.77320776331966
P	-0.43187129305977	5.00161254681378	0.40235275608072
N	-2.06279991706372	1.01929479177039	0.52692811917487
N	3.05612299944493	4.19984483954987	-0.35579447741608

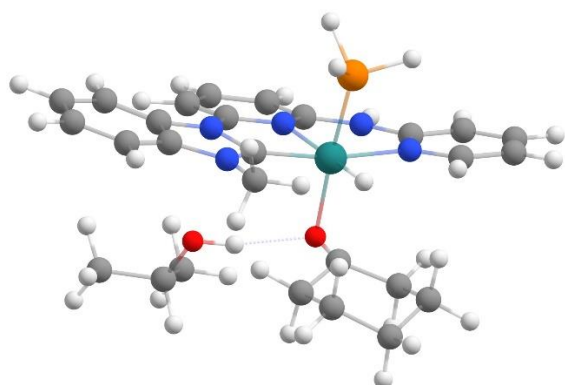
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N	2.38394067574279	2.48507164065685	0.87363916191241
N	0.20119334281951	1.73333128692610	0.78853819935684
C	3.69668204011259	2.78191509894629	1.31168073837631
C	-2.66008243063122	1.84153320032185	-0.43213856845422
C	1.72071302284788	0.50611422654749	2.23190408436000
H	2.73037328166578	0.33709354226419	2.62719651824497
C	-4.03147870517261	3.42320417667617	-2.26963246707330
H	-4.52555074659656	4.07991856351609	-3.00444277765781
C	-2.67174742157100	3.57595501814625	-2.00133140363315
H	-2.06904629763768	4.34406470653758	-2.51437908507090
C	0.66251492550927	-0.35287437016938	2.58600509457487
H	0.84253905641263	-1.18087229932113	3.29292271308944
C	1.44481089416091	1.54682560190766	1.33189832312625
C	-4.04998653782437	1.62230234776472	-0.66172791250780
H	-4.57805494927394	0.82974052896645	-0.10153407651190
C	4.54960861454518	2.26183596380040	2.30192727101887
H	4.26032398479321	1.43567543009950	2.96749217564997
C	1.97922246597353	3.36824635163420	-0.16351827776273
C	4.11812598788808	3.87726745011807	0.50818083696930
C	6.23954635292831	3.92610574957659	1.63139029889847
H	7.24559575854666	4.35799767682158	1.77035498058186
C	5.38595118315913	4.46245173191194	0.64789269905995
H	5.70419887053041	5.30977157493343	0.01773675995366
C	5.82356269218731	2.84966449259944	2.44465017822316

H	6.50768792896557	2.45453489420950	3.21530432445944
C	-0.60644053762705	-0.17380255691987	2.03066337361074
H	-1.43816259424698	-0.85171666803548	2.29022911079097
C	-4.73680646642922	2.41118688712928	-1.58281410383586
H	-5.81314549019269	2.24439802963003	-1.76226205809166
C	-0.80014302935477	0.88334234433045	1.10144115758954
H	-2.72362227262108	0.32738728914560	0.89568518689944
H	0.18118208294169	4.30620585900413	-1.97451736707295
O	0.48518907234557	1.29990033668742	-1.91677655733001
H	-1.72521474668619	5.59565479224821	0.16463279250749
H	0.36079726488616	6.19967340453926	0.30337523835424
H	-0.49904089599078	4.94939301134278	1.84572881118439
C	3.10101504914479	5.30880002476858	-1.30401699349707
C	0.67078278312706	1.96208046811538	-2.98744062075293
C	2.07542502878316	2.32792292490048	-3.46106922348271
C	-0.40960269650740	2.01044178928938	-4.06519128940384
C	2.13082478520171	3.53499132096030	-4.42337262885068
H	2.42619364473752	1.41311890474480	-4.00826504300834
H	2.75617326974947	2.43702896010519	-2.59034304154584
C	-0.32114166376829	3.22698955968049	-5.01096165337761
H	-0.23781766013779	1.07541613686036	-4.66118919464668
H	-1.41405739419790	1.88818716837406	-3.60848190938807
C	1.10469550170290	3.41062863328589	-5.56678190558374
H	3.16269533334002	3.64138250557492	-4.82956172152402
H	1.91656333320316	4.46545205451758	-3.84774910291380

H	-1.05596733734195	3.10963478707951	-5.83966896877377
H	-0.61839537660161	4.14663730541008	-4.45149082787550
H	1.14944953644305	4.31141618434467	-6.22054995110171
H	1.36854931358826	2.54245405352687	-6.21944242705586
H	2.12059574812095	5.36268240483424	-1.81855213705882
H	3.90427374856640	5.15100919198947	-2.05786905126295
H	3.29635392015528	6.26595738578789	-0.77065744771328

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### PS-C(Me)-PH3



Ru	-0.43746762568256	1.84255675986350	-0.46168626454673
H	-1.04812069857229	3.37702447245006	-0.44890989526299
P	-1.22262090614126	2.00116073691093	1.65057782381665
N	-1.41242536387064	-1.23714005258152	-1.28141582142757
N	2.04078548382702	3.36644754324783	0.73364214514361
N	-2.33965942026752	0.98665752635780	-1.03782735586821
N	2.19648287092015	1.17306075799470	0.50470635887920
N	0.45473204659044	-0.08655889719910	-0.33221393702744
C	3.41183857779096	1.58291164982749	1.09504480035201
C	-2.47813003445256	-0.33559831183261	-1.33080410160770
C	2.56019855668489	-1.24027311228256	0.02656272272221

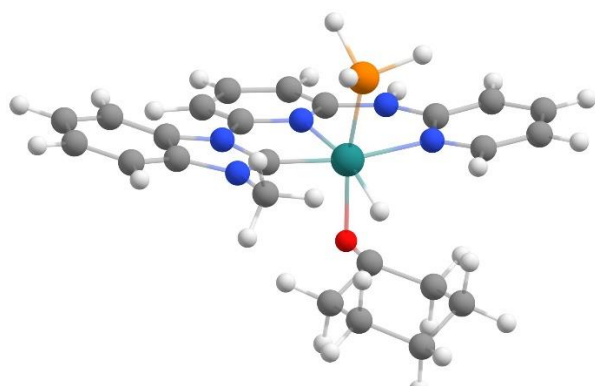
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C	-4.73011973212800	1.30163638562885	-1.40859735509688
H	-5.58875047109084	1.99300503320420	-1.41680174006759
C	-3.46222760685059	1.76895877268812	-1.06642904111554
H	-3.29521438877901	2.82866331213748	-0.80994455926026
C	1.97455214428600	-2.42274126984996	-0.45949998966941
H	2.57423657156807	-3.34729462018858	-0.51770538532122
C	1.76329384174884	-0.08637428561013	0.07387768081554
C	-3.74097166569863	-0.88021270936767	-1.70721018087435
H	-3.82118400239983	-1.95464519083979	-1.95182230242178
C	4.56167745232587	0.91525688590884	1.55313493443613
H	4.68026165162758	-0.17649526583998	1.49971067927404
C	1.35020097752917	2.28288883987493	0.25497433150646
C	3.30134047734973	2.99264633923759	1.23476338691807
C	5.47911532185927	3.09815742169926	2.23730802962654
H	6.30718559528543	3.67561559442403	2.68316746886856
C	4.32231760725275	3.77165661474782	1.79953362439306
H	4.22830270021786	4.86613940401682	1.89719154599728
C	5.59034136760347	1.69553577918408	2.11964182155809
H	6.50289667828055	1.19079092430185	2.48101345161372
C	0.64435031035898	-2.42798169033512	-0.88855568722068
H	0.17942052782680	-3.34881941718000	-1.28140529958071
C	-4.86803290731752	-0.06156960428240	-1.75000612944869
H	-5.84764174874393	-0.48063177232886	-2.03851485527367
C	-0.09551434172062	-1.21818114523372	-0.82421874325589

H	-1.68776880023148	-2.16920405668228	-1.60801432430299
O	0.17977879608929	1.60310809657839	-2.54748511940580
C	-0.20858658803468	2.83373658088003	-2.66986603803959
C	0.81828115662223	3.96492458727501	-2.73336509348074
C	-1.51057222034877	3.12670131546052	-3.41644591502379
C	0.22532378379266	5.37597648553838	-2.53214019564977
H	1.23059918545046	3.89981381992955	-3.77512617771606
H	1.68235657810055	3.75381493524831	-2.06871530219984
C	-2.08089137749006	4.53991664922003	-3.18444840552404
H	-1.22569551069776	3.02769034530529	-4.49712260123849
H	-2.25673911390228	2.32579245692963	-3.23991771086552
C	-1.00947534431459	5.62248015348780	-3.42075647183162
H	1.01185761071952	6.13968408325678	-2.73071133584630
H	-0.07414991371051	5.50230951696413	-1.46579026228332
H	-2.96011383740771	4.70236464948245	-3.84871424614063
H	-2.45699569273168	4.61875480862710	-2.13555747544229
H	-1.43018959222101	6.63416443806772	-3.21989650798884
H	-0.70787552966831	5.62100128619896	-4.49694024700242
C	3.30746801912067	-0.47132396214340	-3.84679850932936
C	3.82357550887651	0.88716127916255	-3.33615133572818
H	3.77582709994686	1.62000169528557	-4.18862775293463
H	2.25082678326213	-0.39796486058421	-4.19313972108622
H	3.91368387999871	-0.83680873280901	-4.70658409475543
H	3.35215592324016	-1.24001043483397	-3.04127703362931
C	5.27637673067715	0.82117039934545	-2.84924962411278

H	5.60856474722743	1.81179859650586	-2.46800009624576
H	5.38205951776803	0.08356863312802	-2.02029656644272
H	5.96163545798317	0.51800299719043	-3.67133600033162
O	3.03117928971644	1.37085400890296	-2.23894813067722
H	2.07618096460325	1.38062371063360	-2.50614546949302
H	-0.94091988045745	0.95391234374012	2.60492744561742
H	-2.64890233617059	2.07615534705506	1.85043732443147
H	-0.83895889058698	3.11490667747678	2.47573216590453
C	1.53685164318108	4.73464612775819	0.77423794649708
H	0.48837520973761	4.72731557173325	0.41604084208458
H	2.14435557456378	5.40151696028569	0.12266303514029
H	1.57114346656599	5.12573379240920	1.81567692196992

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**NPS-TS-II(Me)-PH3**



Ru	-0.29391977974727	1.78930651115871	-0.71500043339327
H	-0.77127121480604	3.34712602378350	-1.32380761177012
P	-1.05416312604311	2.05848328920743	1.41804548754765
N	-1.35010724037239	-1.30330977596791	-1.27868064265333



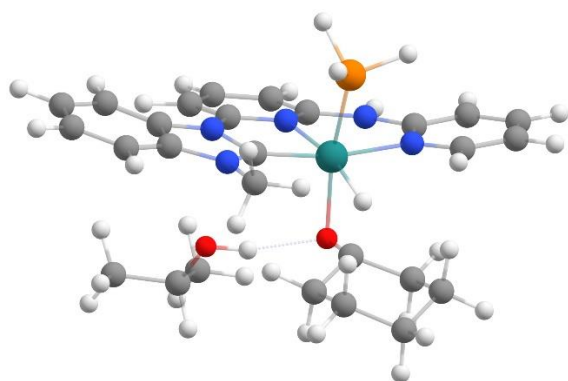
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N	-2.23470621920705	0.93673305978188	-1.17598142278425
N	2.37525289316007	1.18935723633125	0.14727829829903
N	0.56950754576321	-0.08867701971929	-0.51266232235314
C	3.57199799509626	1.61245015806990	0.77280098325588
C	-2.41242875176022	-0.40017736257213	-1.33972785361734
C	2.71087157396230	-1.23309517554088	-0.28050410401181
H	3.78937974603708	-1.19131547776783	-0.08000844143158
C	-4.63640160435744	1.26889218548981	-1.42934455684684
H	-5.48300472586686	1.97466389280720	-1.44920079056743
C	-3.34145273983661	1.73797763804273	-1.20898003828444
H	-3.14802900602721	2.81223730185836	-1.04641708302203
C	2.09866711201253	-2.43651402962202	-0.67595497049958
H	2.69630279755204	-3.36097266702508	-0.74979197937945
C	1.91204971395101	-0.08355887442087	-0.20524618616538
C	-3.70301788052505	-0.95339751652741	-1.58078430671542
H	-3.81516206309052	-2.04416305176724	-1.71568667729853
C	4.73296152568462	0.95921185066255	1.22253663460676
H	4.87832808109869	-0.12761356693637	1.13553166020792
C	1.48827649246834	2.27657731820967	-0.05132179213872
C	3.42132146765418	3.01514145785771	0.94981835603466
C	5.58597964121451	3.14389771930309	1.97984652542748
H	6.39381185190994	3.72902133302229	2.45207396070895
C	4.41791148732178	3.80198654324189	1.54719101736320
H	4.29603096653239	4.89040602640120	1.67667398628819

C	5.73487103631055	1.74856371452004	1.82451253014994
H	6.65567904527472	1.25690281959065	2.18280506123759
C	0.73968485274832	-2.45411682299863	-0.99730096095024
H	0.24879272517328	-3.38759968280360	-1.32311815808346
C	-4.81724483676910	-0.11667374543796	-1.63033584909559
H	-5.82026156047659	-0.53900627617923	-1.81478097785099
C	-0.00520870314078	-1.24799271112876	-0.92310793642388
H	-1.64113839166537	-2.25567473146526	-1.52285398090314
O	0.15163934648072	1.78197043095176	-2.76500131272698
C	-0.28395661480301	3.02962098191380	-2.74651363023067
C	0.75856130140291	4.15943705387524	-2.90220376306477
C	-1.57668307458442	3.32498164085144	-3.53857985813691
C	0.17904096679918	5.57500663147213	-2.69824779340083
H	1.12804186766634	4.05751785620323	-3.95282806013119
H	1.63852967614365	3.96241147005417	-2.25325987891601
C	-2.14352591341257	4.73965701002298	-3.31313755687014
H	-1.27344591039057	3.21045535559092	-4.60917734082986
H	-2.33040169219027	2.52982851548366	-3.36112981435170
C	-1.07308291846769	5.82124496649278	-3.56437471710893
H	0.96278586801201	6.33677925224796	-2.91546358359243
H	-0.09742602491858	5.71609064425898	-1.62463374647199
H	-3.02812233948917	4.90137065288735	-3.97068940300332
H	-2.51992995154254	4.83077397666164	-2.26278460431153
H	-1.48849574462813	6.83452502313247	-3.36048444765228
H	-0.78758608435788	5.81468331781939	-4.64449340826998

H	-0.76060477237350	3.25617089521590	2.16671412111978
H	-2.47834383482904	2.03798331896667	1.65751099688170
H	-0.68143268442645	1.12611746542049	2.46033777961640
C	1.61174839412522	4.72207855492141	0.53043151262781
H	0.57290110944426	4.70692206130183	0.14571698127254
H	2.21575224846862	5.43101053244997	-0.07850730260599
H	1.60731605644318	5.07353945669495	1.58656986504673

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### PS-TS-II(Me)-PH3



Ru	-0.35371087009375	1.76513922624059	-0.58069828268597
H	-0.81046078932076	3.33132173189140	-1.13435509674724
P	-1.16678167635387	2.05038629450228	1.52187656690158
N	-1.37684960401810	-1.31156666511920	-1.26122841090736
N	2.09197477875126	3.32773906681239	0.63899514805499
N	-2.27743053317407	0.91952064746515	-1.11006123070456
N	2.23722750795601	1.12867170175242	0.48894071835610
N	0.48446534693499	-0.12675630302558	-0.32547425639535
C	3.43389669133553	1.54701014053171	1.10907715052713
C	-2.44220372340606	-0.41283622753047	-1.32343226621585
C	2.58740807608079	-1.29141041334103	0.07125233290242

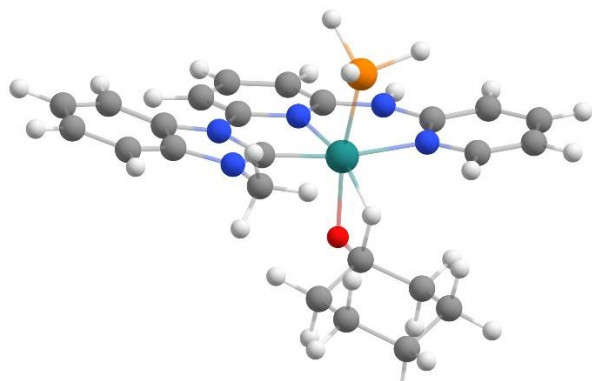
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C	-4.67411091326165	1.24620136759730	-1.41883291835686
H	-5.52448580547977	1.94747900727457	-1.43712369111493
C	-3.38937690332059	1.71427990688033	-1.14469692896458
H	-3.20786196154839	2.78376114652633	-0.94213475119726
C	2.00356732782996	-2.48168418089951	-0.39559035102684
H	2.59934380366945	-3.40951383509328	-0.43388861339080
C	1.79671285487698	-0.13364070436998	0.08990147595968
C	-3.72164830050742	-0.96325157884535	-1.62430229709050
H	-3.82248402037717	-2.04930117039957	-1.79986078468504
C	4.55676934053827	0.88310230759660	1.63368116116412
H	4.66128560613209	-0.21167064310835	1.62428722491602
C	1.41279422712872	2.23245891444149	0.16820874545234
C	3.33137041680407	2.96151475772601	1.19608563381377
C	5.47140077344509	3.07963569405597	2.27592045766278
H	6.28844589207313	3.66451009972186	2.73233218906634
C	4.33876464220261	3.74927139132667	1.77277134631668
H	4.25345767115194	4.84728035245288	1.83091334724284
C	5.57225003961440	1.67280687564448	2.21134229196333
H	6.46499641030574	1.17251556689031	2.62459509252774
C	0.67658380915286	-2.48456922529808	-0.83329297463739
H	0.20818634287139	-3.40909471508491	-1.21307813920249
C	-4.83959464482586	-0.13193279220058	-1.67715813214858
H	-5.83383461863106	-0.55287963594246	-1.90676647592347
C	-0.06319996416674	-1.27459383814227	-0.79790275880933

H	-1.65094388020483	-2.25471866342624	-1.55539048505429
O	0.15833399971530	1.74428170256679	-2.64277473863013
C	-0.28213515193424	2.99510229741824	-2.61465550507012
C	0.75529432097879	4.12656629476548	-2.75315816461436
C	-1.56934945828677	3.28456739427198	-3.40970668033836
C	0.16823148203285	5.53941826429779	-2.55360031921379
H	1.12914132360107	4.03161707244797	-3.80363523724263
H	1.63801346640295	3.92743265139261	-2.10948117412138
C	-2.14609850885784	4.69418749065938	-3.18048366860783
H	-1.25567606539128	3.18213695508180	-4.47895954165796
H	-2.31951524172070	2.48355848028969	-3.24830652168064
C	-1.08069961685618	5.78206469378413	-3.42484561704383
H	0.95190622055080	6.30166385759941	-2.76861177180505
H	-0.11333125749209	5.68227045665223	-1.48218562630845
H	-3.02910502032352	4.85139739618965	-3.84105788749262
H	-2.52624630125356	4.77850331796478	-2.13123468096570
H	-1.50215079835381	6.79247925418761	-3.21954951209070
H	-0.79129623140485	5.78023485930548	-4.50396425343717
C	3.23798653422351	-0.45539070163845	-3.79754586008861
C	3.77939736784309	0.91177934167428	-3.33763579995150
H	3.78384604706619	1.60060649939101	-4.22737497890600
H	2.19453607716892	-0.36871144162605	-4.17852417470876
H	3.85798365211291	-0.88049812688226	-4.61935937564394
H	3.23732203350081	-1.18357320515654	-2.95387632286496
C	5.21349202776946	0.82619293753659	-2.79988004698617

H	5.56757715130527	1.82542585516009	-2.46323592672859
H	5.26802400888239	0.13396190789527	-1.92776723106609
H	5.91397053559311	0.45468001805576	-3.58009839390795
O	2.96841363150463	1.47335172090240	-2.29429068123972
H	2.02361246790300	1.51693967205848	-2.59841565296326
H	-0.82348756903142	1.11814728216725	2.57354151410498
H	-2.59663545496505	2.04000590459728	1.72303644845736
H	-0.87904149215752	3.25164790635690	2.26527902740830
C	1.59496134734116	4.69821846666499	0.63221421430432
H	0.56083167302759	4.69453458566830	0.23572579548404
H	2.23028273043934	5.35045270819400	-0.00740173638316
H	1.58911171165976	5.10965825038172	1.66643049391912

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**NPS-D(Me)-PH3**



Ru	-0.40574970091646	1.52797255614959	-0.87412447543579
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H	-0.68534564627417	3.04315054780019	-1.83201975572040
P	-1.09089903317962	2.11986171481545	1.23167424258775
N	-1.83080683935117	-1.44654722498224	-1.04135123795378
N	2.22746471192038	2.95836724793866	0.05507572193687
N	-2.44009889651915	0.87348551850631	-1.22826090114766
N	2.19090084862395	0.74599454127590	0.04743471819510
N	0.23311372167120	-0.37525828931047	-0.44298344213211
C	3.44370695885091	1.10616628774755	0.59906524362639
C	-2.77923936369827	-0.44073328594903	-1.22851481009812
C	2.22111175286143	-1.73410406354751	-0.04142836311179
H	3.29805496688369	-1.79845121864609	0.16150355507013
C	-4.78250426731289	1.46276226653138	-1.54588818476482
H	-5.53715223905849	2.25802641537153	-1.66086535019548
C	-3.43895214368145	1.79431356829974	-1.37046009115953
H	-3.11668405702258	2.84976536679615	-1.33583864084047
C	1.46260083101809	-2.89585354328377	-0.27231957386186
H	1.94112683249389	-3.88820270728305	-0.21459722601302
C	1.57232421055329	-0.49524385954029	-0.13072536728560
C	-4.12805847920730	-0.85952134967347	-1.41427277790185
H	-4.37325633495189	-1.93673353791576	-1.41689031877053
C	4.53427310358566	0.38849146282989	1.12059775656527
H	4.55368415900093	-0.70974863743687	1.17805192110280
C	1.43069972043132	1.89216260626596	-0.28793465608974
C	3.45769029079856	2.52806621137648	0.58665824915289
C	5.64802713165731	2.54086413359059	1.56907840783242

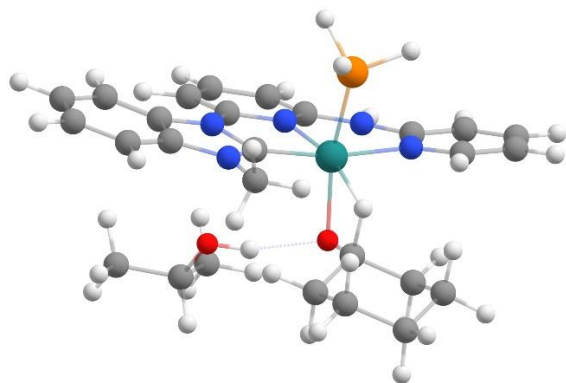
H	6.52852692686265	3.08613765699732	1.95034236189301
C	4.55155860682990	3.26655688853993	1.06311037665504
H	4.55703563971980	4.36925755879314	1.04603199916001
C	5.63412307352959	1.12950614419608	1.60099239498027
H	6.50233356484054	0.58653155134209	2.01250207966875
C	0.10855771269627	-2.78872746209206	-0.59637888275601
H	-0.49697731745529	-3.69009891118487	-0.79469876006460
C	-5.13134747275868	0.09504845792270	-1.57813437266885
H	-6.17921196699603	-0.22118946217803	-1.72098336807100
C	-0.48462759101873	-1.50299009193023	-0.69201643300912
H	-2.23337715465157	-2.38223946359736	-1.15849933334927
O	-0.01948300684336	1.25295087700324	-2.89246002439446
C	-0.31289841173521	2.55843079864056	-3.02843841682383
C	0.87056751280492	3.49589047926007	-3.38001427688176
C	-1.55191105371171	2.87545637221184	-3.90414688253332
C	0.48261725701369	4.98941987641820	-3.40706547673633
H	1.20465282757351	3.17594930965940	-4.39706350039405
H	1.72844363913301	3.29427605104269	-2.70250406098941
C	-1.93330953791282	4.36845479545682	-3.91473381935241
H	-1.26318035005684	2.55086928024834	-4.93378507347494
H	-2.40505141942657	2.22513538768288	-3.61696005911386
C	-0.73564520440558	5.25431589318356	-4.31541783931959
H	1.35565245173095	5.59995621794847	-3.73410388988427
H	0.23928479709091	5.33533654765806	-2.37175928113759
H	-2.79280303964593	4.53488968825250	-4.60385853865104



H	-2.29384253132146	4.67207718462366	-2.89873057491318
H	-1.01827879741470	6.33122155383245	-4.27797093958736
H	-0.46029994207554	5.04226544751669	-5.37717134126125
H	-0.72466423322840	1.31050379322567	2.37368174076065
H	-0.72592800888453	3.38738546169857	1.81942250560871
H	-2.50573757459709	2.19845154847746	1.51327545381799
C	1.83958307577967	4.36201150064160	-0.03468652524838
H	0.79551361295687	4.41921332143547	-0.40137402633946
H	2.50219081940134	4.91515678078668	-0.73676349316225
H	1.90045085699928	4.84365623855948	0.96698563398615

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### PS-D(Me)-PH3



Ru	-0.30267162310570	1.73679687850359	-0.55589649094953
H	-0.75599419182617	3.35697694502750	-1.24870223864700
P	-1.10996065602911	1.92756542428567	1.57195125251252
N	-1.25086623597580	-1.32225794334676	-1.34941782045289
N	2.12871953127879	3.33088867209659	0.68745701754816
N	-2.19908592814624	0.87366321663135	-1.13581661341808
N	2.28846938155901	1.13350078125359	0.54595106207136
N	0.55938360205663	-0.12023444768560	-0.32257159534809

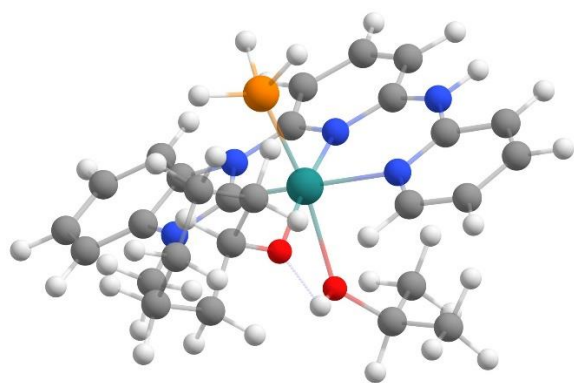
C	3.49536128204139	1.56286932250573	1.14258867418279
C	-2.32848777133694	-0.44355364602032	-1.43498998548438
C	2.63228166015892	-1.29641761264723	0.19700654232937
H	3.66995360978296	-1.27167248125642	0.55129871367624
C	-4.58436138950617	1.18038125671196	-1.52843328303786
H	-5.44812446821887	1.86522780372652	-1.53532277430083
C	-3.32307895560208	1.64993402218082	-1.16205201615964
H	-3.17706432741472	2.70407243337063	-0.86829239293992
C	2.06425722360691	-2.49285715425690	-0.27002780460130
H	2.65132705134118	-3.42661928933768	-0.25336451822745
C	1.85565571950173	-0.13027710407238	0.14837789757861
C	-3.57844733891480	-0.99388985645785	-1.84036663741800
H	-3.64860535942836	-2.06696567881902	-2.09324020155705
C	4.63424532256106	0.91578972486910	1.65514717303844
H	4.75433150383934	-0.17726198028388	1.65882125536494
C	1.45794237434115	2.22845034156692	0.22024442943888
C	3.38425890385770	2.97585032533455	1.21858449485003
C	5.54168523006234	3.12797598069013	2.25602991513127
H	6.36272394546528	3.72487239186156	2.68907820154220
C	4.39257502452890	3.78109057699136	1.76952787816817
H	4.29660132357726	4.87840055426189	1.81933297028380
C	5.65315097324494	1.72137642055712	2.20372461013926
H	6.55860629823133	1.23281372448098	2.60312019200265
C	0.76185242417126	-2.49150263486580	-0.77569015009232
H	0.30327021220817	-3.41880647878096	-1.16050310752212

C	-4.70773953590652	-0.17790974754285	-1.89397451655039
H	-5.68078095886219	-0.59737582395159	-2.20328092722941
C	0.02972456620506	-1.27740974256078	-0.80308666044668
H	-1.48970954337946	-2.26222536941504	-1.68186041666749
O	0.12776115819435	1.87573223696690	-2.60483732901677
C	-0.32751426871694	3.14375500417949	-2.50055666621864
C	0.70871270260368	4.27683188336798	-2.69307332346847
C	-1.60590683459294	3.44513128186961	-3.32707485752055
C	0.12389230680591	5.68342413259010	-2.43989468512731
H	1.01097155638397	4.20757377001749	-3.76708703304777
H	1.63239294966542	4.06622224873643	-2.11155055341688
C	-2.19981455747109	4.84011188947070	-3.05632821614200
H	-1.27867543562914	3.38553184207650	-4.39386052842522
H	-2.35103077831993	2.63254520908908	-3.20106749918277
C	-1.14552717807385	5.94556162379273	-3.27701879170561
H	0.89977104262306	6.45449965245715	-2.65210706931615
H	-0.14173955356264	5.80579657133778	-1.36174399572841
H	-3.08245364006945	5.00801927977285	-3.71515834366084
H	-2.58684247284982	4.89350940157501	-2.00692526784283
H	-1.56933110023449	6.94472985033580	-3.02592066901529
H	-0.87928606172583	5.98634246323462	-4.36113431462723
C	2.91512323589977	-0.49465836904978	-3.75632094754842
C	3.61499443795162	0.81320521302658	-3.33732509789266
H	3.67634473832142	1.47860871188906	-4.24274495869532
H	1.87771188348137	-0.30011337251328	-4.11259761780967

H	3.46236919246977	-1.00040142336123	-4.58438134223507
H	2.85932490021444	-1.20396818136104	-2.89849870392401
C	5.04311138209948	0.57711134542139	-2.82918599453376
H	5.51073540616836	1.53532238128432	-2.51238434716094
H	5.04192476986812	-0.10971500514458	-1.95113779153240
H	5.68143304829414	0.12419882648964	-3.61978795385010
O	2.89317448582116	1.48320252098996	-2.29362272020849
H	1.94913473133660	1.60996019136022	-2.58453074958055
H	-0.72698763232421	0.97471993935517	2.59115833652300
H	-2.53678633119083	1.86236898518480	1.78634903849000
H	-0.85715335532327	3.11447424422283	2.35135136911050
C	1.65950559410740	4.69874772357268	0.64645452162069
H	0.63568559448365	4.72966504369844	0.22510950008290
H	2.31317143574735	5.35315491942694	0.02554133838784
H	1.61735376757521	5.14504815903110	1.66753113541096

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**E(Me)-PH3**



Ru	0.20684980257885	1.48514069958252	-1.12085486578798
H	0.07294429327831	4.76862212009276	-1.15998577075446
P	-0.90202149391447	2.27996830802058	0.66250296996585
N	-1.39995491702313	-1.37686508876910	-0.64894471305364
N	2.91138981176380	2.91469413375159	-0.41750525964046
N	-1.57735002110572	0.61253744392013	-1.99926349229735
N	2.47508694868157	0.99450302476123	0.58644283831527
N	0.60687143107325	-0.21987589257774	-0.02527831005467
C	3.76096740195605	1.37753389006875	1.03856853862010
C	-2.04402724983746	-0.60502663572124	-1.62106585083980
C	2.10054202804825	-1.22923352569357	1.62659356077549
H	2.99865804194006	-1.16737555442576	2.25315278740426
C	-3.41552035967282	0.80859365232921	-3.57880443662653
H	-3.91752757756760	1.40845324192175	-4.35594147252569
C	-2.25342728929353	1.28844805454329	-2.97261420067871
H	-1.78111266805475	2.25113501062258	-3.24095194159397
C	1.26812093037332	-2.36157950327903	1.68354464100243
H	1.52456622061354	-3.20336682771989	2.34873906278261
C	1.74314488185706	-0.18625669450125	0.76052388019414

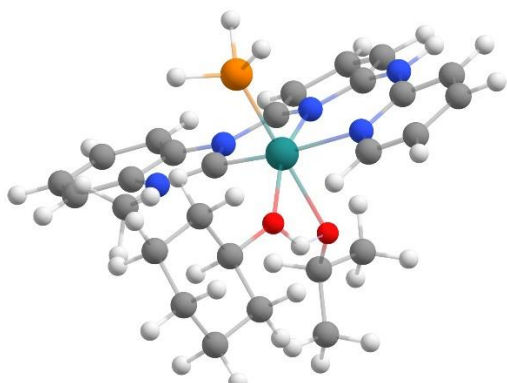
C	-3.22146753542391	-1.16134071117683	-2.19493319063813
H	-3.57800107123508	-2.15407271744095	-1.86594554800883
C	4.71332672392296	0.82016899405795	1.91135411491165
H	4.56171675304718	-0.13282732773296	2.43813113027974
C	1.93958450861084	1.95832375074929	-0.30911726288968
C	4.02454908045288	2.61423060981905	0.38822026097883
C	6.16599489425043	2.76021557505515	1.46337025498351
H	7.11705020699055	3.28920005774032	1.64691404344460
C	5.21864971333105	3.32398532187303	0.58751657786145
H	5.41049774749498	4.28599500257412	0.08358488853280
C	5.91522861873575	1.53041814108993	2.10993644005807
H	6.67445773500312	1.10962797085726	2.79151210173708
C	0.11101538743648	-2.40815444916905	0.90341205445376
H	-0.56145957915035	-3.28282175496539	0.94242323138999
C	-3.91434523983148	-0.44703415376100	-3.17394244029719
H	-4.83051010722158	-0.86943554868180	-3.62246945019623
C	-0.20648414341081	-1.30773428242548	0.06551056681982
H	-1.90495646003352	-2.24909727552756	-0.45991128696654
O	-0.07623591022369	3.09978947882547	-2.42476791864535
C	-0.45384917135441	4.42609317444126	-2.09974539769575
C	-0.02993016226424	5.39005148743943	-3.23630050982189
C	-1.97363419591484	4.59750002132255	-1.83989966115040
C	-0.38118224921704	6.85919654445081	-2.90998400880126
H	-0.54677358659972	5.07035501766557	-4.17470727873364
H	1.06262763587226	5.28664567435067	-3.43691384778695

C	-2.32510862032533	6.05396216330960	-1.46714731847426
H	-2.53372219668510	4.30939995056159	-2.76331576997862
H	-2.31888781685904	3.89569699693839	-1.04381512903647
C	-1.87748500709659	7.03251045598990	-2.57365980934656
H	-0.09466756822061	7.51779554013276	-3.76221671675542
H	0.23359004715856	7.19944060663479	-2.03987145805957
H	-3.41907762876026	6.15107021705709	-1.27712117476114
H	-1.81989900975792	6.32176442502442	-0.50560668639195
H	-2.08775826238333	8.08429501536633	-2.27108206587644
H	-2.48656025477233	6.84753553351377	-3.49262536531613
C	0.29454056284079	-0.21050462308212	-4.84992771633979
C	1.53135412686226	0.02492387507604	-3.97204439514117
H	2.37914059304236	0.34557672899292	-4.62931517999608
H	-0.04735178241075	0.72978059627073	-5.33792462727705
H	0.53852918682900	-0.93173954259771	-5.66194187694936
H	-0.55466013382544	-0.63127617382606	-4.26873560007422
C	1.96612132442599	-1.21806064204005	-3.19211792509224
H	2.84549136870574	-1.00188420441391	-2.54680989968915
H	1.14129515536678	-1.60158852561276	-2.55078210148381
H	2.25122572505321	-2.03003485179519	-3.89620139907764
O	1.34499379772876	1.11043740721376	-3.01479902596098
H	0.98200350431214	1.95469240233798	-3.41990815521765
H	-0.56967077083019	1.72917855033702	1.95817350717412
H	-2.33581779607839	2.13830175409903	0.75395403194124
H	-0.80374452363114	3.67520929184665	1.01297458069150

C	2.84767594894282	4.07846321739844	-1.29772705024445
H	1.99939963132147	3.93236155446593	-1.99364046175632
H	3.79216660709657	4.15781183479734	-1.87920028124620
H	2.70476398298753	5.01462198764550	-0.71305075929050

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**TS-III(Me)-PH3**



Ru	-0.21801305985459	1.30928363627295	-1.00681039491322
H	0.77366555259638	4.53087056178760	-2.51767441836036
P	-1.26613354840858	2.06494112354532	0.86874848666560
N	-1.81272438109533	-1.57933694431955	-0.73128163989138
N	2.33844558619845	2.79867815823342	0.09851940489551
N	-2.15712764904403	0.58360864971162	-1.72431960291867
N	2.22531986786267	0.60392240643688	0.31752640060431
N	0.27044103043993	-0.50301580480164	-0.21476925237881
C	3.45878231372175	0.98041681720722	0.89917989162802
C	-2.60325440005276	-0.66131748494280	-1.42671796058230
C	2.10056999276535	-1.84146684747442	0.70345581633026
H	3.13544458767815	-1.90823383163869	1.05957275632246
C	-4.27989022835283	1.05206398539164	-2.81819521255934
H	-4.90175907811679	1.77258684342436	-3.37473958294502



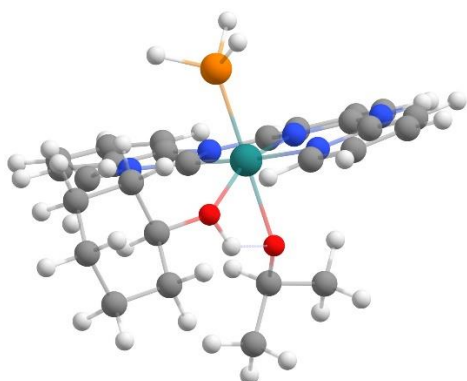
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H	-2.55198280567018	2.39368028749427	-2.65711783683508
C	1.29315482882588	-2.99103816789787	0.63255913591040
H	1.69316192272331	-3.96899909142722	0.94936942379313
C	1.55451953780207	-0.62138153911486	0.28499470889036
C	-3.90384203709499	-1.10178334449302	-1.79912557758540
H	-4.23476808752375	-2.12296010479389	-1.53753953596574
C	4.50974250597461	0.29176125782056	1.53217428384089
H	4.50980519584290	-0.79694371986054	1.68410526925557
C	1.53197920386521	1.72800618632567	-0.20665273496071
C	3.52067201504155	2.39126266662566	0.74377295556102
C	5.66452088723214	2.44939820471309	1.82283253754657
H	6.54344034681121	3.00771112967347	2.18849091702397
C	4.61435126347040	3.14635249868546	1.19469593712668
H	4.65771441193549	4.24015330905026	1.06136448870938
C	5.60845572037797	1.04876414059453	1.98859096778761
H	6.44381166525821	0.52597859270072	2.48541994526747
C	-0.01015659406782	-2.88744283671514	0.14778402729929
H	-0.65846568473173	-3.77789071154462	0.07576875425322
C	-4.74871018570741	-0.23785498614034	-2.49639025885410
H	-5.76029310753532	-0.56833690951400	-2.79004206526818
C	-0.50170580969298	-1.62416367823122	-0.27641018144576
H	-2.28291078348320	-2.48432994876342	-0.62500780614467
O	-0.53996901921621	2.88590014156526	-2.47687442635723
C	-0.30382212687140	4.27853539853574	-2.70801252595783

C	-0.59404808816333	4.61345061193068	-4.18876622709926
C	-1.18614267704414	5.13420592857004	-1.77831066369673
C	-0.40474582116179	6.12051021397790	-4.47124832098821
H	-1.64379169885562	4.31061646261566	-4.42400086021445
H	0.06650846512067	4.00333300216674	-4.84846583084336
C	-1.00465905508462	6.64440093974723	-2.04869824021576
H	-2.25324077282489	4.84537743067583	-1.94306149412607
H	-0.96858471779807	4.89644832396963	-0.70868855370970
C	-1.26827489174579	6.98689333811377	-3.53057273435275
H	-0.64722566109735	6.33720312502492	-5.53667585062067
H	0.67249682231058	6.39053215306552	-4.34156309894329
H	-1.67651343090284	7.23330059407567	-1.38300397873973
H	0.03756051855212	6.94746398245191	-1.77875494904494
H	-1.07873064914692	8.06904722272516	-3.71563244260117
H	-2.34901887742259	6.81777366041486	-3.76056053536864
C	2.11310036414960	1.13181137617127	-4.73614011142422
C	1.82384317676458	0.52156285022783	-3.35252146898849
H	2.54718476105329	0.97137028315871	-2.61873609322212
H	2.02902861354436	2.24208041843467	-4.71589346679432
H	3.14399622184309	0.88107312197653	-5.07313174074460
H	1.39746411985891	0.74360209178919	-5.49594134360071
C	2.01415283067425	-1.00463176103036	-3.35100371107651
H	1.78707396512682	-1.44598002188071	-2.35645848879996
H	1.33932209942881	-1.48275323011992	-4.09685946131116
H	3.06263446047782	-1.27703391778564	-3.60818553487935

O	0.47512938618659	0.84665038783457	-2.97183871831855
H	0.06951979364136	2.06634453808465	-3.07375771158216
H	-1.19434047046278	1.30522148737555	2.09824431084113
H	-2.69791628408841	2.24099423077449	0.83656945872573
H	-0.93685825210014	3.34325162609666	1.45492996179333
C	2.02561085117644	4.20230280512236	-0.13809858441232
H	0.95708733988533	4.29339955711298	-0.40234536778287
H	2.64684712101793	4.62245819517830	-0.96074459271909
H	2.21520877064270	4.78873207137436	0.78771836111764

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### F(Me)-PH3



Ru	-0.18388717946528	1.30764128937043	-1.01042137359650
H	0.76434476838871	4.61215139562711	-2.56803054013015
P	-1.22482105796954	2.05403011335765	0.89278750552287
N	-1.74731394293045	-1.59939272193221	-0.83586590494392
N	2.37016285668502	2.79834496361206	0.08678135420700
N	-2.13819484996829	0.60350831966141	-1.71497094793561
N	2.24194523857772	0.60931334827278	0.34497920410466
N	0.30701825692024	-0.50321000583639	-0.24096523721984
C	3.46270877441549	0.99106145514357	0.94795944396047

C	-2.55916298479503	-0.66251221996418	-1.47679977207877
C	2.13752333935232	-1.84313907746983	0.67774836100516
H	3.16960467639471	-1.90499266739979	1.04353944042922
C	-4.28856532381157	1.09246101536620	-2.74663578959813
H	-4.93263509023625	1.83163025307517	-3.25096581007698
C	-3.00050048908845	1.45227720347832	-2.34491934867989
H	-2.59367362289786	2.45721145330773	-2.53742807130630
C	1.34518833647652	-2.99983873311010	0.56654915948490
H	1.75068710875486	-3.98068759675185	0.86686309798823
C	1.58388115803215	-0.62016374197153	0.27965289718678
C	-3.85609022787802	-1.10766622664760	-1.85855655765884
H	-4.16457372109770	-2.14752597348428	-1.64814408942475
C	4.48808258321869	0.31004971800765	1.62887726127787
H	4.46845308611731	-0.77337763676743	1.81448309480538
C	1.56217626722480	1.72569781586276	-0.20894528261519
C	3.53726081014483	2.39816376464259	0.76364044189109
C	5.65411806602950	2.46447730109191	1.89511266142536
H	6.52832073189257	3.02464802668052	2.26916672222311
C	4.62592625821289	3.15469885762730	1.22412179646591
H	4.68207782945766	4.24478172582962	1.06689099354965
C	5.58105224310761	1.06927547623019	2.09561084224589
H	6.39731338039971	0.55285915646697	2.62945269167684
C	0.04974680256330	-2.89853274577564	0.06116830435676
H	-0.58740528718240	-3.79391061020874	-0.04262495744117
C	-4.72682335947326	-0.22363909615155	-2.49518769950898

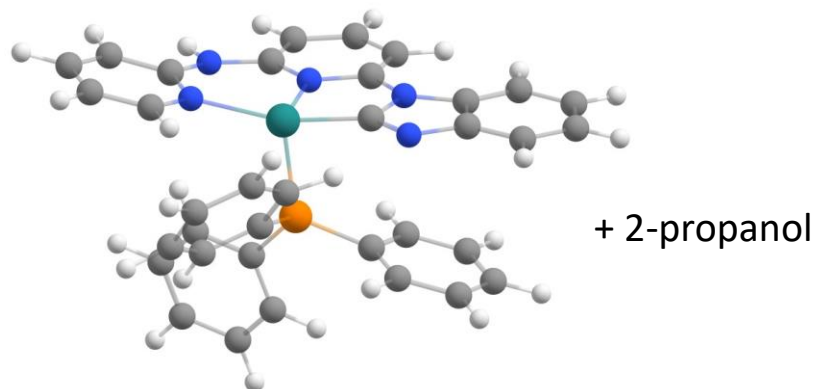
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C	-0.44913062212176	-1.63249915519506	-0.34659931580829
H	-2.19742366429054	-2.51881958453853	-0.77820245302482
O	-0.52899641588678	2.95218626550214	-2.46459898076196
C	-0.31386339839550	4.35404383481496	-2.73440835365144
C	-0.64484855337292	4.65870681694127	-4.21047588160132
C	-1.18547974727457	5.19852582876787	-1.79011628415400
C	-0.48154138731810	6.16525870944788	-4.51416370712197
H	-1.69601309032546	4.33988449338971	-4.41492208234128
H	0.00879068231452	4.04999948133437	-4.87859273096026
C	-1.02718001246766	6.70777165079254	-2.08172322340537
H	-2.25284053226695	4.89754865758545	-1.92843468285053
H	-0.93822245213800	4.97422792537968	-0.72459514674888
C	-1.33119095255341	7.03131820924337	-3.56037404896482
H	-0.75515838665754	6.36515335463374	-5.57509264133705
H	0.59536792897596	6.44909095052665	-4.41706354829856
H	-1.69026250812200	7.29446925674080	-1.40580226274935
H	0.01721180615104	7.02523605185738	-1.83925458149296
H	-1.15810916133496	8.11330092887894	-3.76095532891702
H	-2.41529037941129	6.84839381596186	-3.76176005460491
C	2.16254107863626	1.05660885836042	-4.64340716210525
C	1.79249789051470	0.39968612713973	-3.29840076550525
H	2.54442808810962	0.74816043182759	-2.53641753538021
H	2.16196200321008	2.16751167054555	-4.55983820180151
H	3.17719654673006	0.74613200938944	-4.98099435959250

H	1.43305029550868	0.76800197482247	-5.43424224975560
C	1.87498801854141	-1.13782652856460	-3.38088226537710
H	1.61711681008706	-1.61423672689046	-2.41012341203560
H	1.16640802926064	-1.52530625123163	-4.14812814411172
H	2.90057560651575	-1.47448358137174	-3.65603143553175
O	0.47793085900177	0.82088729222238	-2.93083453592688
H	0.00162363544053	2.27774497845152	-3.08105031748376
H	-1.12729258431516	1.29543717552610	2.12149029412926
H	-2.65952019454422	2.21447936193095	0.88862169866396
H	-0.90694536902314	3.33496147893277	1.48219168674965
C	2.06843608300285	4.19512814623883	-0.19606629435769
H	0.99504973624957	4.28685347990229	-0.44094319754332
H	2.67710402462344	4.57798753546164	-1.04617690372976
H	2.28171017299926	4.81419387388142	0.70266031306927

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**Why does the 2-propanol fail to protonate the anionic NHC?**

**MLC A'**



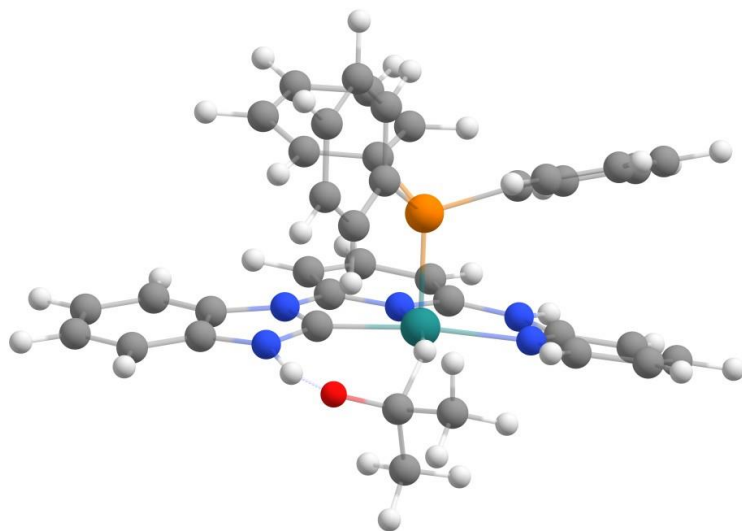
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P	-0.93708740789973	0.78163683439316	2.19785824522786
N	-2.58993756006367	0.57515199175044	-1.90837381941760
N	2.38087137212906	1.73410311795290	1.34957606981400
N	-2.36843462705160	2.50802275545702	-0.50989666879883
N	1.75865914655880	0.13882258626022	-0.14204060054279
N	-0.37759669279964	0.30143239119588	-1.00384926890249
C	0.39269278655691	-0.14649801878862	3.03427754735574
C	3.07469549889329	-0.19869705304548	0.23960961561043
C	-3.04051251009291	1.81914807950899	-1.47513034826938
C	0.99904805206296	-1.57872790492082	-1.75409273539924
C	-2.48090823806714	-0.16169917439597	2.49023102043341
C	-4.02863397877679	4.28121081019138	-0.63368699346234
C	-1.12883924585980	2.49785604812995	2.80841388161618
C	-2.86048649099331	3.72437319140844	-0.11750857740734
C	-3.63122092053373	0.11013720959329	1.71144614510788
C	-0.06377119584789	-2.02417135766407	-2.55753607370065
C	0.82447429271428	-0.41499923394414	-0.98699467490943
C	-4.24061050970478	2.32599782653259	-2.04797082995867

C	3.95332375718974	-1.24652416629962	-0.07743823666059
C	0.75900264396749	-1.40353264753015	2.49313923042424
C	1.37795981118885	1.32459187617448	0.59354672537736
C	3.43684549189775	0.83241213606297	1.17258324292102
C	-0.28164341343404	4.79854645495513	2.65550303470012
C	5.57378915411560	-0.24689123703080	1.49012538551121
C	1.14317240396521	0.41919988267252	4.08789650731362
C	4.69704934027868	0.81051831923392	1.79719672712096
C	-3.73993734028376	-1.83395422563576	3.74849582706662
C	5.20791553424944	-1.25655244862308	0.56984401907475
C	-0.05245576247449	3.40502882893182	2.52656636010305
C	-1.26065958729874	-1.30242653680936	-2.59731604736933
C	2.63567460358336	-1.51211190099852	4.04402091583502
C	-2.38434631807212	3.00085575630844	3.25426261248383
C	-4.73718226713344	3.55790318289271	-1.62039897493259
C	2.26111658550173	-0.27047396160141	4.59131059516445
C	-4.82754817025356	-0.58526770580941	1.95600574052486
C	-1.52457219156245	5.28509169524578	3.08902780715133
C	1.88003223289906	-2.08167156460313	3.00036333287818
C	-2.53943888506659	-1.13945669588952	3.51281256492666
C	-4.88244531334461	-1.56035802690573	2.97193380114263
C	-1.38738432807778	-0.12813250336401	-1.81356155477226
C	-2.56795332879992	4.38106359397913	3.40816129998728
H	1.95232700825987	-2.12334475020930	-1.72329897729402
H	-4.37733864572552	5.26268634615654	-0.27296600779844



H	-2.26976578240217	4.25075673059466	0.65220068002715
H	-3.58851536258666	0.87728620950214	0.92232668088026
H	0.05008914059800	-2.93757777025131	-3.16594455770306
H	-4.76483398277124	1.74892086309378	-2.83058039163105
H	3.70436234695264	-2.04714261189794	-0.79226382941375
H	0.17163648756046	-1.85240912707355	1.67062193138681
H	0.54664783618151	5.49771510017164	2.44313644184369
H	6.56658766099654	-0.28964305843458	1.97169746229442
H	0.86481693077297	1.40112068938758	4.50758576095936
H	4.97184305941044	1.60370754651925	2.51308738923381
H	-3.78189804187843	-2.59488486298553	4.54772407839862
H	5.91764468644014	-2.07214364157239	0.34593023324553
H	0.97490287947116	3.03826293189984	2.31861928699234
H	-2.09836368193034	-1.62819677099435	-3.23776165208254
H	3.52478389299369	-2.03997382767476	4.43066357425082
H	-3.20773469241102	2.30242579021785	3.48460928119629
H	-5.66600499019698	3.96146954242128	-2.05971060475916
H	2.85059503283789	0.17338317372155	5.41260027047099
H	-5.72406837632423	-0.36605940734000	1.34932637060092
H	-1.68454885326260	6.37184268286925	3.20415556062576
H	2.17156493723748	-3.05676505198876	2.57289502246240
H	-1.64853539443869	-1.35693330520206	4.12714751631077
H	-5.82182236931188	-2.10992284109118	3.16008990350347
H	-3.53443849434801	4.76524953621438	3.78058828366358
H	-3.23889257417963	0.13046005420389	-2.56638387636826

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**MLC-TS-I'**

Ru	-0.54655907449814	1.76092272356456	-0.28686962311069
H	-0.73579187104650	3.51244106507518	0.05059772960748
P	-1.08144553798674	1.28859405711628	1.83055880973914
N	-2.12417195997047	-0.78220587533715	-1.68970199082052
N	2.27919640633970	2.72652967216742	0.43082300521496
N	-2.51457149943759	1.53003443406335	-1.10768503873651
N	2.02891329454394	0.53174369291258	0.07456061595167
N	-0.01813360226294	-0.18824508904186	-0.72229886632220
C	-0.28170430006008	-0.28314673366845	2.41344410372693
C	3.40229449679912	0.71898719141213	0.35804472328526
C	-2.92426007338599	0.36448654207150	-1.68133448548750
C	1.72386155867558	-1.87462269285381	-0.45469144681607
C	-2.92430948132128	1.18131448544021	1.98384966356885
C	-4.70735556984599	2.49411423520844	-1.55626681465411
C	-0.62496341164639	2.42686694967384	3.21096590742098

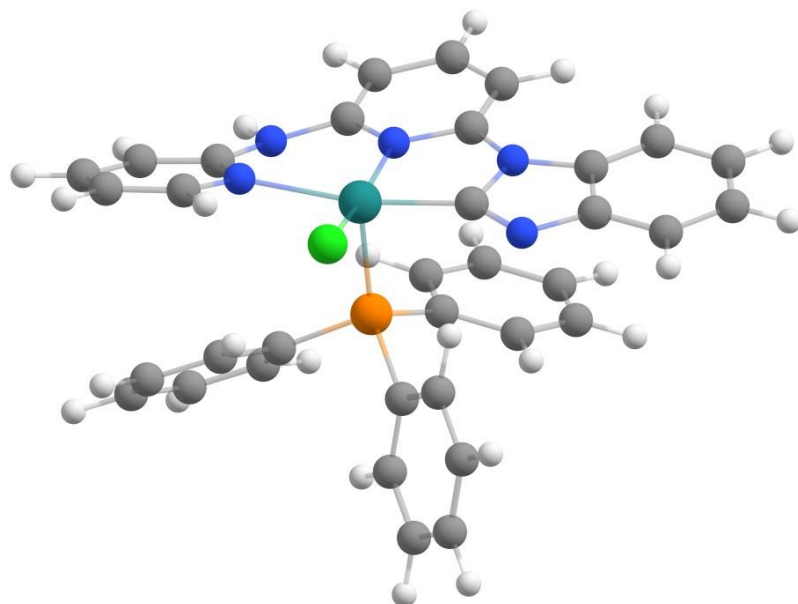
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C	-3.62022637597321	2.28404314148865	2.53632371887727
C	0.84112537438482	-2.84491474264475	-0.96297297513590
C	1.27226146513635	-0.55189979865761	-0.36198000791123
C	-4.21540588766107	0.23798208876393	-2.26720404841947
C	4.51051088146333	-0.13913365480741	0.45183877397442
C	-0.85837631933402	-1.56893746485501	2.31250519839823
C	1.36413232315696	1.78625511253828	0.15690721849062
C	3.53914369437230	2.12949176769532	0.57145663605856
C	0.30400819565869	4.49470466894110	4.10612242264126
C	5.89480058166753	1.83417532082564	0.97067728283536
C	1.05135528059727	-0.16373978675104	2.88201302006172
C	4.78741574622336	2.69822155382975	0.87660625702923
C	-5.07458034397842	0.16497940313034	1.39321941562579
C	5.75753533423670	0.44258289535893	0.76289495288083
C	-0.00139695302751	3.67259647722576	3.00152610377119
C	-0.44310767625394	-2.47982243608661	-1.37526553965479
C	1.21493061680497	-2.58620629088175	3.10745127131517
C	-0.93896800339916	2.00440435583506	4.52835550650528
C	-5.10930719516086	1.30564462521435	-2.20444031085009
C	1.79338920363164	-1.30702008421921	3.22289674408343
C	-5.02711669693598	2.31982042207289	2.52207188957475
C	-0.01185391091670	4.07978740225159	5.41163251487967
C	-0.11329037652601	-2.71162519443660	2.66084781964920
C	-3.66996762514527	0.12918380409085	1.39829247185461

C	-5.75878875024126	1.26035763332481	1.95553743251405
C	-0.84654572540653	-1.12532336005944	-1.24595673954061
C	-0.63471759104806	2.83134946554735	5.62123554270250
H	1.80157662246975	3.87827228826210	0.29569925146310
H	2.73514990332191	-2.14798901971951	-0.12703311567412
H	-5.38331845912899	3.35881993095040	-1.45727723640505
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H	-3.06027016964495	3.12370379949436	2.98239693555748
H	1.16631124623891	-3.89635978110971	-1.04034920724410
H	-4.50751260470617	-0.71078098164169	-2.75211773669649
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H	-1.90241087651974	-1.69923027887110	1.98867366339772
H	0.79790294140603	5.46721974280481	3.93310594336682
H	6.88830992253445	2.25024862864297	1.21243641807798
H	1.51334921944847	0.83336371145385	2.99336394742505
H	4.88696184023549	3.78481868422783	1.03882195977966
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H	-1.42307726974126	1.02596196012052	4.70175737023480
H	-6.11588185180549	1.21243279284442	-2.64775474450675
H	2.82914314165786	-1.19365905270754	3.58897766715275
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H	-0.58276277305840	-3.70879122480499	2.58895621769812
H	-3.16060347505954	-0.72044925837483	0.91586965932438
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H	-0.88256556179468	2.49868903480867	6.64489970878703
H	-2.59963540376194	-1.57674889598073	-2.13035640029847
C	-0.09843487716082	4.56350590396048	-0.53003202597819
O	0.99320599760697	4.84607735777283	0.16409150594254
C	-1.22060515316438	5.60065413160731	-0.32027926770811
H	-0.84931826651866	6.58517945212394	-0.68567210884867
H	-2.14759752551876	5.35589707489060	-0.88275942452560
H	-1.46085660082098	5.70986819457061	0.75878294384967
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H	0.85178034319976	3.34891463399403	-2.14007762627512
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**1a'**



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N	-2.51050580535749	1.54278285195482	-1.28693923706670
N	2.03355245707215	0.45405131657866	-0.11988580808994
N	-0.06146990599563	-0.18904382278255	-0.82250130041570
C	-0.15251922686872	-0.20786332251325	2.33416660799597
C	3.36017858480029	0.52213113088922	0.33449594398347
C	-3.07036023832903	0.31228518611935	-1.42253374365401
C	1.73122343961685	-1.84777714575867	-0.98140772331479
C	-2.85649884286820	1.06768224154614	1.94440041301268
C	-4.62877545284767	2.54293813942285	-1.94734390389637
C	-0.67515442945142	2.54732206995162	3.04799482901593
C	-3.28330851381197	2.62807048617247	-1.58307520860895
C	-3.65132628247886	2.18201840462052	1.57587086819468

C	0.81081327619945	-2.79332072091781	-1.45791109850727
C	1.26839756077577	-0.56061214939615	-0.64844154551794
C	-4.44808644641302	0.14606338415832	-1.73534238133469
C	4.43303811710816	-0.38334559050842	0.39595705612446
C	-0.52771790242082	-1.51135499086947	1.92738512020869
C	1.39255436946559	1.74964192669466	0.15065165871551
C	3.48084156750727	1.86379178356719	0.83990587532783
C	0.47832062505463	4.50342589852444	3.92679264343034
C	5.77229685821987	1.38880619466344	1.46342370362345
C	1.06844941208335	-0.03160610244866	3.02802537243400
C	4.69733222445228	2.29658317593205	1.40353350990736
C	-4.89231440871255	-0.16884950916809	2.49801044564428
C	5.64135488267677	0.07050451361028	0.96951414848856
C	0.22624504077531	3.61656277826768	2.86073079533429
C	-0.54124298702291	-2.44713027783187	-1.58153814273764
C	1.51027327971377	-2.42865339833457	2.90621507000721
C	-1.31496530597897	2.37262404172936	4.29998176140988
C	-5.23338422044434	1.27008266521259	-1.99445012507013
C	1.89605908932381	-1.13455321653902	3.30423592131448
C	-5.05111288775049	2.10972737829663	1.65285411430532
C	-0.15821868043929	4.33309119380942	5.16939911069355
C	0.29351231660976	-2.61382188650759	2.22264394651339
C	-3.48616562093460	-0.10148160989800	2.42469754466841
C	-5.67746858483481	0.92955542684494	2.10289158420651
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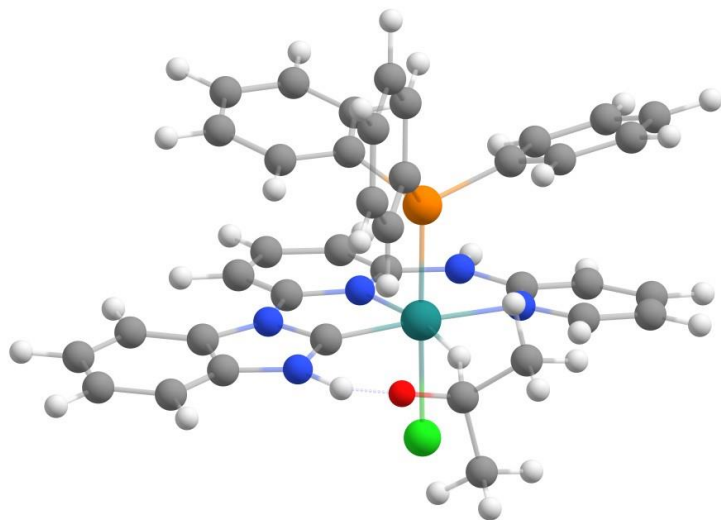
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H	-3.15885050826087	3.10987826473891	1.22882637222464
H	1.15094391753562	-3.80670114334517	-1.73250958902905
H	-4.88114295332908	-0.86932737586862	-1.78415706815406
H	4.36454327252155	-1.42031194265017	0.02979289854499
H	-1.45737568382206	-1.67044378295949	1.35683781597749
H	1.18493411634408	5.33917035403587	3.77507279447765
H	6.73346671070732	1.70886348670427	1.90459973045007
H	1.38916788021729	0.97990540920313	3.33135707218966
H	4.78399405064911	3.32695197857696	1.78972421373894
H	-5.37474091658285	-1.08760102962066	2.87850820432862
H	6.49773838323904	-0.62448226147062	1.03254001415001
H	0.75196589575534	3.74439583734282	1.89966041911533
H	-1.28650842109963	-3.17558868136773	-1.94597860919097
H	2.16300476921260	-3.29359389224713	3.12155878194469
H	-2.02346881700527	1.53864717757482	4.45299068188286
H	-6.30335454861468	1.15338797014938	-2.24156534239264
H	2.85576279232799	-0.97540658769423	3.82670393498236
H	-5.65900369797069	2.98399117197669	1.35887389166174
H	0.04269445859966	5.03646340737096	5.99803869227081
H	-0.01357431063190	-3.62403315148673	1.89731801167524
H	-2.88539507255942	-0.95898416026032	2.77055884073273



H	-6.77954658691188	0.87256676911174	2.15862829135831
H	-1.55971449015666	3.12010972042632	6.32927562302517
H	-2.87480947017437	-1.69479465052994	-1.42885446477909
Cl	-0.75886121550657	4.10689805289624	-0.32870106583886

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**TS-1-Cl**



Ru	-0.53779320998570	1.68452821098464	-0.42770439436212
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N	-2.13873200281636	-0.96842700382879	-1.47078258292200
N	2.24347988230977	2.77116301594275	0.25426164239820
N	-2.54336453885108	1.38063287021363	-1.11616487023423
N	2.05703012649857	0.56249921900727	-0.02371176191236
N	-0.00044039159994	-0.26780146370824	-0.65545262820025
C	-0.37459908398511	-0.25216359685772	2.38794797933035
C	3.41560049183049	0.79635724775147	0.27588844275531
C	-2.94593824359756	0.16966948376804	-1.57500496327160
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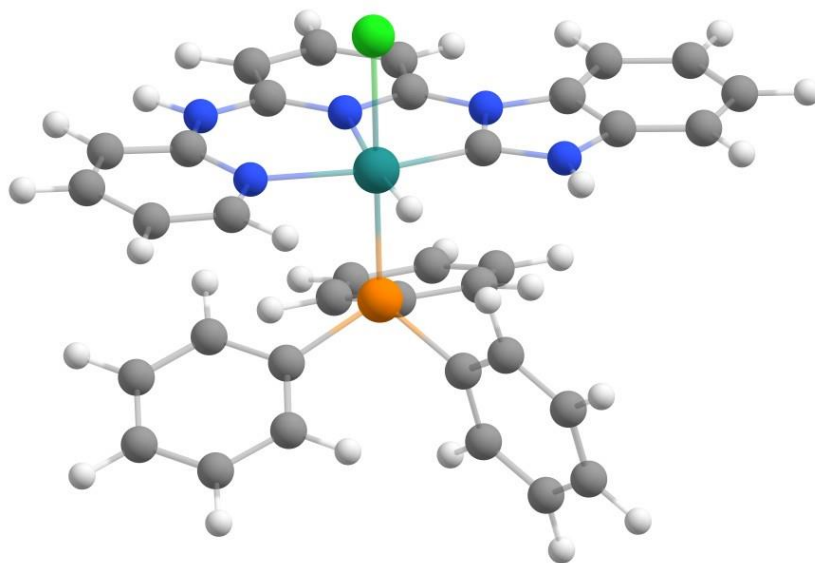
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C	-3.42180633157604	2.41715391771736	-1.17590268369374
C	-3.62570887722923	2.47195151913599	2.43583197070302
C	0.95473896294554	-2.88933466583221	-0.90205864251867
C	1.32246981961795	-0.56499062705051	-0.38250339195521
C	-4.23881878990428	-0.01714486154040	-2.13918817231967
C	4.54230541937429	-0.02735843921999	0.43183966294880
C	-0.96132080395781	-1.53354322686151	2.29575218729397
C	1.35152572516884	1.79924371481793	-0.00488717767087
C	3.51222189952150	2.21828514912958	0.44363743370088
C	0.51990045817265	4.28121822990184	4.24774069318633
C	5.86725254802656	1.99329969442977	0.90980036394954
C	0.97297261428825	-0.15790318923374	2.82187126044800
C	4.73929768130023	2.82499906973239	0.75920379963337
C	-5.18397662445644	0.34873565522075	1.46227907383072
C	5.76998546492350	0.59331447136406	0.75088700685425
C	0.15090218291509	3.54966447687078	3.09765383333924
C	-0.36729200471926	-2.58361910964970	-1.23848439173430
C	1.11969589266258	-2.58333495756595	3.02928034119344
C	-1.08317985321317	1.99007096181468	4.51765514708675
C	-5.12851571691853	1.05668147873971	-2.19166679216995
C	1.71177270818038	-1.31005390856254	3.13779443658782
C	-5.02811470441754	2.58017513821102	2.41057439012352

C	0.09252904324604	3.87433313447526	5.52278790498803
C	-0.22026379303298	-2.68797827766249	2.61578656753642
C	-3.78174852441169	0.24368926590917	1.47765948283513
C	-5.81442974509132	1.51770846181965	1.92767869821868
C	-0.81665388995430	-1.24347795342847	-1.11627293515950
C	-0.71402038567248	2.72376296372439	5.65592040778835
H	1.77970755034561	3.86894511117120	0.26315164992702
H	2.87088602352413	-2.09039457347473	-0.22484226756356
H	-5.37978485526007	3.18744471619901	-1.70078889827535
H	-3.04236184552871	3.37258258322737	-0.77817506860206
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H	-4.53228896190303	-1.01073771839914	-2.52404119080875
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H	-2.01183826570781	-1.65299746679628	1.98806131027706
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H	6.84411437206535	2.44496828275392	1.15794096814974
H	1.45361330763877	0.83181493181583	2.91829988887884
H	4.80750501940606	3.91905414795779	0.88410337388735
H	-5.78813157676818	-0.48875516191281	1.06947980823859
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H	-1.05740286303526	-3.36705154049039	-1.59791872868407
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H	-0.70165038392976	-3.67972617899070	2.53956628559413
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H	-6.91572520153438	1.60234381652313	1.90809493911286
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H	-2.61080028146068	-1.80212547297189	-1.83321723025926
C	-0.23792827862093	4.76840231767982	-0.26498416307938
O	0.91701062552406	4.89302743036411	0.38173743261426
C	-1.42669830587107	5.43172373949443	0.47330440736406
H	-1.24546789622563	6.53066145481057	0.51765769174932
H	-2.39733422176256	5.26700306428591	-0.04638899715146
H	-1.51098943581891	5.05954813611084	1.51631202092083
C	-0.19750744955554	5.10641600926877	-1.76570883375335
H	0.56351765426274	4.49515150126279	-2.29304789949552
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2b



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H	1.83284689897393	-3.43842331982925	3.18981663513569
H	-0.90872614734278	1.16169454226294	4.74833798800151
H	-6.12499823197268	1.13397468105029	-2.64317071763311
H	2.86444410117177	-1.14296480006406	3.39077787602590
H	-5.63551050237349	2.90387821044788	3.36753932755583

H	0.31568842319228	5.19401589284036	5.83290516982656
H	-0.59309356709767	-3.65178413262189	2.54545165536926
H	-3.17215486187817	-0.63441358680670	0.80989632437127
H	-6.91131019277102	1.06539633617466	2.21124450277219
H	-0.28407145731368	2.84160069742119	6.49690002656619
H	-2.62735431442445	-1.65912928773526	-2.11931379366087
Cl	0.03003612963561	2.35495541500666	-2.67438446424527