

Supporting Information

**Palladium-Catalyzed Decarboxylative Allylation of Vinyloxazolidin-2-ones with Sodium Sulfinates: Stereoselective Assembly of Highly Functionalized (Z)-Allylic Amines**

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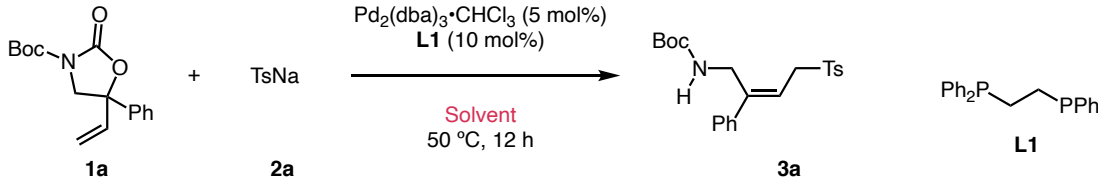
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## 1. Supporting Figures and Tables.

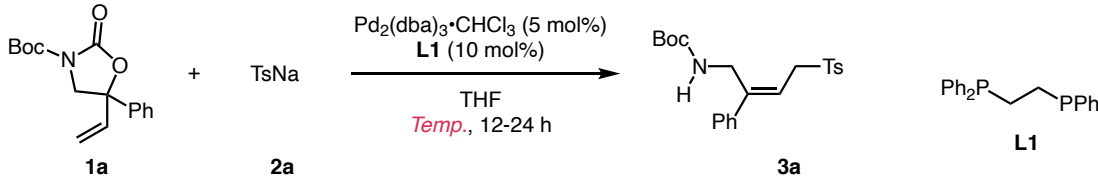
**Table S1.** Effect of solvents.



Entry <sup>a</sup>	Solvent	Yield (%) <sup>b</sup>	Z/E <sup>b</sup>
1	DCE	58	82:18
2	THF	82	77:23
3	toluene	57	80:20
4	MeCN	59	90:10

<sup>a</sup> Reactions were performed with **1** (0.12 mmol) and **2** (0.18 mmol, 1.5 equiv.) in THF (6 ml). <sup>b</sup> Z:E ratios were determined by <sup>1</sup>H NMR.

**Table S2.** Effect of reaction temperature.



Entry <sup>a</sup>	Temp (°C)	Time (h)	Yield (%) <sup>b</sup>	Z/E <sup>b</sup>
1	20	24	22	n.d.
2	30	24	36	n.d.
3	40	12	75	79:21
4	50	12	83	77:23
5	60	12	32	n.d.

<sup>a</sup> Reactions were performed with **1** (0.12 mmol) and **2** (0.18 mmol, 1.5 equiv.) in THF (6 ml). <sup>b</sup> Z:E ratios were determined by <sup>1</sup>H NMR.

## 2. General Procedures.

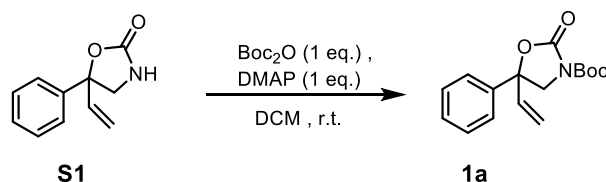
All commercial solvents and chemicals were purchased from Bidepharm, Leyan, Energy Chemical, and TCI and used as received. All reactions were performed in oven-dried glassware under a positive pressure of nitrogen.

Analytical thin-layer chromatography (TLC) was carried out using 0.2 mm commercial silica gel plates impregnated with a fluorescent indicator (254 nm). TLC plates were visualized by exposure to UV light (254 nm). Flash column chromatography was performed using granular silica gel (60-Å pore size, 40–63  $\mu\text{m}$ , 4–6%  $\text{H}_2\text{O}$  content, Synthware).

$^1\text{H}$  NMR spectra were recorded with a Bruker AM400 (400 MHz) spectrometer. Chemical shifts are reported in parts per million (ppm) units on the delta ( $\delta$ ) scale, and are referenced from the residual protium in the  $\text{CDCl}_3$  (7.26 ppm). Data are reported as follows: chemical shift, [multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet), coupling constant(s) in Hertz (Hz)].  $^{13}\text{C}$  NMR spectra were recorded with a Bruker AM 400 (100 MHz) spectrometer. Chemical shifts are reported in parts per million (ppm) units on the delta ( $\delta$ ) scale, and are referenced from the carbon resonances of  $\text{CDCl}_3$  (77.23 ppm).  $^{19}\text{F}$  NMR spectra were recorded with a Bruker AM400 (376 MHz) spectrometer. High resolution mass spectra (HRMS) were recorded on a Bruker microTOF Q III spectrometer with electrospray ionization (ESI). Melting points (mp) were recorded on an SRS–optic melting point apparatus.

### 3 Preparation of vinyloxazolidin2-ones 1

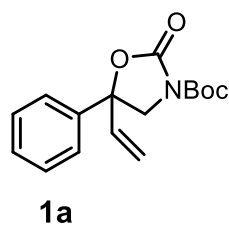
#### 3.1 General procedure for preparation of vinyloxazolidin2-ones 1.



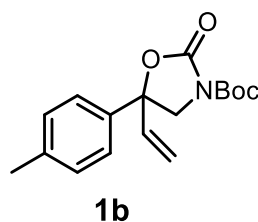
Vinyloxazolidin2-ones (**1a-1o**) were prepared following previously reported procedures:<sup>[1]</sup>

To a solution of S1 (567.6 mg, 3.00 mmol) in DCM (12 ml) was added Boc<sub>2</sub>O (654.8 mg, 3.00 mmol) and DMAP (366.5 mg, 3.00 mmol) at room temperature. The mixture was stirred for 30 min. The reaction mixture was concentrated under reduced pressure, and the residue was purified by column chromatography on silica gel (Petroleum ether/EtOAc = 10:1 as eluent) to afford **1a** (607.6 g, 2.10 mmol, 70% yield) as a light yellow oil.

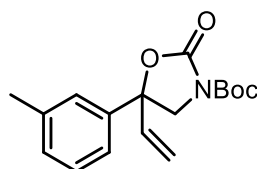
#### 3.2. Characterization Data of Vinyloxazolidin2-ones 1



(**1a**): 70% yield, 607.6 mg. Light yellow liquid. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.45 – 7.31 (m, 5H), 6.11 (dd, *J* = 17.1, 10.7 Hz, 1H), 5.43 – 5.29 (m, 2H), 4.24 – 4.08 (m, 2H), 1.53 (s, 9H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 152.3, 149.4, 140.1, 138.5, 129.0, 128.6, 125.0, 117.9, 85.1, 82.4, 55.4, 28.1.

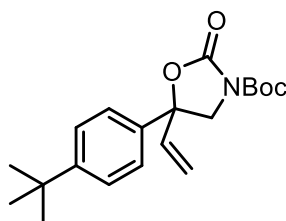


**(1b)**: 73% yield, 663.9 mg. Light yellow liquid.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.42 (d,  $J = 8.3$  Hz, 2H), 7.35 (d,  $J = 8.1$  Hz, 2H), 6.24 (dd,  $J = 17.1, 10.7$  Hz, 1H), 5.57 – 5.43 (m, 2H), 4.35 – 4.20 (m, 2H), 2.50 (s, 3H), 1.67 (s, 9H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  151.3, 149.5, 139.6, 138.2, 137.1, 129.6, 124.4, 116.3, 86.0, 82.1, 56.9, 30.5, 23.2.



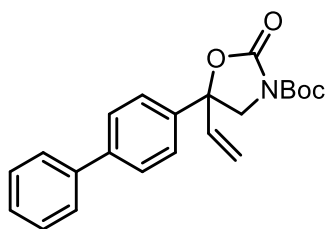
**1c**

**(1c)**: 74% yield, 673.0 mg. Light yellow liquid.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.28 (d,  $J = 10.0$  Hz, 1H), 7.21 (s, 1H), 7.16 (d,  $J = 7.7$  Hz, 2H), 6.10 (dd,  $J = 17.1, 10.6$  Hz, 1H), 5.47 – 5.26 (m, 2H), 4.28 – 3.99 (m, 2H), 2.37 (d,  $J = 1.7$  Hz, 3H), 1.53 (s, 9H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  151.3, 149.5, 140.1, 138.8, 138.2, 129.3, 128.9, 125.6, 122.0, 116.3, 84.2, 81.3, 54.9, 28.1, 21.7.



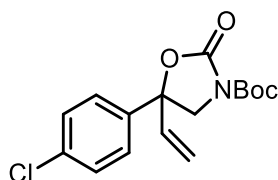
**1d**

**(1d)**: 65% yield, 673.1 mg. Yellow solid. Mp = 75.4-76.9 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.42 (d,  $J = 8.6$  Hz, 2H), 7.31 (d,  $J = 8.6$  Hz, 2H), 6.10 (dd,  $J = 17.1, 10.7$  Hz, 1H), 5.44 – 5.28 (m, 2H), 4.21 – 4.07 (m, 2H), 1.53 (s, 9H), 1.31 (s, 9H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  151.7, 151.4, 149.5, 138.1, 137.0, 126.0, 125.9, 124.8, 116.2, 84.2, 81.3, 54.8, 34.7, 31.4, 28.1.



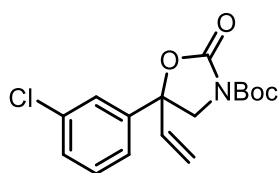
**1e**

(**1e**): 75% yield, 821.6 mg. Light yellow solid. Mp = 86.3-87.4 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.64 – 7.53 (m, 4H), 7.48 – 7.39 (m, 4H), 7.35 (d, *J* = 7.3 Hz, 1H), 6.14 (dd, *J* = 17.1, 10.6 Hz, 1H), 5.50 – 5.30 (m, 2H), 4.28 – 4.11 (m, 2H), 1.54 (s, 9H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 151.3, 149.5, 141.6, 140.3, 139.0, 138.0, 129.0, 127.8, 127.7, 127.2, 125.5, 116.6, 84.3, 81.2, 54.8, 28.1.



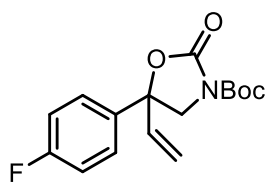
**1f**

(**1f**): 71% yield, 688.2 mg. Light yellow liquid. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.43 – 7.31 (m, 4H), 6.10 (dd, *J* = 17.1, 10.7 Hz, 1H), 5.44 – 5.28 (m, 2H), 4.24 – 4.07 (m, 2H), 1.54 (s, 9H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 150.8, 149.0, 138.4, 137.4, 134.3, 128.9, 126.3, 116.6, 84.1, 80.6, 54.5, 27.8.



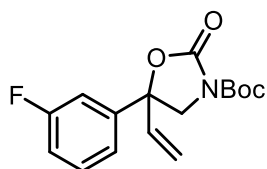
**1g**

(**1g**): 78% yield, 756.0 mg. Brown liquid. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.39 (s, 1H), 7.36 – 7.32 (m, 2H), 7.28 (dd, *J* = 4.3, 1.9 Hz, 1H), 6.08 (dd, *J* = 17.1, 10.7 Hz, 1H), 5.45 – 5.33 (m, 2H), 4.24 – 4.03 (m, 2H), 1.54 (s, 9H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 150.9, 149.2, 142.1, 137.4, 135.0, 130.3, 128.8, 125.3, 123.1, 117.0, 84.4, 80.6, 54.7, 28.0.



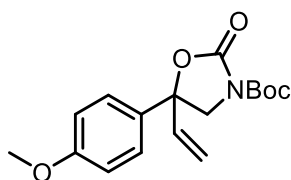
**1h**

(**1h**): 70% yield, 645.0 mg. Light yellow liquid.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.40 – 7.30 (m, 2H), 7.09 – 6.98 (m, 2H), 6.06 (dd,  $J = 17.1, 10.7$  Hz, 1H), 5.39 – 5.26 (m, 2H), 4.24 – 3.97 (m, 2H), 1.48 (s, 9H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  162.5 (d,  $J = 247.9$  Hz), 151.6, 150.0, 138.2, 135.7 (d,  $J = 3.2$  Hz), 126.9 (d,  $J = 8.3$  Hz), 116.6, 115.8 (d,  $J = 21.8$  Hz), 84.2, 80.8, 54.7, 27.9.  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -113.1.



**1i**

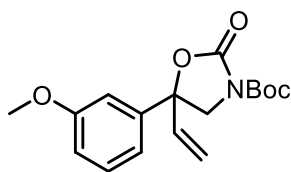
(**1i**): 79% yield, 727.9 mg. White crystal. Mp = 62.2-63.5 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.39 (s, 1H), 7.19 – 7.01 (m, 3H), 6.08 (dd,  $J = 17.1, 10.7$  Hz, 1H), 5.45 – 5.31 (m, 2H), 4.25 – 4.01 (m, 2H), 1.53 (s, 9H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  164.1, 161.7, 150.0 (d,  $J = 166.1$  Hz), 142.6 (d,  $J = 7.1$  Hz), 137.4, 130.7 (d,  $J = 8.3$  Hz), 120.5 (d,  $J = 3.1$  Hz), 116.8, 115.5 (d,  $J = 21.1$  Hz), 112.4 (d,  $J = 23.5$  Hz), 84.3, 80.6, 54.6, 28.0.  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -111.1.



**1j**

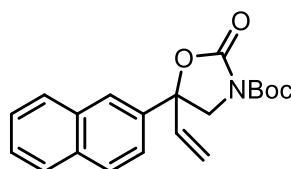
(**1j**): 71% yield, 679.8 mg. Light yellow liquid.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.30 (d,  $J = 8.8$  Hz, 2H), 6.91 (d,  $J = 8.9$  Hz, 2H), 6.08 (dd,  $J = 17.1, 10.7$  Hz, 1H), 5.45 – 5.22 (m, 2H), 4.22 – 4.03 (m, 2H), 3.80 (s, 3H), 1.52 (s, 9H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  159.7, 151.3, 149.5, 138.1, 131.8, 126.5, 116.3, 114.2, 84.2, 81.2, 55.5, 54.8, 28.1.





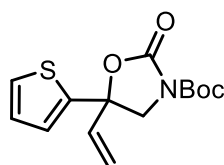
**1k**

(**1k**): 70% yield, 670.2 mg. White solid. Mp = 101.7-102.6 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.24 (s, 1H), 6.94 – 6.74 (m, 3H), 6.02 (dd, *J* = 17.1, 10.7 Hz, 1H), 5.43 – 5.16 (m, 2H), 4.17 – 3.95 (m, 2H), 3.73 (s, 3H), 1.45 (s, 9H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 156.0, 151.1, 149.3, 141.6, 137.9, 130.0, 117.0, 116.3, 113.9, 110.7, 84.1, 81.1, 55.4, 54.8, 28.0.



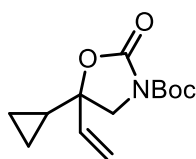
**1l**

(**1l**): 73% yield, 742.7 mg. Light yellow liquid. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.95 – 7.80 (m, 4H), 7.57 – 7.49 (m, 2H), 7.42 (dd, *J* = 8.6, 2.0 Hz, 1H), 6.20 (dd, *J* = 17.1, 10.6 Hz, 1H), 5.49 – 5.35 (m, 2H), 4.32 – 4.18 (m, 2H), 1.53 (s, 9H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 151.3, 149.5, 137.9, 137.2, 133.1, 133.0, 129.0, 128.4, 127.8, 126.9, 124.1, 122.7, 116.9, 84.3, 81.4, 54.8, 28.1.



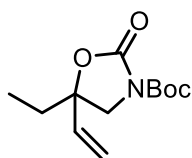
**1m**

(**1m**): 81% yield, 717.1 mg. Orange solid. Mp = 67.3-68.6 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.37 (d, *J* = 5.1 Hz, 1H), 7.10 (d, *J* = 1.5 Hz, 1H), 7.02 (dd, *J* = 8.8, 2.1 Hz, 1H), 6.16 (dd, *J* = 17.0, 10.6 Hz, 1H), 5.61 – 5.37 (m, 2H), 4.25 – 4.11 (m, 2H), 1.54 (s, 9H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 150.8, 149.3, 142.7, 136.9, 127.3, 127.0, 126.1, 117.1, 84.3, 79.2, 55.4, 28.0.



**1n**

(**1n**): 50% yield, 379.7 mg. Light yellow liquid.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  5.80 (dd,  $J = 17.2, 10.8$  Hz, 1H), 5.52 – 5.19 (m, 2H), 3.84 – 3.73 (m, 2H), 1.53 (s, 9H), 1.17 (tt,  $J = 8.3, 5.3$  Hz, 1H), 0.63 – 0.43 (m, 4H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  151.6, 149.6, 136.5, 116.5, 84.0, 80.0, 53.3, 28.1, 18.3, 1.2, 0.9.

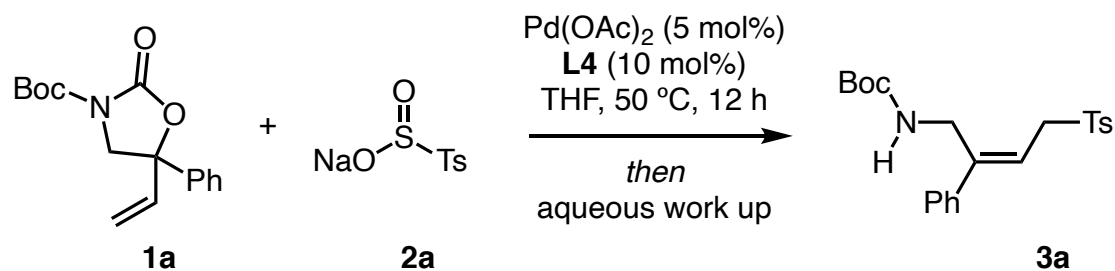


**1o**

(**1o**): 80% yield, 482.2 mg. Orange liquid.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  5.78 (dd,  $J = 17.2, 11.0$  Hz, 1H), 5.52 – 5.13 (m, 2H), 3.94 – 3.53 (m, 2H), 1.78 (td,  $J = 14.4, 6.9$  Hz, 2H), 1.49 (s, 9H), 0.92 (t,  $J = 7.5$  Hz, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  151.6, 149.5, 137.1, 115.9, 83.9, 80.9, 52.8, 31.9, 28.0, 7.4.

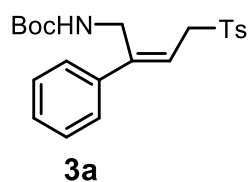
## 4. Synthesis of (Z)-allylic amines 3

### 4.1. General Procedure of Decarboxylative Allylation

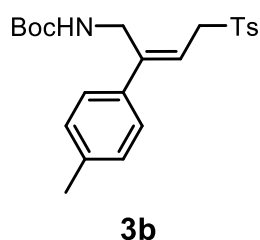


To a mixture of vinyloxazolidin-2-one **1a** (34.7 mg, 0.12 mmol), sodium p-toluene sulfonate (**2a**) (42.8 mg, 0.24 mmol), Pd(OAc)<sub>2</sub> (1.3 mg, 0.006 mmol) and dppp (5.3 mg, 0.012 mmol) was added THF (6 ml). The reaction was heated at 50 °C for 12 h. The reaction was cooled to room temperature and quenched with saturated aqueous NH<sub>4</sub>Cl solution (10 mL). The mixture was extracted with EtOAc, and the combined organic phases were washed with brine and dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>. The solvent was removed under reduced pressure and the residue was purified by flash chromatography on silica gel (Petroleum ether/EtOAc= 2:1) to give desired products.

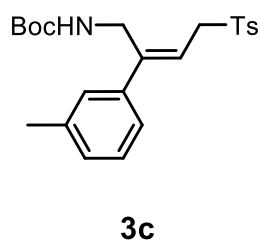
## 4.2. Characterization Data of Allylic Amines 3.



(**3a**): Light yellow liquid (43.5 mg, 91%). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.80 (d, *J* = 8.2 Hz, 2H), 7.42 – 7.25 (m, 7H), 5.79 (t, *J* = 8.2 Hz, 1H), 4.50 (s, 1H), 4.11 (d, *J* = 8.3 Hz, 2H), 3.98 (d, *J* = 5.7 Hz, 2H), 2.46 (s, 3H), 1.37 (s, 9H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 155.7, 145.8, 145.2, 139.4, 135.9, 130.0, 128.7, 128.6, 128.5, 126.7, 116.3, 79.7, 56.3, 39.0, 28.5, 21.8. HRMS(ESI): calcd for C<sub>22</sub>H<sub>28</sub>NO<sub>4</sub>S<sup>+</sup> [M+H]<sup>+</sup>: 402.1730; Found: 402.1734.

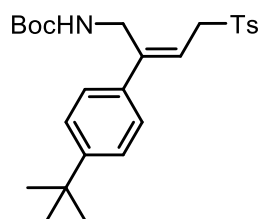


(**3b**): Light yellow liquid (46.2 mg, 93%). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.79 (d, *J* = 8.2 Hz, 2H), 7.35 (d, *J* = 8.0 Hz, 2H), 7.23 (d, *J* = 8.0 Hz, 2H), 7.14 (d, *J* = 7.8 Hz, 2H), 5.78 (t, *J* = 8.2 Hz, 1H), 4.47 (s, 1H), 4.09 (d, *J* = 7.1 Hz, 2H), 3.95 (d, *J* = 5.7 Hz, 2H), 2.45 (s, 3H), 2.34 (s, 3H), 1.37 (s, 9H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 155.8, 145.5, 145.1, 138.5, 136.3, 135.9, 130.0, 129.4, 128.6, 126.51, 115.5, 79.6, 56.3, 38.9, 28.5, 21.8, 21.3. HRMS(ESI): calcd for C<sub>23</sub>H<sub>29</sub>NNaO<sub>4</sub>S<sup>+</sup> [M+Na]<sup>+</sup>: 438.1712; Found: 438.1710.



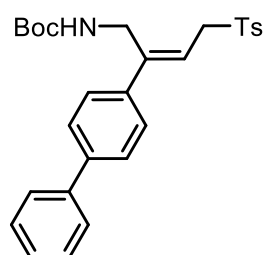
(**3c**): Light yellow liquid (47.7 mg, 96%). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.83 – 7.75 (m, 2H), 7.36 (d, *J* = 8.0 Hz, 2H), 7.22 (t, *J* = 7.6 Hz, 1H), 7.12 (d, *J* = 8.1 Hz, 3H),

5.79 (t,  $J = 8.3$  Hz, 1H), 4.48 (s, 1H), 4.10 (d,  $J = 7.3$  Hz, 2H), 3.96 (d,  $J = 5.8$  Hz, 2H), 2.46 (s, 3H), 2.34 (s, 3H), 1.37 (s, 9H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  155.7, 145.8, 145.1, 139.3, 138.3, 130.0, 129.3, 128.6, 128.6, 127.5, 123.7, 116.1, 79.6, 56.3, 39.0, 28.5, 21.8, 21.6. HRMS(ESI): calcd for  $\text{C}_{23}\text{H}_{29}\text{NNaO}_4\text{S}^+$   $[\text{M}+\text{Na}]^+$ : 438.1706; Found: 438.1710.



**3d**

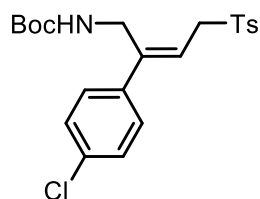
(**3d**): Light yellow liquid (51.0 mg, 93%).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.79 (d,  $J = 8.3$  Hz, 2H), 7.36 (dd,  $J = 8.3, 3.3$  Hz, 4H), 7.27 (d,  $J = 8.2$  Hz, 2H), 5.79 (t,  $J = 8.2$  Hz, 1H), 4.51 (s, 1H), 4.10 (d,  $J = 8.8$  Hz, 2H), 3.96 (d,  $J = 5.8$  Hz, 2H), 2.46 (s, 3H), 1.37 (s, 9H), 1.31 (s, 9H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  155.8, 151.7, 145.4, 145.1, 136.3, 135.9, 130.0, 128.6, 126.3, 125.6, 115.6, 79.6, 56.3, 38.9, 34.7, 31.4, 28.5, 21.8. HRMS(ESI): calcd for  $\text{C}_{26}\text{H}_{36}\text{NO}_4\text{S}^+$   $[\text{M}+\text{H}]^+$ : 458.2358; Found: 458.2360.



**3e**

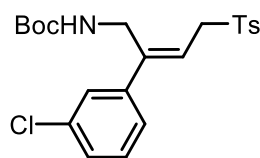
(**3e**): Light yellow solid (52.2 mg, 91%). Mp = 156.2-157.5 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.81 (d,  $J = 8.3$  Hz, 2H), 7.58 (dd,  $J = 7.9, 6.2$  Hz, 4H), 7.49 – 7.32 (m, 7H), 5.87 (t,  $J = 8.3$  Hz, 1H), 4.55 (s, 1H), 4.13 (d,  $J = 8.4$  Hz, 2H), 4.03 (d,  $J = 5.7$  Hz, 2H), 2.47 (s, 3H), 1.38 (s, 9H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  155.8, 145.3, 145.2, 141.3, 140.5, 138.1, 136.0, 130.0, 129.0, 128.6, 127.7, 127.4, 127.1, 127.1, 116.2, 79.7, 56.3, 38.9, 28.5, 21.8. HRMS(ESI): calcd for  $\text{C}_{28}\text{H}_{31}\text{NNaO}_4\text{S}^+$   $[\text{M}+\text{Na}]^+$ :

500.1872; Found: 500.1866.



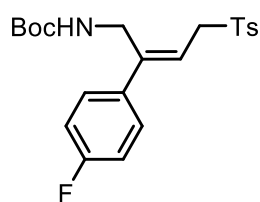
**3f**

(**3f**): Light yellow liquid (41.7 mg, 80%).  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.84 – 7.73 (m, 2H), 7.37 (d,  $J = 8.1$  Hz, 2H), 7.33 – 7.27 (m, 4H), 5.77 (t,  $J = 8.3$  Hz, 1H), 4.50 (s, 1H), 4.08 (d,  $J = 8.3$  Hz, 2H), 3.99 (d,  $J = 5.8$  Hz, 2H), 2.46 (s, 3H), 1.37 (s, 9H).  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  155.7, 145.3, 145.0, 137.7, 135.9, 134.5, 130.1, 128.9, 128.6, 128.0, 116.6, 79.8, 56.1, 38.9, 28.4, 21.8. HRMS(ESI): calcd for  $\text{C}_{22}\text{H}_{26}\text{ClNNaO}_4\text{S}^+$   $[\text{M}+\text{Na}]^+$ : 458.1158, 460.1134; Found: 458.1163, 460.1141.



**3g**

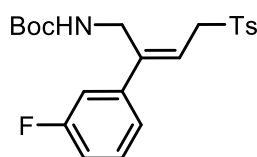
(**3g**): Light yellow liquid (49.5 mg, 95%).  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.79 (d,  $J = 8.4$  Hz, 2H), 7.38 (d,  $J = 8.0$  Hz, 2H), 7.31 – 7.16 (m, 4H), 5.77 (t,  $J = 8.3$  Hz, 1H), 4.54 (s, 1H), 4.09 (d,  $J = 7.2$  Hz, 2H), 3.98 (d,  $J = 5.9$  Hz, 2H), 2.46 (s, 3H), 1.37 (s, 9H).  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  155.7, 145.3, 144.9, 141.3, 135.9, 134.6, 130.1, 129.9, 128.6, 128.5, 127.0, 124.9, 117.3, 79.8, 56.1, 38.94, 28.4, 21.8. HRMS(ESI): calcd for  $\text{C}_{22}\text{H}_{26}\text{ClNNaO}_4\text{S}^+$   $[\text{M}+\text{Na}]^+$ : 458.1165, 460.1142; Found: 458.1163, 460.1141.



**3h**

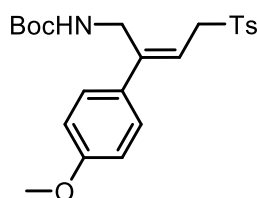
(**3h**): Light yellow liquid (44.4 mg, 88%).  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.85 – 7.74

(m, 2H), 7.37 (d,  $J = 8.1$  Hz, 2H), 7.31 (dd,  $J = 8.6, 5.3$  Hz, 2H), 7.09 – 6.93 (m, 2H), 5.73 (t,  $J = 8.3$  Hz, 1H), 4.52 (s, 1H), 4.08 (d,  $J = 8.3$  Hz, 2H), 3.99 (d,  $J = 5.9$  Hz, 2H), 2.46 (s, 3H), 1.37 (s, 9H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  162.9 (d,  $J = 247.9$  Hz), 155.8, 145.2 (d,  $J = 12.9$  Hz), 136.0, 135.4, 130.1, 128.6, 128.5 (d,  $J = 8.2$  Hz), 116.1, 115.6 (d,  $J = 21.5$  Hz), 79.7, 56.2, 39.0, 28.4, 21.8.  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -113.5. HRMS(ESI): calcd for  $\text{C}_{22}\text{H}_{26}\text{FNNaO}_4\text{S}^+$   $[\text{M}+\text{Na}]^+$ : 442.1459; Found: 442.1459.



**3i**

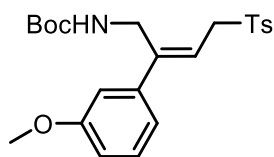
**(3i)**: Light yellow liquid (42.3 mg, 84%).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.86 – 7.74 (m, 2H), 7.38 (d,  $J = 8.0$  Hz, 2H), 7.30 (td,  $J = 8.0, 6.0$  Hz, 1H), 7.16 – 7.08 (m, 1H), 7.06 – 6.95 (m, 2H), 5.80 (t,  $J = 8.3$  Hz, 1H), 4.54 (s, 1H), 4.10 (d,  $J = 8.3$  Hz, 2H), 3.98 (d,  $J = 5.9$  Hz, 2H), 2.47 (s, 3H), 1.37 (s, 9H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  163.0 (d,  $J = 246.2$  Hz), 155.7, 145.3, 145.0, 141.7 (d,  $J = 7.5$  Hz), 135.9, 130.2 (d,  $J = 8.4$  Hz), 130.1, 128.6, 122.4, 117.3, 115.4 (d,  $J = 21.2$  Hz), 113.8 (d,  $J = 22.3$  Hz), 79.8, 56.1, 39.0, 28.4, 21.8.  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -112.7. HRMS(ESI): calcd for  $\text{C}_{22}\text{H}_{26}\text{FNNaO}_4\text{S}^+$   $[\text{M}+\text{Na}]^+$ : 442.1453; Found: 442.1459.



**3j**

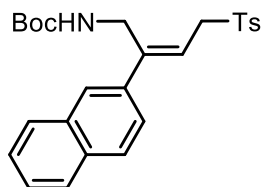
**(3j)**: Light yellow liquid (42.0 mg, 81%).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.85 – 7.74 (m, 2H), 7.36 (d,  $J = 8.1$  Hz, 2H), 7.28 (d,  $J = 8.5$  Hz, 2H), 6.91 – 6.82 (m, 2H), 5.73 (t,  $J = 8.3$  Hz, 1H), 4.49 (s, 1H), 4.08 (d,  $J = 8.4$  Hz, 2H), 3.96 (d,  $J = 5.7$  Hz, 2H), 3.81 (s, 3H), 2.46 (s, 3H), 1.37 (s, 9H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  159.9, 155.8, 145.1, 136.0, 131.6, 130.0, 128.6, 127.9, 114.5, 114.1, 79.6, 56.3, 55.4, 38.8, 28.5,

21.8. HRMS(ESI): calcd for  $C_{23}H_{30}NO_5S^+$   $[M+H]^+$ : 432.1836; Found: 432.1839.



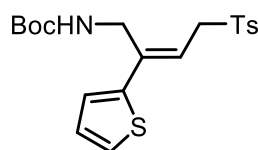
**3k**

(**3k**): Light yellow liquid (48.6 mg, 94%).  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  7.79 (d,  $J = 8.3$  Hz, 2H), 7.36 (d,  $J = 8.0$  Hz, 2H), 7.23 (d,  $J = 7.7$  Hz, 1H), 6.91 (d,  $J = 8.0$  Hz, 1H), 6.88 – 6.82 (m, 2H), 5.80 (t,  $J = 8.3$  Hz, 1H), 4.52 (s, 1H), 4.10 (d,  $J = 6.8$  Hz, 2H), 3.96 (d,  $J = 5.8$  Hz, 2H), 3.81 (s, 3H), 2.46 (s, 3H), 1.37 (s, 9H).  $^{13}C$  NMR (100 MHz,  $CDCl_3$ )  $\delta$  159.8, 155.7, 145.7, 145.2, 140.8, 135.9, 130.0, 129.7, 128.6, 119.0, 116.4, 114.1, 112.3, 79.6, 56.2, 55.4, 39.0, 28.5, 21.8. HRMS(ESI): calcd for  $C_{23}H_{29}NNaO_5S^+$   $[M+Na]^+$ : 454.1659; Found: 454.1659.



**3l**

(**3l**): Light yellow liquid (42.3 mg, 78%).  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  7.94 – 7.71 (m, 6H), 7.54 – 7.43 (m, 3H), 7.37 (d,  $J = 8.0$  Hz, 2H), 5.96 (t,  $J = 8.2$  Hz, 1H), 4.53 (s, 1H), 4.20 – 4.07 (m, 4H), 2.46 (s, 3H), 1.36 (s, 9H).  $^{13}C$  NMR (100 MHz,  $CDCl_3$ )  $\delta$  155.8, 145.7, 145.2, 136.4, 135.9, 133.4, 133.2, 130.0, 128.7, 128.43, 128.37, 127.7, 126.59, 126.57, 126.0, 124.4, 116.6, 79.7, 56.4, 38.9, 28.4, 21.8. HRMS(ESI): calcd for  $C_{26}H_{30}NO_4S^+$   $[M+H]^+$ : 452.1886; Found: 452.1890.

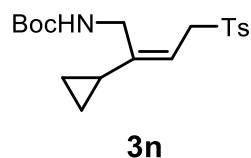


**3m**

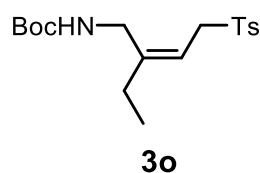
(**3m**): Yellow liquid (44.1 mg, 90%).  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  7.78 (d,  $J = 8.0$



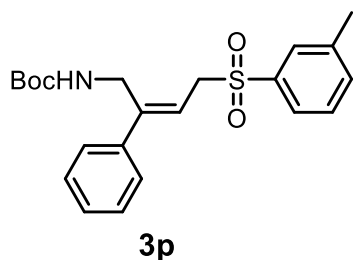
Hz, 2H), 7.36 (d,  $J = 8.0$  Hz, 2H), 7.24 – 7.16 (m, 2H), 6.99 (dd,  $J = 5.1, 3.6$  Hz, 1H), 5.86 (t,  $J = 8.3$  Hz, 1H), 4.85 (s, 1H), 4.20 – 4.07 (m, 4H), 2.46 (s, 3H), 1.41 (s, 9H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  155.8, 145.2, 143.1, 139.5, 135.9, 130.1, 128.6, 128.0, 125.7, 125.5, 114.2, 79.8, 56.2, 38.9, 28.5, 21.8. HRMS(ESI): calcd for  $\text{C}_{20}\text{H}_{25}\text{NNaO}_4\text{S}_2^+$  [ $\text{M}+\text{Na}$ ] $^+$ : 430.1116; Found: 430.1117.



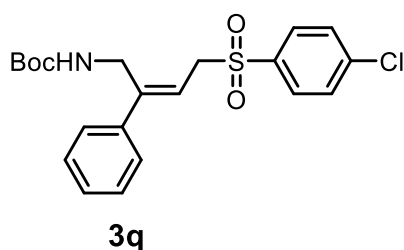
**(3n)**: Colorless liquid (24.6 mg, 56%).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.73 (d,  $J = 8.2$  Hz, 2H), 7.35 (d,  $J = 8.0$  Hz, 2H), 5.17 (t,  $J = 8.3$  Hz, 1H), 4.72 (s, 1H), 3.86 (d,  $J = 8.2$  Hz, 2H), 3.57 (d,  $J = 5.9$  Hz, 2H), 2.46 (s, 3H), 1.43 (s, 9H), 1.31 – 1.21 (m, 1H), 0.75 – 0.62 (m, 2H), 0.51 – 0.37 (m, 2H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  159.3, 148.6, 145.0, 136.0, 129.9, 128.6, 110.8, 79.6, 55.5, 39.8, 28.6, 21.8, 16.1, 6.2. HRMS(ESI): calcd for  $\text{C}_{19}\text{H}_{28}\text{NO}_4\text{S}^+$  [ $\text{M}+\text{H}$ ] $^+$ : 366.1731; Found: 366.1734.



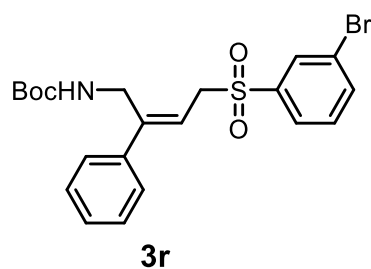
**(3o)**: Light yellow liquid (36.1 mg, 51.1%).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.71 (d,  $J = 8.3$  Hz, 2H), 7.32 (d,  $J = 8.2$  Hz, 2H), 5.22 (t,  $J = 8.1$  Hz, 1H), 4.70 (s, 1H), 3.85 (d,  $J = 8.2$  Hz, 2H), 3.53 (d,  $J = 6.1$  Hz, 2H), 2.41 (s, 3H), 2.24 – 1.96 (m, 2H), 1.39 (s, 9H), 0.96 (t,  $J = 7.4$  Hz, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  156.1, 149.2, 145.0, 135.8, 129.8, 128.5, 112.0, 79.4, 55.4, 39.4, 28.4, 21.7, 12.3. HRMS(ESI): calcd for  $\text{C}_{18}\text{H}_{28}\text{NO}_4\text{S}^+$  [ $\text{M}+\text{H}$ ] $^+$ : 354.1718; Found: 354.1734.



**(3p):** White crystal (42.9 mg, 89%). Mp = 82.1-83.6 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.81 – 7.65 (m, 2H), 7.51 – 7.42 (m, 2H), 7.35 – 7.31 (m, 5H), 5.80 (t, *J* = 8.3 Hz, 1H), 4.49 (s, 1H), 4.11 (d, *J* = 8.3 Hz, 2H), 3.97 (d, *J* = 5.9 Hz, 2H), 2.44 (s, 3H), 1.36 (s, 9H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 155.8, 146.0, 139.7, 139.4, 138.7, 134.9, 129.3, 128.9, 128.7, 128.5, 126.7, 125.7, 116.2, 79.6, 56.2, 38.9, 28.4, 21.4. HRMS(ESI): calcd for C<sub>22</sub>H<sub>28</sub>NO<sub>4</sub>S<sup>+</sup> [M+H]<sup>+</sup>: 402.1720; Found: 402.1734.

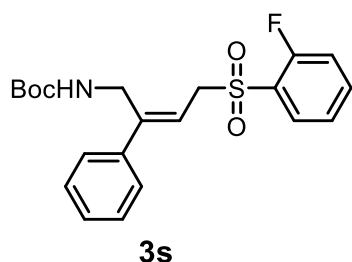


**(3q):** White solid (47.1 mg, 93%). Mp = 108.4-109.3 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.94 – 7.79 (m, 2H), 7.55 (dd, *J* = 8.8, 2.2 Hz, 2H), 7.40 – 7.27 (m, 5H), 5.78 (t, *J* = 8.3 Hz, 1H), 4.58 (s, 1H), 4.16 (d, *J* = 8.2 Hz, 2H), 4.00 (d, *J* = 5.8 Hz, 2H), 1.37 (s, 9H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 155.7, 146.3, 140.9, 139.2, 137.3, 130.1, 129.8, 129.7, 128.8, 128.7, 126.7, 115.7, 79.8, 56.3, 39.0, 28.4. HRMS(ESI): calcd for C<sub>21</sub>H<sub>24</sub>ClNNaO<sub>4</sub>S<sup>+</sup> [M+Na]<sup>+</sup>: 444.1015, 446.0993; Found: 444.1007, 446.0984.

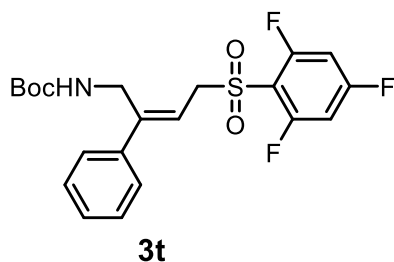


**(3r):** White solid (53.1 mg, 95%). Mp = 109.2-110.7 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)

$\delta$  8.06 (d,  $J = 1.9$  Hz, 1H), 7.94 – 7.73 (m, 2H), 7.47 (t,  $J = 7.9$  Hz, 1H), 7.38 – 7.30 (m, 5H), 5.77 (t,  $J = 8.2$  Hz, 1H), 4.58 (s, 1H), 4.16 (d,  $J = 8.2$  Hz, 2H), 3.98 (d,  $J = 5.8$  Hz, 2H), 1.37 (s, 9H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  155.7, 146.6, 140.7, 139.2, 137.2, 131.6, 131.0, 128.8, 128.7, 127.1, 126.8, 123.4, 115.5, 79.8, 56.3, 39.0, 28.4. HRMS(ESI): calcd for  $\text{C}_{21}\text{H}_{24}\text{BrNNaO}_4\text{S}^+$   $[\text{M}+\text{Na}]^+$ : 466.0692, 468.0672; Found: 466.0682, 468.0664.

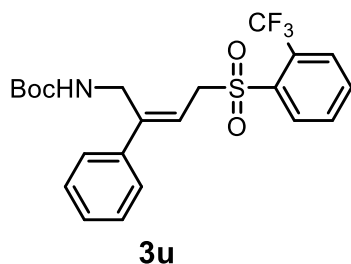


(**3s**): Light yellow liquid (44.7 mg, 92%).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.86 (td,  $J = 7.4, 1.8$  Hz, 1H), 7.60 (qd,  $J = 7.4, 1.8$  Hz, 1H), 7.34 – 7.16 (m, 7H), 5.73 (t,  $J = 8.2$  Hz, 1H), 4.60 (s, 1H), 4.27 (d,  $J = 8.2$  Hz, 2H), 4.08 (d,  $J = 5.9$  Hz, 2H), 1.30 (s, 9H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  161.0, 157.1 (d,  $J = 270.9$  Hz), 146.8, 139.3, 136.6 (d,  $J = 8.4$  Hz), 131.1, 128.6 (d,  $J = 12.5$  Hz), 126.8, 125.0 (d,  $J = 3.8$  Hz), 117.4 (d,  $J = 21.2$  Hz), 115.0, 79.6, 55.5, 39.2, 28.4.  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -108.4. HRMS(ESI): calcd for  $\text{C}_{21}\text{H}_{25}\text{FNO}_4\text{S}^+$   $[\text{M}+\text{H}]^+$ : 406.1480; Found: 406.1483.

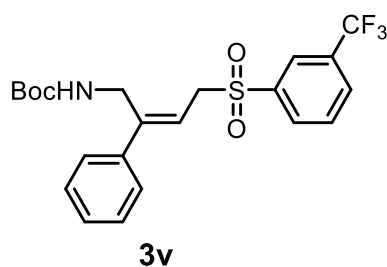


(**3t**): White solid (48.6 mg, 92%). Mp = 62.1-63.3 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.80 (td,  $J = 8.6, 6.1$  Hz, 1H), 7.42 – 7.29 (m, 5H), 7.16 (td,  $J = 9.1, 5.8$  Hz, 1H), 5.79 (t,  $J = 8.1$  Hz, 1H), 4.66 (s, 1H), 4.37 (d,  $J = 8.2$  Hz, 2H), 4.17 (d,  $J = 5.8$  Hz, 2H), 1.37 (s, 9H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  171.2, 155.5 (dd,  $J = 255.8, 10.9, 9.5$  Hz), 155.7, 152.9 (dt, 259.3, 14.2, 13.2 Hz), 146.7 (dd,  $J = 239.1$  Hz), 147.3, 139.1,

128.7, 128.60, 126.7, 123.6 (dd,  $J = 17.4$  Hz), 119.4 (dt,  $J = 21.8, 2.4$  Hz), 114.2, 107.8 (dd,  $J = 27.6, 21.8$  Hz), 79.6, 60.4, 55.7, 28.3.  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -108.7 (dd,  $J = 16.0, 9.0$  Hz), -121.3 (dd,  $J = 20.8, 9.0$  Hz), -138.1 (dd,  $J = 20.8, 16.0$  Hz). HRMS(ESI): calcd for  $\text{C}_{21}\text{H}_{23}\text{F}_3\text{NO}_4\text{S}^+$   $[\text{M}+\text{H}]^+$ : 442.1296; Found: 442.1294.



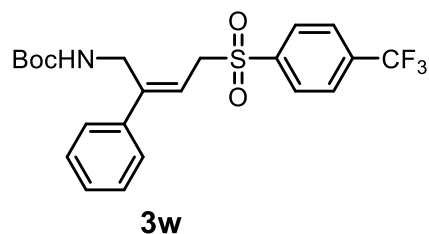
(**3u**): White solid (45.9 mg, 84%). Mp = 125.4-126.4 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.23 (d,  $J = 8.6$  Hz, 1H), 7.96 (d,  $J = 7.5$  Hz, 1H), 7.87 – 7.69 (m, 2H), 7.42 – 7.29 (m, 5H), 5.81 (t,  $J = 8.3$  Hz, 1H), 4.64 (s, 1H), 4.30 (d,  $J = 8.3$  Hz, 2H), 4.11 (d,  $J = 6.6$  Hz, 2H), 1.37 (s, 9H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  155.7, 146.9, 139.2, 137.8, 134.2, 133.5, 132.6, 129.2 (q,  $J = 33.1$  Hz), 128.64 (q,  $J = 12.0$  Hz), 128.62, 128.5, 126.7, 122.7 (q,  $J = 273.9$  Hz), 115.0, 79.5, 56.4, 39.1, 28.3.  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -56.5. HRMS(ESI): calcd for  $\text{C}_{22}\text{H}_{25}\text{F}_3\text{NO}_4\text{S}^+$   $[\text{M}+\text{H}]^+$ : 456.1459; Found: 456.1451.



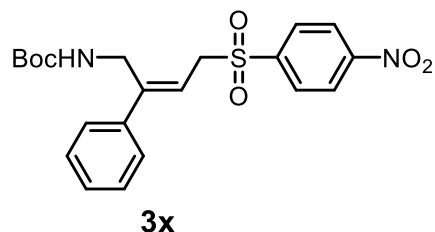
(**3v**): White solid (51.9 mg, 95%). Mp = 120.3-121.1 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.28 – 8.08 (m, 2H), 7.94 (d,  $J = 7.8$  Hz, 1H), 7.75 (t,  $J = 7.8$  Hz, 1H), 7.40 – 7.27 (m, 5H), 5.77 (t,  $J = 8.2$  Hz, 1H), 4.59 (s, 1H), 4.21 (d,  $J = 8.2$  Hz, 2H), 3.97 (d,  $J = 5.9$  Hz, 2H), 1.36 (s, 9H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  155.7, 146.7, 140.1, 139.1, 131.8, 132.0 (q,  $J = 33.4$  Hz), 130.8, 130.7 (q,  $J = 3.8$  Hz), 130.3, 128.7, 126.6, 125.7 (q,  $J = 4.0$  Hz), 123.1 (q,  $J = 273.1$  Hz), 115.3, 79.6, 56.1, 38.9, 28.3.  $^{19}\text{F}$  NMR (376

MHz, CDCl<sub>3</sub>) δ -62.7. HRMS(ESI): calcd for C<sub>22</sub>H<sub>25</sub>F<sub>3</sub>NO<sub>4</sub>S<sup>+</sup> [M+H]<sup>+</sup>: 456.1442;

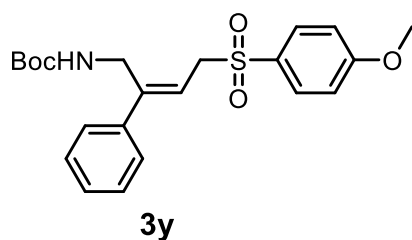
Found: 456.1451.



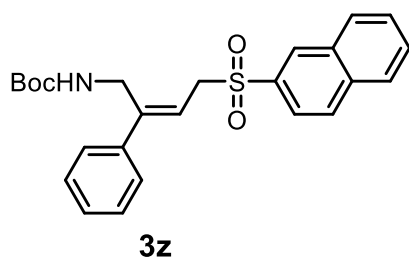
(**3w**): White solid (47.4 mg, 87%). Mp = 135.7-136.9 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.08 (d, *J* = 8.1 Hz, 2H), 7.85 (d, *J* = 8.1 Hz, 2H), 7.42 – 7.29 (m, 5H), 5.77 (t, *J* = 8.1 Hz, 1H), 4.63 (s, 1H), 4.22 (d, *J* = 8.1 Hz, 2H), 4.02 (d, *J* = 5.9 Hz, 2H), 1.37 (s, 9H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 155.7, 146.7, 142.5, 139.2, 135.6 (q, *J* = 33.1 Hz), 129.2, 128.9, 128.8, 128.7, 128.6, 126.6, 126.4 (q, *J* = 3.8 Hz), 123.2 (q, *J* = 273.2 Hz), 115.2, 79.7, 56.0, 39.0, 28.3. <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ -63.1. HRMS(ESI): calcd for C<sub>22</sub>H<sub>25</sub>F<sub>3</sub>NO<sub>4</sub>S<sup>+</sup> [M+H]<sup>+</sup>: 456.1448; Found 456.1451.



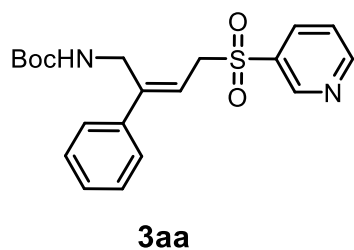
(**3x**): White solid (40.8 mg, 79%). Mp = 161.2-162.3 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.53 – 8.37 (m, 2H), 8.14 (d, *J* = 8.7 Hz, 2H), 7.41 – 7.27 (m, 5H), 5.77 (t, *J* = 8.1 Hz, 1H), 4.58 (s, 1H), 4.27 (d, *J* = 8.1 Hz, 2H), 4.00 (d, *J* = 5.9 Hz, 2H), 1.35 (s, 9H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 155.7, 151.1, 146.9, 144.6, 139.0, 130.1, 128.94, 128.85, 126.7, 124.5, 114.9, 80.0, 56.2, 39.1, 28.4. HRMS(ESI): calcd for C<sub>21</sub>H<sub>24</sub>N<sub>2</sub>NaO<sub>6</sub>S<sup>+</sup> [M+Na]<sup>+</sup>: 455.1244; Found: 455.1247.



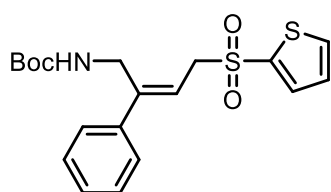
(**3y**): Yellow liquid (13.2 mg, 40%). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.95 – 7.66 (m, 2H), 7.37 – 7.29 (m, 5H), 7.10 – 6.91 (m, 2H), 5.79 (t, *J* = 8.4 Hz, 1H), 4.57 (s, 1H), 4.10 (d, *J* = 8.3 Hz, 2H), 3.98 (d, *J* = 5.9 Hz, 2H), 3.88 (s, 3H), 1.36 (s, 9H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 164.1, 155.7, 145.7, 139.4, 130.7, 130.3, 128.7, 128.50, 126.6, 116.5, 114.5, 79.6, 56.4, 55.8, 38.9, 28.4. HRMS(ESI): calcd for C<sub>22</sub>H<sub>28</sub>NO<sub>5</sub>S<sup>+</sup> [M+H]<sup>+</sup>: 418.1675; Found: 418.1683.



(**3z**): White solid (40.8 mg, 78%). Mp = 92.4-93.5 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.49 (s, 1H), 8.14 – 7.83 (m, 4H), 7.78 – 7.61 (m, 2H), 7.39 – 7.28 (m, 5H), 5.83 (t, *J* = 8.3 Hz, 1H), 4.56 (s, 1H), 4.22 (d, *J* = 8.2 Hz, 2H), 3.97 (d, *J* = 5.8 Hz, 2H), 1.34 (s, 9H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 155.7, 146.1, 139.3, 135.7, 135.5, 132.2, 130.5, 129.64, 129.56, 129.5, 128.7, 128.5, 128.2, 128.0, 126.7, 123.0, 116.1, 79.6, 56.3, 39.0, 28.4. HRMS(ESI): calcd for C<sub>25</sub>H<sub>28</sub>NO<sub>4</sub>S<sup>+</sup> [M+H]<sup>+</sup>: 438.1730; Found: 438.1734.

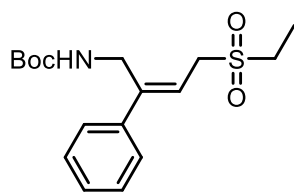


**(3aa)**: White solid (14.4 mg, 31%). Mp =124.3-125.7 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 9.11 (s, 1H), 8.89 (d, *J* = 4.9 Hz, 1H), 8.22 (d, *J* = 10.1 Hz, 1H), 7.53 (dd, *J* = 8.0, 4.9 Hz, 1H), 7.49 – 7.23 (m, 5H), 5.78 (t, *J* = 8.1 Hz, 1H), 4.63 (s, 1H), 4.23 (d, *J* = 8.3 Hz, 2H), 3.97 (d, *J* = 6.0 Hz, 2H), 1.36 (s, 7H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 154.6, 149.6, 146.8, 139.2, 136.4, 135.4, 128.9, 128.7, 126.7, 124.0, 115.2, 79.8, 56.6, 39.1, 28.4. HRMS(ESI): calcd for C<sub>20</sub>H<sub>25</sub>N<sub>2</sub>O<sub>4</sub>S<sup>+</sup> [M+H]<sup>+</sup>: 389.1531; Found: 389.1530.



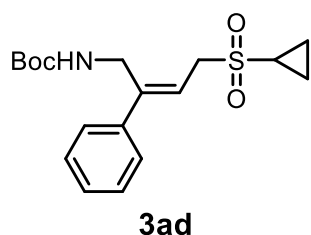
**3ab**

**(3ab)**: Colorless liquid (39.6 mg, 84%). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.75 (dd, *J* = 4.9, 1.3 Hz, 1H), 7.70 (dd, *J* = 3.8, 1.3 Hz, 1H), 7.34 (d, *J* = 6.9 Hz, 5H), 7.21 – 7.14 (m, 1H), 5.85 (t, *J* = 8.2 Hz, 1H), 4.53 (s, 1H), 4.24 (d, *J* = 8.3 Hz, 2H), 4.02 (d, *J* = 5.8 Hz, 2H), 1.37 (s, 9H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 155.7, 146.4, 139.6, 139.2, 134.8, 134.7, 128.8, 128.6, 128.2, 126.7, 117.1, 79.7, 57.4, 38.9, 28.4. HRMS(ESI): calcd for C<sub>19</sub>H<sub>24</sub>NO<sub>4</sub>S<sub>2</sub><sup>+</sup> [M+H]<sup>+</sup>: 394.1133; Found: 394.1141.



**3ac**

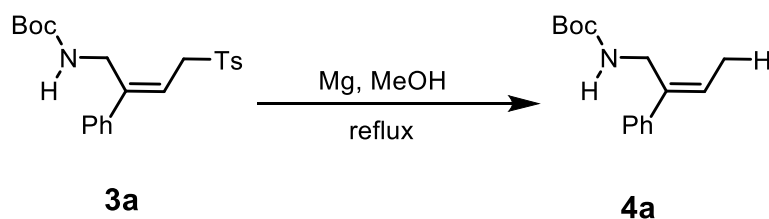
**(3ac)**: Light yellow liquid (29.7 mg, 73%). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.50 – 7.31 (m, 5H), 5.91 (t, *J* = 8.1 Hz, 1H), 4.85 (s, 1H), 4.25 (d, *J* = 6.0 Hz, 2H), 4.08 (d, *J* = 8.1 Hz, 2H), 3.06 (q, *J* = 7.5 Hz, 2H), 1.47 – 1.35 (m, 12H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 147.1, 145.2, 139.1, 129.3, 128.8, 127.6, 116.0, 79.7, 56.4, 39.0, 29.8, 28.4, 14.3. HRMS(ESI): calcd for C<sub>17</sub>H<sub>26</sub>NO<sub>4</sub>S<sup>+</sup> [M+H]<sup>+</sup>: 340.1577; Found: 340.1577.



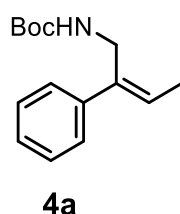
**(3ad)**: White solid (29.4 mg, 70%). Mp = 98.1-99.9 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.45 – 7.30 (m, 5H), 5.96 (t, *J* = 8.2 Hz, 1H), 4.83 (s, 1H), 4.27 (d, *J* = 5.9 Hz, 2H), 4.12 (d, *J* = 8.2 Hz, 2H), 2.47 (td, *J* = 8.0, 4.0 Hz, 1H), 1.38 (s, 9H), 1.29 (dt, *J* = 6.4, 3.0 Hz, 2H), 1.11 – 1.01 (m, 2H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 155.8, 145.6, 139.5, 128.8, 128.6, 126.8, 116.1, 79.8, 53.9, 39.3, 29.5, 28.5, 5.0. HRMS(ESI): calcd for C<sub>18</sub>H<sub>26</sub>NO<sub>4</sub>S<sup>+</sup> [M+H]<sup>+</sup>: 352.1573; Found: 352.1577.

## 5. Synthetic transformations of 3a

### 5.1. Reductive desulfonation of 3a.



To a solution of 3a (120.3 mg, 0.30 mmol) in MeOH (3 mL) was added Magnesium turnings (72.9 mg, 3.00 mmol) at room temperature under air. The mixture was heated at 90 °C and refluxed overnight. The solvent was removed under reduced pressure and the residue was purified by flash chromatography on silica gel (Petroleum ether/EtOAc= 10:1) to give **4a**.

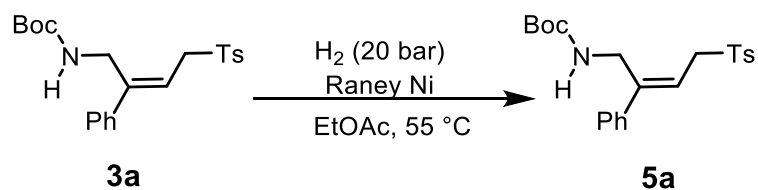


**(4a)**: White solid (45.1 mg, 61%). Mp = 39.1-40.7 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.45 – 7.15 (m, 5H), 5.97 (q, *J* = 7.0 Hz, 1H), 4.40 (s, 1H), 4.28 – 4.18 (m, 2H), 1.89 (d, *J* = 7.0 Hz, 3H), 1.41 (s, 9H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 155.9, 128.9, 128.6,

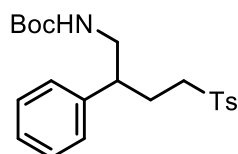


127.9, 127.2, 126.8, 126.3, 79.4, 38.9, 28.5, 14.3. HRMS calcd for  $C_{15}H_{22}NO_2^+$   
[M+H]<sup>+</sup>: 248.1644; Found 248.1645.

## 5.2. Selective hydrogenation of 3a



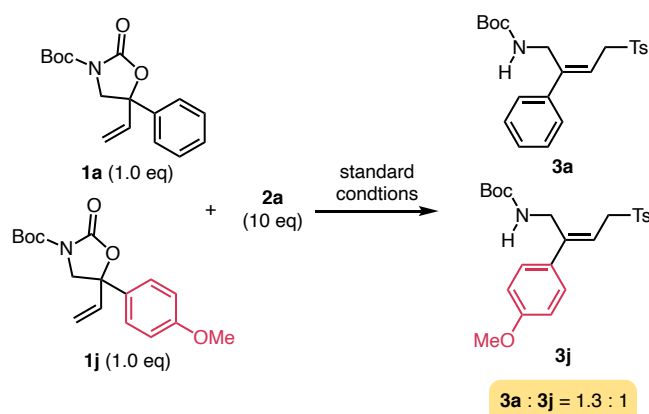
To a solution of 3a (120.3 mg, 0.30 mmol) in ethyl acetate (3 mL) was added Raney Ni at room temperature under air. The mixture was placed in an autoclave, pressurized to 20 bar of H<sub>2</sub>, and heated to 50 °C for 17 h. Then the solvent was removed under reduced pressure and the residue was purified by flash chromatography on silica gel (Petroleum ether/EtOAc= 2:1) to give desired products.



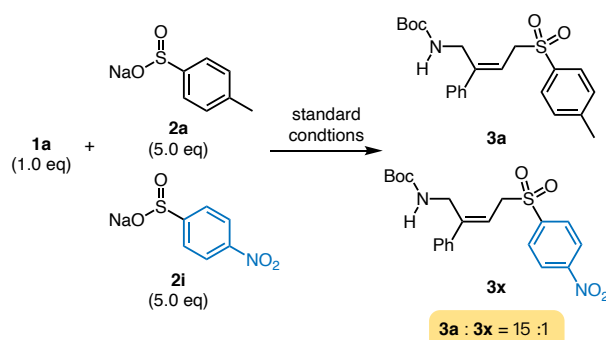
**5a**

(**5a**): White solid (26.1 mg, 64%). Mp = 102.4-103.5 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.72 – 7.57 (m, 2H), 7.33 – 7.11 (m, 5H), 7.06 – 6.93 (m, 2H), 4.37 (s, 1H), 3.43 – 3.00 (m, 2H), 2.89 (ddd, *J* = 13.9, 11.0, 5.4 Hz, 1H), 2.82 – 2.65 (m, 2H), 2.37 (s, 3H), 2.10 – 1.81 (m, 2H), 1.31 (s, 9H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 155.9, 144.8, 140.5, 136.1, 130.0, 129.1, 128.1, 127.8, 127.5, 79.5, 54.4, 46.2, 44.9, 28.4, 26.2, 21.7. HRMS calcd for C<sub>22</sub>H<sub>29</sub>NNaO<sub>4</sub>S<sup>+</sup> [M+Na]<sup>+</sup>: 426.1701; Found 426.1710.

## 6. Competition experiments



To a mixture of **1a** (34.7 mg, 0.12 mmol), **1e** (38.4 mg, 0.12 mmol), **2a** (213.9 mg, 1.20 mmol), Pd(OAc)<sub>2</sub> (1.3 mg, 0.006 mmol) and dpppe (5.3 mg, 0.012 mmol) was added THF (6 ml). The reaction allowed to heat at 50 °C for 12 h. The reaction was heated at 50 °C for 12 h. The reaction was cooled to room temperature and quenched with saturated aqueous NH<sub>4</sub>Cl solution (10 mL). The mixture was extracted with EtOAc, and the combined organic phases were washed with brine and dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>. The solvent was removed under reduced pressure and the ratio of the products was analyzed by <sup>1</sup>H NMR. Further purification by flash chromatography on silica gel (Petroleum ether/EtOAc= 2:1) afforded product **3a** (40.8 mg) and **3j** (33.6 mg).



To a mixture of **1a** (34.7 mg, 0.12 mmol), **2a** (106.8 mg, 0.60 mmol), **2i** (125.4 mg, 0.60 mmol), Pd(OAc)<sub>2</sub> (1.3 mg, 0.006 mmol) and dppp (5.3 mg, 0.012 mmol) was added THF (6 ml). The reaction allowed to heat at 50 °C for 12 h. The reaction was

cooled to room temperature and quenched with saturated aqueous  $\text{NH}_4\text{Cl}$  solution (10 mL). The mixture was extracted with EtOAc, and the combined organic phases were washed with brine and dried over anhydrous  $\text{Na}_2\text{SO}_4$ . The solvent was removed under reduced pressure and the ratio of the products was analyzed by  $^1\text{H}$  NMR. Further purification by flash chromatography on silica gel (Petroleum ether/EtOAc= 2:1) afforded product **3a** (2.2 mg) and **3x** (40.1 mg).

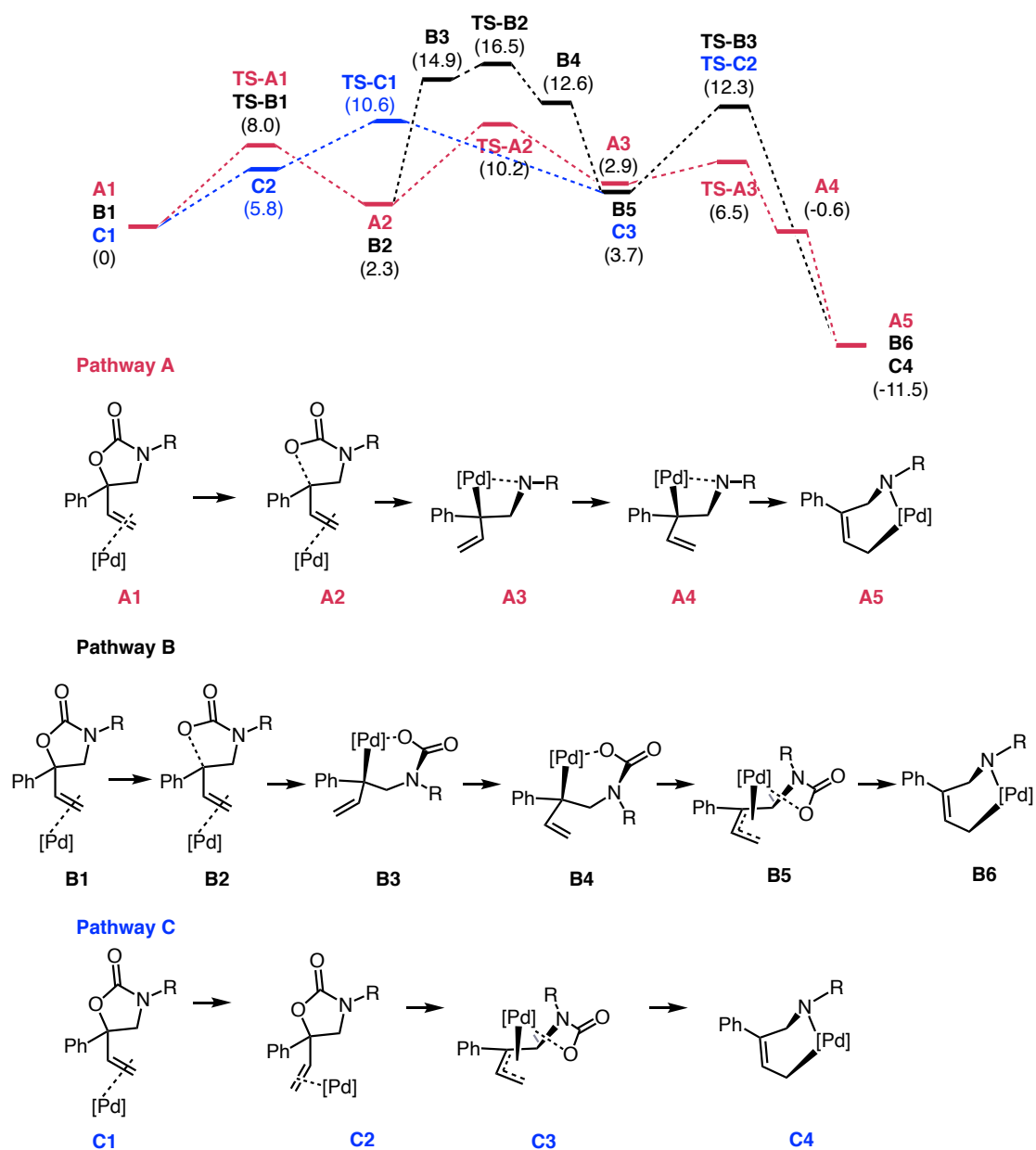
## **7. Computational Details**

### **7.1 Computational Methods**

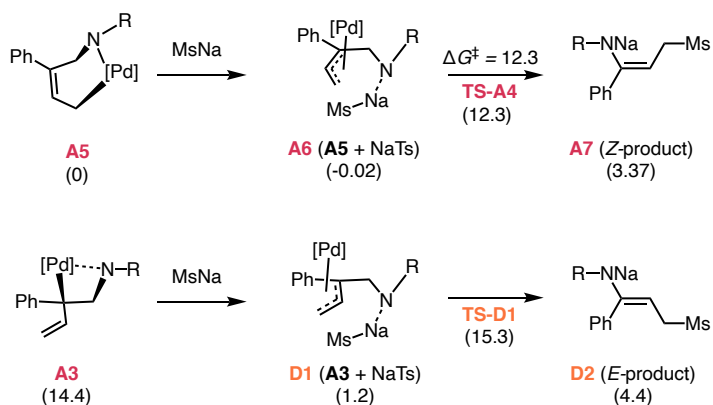
Density functional theory (DFT) calculations were performed using the Gaussian 16<sup>[2]</sup> and ORCA 5.0.3.<sup>[3]</sup> Geometries of intermediates and transition states were optimized using the dispersion-corrected B3LYP-D3(BJ)<sup>[4, 5]</sup> functional and the def2-svp basis set.<sup>[6]</sup> Vibrational frequency calculations and IRC calculations<sup>[7]</sup> at the same level of theory of the optimization were performed to confirm if each structure is a local minimum or a transition state. Single-point energy calculations were carried out using the B3LYP-D3(BJ) functional with the def2-tzvpp basis set. The CPCM solvation mode was employed with dichloroethane as solvent. A conformation search was performed by manually exchanging the coordinating groups on the metal center of the intermediates and transition states, and the structures were fully optimized using DFT. The structures were visualized using CYLview<sup>[8]</sup>.

## 7.2 Discussions on Reaction Pathways.

We examined three possible pathways using DFT calculations, as illustrated in **Figure S1**. The energetically favorable **Pathway A** is also depicted in **Scheme 5A** in the manuscript. The **Pathway B** represents the reaction mechanism in which the *cis-trans* isomerization transpires subsequent the generation of allyl-Pd intermediate and prior to the decarboxylation step. In the **Pathway C**, isomerization occurred prior to the formation of allyl-Pd species.



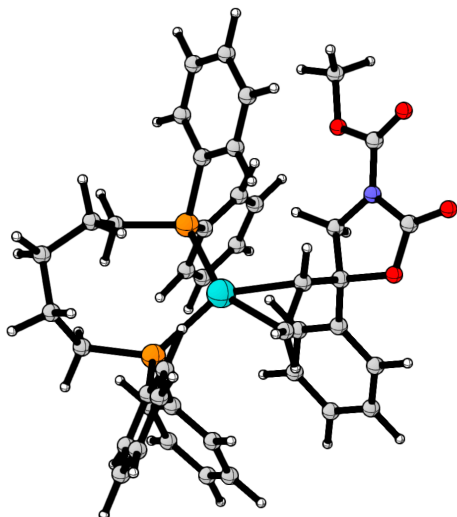
**Figure S1.** Energy diagram for the formation of A5.



**Figure S2.** Energy Profiles for the substitution step.

### 9.3 Cartesian Coordinate of Calculated Structures

A1



Energy: -2791.43045194

Zero point energy correction: 0.756214

Atom Coordinates:

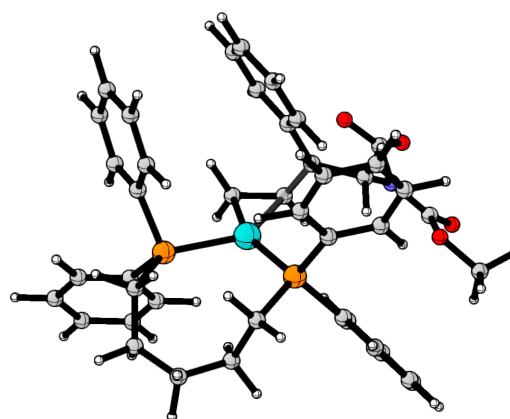
C	-3.96042900	-0.95874600	-1.40384900
C	-3.46398400	-1.39409500	-2.64144300
H	-2.39547000	-1.59711900	-2.74523000
C	-4.32320100	-1.56033200	-3.73257000
H	-3.92485400	-1.90157400	-4.69100200
C	-5.68616200	-1.28263700	-3.59740300
H	-6.35761100	-1.40439700	-4.45072400
C	-6.18948100	-0.84471500	-2.36659000
H	-7.25422400	-0.62443700	-2.25773700
C	-5.33286600	-0.68854500	-1.27501200
H	-5.73382000	-0.34357000	-0.31891600
C	-3.39266700	0.67004900	0.91121200

C	-3.68237900	1.83878300	0.18415600
H	-3.62381900	1.82601500	-0.90601100
C	-4.04207500	3.01434400	0.84159800
H	-4.26140600	3.91283700	0.26061700
C	-4.10655600	3.04981700	2.23885900
H	-4.38015400	3.97411800	2.75277200
C	-3.80853000	1.89922800	2.97159200
H	-3.85228900	1.91610300	4.06329200
C	-3.45623500	0.71603500	2.31319900
H	-3.23467900	-0.17191200	2.90725000
C	2.27405100	-2.36558300	0.37992200
C	3.08194900	-3.14157100	1.22882600
H	2.82245300	-3.24972500	2.28469100
C	4.22564800	-3.77043700	0.73401300
H	4.84884400	-4.36970500	1.40203300
C	4.57484000	-3.63307600	-0.61511000
H	5.47206800	-4.12389200	-0.99943100
C	3.77807800	-2.86384600	-1.46606400
H	4.04997500	-2.74659300	-2.51751500
C	2.63185900	-2.23556600	-0.96933500
H	2.00350100	-1.63171300	-1.62649700
C	1.28324800	-0.55094600	2.41743800
C	2.61102400	-0.12778800	2.59057000
H	3.39233900	-0.48172700	1.91733200
C	2.94104600	0.77336700	3.60801300
H	3.97801200	1.09815000	3.72262900
C	1.95473800	1.26024100	4.46962100
H	2.21534600	1.96643600	5.26118400
C	0.62894700	0.84269200	4.30679000

H	-0.15303600	1.22264000	4.96846700
C	0.29610700	-0.04864200	3.28648400
H	-0.74990300	-0.32876200	3.15007900
P	-2.79605500	-0.82294500	0.01824500
P	0.73644100	-1.54689100	0.97154600
Pd	-0.56644700	-0.35529800	-0.57064300
C	2.63360100	1.44323200	-0.49142600
C	1.40904100	1.98384900	-1.25871300
H	2.93146900	2.10367300	0.33607400
H	2.45081400	0.44290700	-0.10012100
C	0.59395500	0.87371000	-1.89946500
C	-0.77701800	1.00161300	-2.21962300
H	1.21440100	0.23199300	-2.53767800
C	0.58384500	2.95084400	-0.43839500
C	0.17908600	4.18996400	-0.94489900
C	0.17964000	2.57447200	0.85085600
C	-0.61965600	5.04018500	-0.17030200
H	0.49187800	4.49007000	-1.94526100
C	-0.61938200	3.41866400	1.62001700
H	0.47772400	1.60761300	1.25280200
C	-1.02270900	4.65699200	1.11073300
H	-0.93009400	6.00604500	-0.57644700
H	-0.93965900	3.09770600	2.61279300
H	-1.65718800	5.31537800	1.70817500
C	3.30356900	2.27272400	-2.58897400
O	3.96441000	2.58553600	-3.54161300
H	-1.32928100	1.89661900	-1.92003700
H	-1.18144800	0.47806400	-3.09018300
C	-3.45897000	-2.20951600	1.08672200
H	-4.52357400	-1.98070000	1.24791000
H	-2.98062500	-2.15576600	2.07459100
C	-3.30454400	-3.61894400	0.47584800
H	-4.23166700	-4.17657100	0.68476100
H	-3.25547100	-3.54387200	-0.62409000
C	-0.19365800	-2.94638500	1.74452500
H	-1.01424200	-2.47055300	2.29678500
H	0.42408200	-3.46842600	2.49107900
C	-0.72805500	-3.91271200	0.67250500
H	-0.00854100	-4.73842000	0.56119600
H	-0.75457100	-3.40499200	-0.30837400
C	-2.12723400	-4.47472800	0.96528300
H	-2.22171500	-5.45933000	0.47801900
H	-2.22934000	-4.66423200	2.04915400
O	2.05723800	2.72475800	-2.36061600

N	3.65208800	1.42043000	-1.53220900
C	4.86207800	0.75106100	-1.41367100
O	5.71992800	0.67992300	-2.25873500
O	4.93236100	0.18024400	-0.19899700
C	6.12694000	-0.55110700	0.08793900
H	6.98647800	0.13152700	0.15750100
H	5.95130200	-1.04623600	1.04926000
H	6.31765600	-1.30079300	-0.69060500

#### TS-A1



Energy: -2791.40851275

Zero point energy correction: 0.755104

Atom Coordinates:

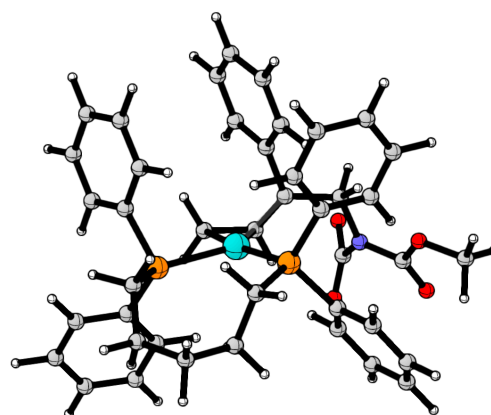
C	-3.73503700	-1.37029900	-1.23572800
C	-3.04488600	-2.00797000	-2.27691600
H	-1.95283000	-2.03356900	-2.25608100
C	-3.74532400	-2.60761800	-3.32824000
H	-3.19747400	-3.10171700	-4.13377000
C	-5.14196500	-2.57213400	-3.34639700
H	-5.69086400	-3.03659300	-4.16890500
C	-5.83837400	-1.94189100	-2.30820700
H	-6.93041400	-1.91387700	-2.31924800
C	-5.14010400	-1.34835700	-1.25547000
H	-5.69422000	-0.85917600	-0.45118300
C	-3.46560300	1.01813000	0.42664200
C	-4.12154800	1.72978300	-0.58998200
H	-4.31475900	1.25522600	-1.55298400
C	-4.52560000	3.05123900	-0.37798200
H	-5.03527500	3.59357400	-1.17789700
C	-4.27713400	3.67750900	0.84586800
H	-4.58762500	4.71229600	1.00643200
C	-3.61267600	2.97873300	1.85852000
H	-3.39678600	3.46664500	2.81126700



C	-3.20432000	1.66073300	1.64982000
H	-2.66052300	1.13851000	2.44020900
C	2.03167800	-2.40280400	0.66656700
C	2.84860200	-3.17687600	1.50813800
H	2.75451200	-3.09241200	2.59347200
C	3.78823000	-4.05398000	0.96407700
H	4.42036200	-4.65144800	1.62508000
C	3.91889400	-4.16900800	-0.42524400
H	4.65602500	-4.85479900	-0.84917300
C	3.11350600	-3.39969900	-1.26784600
H	3.21869000	-3.47822200	-2.35211000
C	2.17483100	-2.51884600	-0.72322000
H	1.54269200	-1.91438700	-1.37722200
C	1.60249100	-0.23690700	2.55487900
C	2.97307300	0.05002600	2.44425100
H	3.57808100	-0.44276600	1.68217600
C	3.56931200	0.98512200	3.29533700
H	4.63409100	1.20575900	3.19101100
C	2.80992300	1.63616400	4.27167900
H	3.27786800	2.36839000	4.93335800
C	1.44621700	1.34768200	4.39522800
H	0.84472300	1.85361700	5.15385300
C	0.84515500	0.42374400	3.53927400
H	-0.22700100	0.23525800	3.62733600
P	-2.77657200	-0.66265100	0.15692700
P	0.73265100	-1.29707400	1.34053000
Pd	-0.53814000	-0.22102800	-0.31846800
C	2.64714900	1.37738500	-0.76464600
C	1.21608300	1.74548500	-1.11161700
H	3.07987500	2.16050200	-0.12424000
H	2.67744200	0.43896300	-0.20923600
C	0.46604800	0.87615900	-1.94479900
C	-0.95205500	0.88590400	-2.08772700
H	1.05036300	0.17856000	-2.55230400
C	0.56423200	2.81050500	-0.30629700
C	-0.27903400	3.75985800	-0.90969800
C	0.79118300	2.88984500	1.07777900
C	-0.90337300	4.74098500	-0.14049700
H	-0.41208400	3.73904000	-1.99082100
C	0.15555600	3.86554600	1.84776200
H	1.44784500	2.17168600	1.56445800
C	-0.69679400	4.79164800	1.24226600
H	-1.55681800	5.47107300	-0.62303100
H	0.32936200	3.89468500	2.92556400

H	-1.19732000	5.55382400	1.84361700
C	3.11893400	2.27726700	-2.97308500
O	3.77988500	2.38608500	-3.99516400
H	-1.53719800	1.75515200	-1.78632200
H	-1.38781100	0.30174300	-2.90190000
C	-3.50153300	-1.60449000	1.60472500
H	-4.53571100	-1.23549800	1.67937100
H	-2.99401800	-1.26962200	2.52121100
C	-3.51461700	-3.14163700	1.48005000
H	-4.43543500	-3.50053100	1.96767200
H	-3.62519700	-3.41646400	0.41800800
C	-0.27454900	-2.43032500	2.39212000
H	-1.02200900	-1.79190800	2.88252700
H	0.34370200	-2.86245200	3.19375300
C	-0.94931800	-3.52539700	1.55063900
H	-0.28307000	-4.40075000	1.52462200
H	-1.04167300	-3.19539600	0.50055200
C	-2.33693900	-3.92593700	2.07308900
H	-2.51550000	-4.99041300	1.85005900
H	-2.34863500	-3.84436700	3.17444200
O	2.13679400	2.98753700	-2.58247900
N	3.41279900	1.23039800	-1.99167300
C	4.46400000	0.34483400	-2.08072700
O	5.12592400	0.09365500	-3.06220600
O	4.68726300	-0.24972100	-0.87739000
C	5.76586600	-1.17999100	-0.83311000
H	6.72716000	-0.66730000	-0.98905600
H	5.73378900	-1.63388400	0.16413200
H	5.64732800	-1.95778200	-1.59901100

A2



Energy: -2791.41548617

Zero point energy correction: 0.756378

## Atom Coordinates:

C	-3.48031900	-1.91148400	-0.48044700	H	-0.01569100	1.52825600	3.46314900
C	-2.70617800	-2.73938700	-1.30780300	P	-2.63885300	-0.65083900	0.54123900
H	-1.62539100	-2.58849300	-1.36119200	P	0.90497500	-0.51580300	1.57375200
C	-3.31053900	-3.75267300	-2.05723300	Pd	-0.50316700	-0.07345700	-0.24293200
H	-2.69845900	-4.39098300	-2.69804000	C	2.34369500	1.27051300	-1.81042500
C	-4.69266200	-3.94529200	-1.98525000	C	0.83121700	1.31046800	-1.68307100
H	-5.16638900	-4.73443500	-2.57354300	H	2.59225000	2.10118500	-2.49775900
C	-5.47017400	-3.12889800	-1.15581000	H	2.80454200	1.51183400	-0.84675700
H	-6.55031800	-3.27946200	-1.09505600	C	0.00202300	0.37974700	-2.33911600
C	-4.86805500	-2.12087200	-0.40118100	C	-1.40464800	0.36188300	-2.16843900
H	-5.48586600	-1.49549300	0.24667400	H	0.47081500	-0.48764900	-2.80758000
C	-3.50896800	0.94551400	0.29007400	C	0.30798800	2.64628800	-1.25382800
C	-4.44773600	1.16376600	-0.72784000	C	-0.54282200	3.38980200	-2.09308300
H	-4.76198300	0.34276900	-1.37319200	C	0.69801200	3.21346300	-0.02860100
C	-4.96912000	2.44469300	-0.93862200	C	-1.02823300	4.63613000	-1.69279900
H	-5.69648400	2.60451200	-1.73788000	H	-0.81888600	2.99060200	-3.07009300
C	-4.55767100	3.51490100	-0.14074000	C	0.20860800	4.45685200	0.37380100
H	-4.96025600	4.51524800	-0.31461300	H	1.37069400	2.66732100	0.62698500
C	-3.61635800	3.30380900	0.87284500	C	-0.66492800	5.16954500	-0.45242700
H	-3.27449300	4.13832100	1.48824000	H	-1.69309500	5.19402600	-2.35617900
C	-3.09170900	2.02891200	1.08475300	H	0.51115200	4.86308000	1.34144700
H	-2.32680000	1.88406900	1.85167200	H	-1.05387300	6.14029500	-0.13658500
C	2.20633500	-1.73470100	1.17701400	C	2.47372700	-0.33401900	-3.75123100
C	3.11628900	-2.16649700	2.15706700	O	2.23081200	-1.53486800	-3.91670400
H	3.09889900	-1.72649800	3.15709100	H	-1.96165400	1.27754600	-1.97594500
C	4.04948600	-3.15893800	1.85532300	H	-1.97197700	-0.43831500	-2.64679500
H	4.75610100	-3.49037300	2.61967800	C	-3.23107800	-1.10652900	2.25805200
C	4.08418500	-3.72373500	0.57412300	H	-4.29483400	-0.82482600	2.23104500
H	4.82139500	-4.49466300	0.33824300	H	-2.76050400	-0.42189400	2.97830700
C	3.18694600	-3.29197400	-0.40495400	C	-3.11357200	-2.58200200	2.68105500
H	3.22684400	-3.70108900	-1.41534100	H	-3.95379100	-2.78973100	3.36327700
C	2.24568500	-2.30416200	-0.10261900	H	-3.29185900	-3.21927800	1.79969000
H	1.56002300	-1.95728100	-0.87648500	C	0.02315700	-1.30736000	2.98265500
C	1.74442900	0.91041900	2.34536600	H	-0.77895900	-0.61405000	3.26685300
C	3.06105900	1.24760900	1.99718100	H	0.69995500	-1.37293300	3.84815000
H	3.62010200	0.60658600	1.31773200	C	-0.53284900	-2.69009700	2.61113100
C	3.63890400	2.42183500	2.48756300	H	0.24592100	-3.44002900	2.81378400
H	4.66190300	2.67845300	2.20291400	H	-0.72110900	-2.75511300	1.52471900
C	2.91013400	3.26799100	3.32852800	C	-1.82074800	-3.03398500	3.36944300
H	3.36128000	4.18830600	3.70609700	H	-1.88755800	-4.12555400	3.50384000
C	1.59835600	2.93341900	3.68290300	H	-1.76631600	-2.60755700	4.38654900
H	1.02254500	3.59086500	4.33816000	O	2.35850500	0.64371600	-4.49958200
C	1.01595400	1.76296200	3.19326300	N	2.90421000	0.04253200	-2.33501500

O	4.76266600	-1.30345500	-2.45266700
O	4.46935800	0.07096100	-0.69162400
C	5.70829300	-0.40457100	-0.17352400
H	6.53415700	-0.19085800	-0.86792900
H	5.86761400	0.12862600	0.77235200
H	5.66491600	-1.48629300	0.01141300

H	-2.45957100	1.95400800	1.77351800
C	2.21221100	-1.61067200	1.40670200
C	3.08789500	-1.92214700	2.46137000
H	3.01538200	-1.38953800	3.41269800
C	4.05845600	-2.90990200	2.29402000
H	4.73925400	-3.14799400	3.11469800

C	4.16217500	-3.59092400	1.07407600
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H	4.92875800	-4.35837700	0.94278500
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C	3.29864900	-3.27944900	0.02267200
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H	3.39686600	-3.78015800	-0.94086200
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C	2.32111100	-2.29374700	0.18968500
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H	1.66713900	-2.02537700	-0.63995900
---	------------	-------------	-------------

C	1.70091900	1.10716000	2.29652000
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C	3.01744600	1.42265200	1.92287300
---	------------	------------	------------

H	3.58642200	0.74202800	1.28869700
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C	3.58906400	2.63234400	2.32751500
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H	4.61035000	2.87192500	2.02229600
---	------------	------------	------------

C	2.85804000	3.53418800	3.10629700
---	------------	------------	------------

H	3.30617300	4.48083400	3.41661700
---	------------	------------	------------

C	1.54766600	3.22125700	3.48517500
---	------------	------------	------------

H	0.96993200	3.92198400	4.09223500
---	------------	------------	------------

C	0.96983100	2.01647600	3.08078500
---	------------	------------	------------

H	-0.06087800	1.79735900	3.36718700
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P	-2.66754000	-0.64059300	0.53545900
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P	0.87750700	-0.38313600	1.63636800
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Pd	-0.51342700	-0.12934100	-0.24311300
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C	2.33600200	1.16870600	-1.68543000
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C	0.82229200	1.24758000	-1.69521100
---	------------	------------	-------------

H	2.65844200	2.02018700	-2.33287100
---	------------	------------	-------------

H	2.68749900	1.45848600	-0.67959600
---	------------	------------	-------------

C	0.07561500	0.24235600	-2.33923100
---	------------	------------	-------------

C	-1.33476000	0.13600300	-2.23471800
---	-------------	------------	-------------

H	0.65190200	-0.59636300	-2.73432200
---	------------	-------------	-------------

C	0.23679900	2.57984800	-1.36096600
---	------------	------------	-------------

C	-0.66388600	3.21710400	-2.23667700
---	-------------	------------	-------------

C	0.61634000	3.26064700	-0.19022300
---	------------	------------	-------------

C	-1.20223400	4.46639600	-1.92577700
---	-------------	------------	-------------

H	-0.93302300	2.73458900	-3.17688900
---	-------------	------------	-------------

C	0.07493400	4.50817700	0.12270000
---	------------	------------	------------

H	1.32377500	2.79923700	0.49266500
---	------------	------------	------------

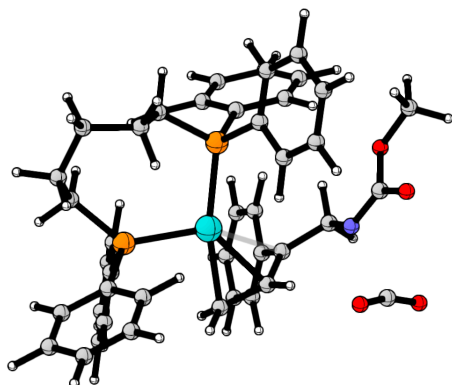
C	-0.84451000	5.11315500	-0.73887000
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H	-1.90414700	4.93825100	-2.61715100
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H	0.37312900	5.00291300	1.04975000
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H	-1.27450000	6.08655900	-0.49180000
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TS-A2



Energy: -2791.39602242

Zero point energy correction: 0.751858

Atom Coordinates:

C	-3.51714400	-1.95210100	-0.41526700
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C	-2.74195200	-2.85412900	-1.15922900
---	-------------	-------------	-------------

H	-1.65741100	-2.72684000	-1.19410400
---	-------------	-------------	-------------

C	-3.34965200	-3.90757700	-1.84831900
---	-------------	-------------	-------------

H	-2.73644000	-4.60436300	-2.42388800
---	-------------	-------------	-------------

C	-4.73718600	-4.06569900	-1.79930000
---	-------------	-------------	-------------

H	-5.21386900	-4.88627200	-2.34039800
---	-------------	-------------	-------------

C	-5.51657900	-3.17367900	-1.05361500
---	-------------	-------------	-------------

H	-6.60118200	-3.29639800	-1.01160700
---	-------------	-------------	-------------

C	-4.91067200	-2.12553300	-0.35884200
---	-------------	-------------	-------------

H	-5.52952200	-1.43948100	0.22339300
---	-------------	-------------	------------

C	-3.52485600	0.94229800	0.17231600
---	-------------	------------	------------

C	-4.39831800	1.11438600	-0.91122200
---	-------------	------------	-------------

H	-4.66778700	0.26616800	-1.54164800
---	-------------	------------	-------------

C	-4.91515900	2.38108900	-1.20354500
---	-------------	------------	-------------

H	-5.59162000	2.50300900	-2.05268000
---	-------------	------------	-------------

C	-4.56458500	3.48467000	-0.42235200
---	-------------	------------	-------------

H	-4.96249400	4.47381300	-0.65942300
---	-------------	------------	-------------

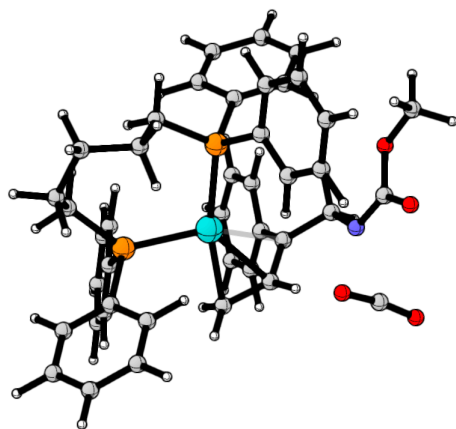
C	-3.68931400	3.32034500	0.65639700
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H	-3.39432400	4.18033500	1.26085400
---	-------------	------------	------------

C	-3.16980900	2.05957500	0.95004000
---	-------------	------------	------------

C	2.75760000	-0.91207900	-4.35334200
O	2.08392000	-1.85816700	-4.17851100
H	-1.96458500	1.01789600	-2.12500800
H	-1.82279100	-0.72761200	-2.69105700
C	-3.29092600	-0.98634600	2.26725200
H	-4.35962300	-0.73046300	2.20392700
H	-2.84696900	-0.24763000	2.95032600
C	-3.14489800	-2.42761300	2.78883600
H	-4.00543100	-2.62250000	3.44920500
H	-3.26304700	-3.12714800	1.94490700
C	-0.03761100	-1.05697600	3.08710000
H	-0.86155800	-0.35884600	3.28031100
H	0.60863000	-1.03472500	3.97765400
C	-0.56007100	-2.47589200	2.81718200
H	0.22390600	-3.19201900	3.10439500
H	-0.71213400	-2.62992000	1.73418600
C	-1.86763500	-2.78413100	3.55796400
H	-1.91453900	-3.86125300	3.78573900
H	-1.86152200	-2.26879000	4.53461300
O	3.39640600	-0.07705000	-4.87295700
N	2.85846800	-0.07368400	-2.14878900
C	4.03406300	-0.50893500	-1.73677800
O	4.65641100	-1.48282700	-2.18406500
O	4.61317800	0.22053800	-0.68699100
C	5.84005700	-0.27459900	-0.18707000
H	6.59705000	-0.36141800	-0.98265100
H	6.18340400	0.44444000	0.57165200
H	5.71804900	-1.26476000	0.28012700

A3



Energy: -2791.39827717

Zero point energy correction: 0.752391

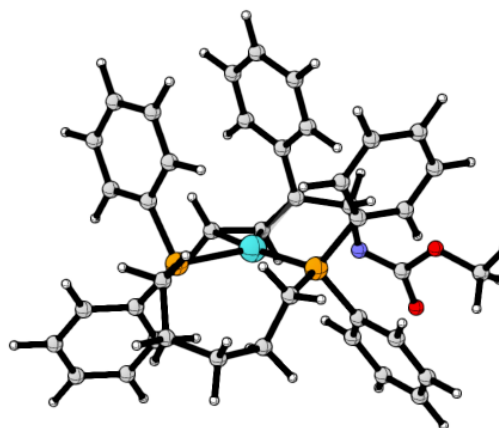
Atom Coordinates:

C	3.37927800	-2.13179200	0.06786200
C	2.56200700	-3.08854100	0.68847900
H	1.48789700	-2.90628000	0.76988600
C	3.11444500	-4.26880600	1.19441700
H	2.46868500	-5.00718500	1.67466900
C	4.48808100	-4.50033800	1.08479300
H	4.92152900	-5.42058700	1.48309500
C	5.30883200	-3.55380400	0.46054900
H	6.38256000	-3.73341600	0.37085100
C	4.75785700	-2.37825900	-0.05194600
H	5.40821500	-1.65033300	-0.54162900
C	3.56889500	0.81091000	-0.08162300
C	4.46951400	0.76025500	0.99193200
H	4.69089800	-0.18995200	1.47933200
C	5.07309400	1.93265700	1.45903900
H	5.77055400	1.88121800	2.29836100
C	4.78187700	3.16228500	0.86384800
H	5.24740600	4.07696000	1.23753700
C	3.87819900	3.22005400	-0.20249600
H	3.62843700	4.17949600	-0.65956200
C	3.27293100	2.05381600	-0.67072300
H	2.54107200	2.11910000	-1.47948000
C	-2.32470000	-1.18536000	-1.52646300
C	-3.20325800	-1.32550300	-2.61608600
H	-3.10547200	-0.67750700	-3.49052100
C	-4.20708500	-2.29290200	-2.58306200
H	-4.88812600	-2.39882700	-3.43093400
C	-4.34227000	-3.12471600	-1.46323700
H	-5.13282400	-3.87877000	-1.43861600
C	-3.48102100	-2.97879200	-0.37510500
H	-3.59669600	-3.59124500	0.51814800
C	-2.47125300	-2.01166800	-0.40673300
H	-1.82696100	-1.87772800	0.46162800
C	-1.69133500	1.60510400	-2.02211300
C	-2.98380100	1.92362900	-1.57415500
H	-3.57438300	1.18516500	-1.03040300
C	-3.50238100	3.20415700	-1.78698100
H	-4.50470800	3.44446100	-1.42479800
C	-2.74234300	4.17370100	-2.44763100
H	-3.14904500	5.17472500	-2.60837800
C	-1.45628100	3.85848600	-2.90095500
H	-0.85636200	4.61184200	-3.41662500
C	-0.93074600	2.58293000	-2.68696800

H	0.08343000	2.36004700	-3.02543000
P	2.60146800	-0.64154200	-0.65489300
P	-0.93374400	-0.00292900	-1.60281000
Pd	0.50373700	-0.11074200	0.25592000
C	-2.23126900	1.13760400	1.94308500
C	-0.71392800	1.12537100	1.92036200
H	-2.48307500	1.94057800	2.67858000
H	-2.58167500	1.55428600	0.98117600
C	-0.02932600	-0.00863800	2.39618500
C	1.36793800	-0.19626800	2.24387300
H	-0.67431000	-0.84654900	2.67066600
C	-0.04964400	2.45102900	1.75596300
C	0.90189000	2.90872200	2.68795200
C	-0.40640000	3.30587100	0.69760400
C	1.50605200	4.15812000	2.53892200
H	1.15995600	2.28477400	3.54457000
C	0.20118300	4.55276100	0.54592700
H	-1.14862000	2.98071700	-0.02584000
C	1.16636200	4.98191800	1.46139600
H	2.24618200	4.48993600	3.27071300
H	-0.08159900	5.18679700	-0.29744300
H	1.64690500	5.95560900	1.34085100
C	-2.71019600	-2.59500800	3.61847700
O	-2.13802700	-3.09352500	2.73161500
H	2.05836500	0.64657500	2.25194500
H	1.79968000	-1.14937800	2.55703000
C	3.17819300	-0.76439800	-2.43272000
H	4.26294700	-0.59558800	-2.35384800
H	2.78189200	0.09805800	-2.98783400
C	2.92619800	-2.09647200	-3.16159100
H	3.76101800	-2.24394400	-3.86585000
H	3.00997900	-2.92208600	-2.43585300
C	-0.08242400	-0.49850400	-3.16032700
H	0.78288100	0.16891200	-3.26420600
H	-0.73764400	-0.29647600	-4.02110200
C	0.34481500	-1.97402400	-3.12828500
H	-0.49173100	-2.58093400	-3.50479300
H	0.50042900	-2.31043800	-2.08749500
C	1.61568500	-2.24907700	-3.94133700
H	1.58579500	-3.28009100	-4.32933100
H	1.62801400	-1.59286000	-4.82960900
O	-3.20075700	-2.22313500	4.60638500
N	-2.80762400	-0.11525400	2.29710900
C	-3.98502800	-0.46155200	1.83202600

O	-4.61636200	-1.49998900	2.10331000
O	-4.58055000	0.44322600	0.92906700
C	-5.80038200	0.03367800	0.34561300
H	-6.54756700	-0.23513100	1.10916200
H	-6.16947700	0.88489100	-0.24667100
H	-5.66281200	-0.83532400	-0.31811000

### A3' (CO<sub>2</sub> removed)



Energy: -2602.93645020

Zero point energy correction: 0.739203

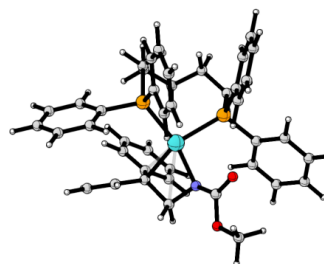
Atom Coordinates:

C	-3.48358000	-1.86260800	-0.43273000
C	-2.83540800	-2.70705400	-1.34651300
H	-1.75887800	-2.60461300	-1.50235000
C	-3.55832600	-3.67458800	-2.05040300
H	-3.04357500	-4.32719800	-2.75891700
C	-4.93470800	-3.80371400	-1.84686000
H	-5.50133600	-4.55676700	-2.39931700
C	-5.58712400	-2.96989100	-0.93132800
H	-6.66244300	-3.07060100	-0.76778100
C	-4.86551400	-2.00847600	-0.22184200
H	-5.38533600	-1.36712900	0.49316500
C	-3.33347700	0.95811400	0.42190400
C	-4.32339800	1.24806700	-0.52794300
H	-4.68215700	0.46927900	-1.20184700
C	-4.84320400	2.54287700	-0.62884100
H	-5.61241500	2.75743500	-1.37438500
C	-4.37959900	3.55729000	0.21220600
H	-4.78179200	4.56905600	0.12512200
C	-3.38665100	3.27575400	1.15651500
H	-3.00431400	4.06703800	1.80433300
C	-2.86353400	1.98673100	1.25870200

H	-2.06281000	1.79033300	1.97549300
C	2.42190800	-1.83313300	0.68790900
C	3.36267200	-2.31912900	1.61350400
H	3.38891000	-1.92548800	2.63239700
C	4.27361000	-3.30344900	1.23087300
H	5.00440300	-3.67767300	1.95181500
C	4.25429400	-3.80631100	-0.07688200
H	4.97522100	-4.57100000	-0.37610100
C	3.32856300	-3.31946100	-1.00067900
H	3.33634500	-3.67146600	-2.03188600
C	2.40951200	-2.33692600	-0.61756200
H	1.71453200	-1.92360100	-1.34886300
C	2.15196900	0.79300700	1.87771100
C	3.43057400	1.08607900	1.37556300
H	3.88429000	0.44716300	0.61686000
C	4.11124800	2.22441200	1.81703000
H	5.10038600	2.44926300	1.41131300
C	3.52884300	3.07450000	2.76174700
H	4.06243300	3.96499200	3.10173600
C	2.25752600	2.78267300	3.26898400
H	1.79571800	3.44397500	4.00570100
C	1.56978700	1.65119900	2.82687400
H	0.56762600	1.45064900	3.21161900
P	-2.48258400	-0.66658000	0.52457400
P	1.17871800	-0.59176400	1.19166100
Pd	-0.42567800	-0.11403500	-0.46639600
C	2.27403100	1.25038200	-2.09264200
C	0.77288600	1.37907800	-1.91216000
H	2.56499900	2.18879900	-2.62627700
H	2.74436500	1.37111000	-1.09928600
C	-0.07114200	0.46462500	-2.57134200
C	-1.46144600	0.35839300	-2.31553400
H	0.46370400	-0.31598200	-3.12048700
C	0.28028200	2.67453900	-1.36045500
C	-0.71904100	3.41552500	-2.02184800
C	0.84582900	3.22101000	-0.19388700
C	-1.17027400	4.63115400	-1.50637000
H	-1.13600800	3.04191100	-2.95758100
C	0.39134700	4.43437800	0.32414500
H	1.63357200	2.68160200	0.32407400
C	-0.62584000	5.14100800	-0.32370100
H	-1.95146800	5.18371100	-2.03338300
H	0.83577000	4.82311400	1.24316100
H	-0.98697200	6.08760900	0.08503600

H	-2.05795600	1.22897700	-2.04498800
H	-2.01627800	-0.45006700	-2.79681700
C	-2.90871600	-1.16679200	2.27887000
H	-3.97050900	-0.88982000	2.36464000
H	-2.36996600	-0.50338500	2.97085500
C	-2.74361600	-2.65217700	2.64697100
H	-3.52385700	-2.89174900	3.38757200
H	-2.98242500	-3.26843000	1.76441800
C	0.41654200	-1.36874600	2.67959500
H	-0.35429800	-0.67040000	3.02998200
H	1.16195100	-1.44146900	3.48597300
C	-0.17910100	-2.74581300	2.35058300
H	0.61253700	-3.50019300	2.46912700
H	-0.46874400	-2.79320000	1.28586500
C	-1.39359900	-3.09996800	3.21781200
H	-1.44213400	-4.19270000	3.35172300
H	-1.25411800	-2.67789000	4.22880300
N	2.66513700	0.07888900	-2.80238500
C	3.86028300	-0.43380600	-2.61252800
O	4.36678200	-1.40522000	-3.19498300
O	4.63960600	0.20526800	-1.61472900
C	5.88193400	-0.39320600	-1.31586300
H	6.50074800	-0.52648900	-2.21791100
H	6.39816400	0.27831900	-0.61232300
H	5.75817600	-1.38212200	-0.84270300

### A3



Energy: -2602.94622331

Zero point energy correction: 0.739957

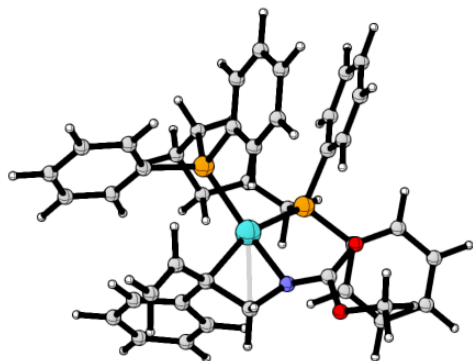
Atom Coordinates:

C	-1.09411600	2.61906100	0.31555400
C	-1.29318600	3.86953800	-0.28901900
H	-1.77568300	3.94625000	-1.26423900
C	-0.87994300	5.03883000	0.35602400
H	-1.03148800	6.00542700	-0.13015500
C	-0.28339800	4.97466700	1.61832900
H	0.03515200	5.89081900	2.12089300

C -0.08438900 3.73345700 2.22817500  
H 0.39616100 3.67207600 3.20718800  
C -0.47391100 2.56322700 1.57540800  
H -0.28403700 1.59159700 2.03796800  
C -3.39389200 0.94371100 0.23506900  
C -4.45073400 0.44071500 -0.53983700  
H -4.28479200 0.13327900 -1.57172000  
C -5.73646300 0.32700300 -0.00352400  
H -6.54464500 -0.06866600 -0.62318200  
C -5.98873600 0.72373600 1.31171300  
H -6.99478700 0.63862700 1.72885400  
C -4.94350600 1.22999300 2.08936200  
H -5.12785100 1.54423500 3.11939900  
C -3.65694600 1.33301300 1.55848800  
H -2.85440900 1.72800100 2.18202500  
C 2.28115600 1.88261800 -1.01042300  
C 2.40603400 2.68795700 -2.15293400  
H 2.25357700 2.27134400 -3.14850800  
C 2.73403900 4.04197600 -2.02794700  
H 2.82291800 4.66103500 -2.92389800  
C 2.95165100 4.59835000 -0.76510600  
H 3.20620700 5.65649800 -0.66897200  
C 2.83999800 3.79591800 0.37579700  
H 3.00451200 4.22692100 1.36562900  
C 2.49849800 2.44899700 0.25880000  
H 2.40902600 1.81355300 1.14256400  
C 3.28011700 -0.81919100 -0.61987600  
C 4.52518900 -0.21399300 -0.40725400  
H 4.62514300 0.86986900 -0.47873300  
C 5.64129800 -0.99177100 -0.08708400  
H 6.60658300 -0.50805000 0.08196600  
C 5.52483000 -2.38111600 0.01921100  
H 6.39727700 -2.98761300 0.27417600  
C 4.28637000 -2.99120500 -0.20681100  
H 4.18665300 -4.07661700 -0.12869700  
C 3.16928600 -2.21528600 -0.52234000  
H 2.20167100 -2.69493100 -0.67312500  
P -1.67941200 1.04323100 -0.43528800  
P 1.76931400 0.12951600 -1.06053800  
Pd -0.13588000 -0.55916200 0.24771300  
C -0.17043000 -2.49563000 2.09571400  
C -1.35724200 -2.08093700 1.19872300  
H -0.38242400 -2.24075600 3.14725100  
H -0.00004000 -3.59066500 2.07547800

C -2.53336700 -1.68318300 2.00007000  
H -2.30937900 -0.92120400 2.75517700  
C -1.53340800 -2.85683400 -0.06277200  
C -0.54025200 -3.75104900 -0.52728200  
C -2.65656900 -2.66097800 -0.90136100  
C -0.66350600 -4.40667400 -1.75454200  
H 0.35620900 -3.91658900 0.06921600  
C -2.78041400 -3.31965300 -2.12216500  
H -3.42975100 -1.95935600 -0.59560200  
C -1.78474900 -4.20017300 -2.56243400  
H 0.13026700 -5.08370000 -2.08102300  
H -3.66087900 -3.13475400 -2.74330700  
H -1.87982700 -4.71177600 -3.52296500  
C -1.94898000 1.46919500 -2.22083100  
H -1.09486800 2.10725900 -2.49137100  
H -2.84615600 2.10250500 -2.28699900  
C -2.05243100 0.29134600 -3.20297500  
H -2.25097500 0.71828600 -4.20160300  
H -2.92468800 -0.33501400 -2.96325800  
C -0.81439000 -0.60319500 -3.26263100  
H -1.00262600 -1.42539800 -3.96960600  
H -0.68543500 -1.09112500 -2.28423800  
C 0.47532500 0.13802500 -3.65242900  
H 0.35147300 1.22395900 -3.52746900  
H 0.67935600 -0.00506100 -4.72614800  
C 1.70139900 -0.32476800 -2.86589900  
H 1.75824700 -1.42467000 -2.87440300  
H 2.63860400 0.03665900 -3.31791700  
C -3.78105800 -2.17819000 1.97950000  
H -4.53668400 -1.79824200 2.67082800  
H -4.09336200 -2.95947700 1.28391500  
N 0.92894000 -1.70809500 1.57210900  
C 1.89523700 -1.23444300 2.36334900  
O 2.57429700 -0.22131300 2.18997700  
O 2.10781500 -2.03397600 3.46356900  
C 3.13241000 -1.61445300 4.35030200  
H 2.92837800 -0.61188800 4.75899500  
H 3.15765800 -2.34899700 5.16652700  
H 4.11130100 -1.58611300 3.84588500

**TS-A3**



Energy: -2602.93981858

Zero point energy correction: 0.739174

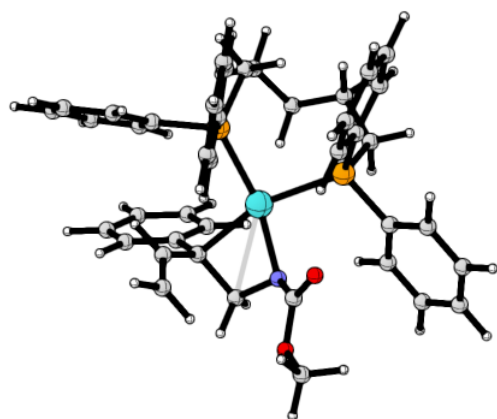
Atom Coordinates:

C	-0.78433300	2.57546900	0.71208200
C	-0.66952200	3.91963300	0.32921700
H	-0.95785200	4.24062400	-0.67159800
C	-0.17205000	4.86931500	1.22558700
H	-0.07455600	5.91027000	0.90914700
C	0.20381000	4.49066300	2.51646900
H	0.59459600	5.23509900	3.21406600
C	0.08712200	3.15333200	2.90902100
H	0.38619600	2.84669900	3.91387500
C	-0.39662600	2.20151700	2.01121500
H	-0.45842700	1.15202400	2.30800300
C	-3.22445800	1.24475600	-0.07150600
C	-4.03121900	0.35258400	-0.79651900
H	-3.58255100	-0.32437300	-1.52208400
C	-5.40805000	0.29699500	-0.57090500
H	-6.02009600	-0.40549500	-1.14145200
C	-5.99430100	1.11880400	0.39572700
H	-7.06983500	1.06797700	0.58039500
C	-5.19664400	2.00235600	1.12993300
H	-5.64741700	2.64517400	1.88973500
C	-3.82054800	2.06953300	0.89660500
H	-3.20844500	2.76252400	1.47509100
C	2.36557500	1.69951700	-1.04183100
C	2.60775200	2.54456900	-2.13527400
H	2.50422300	2.17820500	-3.15672200
C	2.99316200	3.87356800	-1.92626900
H	3.17016300	4.52594700	-2.78467600
C	3.15671700	4.36102600	-0.62752900
H	3.45357900	5.40009500	-0.46630700
C	2.94209400	3.51396100	0.46561600
H	3.07201500	3.88839300	1.48275900
C	2.54186200	2.19393700	0.26432800
H	2.38150500	1.52313100	1.11039700
C	3.21726100	-1.07327600	-0.85469600
C	4.50616900	-0.54788600	-0.69876900
H	4.66628900	0.53005600	-0.75325700
C	5.58772800	-1.39823500	-0.45460200
H	6.58848600	-0.97781300	-0.32789600
C	5.39174100	-2.78018100	-0.36912800
H	6.23767500	-3.44355200	-0.17349000
C	4.10813200	-3.30986300	-0.53843300
H	3.94655900	-4.38867300	-0.47446500
C	3.02552400	-2.46113800	-0.77806900
H	2.02352900	-2.87819600	-0.88409200
P	-1.41989100	1.26290200	-0.40766600
P	1.75491300	-0.01541700	-1.19671000
Pd	-0.13105500	-0.57328500	0.17081800
C	-0.32922500	-2.45662000	2.07150400
C	-1.49892700	-1.81193600	1.28246200
H	-0.40355300	-2.21059400	3.14213700
H	-0.34158300	-3.56192400	1.99346200
C	-2.53271800	-1.17443100	2.16984400
H	-2.61631800	-0.08427000	2.16994600
C	-2.00134300	-2.65297500	0.15375900
C	-1.10837900	-3.46568900	-0.59075200
C	-3.35559000	-2.66846600	-0.23877200
C	-1.54033900	-4.20236100	-1.69243200
H	-0.05629100	-3.49931000	-0.30670100
C	-3.78713600	-3.40661400	-1.34359200
H	-4.07806300	-2.09544200	0.33798900
C	-2.88360200	-4.17004000	-2.08812400
H	-0.81990900	-4.80844200	-2.24827100
H	-4.84488100	-3.38606000	-1.62057200
H	-3.22125800	-4.74368800	-2.95451200
C	-1.35209600	2.05700700	-2.08246600
H	-0.31147200	2.39326200	-2.21424300
H	-1.98003300	2.95918600	-2.04296800
C	-1.79506500	1.16943700	-3.25104300
H	-1.76904500	1.78756500	-4.16537800
H	-2.84878400	0.88188500	-3.12084900
C	-0.92928500	-0.07459900	-3.46539800
H	-1.38818300	-0.69411400	-4.25140400
H	-0.93904600	-0.69518600	-2.55382500
C	0.52130200	0.27667600	-3.85547100



H	0.65571500	1.36882000	-3.84114000
H	0.69979900	-0.01567000	-4.90282300
C	1.61585300	-0.38606900	-3.01840500
H	1.49040600	-1.48074200	-3.04246200
H	2.60915400	-0.18330100	-3.45021100
C	-3.34533200	-1.85768700	2.98483500
H	-4.06185300	-1.34504100	3.63378300
H	-3.33049200	-2.95211000	3.02873800
N	0.83868900	-1.84293900	1.46290800
C	1.89336600	-1.48253100	2.20140400
O	2.68975500	-0.57087800	1.97598400
O	2.05000500	-2.27859300	3.31414000
C	3.14055100	-1.95709300	4.16204500
H	3.05623600	-0.93261600	4.55900200
H	3.11357600	-2.67779000	4.99050300
H	4.10094600	-2.03915300	3.62904300

A4



Energy: -2602.95640037

Zero point energy correction: 0.740488

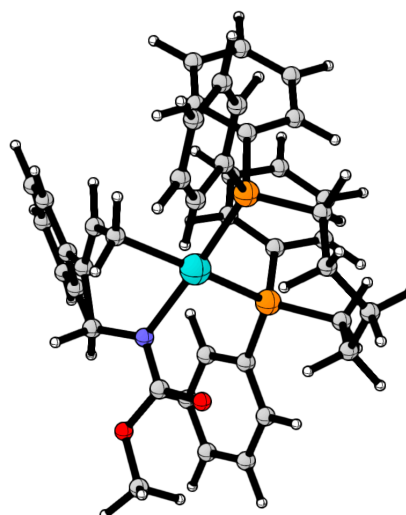
Atom Coordinates:

C	-0.59879800	2.46552700	0.90005700
C	-0.41470300	3.83203600	0.64367600
H	-0.67320200	4.25902600	-0.32503600
C	0.11350200	4.67010700	1.62944900
H	0.26360200	5.72998400	1.41177200
C	0.45113800	4.15702700	2.88395900
H	0.86425000	4.81504900	3.65204000
C	0.26824000	2.79620400	3.14768800
H	0.53633300	2.38314200	4.12290200
C	-0.24516900	1.95385500	2.16092000
H	-0.37269300	0.89058500	2.37043000

C	-3.09580300	1.30907000	0.03761600
C	-3.96511800	0.56047500	-0.77257700
H	-3.56988200	-0.07540500	-1.56440000
C	-5.34328900	0.59256100	-0.55019900
H	-6.00222400	0.00421000	-1.19106500
C	-5.86911300	1.34239300	0.50460200
H	-6.94648600	1.35592000	0.68555900
C	-5.00765500	2.06534000	1.33590400
H	-5.40879700	2.64700500	2.16939400
C	-3.63048500	2.05651500	1.10087700
H	-2.97139900	2.63539900	1.74874300
C	2.53813800	1.67628200	-0.81769900
C	2.83295600	2.67901000	-1.75295300
H	2.72467000	2.49404400	-2.82194400
C	3.28044800	3.93275200	-1.32147100
H	3.50030000	4.71034800	-2.05684700
C	3.45245200	4.18574300	0.04130200
H	3.80043500	5.16575000	0.37629600
C	3.17598700	3.18183200	0.97653200
H	3.30638300	3.37556600	2.04273100
C	2.71201900	1.93728200	0.55455500
H	2.49484700	1.14662300	1.27598000
C	3.29339300	-1.11598900	-1.01799600
C	4.57324400	-0.67360600	-0.65837400
H	4.75814700	0.38876200	-0.49447200
C	5.61553800	-1.59001900	-0.49476900
H	6.60858200	-1.23374100	-0.20993700
C	5.38959500	-2.95570700	-0.69167800
H	6.20411300	-3.67182800	-0.55866500
C	4.11653000	-3.40080500	-1.06309100
H	3.93198600	-4.46632400	-1.21999100
C	3.07276200	-2.48730100	-1.22362900
H	2.07623600	-2.84523800	-1.48489600
P	-1.29652600	1.29728000	-0.33525200
P	1.87931300	0.03145800	-1.25797700
Pd	-0.07085800	-0.65396900	-0.04308400
C	-0.39398100	-3.04023000	1.05481500
C	-1.49091200	-1.95201700	0.96726700
H	-0.40462500	-3.58744900	2.01376300
H	-0.53907600	-3.78286800	0.25335700
C	-1.82367900	-1.28637200	2.23915200
H	-2.63481400	-0.55185700	2.17199600
C	-2.63908700	-2.29944900	0.07786600
C	-2.42765700	-2.62221500	-1.28072500

C	-3.95728500	-2.37394300	0.56149100
C	-3.48481500	-2.96761900	-2.11976400
H	-1.41323500	-2.57269500	-1.68335200
C	-5.01979600	-2.72924500	-0.27540000
H	-4.15737200	-2.15279100	1.61102200
C	-4.79448000	-3.01890900	-1.62183500
H	-3.28886900	-3.19491000	-3.17086600
H	-6.03376600	-2.76930700	0.13068300
H	-5.62581300	-3.28636100	-2.27843100
C	-1.22286400	2.26035200	-1.91818500
H	-0.18126800	2.60858900	-2.00163600
H	-1.85278200	3.15281600	-1.78951400
C	-1.64274000	1.50271700	-3.18274800
H	-1.63958800	2.22444000	-4.01802200
H	-2.68492300	1.16360000	-3.08720100
C	-0.73513200	0.32218500	-3.53650400
H	-1.16103500	-0.21000200	-4.40131000
H	-0.74375100	-0.40186900	-2.70555800
C	0.71280200	0.75439300	-3.84429800
H	0.83777800	1.82621500	-3.62879900
H	0.90556800	0.65789700	-4.92495100
C	1.79742200	-0.04177700	-3.11773200
H	1.67762800	-1.11627800	-3.33108700
H	2.79932800	0.23263500	-3.48480200
C	-1.22648400	-1.44439600	3.43755700
H	-1.54376500	-0.84859800	4.29721300
H	-0.39343100	-2.13396500	3.59380500
N	0.81968100	-2.27667400	0.82886500
C	1.74858700	-2.09515100	1.77450100
O	2.49028800	-1.12048200	1.90472700
O	1.85506700	-3.16598800	2.63204600
C	2.83537100	-3.05223000	3.65185800
H	2.62713000	-2.19881500	4.31667400
H	2.79411700	-3.98695600	4.22695400
H	3.84194800	-2.92043900	3.22546300

**A5**



Energy: -2602.97274187

Zero point energy correction: 0.741109

Atom Coordinates:

C	-3.85506200	-0.50687600	-0.99147200
C	-3.72680500	-1.47192000	-2.00194900
H	-2.76864900	-1.97800200	-2.14045500
C	-4.81049900	-1.77094500	-2.83152100
H	-4.70200900	-2.52353700	-3.61587900
C	-6.02611800	-1.10013900	-2.66469500
H	-6.87085100	-1.32760500	-3.31915500
C	-6.15797200	-0.13307500	-1.66228900
H	-7.10544500	0.39491400	-1.53116200
C	-5.07856700	0.16123800	-0.82578500
H	-5.18726900	0.91638100	-0.04419700
C	-2.64471300	1.50407200	0.71499200
C	-2.58660400	2.52886600	-0.24566800
H	-2.51513500	2.27757900	-1.30576400
C	-2.61945100	3.86688300	0.14560300
H	-2.57331700	4.65401000	-0.61044500
C	-2.70304700	4.19833500	1.50282200
H	-2.71699100	5.24627000	1.81085200
C	-2.76119100	3.18547300	2.46178900
H	-2.81764400	3.43684000	3.52288300
C	-2.73435900	1.84359600	2.07220800
H	-2.76800700	1.06925500	2.83822500
C	2.44781700	-1.31858400	1.37056000
C	3.32311000	-0.30286100	0.95675800
H	2.94044200	0.69748000	0.75316600
C	4.68557100	-0.56025700	0.79839400
H	5.35484400	0.24370800	0.48263100

C	5.19270400	-1.84063200	1.04447500
H	6.25878600	-2.04373500	0.91909900
C	4.32603500	-2.85769600	1.45171800
H	4.71090100	-3.86201300	1.64400600
C	2.96104900	-2.60104100	1.61173800
H	2.30199500	-3.41698600	1.90661700
C	0.61950700	0.69205900	2.26837100
C	0.62764700	1.81574100	1.42212500
H	0.60819800	1.67850600	0.33903600
C	0.64653700	3.10501800	1.95377500
H	0.65079000	3.96475000	1.28083800
C	0.63296900	3.29151500	3.33888000
H	0.62979500	4.30097800	3.75649200
C	0.61260900	2.18176800	4.18844200
H	0.60069800	2.32100800	5.27211800
C	0.61467800	0.88799300	3.65783600
H	0.61860600	0.03575800	4.33931300
P	-2.44696000	-0.22112000	0.14796900
P	0.64380200	-0.97457500	1.48808900
Pd	-0.37072700	-0.69152200	-0.65819800
C	2.15197600	-0.22585900	-2.40460700
C	1.51230500	1.14593800	-2.37009100
H	2.17824400	-0.57108200	-3.45826100
H	3.20576100	-0.18049000	-2.09536000
C	0.15119600	1.23282300	-2.45665000
C	-0.77687700	0.10545200	-2.57418500
H	-0.30558900	2.21572700	-2.30741200
C	2.33976800	2.35287000	-2.15961400
C	1.85880900	3.64120100	-2.49440500
C	3.62495200	2.28821100	-1.57726600
C	2.59411900	4.79224300	-2.21766700
H	0.89496900	3.74085100	-2.99603100
C	4.36370900	3.44088100	-1.30149300
H	4.05299900	1.32190800	-1.31689400
C	3.85323400	4.70391300	-1.61137600
H	2.18608300	5.76888700	-2.49103400
H	5.34901900	3.34608500	-0.83758500
H	4.43173200	5.60574000	-1.39809000
H	-0.47855800	-0.69378200	-3.26466800
H	-1.81623400	0.40409000	-2.74673700
C	-2.87827100	-1.29256700	1.58157600
H	-3.90283700	-1.06797400	1.91389800
H	-2.20982200	-0.99884700	2.39961300
C	-2.70737300	-2.78426200	1.21531700

H	-3.70374700	-3.21057300	1.02448800
H	-2.15456600	-2.87989500	0.26486500
C	0.09078300	-2.14174700	2.82352100
H	-0.66107200	-1.62411600	3.43523500
H	0.95655500	-2.29645300	3.48310300
C	-0.45211100	-3.49324700	2.30899300
H	-0.06508200	-4.28284500	2.97295800
H	-0.03887400	-3.70365600	1.30880400
C	-1.98151000	-3.63268800	2.26671800
H	-2.20688000	-4.69174700	2.05854600
H	-2.40015800	-3.42406000	3.26824200
N	1.42530100	-1.19570200	-1.58998900
C	1.83999400	-2.45332400	-1.49286600
O	1.25510500	-3.36715400	-0.89412100
O	3.03921400	-2.69382500	-2.12580900
C	3.54936000	-4.01190100	-2.02072300
H	2.83668100	-4.75389600	-2.41379500
H	4.47332300	-4.03473900	-2.61483700
H	3.77800400	-4.27031400	-0.97538500

CO<sub>2</sub>

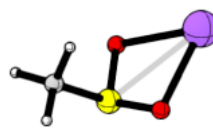
Energy: -188.446954372

Zero point energy correction: 0.011697

Atom Coordinates:

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.16299500
O	0.00000000	0.00000000	-1.16299500

MsNa (7)



Energy: -750.606124947

Zero point energy correction: 0.045296

Atom Coordinates:

S	-0.57695400	-0.00027700	-0.58163300
O	0.26712700	-1.25016300	-0.21823200
O	0.26688100	1.25011100	-0.21939300
C	-1.82030600	0.00022600	0.76944400
H	-1.25768900	0.00072500	1.71566800
H	-2.44230000	0.90338800	0.68620900
H	-2.44211700	-0.90313900	0.68705100
Na	2.03897300	0.00045000	0.46492500

Filename: A1B1C1-10-TS.log

Energy: -3353.57005079

Zero point energy correction: 0.787219

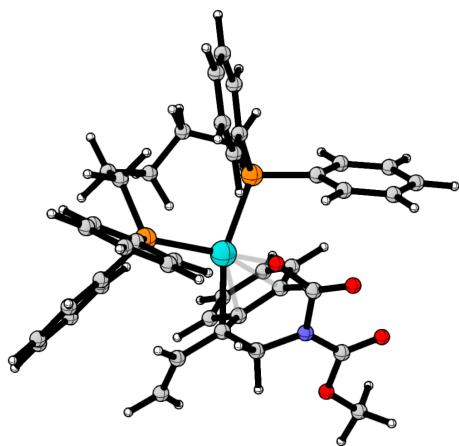
Atom Coordinates:

C -3.52622700 1.58418800 -0.90255000  
C -4.91776000 1.45489600 -0.80098400  
H -5.40049700 1.38460900 0.17428900  
C -5.70843900 1.39783200 -1.95369100  
H -6.79110900 1.28676700 -1.85967900  
C -5.11939300 1.47617700 -3.21752800  
H -5.73909200 1.42869800 -4.11582800  
C -3.72958800 1.60676700 -3.32872100  
H -3.26003100 1.66166700 -4.31344600  
C -2.93935100 1.65001800 -2.18049500  
H -1.85150500 1.71709200 -2.26959900  
C -1.87706300 3.32182400 0.73797700  
C -1.02136400 3.62000300 1.81551800  
H -0.75502000 2.83881900 2.53245100  
C -0.47556800 4.89531400 1.95929300  
H 0.19236600 5.10757000 2.79730000  
C -0.76928200 5.89419000 1.02243500  
H -0.33113400 6.88940700 1.12557800  
C -1.62414200 5.60877800 -0.04506100  
H -1.86245300 6.38354500 -0.77773700  
C -2.17956800 4.33176200 -0.18637000  
H -2.83894100 4.12290500 -1.03003300  
C -2.73409700 -2.60708800 -0.31328400  
C -3.40146100 -3.76946000 0.10753000  
H -2.96749800 -4.40811300 0.87929200  
C -4.62736800 -4.12211900 -0.46164000  
H -5.14278000 -5.02353500 -0.12161800  
C -5.19282900 -3.32726000 -1.46574200  
H -6.15251700 -3.60554800 -1.90764400  
C -4.52641800 -2.17867800 -1.90079800  
H -4.95724200 -1.54963600 -2.68223400  
C -3.30570100 -1.81930900 -1.32263700  
H -2.79660700 -0.91341700 -1.65079600  
C 0.03087000 -3.20294300 -0.53953900  
C 0.01021400 -3.14680600 -1.94514100  
H -0.71044900 -2.50113100 -2.45284800  
C 0.90467600 -3.90464400 -2.69895900  
H 0.87535600 -3.85094100 -3.78983700

C 1.84345300 -4.72390200 -2.06014800  
H 2.55217800 -5.30958400 -2.64988700  
C 1.87349700 -4.78123100 -0.66665800  
H 2.60910300 -5.40982700 -0.15919400  
C 0.97216400 -4.02784400 0.09319500  
H 1.02491500 -4.08124700 1.17927300  
P -2.38360000 1.56563600 0.52748600  
P -1.11064800 -2.09845000 0.38448900  
Pd -0.50705100 0.16382600 0.29039700  
C 2.32449200 -0.53215700 -0.94467300  
C 1.78787400 -0.02253100 0.38833100  
H 2.19845400 -1.62122600 -0.99446500  
H 1.69053000 -0.12775400 -1.75482000  
C 1.40272900 1.35013500 0.51565500  
H 1.38164900 1.80342000 1.50859600  
C 2.14774600 -0.77545900 1.61911000  
C 2.95474100 -1.92966800 1.55671400  
C 1.65928200 -0.39470100 2.89066500  
C 3.24525900 -2.67078400 2.70555500  
H 3.35734900 -2.25982900 0.60154300  
C 1.94845700 -1.13566200 4.03455100  
H 1.00715500 0.47421000 2.98296300  
C 2.74369600 -2.28544200 3.95082500  
H 3.86990000 -3.56375000 2.61967400  
H 1.53997500 -0.81959600 4.99769400  
H 2.96653200 -2.87107800 4.84577900  
C -1.07917700 -2.78593400 2.10329100  
H -0.09123500 -2.49537900 2.49465300  
H -1.08960800 -3.88518800 2.04675300  
C -2.17304200 -2.30036400 3.06821400  
H -1.90796900 -2.69644300 4.06136900  
H -3.13464600 -2.77181100 2.80603800  
C -2.35586400 -0.77469300 3.14750600  
H -1.42895000 -0.28074100 2.80767700  
H -2.49047000 -0.46401700 4.19656400  
C -3.54696500 -0.24561500 2.33387400  
H -4.47850000 -0.43474200 2.89234100  
H -3.64940800 -0.80817300 1.39266200  
C -3.42797600 1.25194500 2.02618100  
H -4.40519200 1.73770800 1.89104200  
H -2.93864500 1.77903700 2.85957800  
N 3.69318600 -0.10217600 -1.12446400  
C 4.66172700 -0.95431700 -1.35938800  
O 5.87267800 -0.63425000 -1.49133000

O	4.32562600	-2.29651000	-1.46231600
C	5.38333100	-3.21066500	-1.67294600
H	5.92572700	-2.99649900	-2.60776100
H	6.11092300	-3.19000300	-0.84523000
H	4.92352800	-4.20699400	-1.73329100
C	1.11798400	2.21450900	-0.55735300
H	1.14176500	1.86770000	-1.59054100
H	0.57908500	3.14108600	-0.36516000
Na	5.30742900	1.59078300	-1.01923300
O	4.02900700	3.31905800	-2.07969300
S	3.21472900	3.48100800	-0.80321100
O	4.02739800	3.08606700	0.42084400
C	2.98311900	5.28158500	-0.62640800
H	2.40830700	5.46464400	0.29154800
H	3.98740100	5.72483800	-0.56408700
H	2.44002700	5.65038500	-1.50692400

**B3**



Energy: -2791.40695417

Zero point energy correction: 0.756166

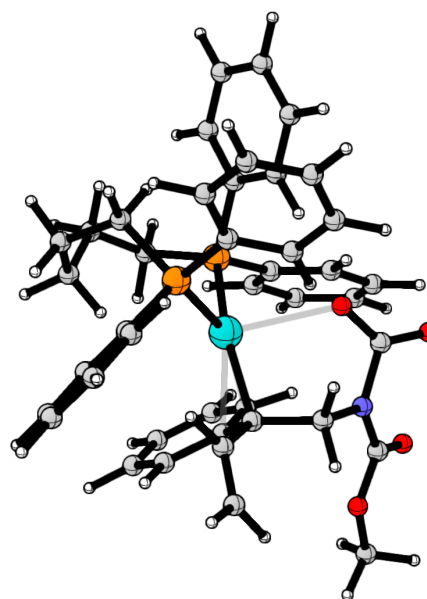
Atom Coordinates:

C	-2.84880500	0.73933100	1.51678200
C	-4.13290800	1.28825000	1.68415500
H	-4.80798400	1.39687600	0.83334800
C	-4.56912100	1.69377600	2.94670100
H	-5.56852500	2.11943300	3.06298900
C	-3.72935200	1.55588000	4.05765900
H	-4.07062900	1.87797500	5.04436000
C	-2.45407300	1.00838000	3.89848100
H	-1.78881900	0.90437800	4.75889000
C	-2.01268200	0.60119200	2.63535400

H	-0.99802300	0.21597000	2.51323400
C	-3.29115000	-1.21937600	-0.59413500
C	-3.01311300	-1.88417600	-1.80113900
H	-2.18744200	-1.55082300	-2.42897200
C	-3.75981800	-2.99589000	-2.19016500
H	-3.52837100	-3.49926300	-3.13172500
C	-4.78434500	-3.47583100	-1.36838800
H	-5.36206600	-4.35389000	-1.66618200
C	-5.05677100	-2.83268300	-0.15832200
H	-5.84776400	-3.20679700	0.49595200
C	-4.31821000	-1.70936700	0.22620700
H	-4.53673700	-1.22559000	1.17833100
C	0.24781500	3.26142500	-0.31229400
C	0.13458900	4.49442900	-0.97465400
H	0.49000800	4.61110100	-1.99976700
C	-0.43919400	5.59058700	-0.32484200
H	-0.53172600	6.54334200	-0.85146500
C	-0.89448500	5.46907300	0.99236400
H	-1.34892900	6.32631100	1.49467500
C	-0.76111500	4.25013400	1.66410900
H	-1.10697700	4.14734900	2.69535400
C	-0.19352700	3.14991100	1.01725300
H	-0.07286700	2.20475600	1.54820600
C	2.73771800	1.88606200	-0.79954000
C	3.17792400	1.91762900	0.53381600
H	2.45530200	1.90976900	1.34850400
C	4.54144400	1.90912900	0.82859400
H	4.85610200	1.89864300	1.87354400
C	5.48553200	1.88602500	-0.20281800
H	6.55335500	1.87494300	0.02810500
C	5.05528500	1.87225100	-1.53233000
H	5.78459400	1.85748800	-2.34586900
C	3.68928400	1.86884300	-1.83265500
H	3.38373400	1.84150700	-2.87829100
P	-2.22051000	0.20080000	-0.12234300
P	0.93004400	1.75820000	-1.11245000
Pd	0.07618200	-0.27382700	-0.20023900
C	0.73170900	-2.34242200	1.93994100
C	0.06311000	-2.32736200	0.54705000
H	0.02052800	-1.89809100	2.64732900
H	0.82361300	-3.40270600	2.20924900
C	-1.21255700	-3.07278200	0.72524800
H	-1.93593700	-2.56642600	1.37094800
C	0.81312700	-2.36502900	-0.70526900

C	2.00100400	-1.56751600	-0.83836300
C	0.28482600	-2.93740200	-1.90992200
C	2.62519200	-1.40815700	-2.09881200
H	2.52651200	-1.18887000	0.03065300
C	0.91380200	-2.76470600	-3.12485400
H	-0.63843500	-3.50717700	-1.86150000
C	2.09613100	-1.99585700	-3.23097800
H	3.54031900	-0.81782100	-2.15374700
H	0.48490700	-3.22358200	-4.01895400
H	2.58541800	-1.87411200	-4.19977700
C	2.02216800	-0.29876500	2.54296000
O	1.01818400	0.31597200	2.08034000
O	2.93012700	0.12958400	3.24657100
C	-2.82296300	1.55538400	-1.25203000
H	-2.18097000	2.42396700	-1.03945300
H	-3.83426800	1.82378400	-0.91688400
C	-2.86518300	1.23442600	-2.74932300
H	-3.33952200	2.09233300	-3.25703600
H	-3.53982200	0.38192500	-2.91800100
C	-1.50667000	0.96752300	-3.40160200
H	-1.67261600	0.57089200	-4.41535600
H	-0.97721600	0.17103900	-2.85294500
C	-0.61634100	2.22435400	-3.47490200
H	-1.10065500	3.06035400	-2.94668700
H	-0.53024000	2.55586200	-4.52154900
C	0.80304900	2.04193300	-2.93341800
H	1.27489500	1.16013900	-3.39713400
H	1.42820200	2.91082800	-3.18887200
C	-1.50378700	-4.31659200	0.32845400
H	-2.46092400	-4.77036100	0.59642200
H	-0.81553600	-4.92308400	-0.26506700
N	2.02599400	-1.72047100	2.16206700
C	3.19471000	-2.41135900	1.94419200
O	4.31540300	-1.94711400	1.93012900
O	2.94704400	-3.71737100	1.66849300
C	4.08063200	-4.49807900	1.29986100
H	4.82485700	-4.52124200	2.10921800
H	3.70232100	-5.50892500	1.10531500
H	4.55565900	-4.09188900	0.39418900

**TS-B2**



Energy: -2791.40407475

Zero point energy correction: 0.755709

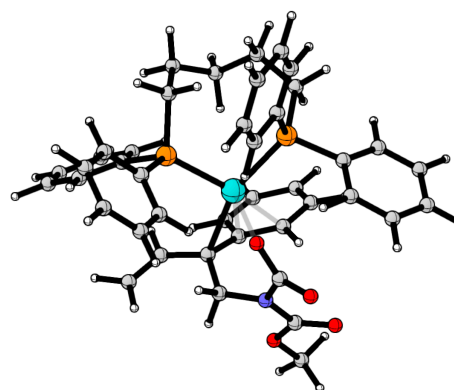
Atom Coordinates:

C	2.88721300	0.56869900	-1.51374500
C	4.18165100	1.09166400	-1.68361900
H	4.85485800	1.20481800	-0.83215600
C	4.63116600	1.46739100	-2.95081300
H	5.63861900	1.87305000	-3.06894900
C	3.79446000	1.32579000	-4.06346900
H	4.14619800	1.62498200	-5.05370400
C	2.50833500	0.80494500	-3.90119400
H	1.84443900	0.70035100	-4.76255800
C	2.05387400	0.42737300	-2.63381500
H	1.02935900	0.07074400	-2.50904600
C	3.24820300	-1.38355400	0.61854600
C	2.91541100	-2.04744900	1.81480500
H	2.07992600	-1.69463700	2.42015300
C	3.61279400	-3.18756000	2.21293300
H	3.33855800	-3.69153900	3.14244100
C	4.64285900	-3.69536200	1.41340400
H	5.18127300	-4.59558200	1.71821700
C	4.97038700	-3.05203100	0.21744800
H	5.76555500	-3.44817900	-0.41832300
C	4.27976700	-1.90163100	-0.17846400
H	4.53799100	-1.42052500	-1.12184900
C	0.01370000	3.24913300	0.25575800
C	0.24911900	4.47605300	0.89694900
H	-0.08337600	4.64239400	1.92281200
C	0.91835000	5.50245700	0.22470700

H	1.10651200	6.44991000	0.73513300
C	1.34796900	5.31741300	-1.09359400
H	1.87910700	6.11870400	-1.61276000
C	1.09031400	4.10749600	-1.74518800
H	1.41478000	3.95612600	-2.77736900
C	0.42538100	3.07699000	-1.07699500
H	0.20864100	2.14077000	-1.59329800
C	-2.58298600	2.10490800	0.75663200
C	-3.01386000	2.09780300	-0.57970400
H	-2.29169200	1.96892500	-1.38455800
C	-4.37059200	2.20563100	-0.88665700
H	-4.67947600	2.15929300	-1.93233900
C	-5.31541200	2.34106500	0.13520300
H	-6.37837800	2.42121300	-0.10434800
C	-4.89261800	2.36789500	1.46697600
H	-5.62218200	2.47627300	2.27316400
C	-3.53472900	2.24713500	1.77990500
H	-3.23776000	2.25413400	2.82825300
P	2.23454800	0.07085000	0.12761500
P	-0.79395600	1.82754000	1.08823300
Pd	-0.08554900	-0.29930500	0.24840900
C	-0.87783500	-2.33310100	-1.89732000
C	-0.26508800	-2.38375300	-0.48542100
H	-0.12248300	-1.91398300	-2.57161500
H	-1.02087600	-3.37816600	-2.19838200
C	0.88063600	-3.35073100	-0.50833900
H	1.87471800	-2.97260800	-0.28048600
C	-1.03773700	-2.28944100	0.74098000
C	-2.09744100	-1.32447400	0.85994100
C	-0.61809700	-2.95681000	1.94095100
C	-2.70276800	-1.08834600	2.12238400
H	-2.58610200	-0.90752700	-0.01479300
C	-1.22052200	-2.69751200	3.15112300
H	0.18626800	-3.68818600	1.87178000
C	-2.27079800	-1.75070700	3.25215000
H	-3.52970100	-0.37997900	2.17654700
H	-0.88814300	-3.23217000	4.04419700
H	-2.74516700	-1.56377600	4.21798500
C	-2.03561100	-0.22452400	-2.55137100
O	-0.98191600	0.32923100	-2.12820900
O	-2.93427800	0.24759700	-3.23981600
C	2.90240000	1.39729000	1.25392300
H	2.30651400	2.29722000	1.04005400
H	3.92591700	1.61120800	0.91766100

C	2.93043700	1.07823600	2.75178200
H	3.46299700	1.90465200	3.25386300
H	3.54730900	0.18345100	2.92218300
C	1.56061900	0.90717200	3.41211000
H	1.70588200	0.51398900	4.43028300
H	0.97796200	0.13939400	2.87648800
C	0.75629100	2.22150200	3.47203800
H	1.30970500	3.02323700	2.95876200
H	0.67057000	2.55489700	4.51812300
C	-0.66180400	2.14520000	2.90316200
H	-1.21673500	1.31949700	3.37835800
H	-1.21244500	3.07106300	3.12746000
C	0.74794100	-4.64742500	-0.80967300
H	1.61705700	-5.31066400	-0.82812500
H	-0.22561600	-5.09784900	-1.02927600
N	-2.12798900	-1.63430500	-2.13252800
C	-3.33369100	-2.24543800	-1.88346300
O	-4.42638300	-1.71898800	-1.87902200
O	-3.15796000	-3.55491000	-1.56609000
C	-4.33073600	-4.25801300	-1.16594900
H	-5.08190500	-4.26366400	-1.96923900
H	-4.00890700	-5.28234200	-0.94241300
H	-4.77488000	-3.79829000	-0.27019500

#### B4



Energy: -2791.41273905

Zero point energy correction: 0.757133

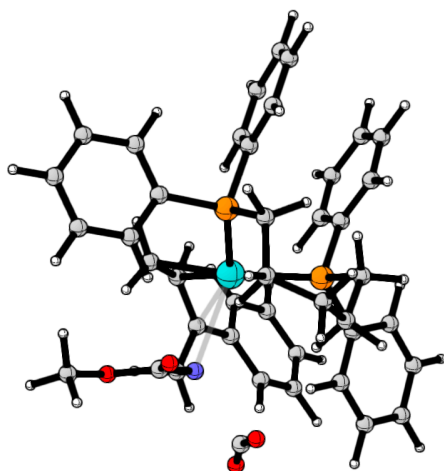
Atom Coordinates:

C	-2.85182600	0.58227100	1.51571800
C	-4.14133100	1.10298500	1.72576700
H	-4.81919800	1.26898700	0.88653900
C	-4.57873200	1.40591000	3.01645300
H	-5.58244900	1.81019600	3.16673800

C	-3.73419100	1.19358100	4.11196200	H	0.04639400	-1.96086500	2.54480600
H	-4.07661300	1.43523100	5.12100500	H	0.83247400	-3.48277300	2.12751400
C	-2.45226600	0.67658000	3.90901800	C	-1.14417900	-3.13510600	0.41791500
H	-1.78251500	0.51710600	4.75735400	H	-1.61054100	-3.23342800	-0.55896400
C	-2.01033200	0.37081900	2.61801700	C	0.92332900	-2.35380100	-0.77337900
H	-0.99097000	0.01108100	2.46438700	C	2.02869600	-1.43756800	-0.87154000
C	-3.29059200	-1.19972600	-0.74982600	C	0.52350300	-3.01972700	-1.97873600
C	-2.99544500	-1.77994600	-1.99808800	C	2.67179400	-1.22509600	-2.11784800
H	-2.14915100	-1.41889100	-2.58331400	H	2.51492000	-1.03844000	0.01216200
C	-3.74371300	-2.85418900	-2.47901600	C	1.16919700	-2.79056200	-3.17434400
H	-3.49751600	-3.29280500	-3.44869900	H	-0.28970100	-3.74261000	-1.94535400
C	-4.79118400	-3.37901900	-1.71324400	C	2.24638700	-1.87577700	-3.25715000
H	-5.37182200	-4.22657000	-2.08437600	H	3.52468900	-0.54707800	-2.15087500
C	-5.08098800	-2.81948500	-0.46701500	H	0.84948200	-3.33084500	-4.06865500
H	-5.88728500	-3.23096200	0.14464300	H	2.75010500	-1.70936000	-4.21169500
C	-4.33624100	-1.73707200	0.01317400	C	2.04840500	-0.40639300	2.52684500
H	-4.56526700	-1.32685300	0.99638700	O	1.02780400	0.21783100	2.12010900
C	0.19365600	3.24700500	-0.14953500	O	2.97892900	-0.00134800	3.21583600
C	0.06036500	4.51982000	-0.72778500	C	-2.82555800	1.61108000	-1.18174100
H	0.40819600	4.71026800	-1.74435400	H	-2.17417300	2.45795700	-0.91895700
C	-0.52497300	5.56194700	-0.00369700	H	-3.82923600	1.86150200	-0.81188500
H	-0.63297300	6.54642500	-0.46489800	C	-2.89273600	1.39654200	-2.69646500
C	-0.97203700	5.34600100	1.30410300	H	-3.37043000	2.28976900	-3.13525900
H	-1.43602900	6.16105600	1.86452100	H	-3.57338700	0.56047400	-2.91518800
C	-0.81706700	4.08731900	1.89267700	C	-1.54575800	1.17275500	-3.38794400
H	-1.15470600	3.91150200	2.91673800	H	-1.73067200	0.84783600	-4.42358800
C	-0.23662600	3.04096500	1.17214000	H	-1.01005000	0.33834900	-2.90562100
H	-0.09485800	2.06636600	1.64028300	C	-0.65248000	2.42970200	-3.38965800
C	2.70452700	1.96634000	-0.73622000	H	-1.14048600	3.23793900	-2.82299000
C	3.14591100	1.90591800	0.59541300	H	-0.55849600	2.81456900	-4.41716000
H	2.42443800	1.81183300	1.40568600	C	0.76458700	2.22186600	-2.85184100
C	4.50956000	1.91698700	0.89005600	H	1.24922400	1.37984700	-3.37305400
H	4.82443400	1.83197300	1.93148100	H	1.38057200	3.11307400	-3.04443100
C	5.45184000	2.00829300	-0.13904400	C	-1.81048300	-3.65844400	1.46274800
H	6.51992000	2.01341800	0.09087500	H	-2.77154700	-4.15006700	1.29980500
C	5.01972400	2.08721300	-1.46580100	H	-1.45441500	-3.61206700	2.49334500
H	5.74761500	2.16125600	-2.27733400	N	2.05147800	-1.81232500	2.08587600
C	3.65411800	2.06254600	-1.76686200	C	3.21614100	-2.49126000	1.82073500
H	3.34850100	2.10671300	-2.81185100	O	4.33769600	-2.02917000	1.81070500
P	-2.22136000	0.17505700	-0.15814300	O	2.96098400	-3.78447600	1.49288700
P	0.89886100	1.81559600	-1.05457100	C	4.08695500	-4.55206500	1.07760900
Pd	0.08305800	-0.28976900	-0.28143300	H	4.83791700	-4.61770900	1.87852500
C	0.75514000	-2.42290700	1.85045600	H	3.70193300	-5.55082800	0.83864700
C	0.12985000	-2.40185100	0.45064600	H	4.55715300	-4.10614400	0.18822100



TS-B3



Energy: -2791.40604521

Zero point energy correction: 0.754219

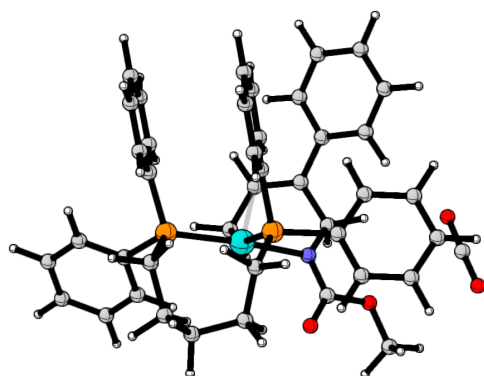
Atom Coordinates:

C	-3.77798300	-0.46965200	-0.24781100
C	-3.85508300	-1.86384000	-0.08019400
H	-3.04888400	-2.40957500	0.41837000
C	-4.95557000	-2.56330600	-0.57955500
H	-5.01778800	-3.64456300	-0.43527000
C	-5.97129700	-1.89107600	-1.26928500
H	-6.82551600	-2.44547800	-1.66490300
C	-5.88444300	-0.50934700	-1.45458200
H	-6.66920300	0.02263900	-1.99776300
C	-4.79467500	0.20246000	-0.94125700
H	-4.74029500	1.28283200	-1.08326700
C	-2.63251300	2.17115900	0.07414600
C	-2.05238500	2.70112700	-1.08957500
H	-1.41334600	2.06951700	-1.70816300
C	-2.26539400	4.03332500	-1.44218300
H	-1.79870800	4.43512000	-2.34337300
C	-3.05010100	4.85629800	-0.62904200
H	-3.20571300	5.90360600	-0.89793800
C	-3.62607500	4.33916700	0.53450200
H	-4.23889300	4.97829000	1.17440600
C	-3.42338100	3.00116800	0.88432500
H	-3.89190600	2.61161100	1.78918100
C	2.80764900	0.61578500	1.30849800
C	3.78753300	1.61668900	1.22144100
H	3.50561900	2.64464600	0.99088300

C	5.13244400	1.30047100	1.42959400
H	5.88870000	2.08518200	1.35139000
C	5.51171300	-0.00958700	1.73890900
H	6.56481000	-0.25124200	1.90056500
C	4.53982900	-1.00955600	1.82855100
H	4.82414500	-2.04031200	2.05086500
C	3.19845900	-0.69715000	1.60455800
H	2.43864000	-1.47227500	1.65657500
C	0.95180500	2.67275400	0.51954800
C	1.45274100	2.90028000	-0.77548700
H	1.89603500	2.07798200	-1.34079400
C	1.39697100	4.17298200	-1.34083100
H	1.79635100	4.33618000	-2.34462900
C	0.82327400	5.23261400	-0.62844000
H	0.76761300	6.22764600	-1.07573000
C	0.31145700	5.01022200	0.65107600
H	-0.14903400	5.82950400	1.20733800
C	0.37947500	3.73770800	1.22749900
H	-0.02574600	3.58726900	2.22841700
P	-2.33612300	0.40982000	0.47094500
P	1.00895900	0.95643700	1.14994600
Pd	-0.31023100	-0.32096200	-0.32036400
C	1.22768800	-2.66914900	-1.60985600
C	1.29716300	-1.22314300	-2.10278700
H	0.70027500	-3.24975500	-2.38212300
H	2.24336500	-3.08118000	-1.56120800
C	0.12378400	-0.58045900	-2.51739200
C	-1.18245400	-1.02910300	-2.17201200
H	0.20508700	0.41572000	-2.95914700
C	2.61686800	-0.58648600	-2.31013600
C	2.79406000	0.49623900	-3.20089100
C	3.74685100	-1.03032800	-1.59242200
C	4.03138000	1.12191000	-3.34251100
H	1.95829900	0.84952700	-3.80587300
C	4.98426400	-0.40188800	-1.73372400
H	3.65359800	-1.85999700	-0.89511400
C	5.13500100	0.68020900	-2.60403800
H	4.13646900	1.95579400	-4.04079500
H	5.83301900	-0.75609300	-1.14618200
H	6.10417800	1.17261300	-2.71206700
C	2.05551300	-3.70876500	1.12324100
O	1.46799400	-3.70114500	2.14401600
H	-1.39023100	-2.09192000	-2.03515400
H	-2.03077500	-0.44310800	-2.53156700

C	-2.66588200	0.26478300	2.28819500
H	-3.75763500	0.31349000	2.41130000
H	-2.26872300	1.17498300	2.75547900
C	-2.08927200	-1.00803800	2.94983300
H	-2.92613700	-1.56437200	3.39895600
H	-1.65584500	-1.68955200	2.19882200
C	0.50635700	1.03952600	2.92695700
H	-0.43324400	1.60206600	2.98270400
H	1.25977300	1.64340200	3.45329800
C	0.36128800	-0.36472900	3.56476700
H	1.05032600	-0.42480400	4.42081400
H	0.69493100	-1.14776300	2.86695300
C	-1.04474000	-0.74625900	4.04505100
H	-0.94322700	-1.67182500	4.63550100
H	-1.42351900	0.02092000	4.74527600
O	2.96931900	-3.89587500	0.39697400
N	0.59820100	-2.79830700	-0.30283000
C	-0.50503100	-3.54748300	-0.16525600
O	-1.20072300	-3.63472000	0.85139900
O	-0.86907500	-4.27528700	-1.28859300
C	-2.01191200	-5.10661300	-1.17285700
H	-2.93693300	-4.51302700	-1.11473900
H	-2.03791400	-5.72701800	-2.07925600
H	-1.95369900	-5.74740200	-0.28058700

**B5**



Zero point energy correction: 0.754017

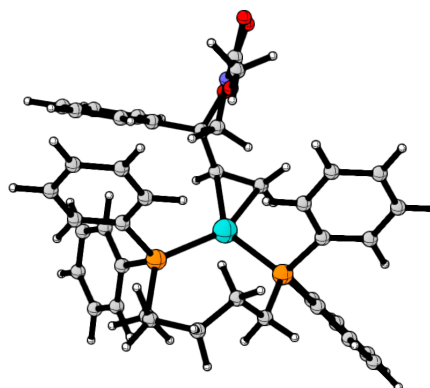
Atom Coordinates:

C	-3.96460200	-1.23237700	-1.04830900
C	-3.60996500	-2.34280600	-1.82942800
H	-2.58053100	-2.70748000	-1.80615200
C	-4.56126400	-2.96634700	-2.64060100
H	-4.27630900	-3.83091500	-3.24451100
C	-5.87058500	-2.47748900	-2.68678700

H	-6.61232600	-2.95936700	-3.32807100
C	-6.22853000	-1.36723400	-1.91452300
H	-7.24993100	-0.98107400	-1.95017600
C	-5.28160400	-0.74849300	-1.09463000
H	-5.56751400	0.11689400	-0.49276500
C	-3.21239500	1.23520600	0.28359900
C	-3.25419000	2.04854100	-0.86215900
H	-3.08668800	1.60931500	-1.84753700
C	-3.51196700	3.41454000	-0.75012600
H	-3.54157400	4.03573600	-1.64821900
C	-3.72572900	3.98651000	0.50913900
H	-3.91781500	5.05811000	0.59847000
C	-3.68593200	3.18419600	1.65091800
H	-3.84243800	3.62523900	2.63738900
C	-3.43139000	1.81449500	1.54147700
H	-3.38922200	1.21045000	2.44775000
C	2.17994600	-0.52724500	1.76916500
C	2.94614600	0.59386600	1.41656300
H	2.45837900	1.51998000	1.11344800
C	4.34151900	0.53940000	1.45418100
H	4.92176000	1.42346400	1.18047200
C	4.98981500	-0.63683000	1.84138900
H	6.08061500	-0.67902900	1.87906200
C	4.23208500	-1.76417400	2.17307900
H	4.72976400	-2.69295500	2.46165300
C	2.83706500	-1.71189500	2.13912300
H	2.26630700	-2.60800200	2.37750800
C	-0.00490800	1.28698400	2.12510200
C	-0.05990100	2.21345800	1.06821800
H	0.06330000	1.86702000	0.04079500
C	-0.27732600	3.56733100	1.32093700
H	-0.31497200	4.27030100	0.48648700
C	-0.46668100	4.01150600	2.63286800
H	-0.65441400	5.06911600	2.83214200
C	-0.42562100	3.09689600	3.68904900
H	-0.57456500	3.43899300	4.71602300
C	-0.18675100	1.74164100	3.43968300
H	-0.13823800	1.04717600	4.28016600
P	-2.71891900	-0.51253900	0.08936800
P	0.34031800	-0.46813600	1.70022500
Pd	-0.53593600	-0.78656300	-0.49516600
C	1.97760600	-0.30578900	-2.23094000
C	1.17686600	0.96963400	-2.39120800
H	1.98735300	-0.83416300	-3.20571800

H	3.02892800	-0.09673000	-2.00465300
C	-0.17380300	0.83972100	-2.56216500
C	-0.90554900	-0.42667700	-2.55699400
H	-0.78611100	1.74554900	-2.55913000
C	1.80538700	2.29208400	-2.20171800
C	1.14098600	3.48805600	-2.56638900
C	3.06745900	2.43064500	-1.58345000
C	1.68121500	4.74068900	-2.28355000
H	0.18342300	3.43652100	-3.08676300
C	3.61016700	3.68663900	-1.30210500
H	3.63356400	1.54683500	-1.29968900
C	2.92018500	4.85328800	-1.63970100
H	1.13372600	5.64021200	-2.57723700
H	4.58442100	3.74845500	-0.80982200
H	3.34413500	5.83557000	-1.41865900
C	5.87214500	-1.05814000	-1.21306300
O	6.30445900	-2.05283700	-0.79521400
H	-0.42654000	-1.26948500	-3.07136800
H	-1.96008800	-0.33994100	-2.83767600
C	-3.12215200	-1.34287500	1.68199200
H	-4.19315200	-1.21168600	1.89718300
H	-2.57682500	-0.79944400	2.46220800
C	-2.72315200	-2.83572500	1.64426500
H	-3.63928900	-3.43604300	1.53870000
H	-2.12363700	-3.04830100	0.74256000
C	-0.14662200	-1.44988100	3.20072100
H	-1.01346400	-0.95592600	3.66121300
H	0.67575600	-1.35115500	3.92362300
C	-0.44647900	-2.93833000	2.91156200
H	0.02770600	-3.53496500	3.70700200
H	0.04077500	-3.23970600	1.96944100
C	-1.93119200	-3.33066200	2.86099700
H	-1.97723400	-4.43236900	2.86250800
H	-2.43296400	-3.00504900	3.79059100
O	5.46986900	-0.05305000	-1.63780400
N	1.38958200	-1.17663800	-1.21001400
C	1.93557700	-2.34119000	-0.88686000
O	1.43307000	-3.19510400	-0.14165100
O	3.17494000	-2.56869500	-1.45420900
C	3.74919300	-3.83898000	-1.18120800
H	3.05228300	-4.65285900	-1.43166400
H	4.65201400	-3.91240600	-1.80027800
H	4.02749100	-3.93302500	-0.12013000

C2



Energy: -2791.41631493

Zero point energy correction: 0.755888

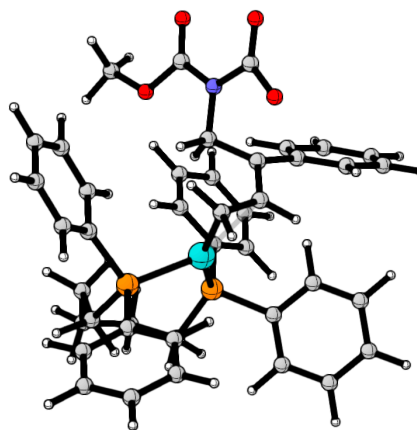
Atom Coordinates:

C	3.10407500	1.79001300	0.41176200
C	2.02785800	2.47847900	1.00441100
H	1.15765900	1.92085900	1.35231100
C	2.04458800	3.86785600	1.12760400
H	1.19244800	4.37885600	1.58092200
C	3.13756500	4.59925000	0.64870900
H	3.14970800	5.68835400	0.73336700
C	4.20690500	3.92827300	0.04990400
H	5.06018000	4.49218000	-0.33490800
C	4.19220300	2.53359500	-0.06911900
H	5.03114800	2.02968600	-0.55058700
C	4.36976300	-0.55108100	-0.79820000
C	4.12871400	-1.06913000	-2.08047200
H	3.09937700	-1.14330700	-2.43689000
C	5.18810300	-1.49289100	-2.88841900
H	4.98499000	-1.89437100	-3.88398100
C	6.50208200	-1.40749600	-2.42018500
H	7.33129000	-1.73988900	-3.04923000
C	6.75350200	-0.89924000	-1.14085300
H	7.77886300	-0.83315900	-0.76930600
C	5.69506100	-0.47497200	-0.33428900
H	5.90979200	-0.07816000	0.66001900
C	-1.66477000	-1.34730500	1.95295700
C	-2.79608200	-2.11645800	2.26182500
H	-2.86726700	-3.14751800	1.91101400
C	-3.84531900	-1.56496100	3.00189400
H	-4.72740300	-2.17040500	3.22340300
C	-3.77331300	-0.24297400	3.45329000

H	-4.59873300	0.18695500	4.02521100
C	-2.63998200	0.52561900	3.16923900
H	-2.57276400	1.55972800	3.51419600
C	-1.59621700	-0.02531600	2.42261600
H	-0.71888800	0.58113400	2.19251600
C	-0.92692300	-3.36531100	-0.00577700
C	-2.08495500	-3.13502900	-0.77052500
H	-2.60189800	-2.17973200	-0.69637500
C	-2.57776900	-4.11743500	-1.62892000
H	-3.48333400	-3.91711600	-2.20581900
C	-1.91257600	-5.34301100	-1.75510200
H	-2.29545500	-6.11002300	-2.43241500
C	-0.75316900	-5.57596100	-1.01203600
H	-0.22241300	-6.52651000	-1.10634200
C	-0.26360600	-4.59607000	-0.14058000
H	0.64647600	-4.80207200	0.42487100
P	2.92695000	-0.03602300	0.21536000
P	-0.22528300	-1.99411100	1.00337600
Pd	0.76664300	-0.50314700	-0.53138400
C	-1.39847400	1.90870500	-0.52310800
C	-1.74653800	0.98840300	-1.69472800
H	-1.72550600	1.51271900	0.43746100
H	-0.31720400	2.08524000	-0.46642400
C	-0.61603700	0.08755200	-2.12106600
C	0.68671500	0.59214700	-2.35631400
H	-0.93275800	-0.80173500	-2.67213700
C	-3.06170400	0.23044000	-1.54472800
C	-3.56057900	-0.44681700	-2.67152400
C	-3.79777000	0.18028000	-0.35609800
C	-4.74249000	-1.18235700	-2.60079100
H	-3.01354600	-0.39411700	-3.61437700
C	-4.98437500	-0.55829700	-0.28204300
H	-3.45252400	0.69325100	0.53857500
C	-5.45717700	-1.24810500	-1.39851000
H	-5.10771900	-1.70816400	-3.48609000
H	-5.53008500	-0.59615700	0.66251900
H	-6.37932700	-1.83059300	-1.33728300
C	-2.34865300	3.18972400	-2.24811500
O	-2.77142400	4.11424400	-2.88917600
H	0.91075500	1.65416500	-2.21063600
H	1.31166200	0.10818700	-3.11295900
C	3.34610600	-0.72269200	1.88371200
H	4.36970300	-0.45274100	2.18403600
H	3.33982000	-1.81225600	1.72273300

C	2.34122300	-0.32510700	2.97550200
H	2.70838900	0.58129000	3.47969100
H	1.38186200	-0.03735700	2.51765200
C	0.66692800	-2.95819200	2.35536200
H	1.64031300	-3.27452100	1.94926000
H	0.06670200	-3.87134500	2.48427700
C	0.82704100	-2.29111900	3.73647000
H	0.81111900	-3.09848500	4.48708100
H	-0.06669900	-1.68346200	3.94960600
C	2.07942900	-1.44354400	3.99856600
H	1.96675800	-1.00497800	5.00348500
H	2.96700200	-2.09785000	4.05660200
O	-2.00750800	2.00288400	-2.77357800
N	-2.09927900	3.13977600	-0.86687800
C	-2.28405500	4.18964600	0.01741800
O	-2.83042200	5.23847900	-0.22026800
O	-1.75879800	3.85474200	1.21293600
C	-1.89578900	4.82542000	2.25320200
H	-1.42531700	4.38389500	3.13915900
H	-1.38807700	5.76142500	1.97938100
H	-2.95672400	5.03644800	2.45020000

#### TS-C1



Energy: -2791.40880706

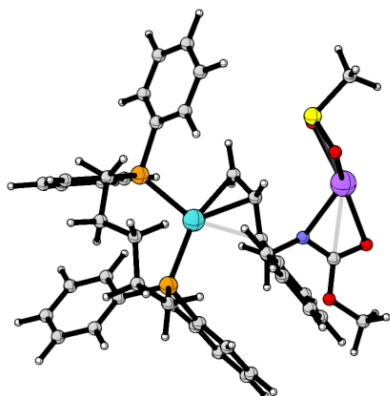
Zero point energy correction: 0.756338

Atom Coordinates:

C	3.31069000	2.42500600	0.22626800
C	2.59497400	3.40719500	0.93481900
H	1.78942200	3.11750100	1.61330300
C	2.89101500	4.75921000	0.75921600
H	2.33066500	5.51272700	1.31724900
C	3.89206000	5.14836000	-0.13865000

H	4.11816700	6.20741300	-0.28136300	H	-1.21352000	2.89924800	-0.82902100
C	4.59225300	4.17800400	-0.85900600	C	-0.27337400	0.82984600	-2.11229000
H	5.36790200	4.47500000	-1.56863600	C	0.84034400	1.65289000	-1.78775700
C	4.30499400	2.82055600	-0.67968400	H	-0.09912600	-0.00270000	-2.79828300
H	4.85622800	2.07353600	-1.25239200	C	-2.51660200	-0.17232000	-1.70897200
C	4.00677800	-0.32947800	-0.49681600	C	-2.54127200	-0.88468300	-2.92388200
C	3.54019600	-1.12349100	-1.55542600	C	-3.48071000	-0.49125600	-0.73481500
H	2.47836400	-1.12253700	-1.80657500	C	-3.46239100	-1.91029900	-3.13482800
C	4.42513500	-1.93262800	-2.27338100	H	-1.84612900	-0.62280900	-3.72196300
H	4.04801800	-2.55260900	-3.08930300	C	-4.39190800	-1.52677800	-0.93808700
C	5.78105900	-1.95563700	-1.93835600	H	-3.49915400	0.05287100	0.20488500
H	6.47256400	-2.58969800	-2.49797300	C	-4.38331900	-2.24705000	-2.13672000
C	6.25366700	-1.16838800	-0.88149800	H	-3.46353800	-2.44737900	-4.08612100
H	7.31312000	-1.18542300	-0.61619900	H	-5.10852000	-1.77159300	-0.15166100
C	5.37274700	-0.35933100	-0.16238400	H	-5.09843600	-3.05683200	-2.29855900
H	5.75498400	0.25357000	0.65656900	C	-3.65190700	2.74874700	-2.23884700
C	-1.62316900	-1.84806100	1.77202200	O	-4.84460200	2.91491200	-2.48704900
C	-2.22328400	-3.11745600	1.78242100	H	0.69890800	2.64634100	-1.35403400
H	-1.69386900	-3.97717800	1.36800200	H	1.75032400	1.54607900	-2.38266900
C	-3.50480200	-3.28513400	2.30842800	C	3.23525300	0.29868800	2.21684700
H	-3.96949100	-4.27368400	2.29881200	H	4.20998400	0.74820600	2.45811100
C	-4.19121800	-2.19136800	2.84693400	H	3.38861100	-0.78831000	2.22836200
H	-5.19464800	-2.32309000	3.25799700	C	2.15728300	0.72254800	3.23434900
C	-3.59245800	-0.92946100	2.85575000	H	2.47647800	1.65841100	3.71603700
H	-4.12683300	-0.07469400	3.27131000	H	1.21044700	0.95756400	2.71790700
C	-2.31591600	-0.75535400	2.31400400	C	1.04992100	-2.20973300	2.63626600
H	-1.86866700	0.24044000	2.29577200	H	2.11283500	-2.27202500	2.36834800
C	0.34501000	-2.90154500	-0.10224600	H	0.70476500	-3.24573500	2.77351300
C	-0.64372500	-3.11556200	-1.07977200	C	0.83555700	-1.40606300	3.93672100
H	-1.60212300	-2.60293300	-1.00918100	H	0.78514100	-2.12765700	4.76728700
C	-0.40414500	-3.98170000	-2.14653600	H	-0.15746300	-0.92862700	3.91399600
H	-1.18260800	-4.13301500	-2.89757900	C	1.88519100	-0.34707200	4.30352900
C	0.82461100	-4.64329600	-2.25488100	H	1.53472300	0.14701300	5.22405100
H	1.01240100	-5.31828000	-3.09300100	H	2.83674000	-0.83974300	4.57060600
C	1.81071600	-4.43547200	-1.28677000	O	-2.65593500	2.70955800	-2.98781700
H	2.77453200	-4.94316300	-1.36605300	N	-3.27001800	2.50571400	-0.80136400
C	1.57519900	-3.56802000	-0.21621100	C	-4.10742900	2.74729100	0.25373500
H	2.36716100	-3.40258000	0.51507500	O	-5.20823900	3.25520300	0.22860600
P	2.82148000	0.67721300	0.46006500	O	-3.54915000	2.34352500	1.44358700
P	0.08584300	-1.59960200	1.16165000	C	-4.31254000	2.63590500	2.60690100
Pd	0.63691800	0.29835100	-0.15080300	H	-3.70123100	2.31759700	3.46083100
C	-1.89395600	2.07158200	-0.58922000	H	-4.52691600	3.71228900	2.68113400
C	-1.50408900	0.87237800	-1.44651200	H	-5.26840700	2.09054000	2.60309600
H	-1.76493000	1.84267300	0.47248600				

A6



Energy: -3353.58437342

Zero point energy correction: 0.787422

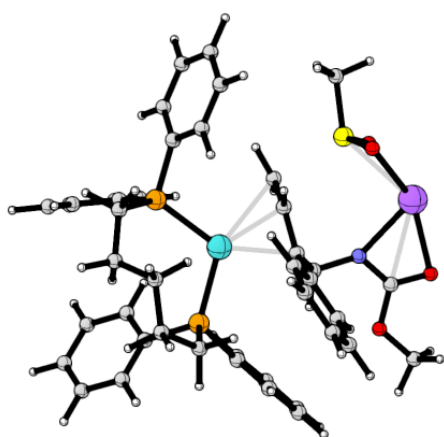
Atom Coordinates:

C	-3.40886000	1.66636700	-1.01751300
C	-4.80005300	1.57007400	-0.88205400
H	-5.26498100	1.55644800	0.10399000
C	-5.61297200	1.47182900	-2.01591300
H	-6.69540400	1.38737300	-1.89717100
C	-5.04556100	1.47305100	-3.29182300
H	-5.68269500	1.39310300	-4.17540600
C	-3.65592500	1.56873600	-3.43510200
H	-3.20454100	1.56552800	-4.42961600
C	-2.84255200	1.65761700	-2.30592300
H	-1.75720800	1.71005000	-2.42277000
C	-1.69623500	3.47663300	0.47081800
C	-0.73897600	3.81025200	1.44617100
H	-0.36594400	3.04280600	2.13036600
C	-0.23012300	5.10590300	1.52377800
H	0.52595800	5.34711000	2.27393800
C	-0.67279900	6.08624800	0.62720300
H	-0.26804700	7.09940500	0.68026400
C	-1.62843200	5.76269700	-0.33852400
H	-1.97810000	6.52393500	-1.03980000
C	-2.14118400	4.46267000	-0.41878500
H	-2.88287900	4.22058000	-1.18118400
C	-2.96230300	-2.36987400	0.01538700
C	-3.75540200	-3.37943300	0.58562700
H	-3.40623300	-3.93347000	1.45829200
C	-5.00094100	-3.68811600	0.03465000
H	-5.61526300	-4.46812600	0.49033200
C	-5.45824300	-3.00759500	-1.09961800

H	-6.43234000	-3.25336600	-1.52875200
C	-4.66579100	-2.01528900	-1.68209300
H	-5.01140600	-1.47780200	-2.56662700
C	-3.42678300	-1.69382100	-1.12190300
H	-2.81924200	-0.90750900	-1.56923300
C	-0.27385500	-3.23337200	-0.18155100
C	-0.39400900	-3.38197400	-1.57503900
H	-1.11475700	-2.77904000	-2.13050500
C	0.40581900	-4.29422700	-2.26138300
H	0.30281100	-4.39632800	-3.34406400
C	1.34180300	-5.07019200	-1.56723900
H	1.97394200	-5.78014900	-2.10526700
C	1.46763400	-4.92579300	-0.18524900
H	2.20343500	-5.51645600	0.36494700
C	0.66576900	-4.01275300	0.50748300
H	0.79836600	-3.90915300	1.58317200
P	-2.25480100	1.72768500	0.39826000
P	-1.29597400	-1.95828800	0.66222000
Pd	-0.45116800	0.21885100	0.22440000
C	2.03777100	-0.94857600	-1.29505100
C	1.78602200	-0.41934800	0.11974900
H	2.02959400	-2.04618500	-1.28251500
H	1.19792100	-0.65591700	-1.95072900
C	1.59924800	0.97706900	0.30470700
H	1.87265500	1.42740300	1.26081400
C	2.32175600	-1.18750600	1.27469300
C	3.22452000	-2.25184600	1.09402100
C	1.93460500	-0.87061800	2.59419900
C	3.71685300	-2.96786900	2.18789700
H	3.54605200	-2.52752000	0.09128700
C	2.41761800	-1.59256500	3.68464100
H	1.21482300	-0.06812700	2.76615500
C	3.31303400	-2.65041900	3.48694500
H	4.41719400	-3.78935800	2.01791600
H	2.08552800	-1.33433500	4.69308300
H	3.68992700	-3.22075800	4.33912800
C	-1.27480500	-2.50738000	2.42711300
H	-0.24840900	-2.28708500	2.75946800
H	-1.38404600	-3.60216600	2.44783800
C	-2.27364600	-1.85129800	3.39170300
H	-1.97043900	-2.15372000	4.40638000
H	-3.27793300	-2.27924200	3.23916600
C	-2.35405900	-0.32075900	3.30180000
H	-1.39355200	0.07437200	2.92709700

H	-2.47921200	0.11230600	4.30724900
C	-3.50431300	0.18077200	2.41596600
H	-4.44610200	0.12482700	2.98570400
H	-3.64983800	-0.48478700	1.55203900
C	-3.28453400	1.61481200	1.93275300
H	-4.22481000	2.15286000	1.74398100
H	-2.74908100	2.20133400	2.69455300
N	3.27159200	-0.36782800	-1.76617700
C	4.33116000	-1.08786900	-2.05208100
O	5.46226500	-0.60738200	-2.30663700
O	4.18349400	-2.46929400	-2.06000600
C	5.35294700	-3.23482500	-2.28498800
H	5.81941700	-2.98775400	-3.25146100
H	6.10298800	-3.07313200	-1.49322400
H	5.04039200	-4.28879200	-2.28318700
C	0.88932600	1.75487600	-0.61602900
H	0.83435800	1.46600400	-1.66808700
H	0.71626700	2.80649800	-0.39911900
Na	4.62743300	1.47019300	-1.32967700
O	3.57776200	3.54411200	-1.41624400
S	3.53071000	3.69643200	0.12308300
O	4.25984100	2.48105600	0.74913500
C	4.76336900	5.03068400	0.39196700
H	4.89734500	5.18577200	1.47264600
H	5.70203900	4.69096100	-0.07187200
H	4.40425100	5.95349100	-0.08688700

#### TS-A4



Energy: -3353.57005079

Zero point energy correction: 0.787219

Atom Coordinates:

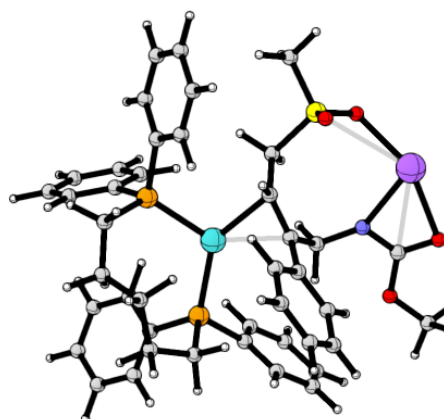
C	-3.52622700	1.58418800	-0.90255000
C	-4.91776000	1.45489600	-0.80098400

H	-5.40049700	1.38460900	0.17428900
C	-5.70843900	1.39783200	-1.95369100
H	-6.79110900	1.28676700	-1.85967900
C	-5.11939300	1.47617700	-3.21752800
H	-5.73909200	1.42869800	-4.11582800
C	-3.72958800	1.60676700	-3.32872100
H	-3.26003100	1.66166700	-4.31344600
C	-2.93935100	1.65001800	-2.18049500
H	-1.85150500	1.71709200	-2.26959900
C	-1.87706300	3.32182400	0.73797700
C	-1.02136400	3.62000300	1.81551800
H	-0.75502000	2.83881900	2.53245100
C	-0.47556800	4.89531400	1.95929300
H	0.19236600	5.10757000	2.79730000
C	-0.76928200	5.89419000	1.02243500
H	-0.33113400	6.88940700	1.12557800
C	-1.62414200	5.60877800	-0.04506100
H	-1.86245300	6.38354500	-0.77773700
C	-2.17956800	4.33176200	-0.18637000
H	-2.83894100	4.12290500	-1.03003300
C	-2.73409700	-2.60708800	-0.31328400
C	-3.40146100	-3.76946000	0.10753000
H	-2.96749800	-4.40811300	0.87929200
C	-4.62736800	-4.12211900	-0.46164000
H	-5.14278000	-5.02353500	-0.12161800
C	-5.19282900	-3.32726000	-1.46574200
H	-6.15251700	-3.60554800	-1.90764400
C	-4.52641800	-2.17867800	-1.90079800
H	-4.95724200	-1.54963600	-2.68223400
C	-3.30570100	-1.81930900	-1.32263700
H	-2.79660700	-0.91341700	-1.65079600
C	0.03087000	-3.20294300	-0.53953900
C	0.01021400	-3.14680600	-1.94514100
H	-0.71044900	-2.50113100	-2.45284800
C	0.90467600	-3.90464400	-2.69895900
H	0.87535600	-3.85094100	-3.78983700
C	1.84345300	-4.72390200	-2.06014800
H	2.55217800	-5.30958400	-2.64988700
C	1.87349700	-4.78123100	-0.66665800
H	2.60910300	-5.40982700	-0.15919400
C	0.97216400	-4.02784400	0.09319500
H	1.02491500	-4.08124700	1.17927300
P	-2.38360000	1.56563600	0.52748600
P	-1.11064800	-2.09845000	0.38448900

Pd	-0.50705100	0.16382600	0.29039700
C	2.32449200	-0.53215700	-0.94467300
C	1.78787400	-0.02253100	0.38833100
H	2.19845400	-1.62122600	-0.99446500
H	1.69053000	-0.12775400	-1.75482000
C	1.40272900	1.35013500	0.51565500
H	1.38164900	1.80342000	1.50859600
C	2.14774600	-0.77545900	1.61911000
C	2.95474100	-1.92966800	1.55671400
C	1.65928200	-0.39470100	2.89066500
C	3.24525900	-2.67078400	2.70555500
H	3.35734900	-2.25982900	0.60154300
C	1.94845700	-1.13566200	4.03455100
H	1.00715500	0.47421000	2.98296300
C	2.74369600	-2.28544200	3.95082500
H	3.86990000	-3.56375000	2.61967400
H	1.53997500	-0.81959600	4.99769400
H	2.96653200	-2.87107800	4.84577900
C	-1.07917700	-2.78593400	2.10329100
H	-0.09123500	-2.49537900	2.49465300
H	-1.08960800	-3.88518800	2.04675300
C	-2.17304200	-2.30036400	3.06821400
H	-1.90796900	-2.69644300	4.06136900
H	-3.13464600	-2.77181100	2.80603800
C	-2.35586400	-0.77469300	3.14750600
H	-1.42895000	-0.28074100	2.80767700
H	-2.49047000	-0.46401700	4.19656400
C	-3.54696500	-0.24561500	2.33387400
H	-4.47850000	-0.43474200	2.89234100
H	-3.64940800	-0.80817300	1.39266200
C	-3.42797600	1.25194500	2.02618100
H	-4.40519200	1.73770800	1.89104200
H	-2.93864500	1.77903700	2.85957800
N	3.69318600	-0.10217600	-1.12446400
C	4.66172700	-0.95431700	-1.35938800
O	5.87267800	-0.63425000	-1.49133000
O	4.32562600	-2.29651000	-1.46231600
C	5.38333100	-3.21066500	-1.67294600
H	5.92572700	-2.99649900	-2.60776100
H	6.11092300	-3.19000300	-0.84523000
H	4.92352800	-4.20699400	-1.73329100
C	1.11798400	2.21450900	-0.55735300
H	1.14176500	1.86770000	-1.59054100
H	0.57908500	3.14108600	-0.36516000

Na	5.30742900	1.59078300	-1.01923300
O	4.02900700	3.31905800	-2.07969300
S	3.21472900	3.48100800	-0.80321100
O	4.02739800	3.08606700	0.42084400
C	2.98311900	5.28158500	-0.62640800
H	2.40830700	5.46464400	0.29154800
H	3.98740100	5.72483800	-0.56408700
H	2.44002700	5.65038500	-1.50692400

A7



Energy: -3353.58676698

Zero point energy correction: 0.789735

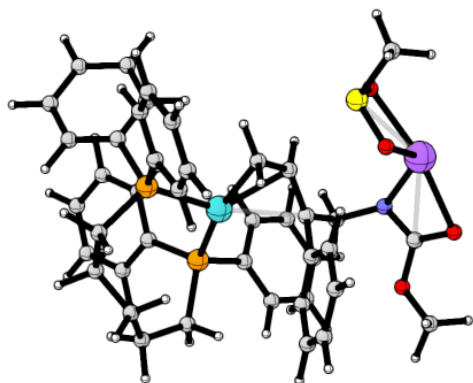
Atom Coordinates:

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C	-4.87023900	1.15815100	-0.73314100
H	-5.32253700	1.08769800	0.25647500
C	-5.68323100	0.99997900	-1.86099200
H	-6.75161800	0.81066300	-1.73308400
C	-5.13431800	1.07708500	-3.14276500
H	-5.77050400	0.94990800	-4.02163000
C	-3.76171500	1.30959900	-3.29540800
H	-3.32214700	1.36538300	-4.29399600
C	-2.94858900	1.45056400	-2.17112000
H	-1.87140800	1.59290400	-2.29421700
C	-1.92800300	3.25633700	0.68339700
C	-1.05244000	3.63998000	1.71746100
H	-0.67923900	2.88963000	2.41862100
C	-0.63887500	4.96533100	1.84871400
H	0.04590200	5.24228800	2.65339600
C	-1.08803600	5.93346500	0.94169400
H	-0.76000200	6.97088100	1.03883300
C	-1.95422800	5.56280500	-0.09053600
H	-2.30872400	6.31175500	-0.80286600



C	-2.37334100	4.23365500	-0.21992500	C	-0.87253000	-2.85249300	2.10427500
H	-3.04971100	3.95892800	-1.03073100	H	0.09359800	-2.49191600	2.49299500
C	-2.54222600	-2.88554700	-0.28632000	H	-0.81830400	-3.95211500	2.08275000
C	-3.02611600	-4.15158100	0.08339200	C	-2.00290000	-2.40536700	3.04486000
H	-2.46081300	-4.77481700	0.77975400	H	-1.76026400	-2.80979100	4.04074500
C	-4.23071000	-4.62763500	-0.43889100	H	-2.94513700	-2.89523700	2.74619300
H	-4.60144500	-5.61102200	-0.13928600	C	-2.21815600	-0.88306900	3.14068500
C	-4.96047900	-3.84990100	-1.34644700	H	-1.30686400	-0.36799400	2.79117400
H	-5.90273100	-4.22475300	-1.75350400	H	-2.34417400	-0.58484900	4.19480600
C	-4.48007200	-2.59496600	-1.72903100	C	-3.42709200	-0.36325700	2.34761400
H	-5.04042800	-1.97799500	-2.43463700	H	-4.35036700	-0.56748300	2.91518100
C	-3.27907200	-2.11475000	-1.19633100	H	-3.53040000	-0.92147300	1.40350300
H	-2.91244800	-1.12862300	-1.48146600	C	-3.32884200	1.13923500	2.04761800
C	0.25572500	-3.26777500	-0.52933200	H	-4.31335700	1.61746900	1.93811300
C	0.22989600	-3.25099500	-1.93616900	H	-2.82345000	1.66371200	2.87350700
H	-0.54248300	-2.67785200	-2.45604900	N	3.80152900	0.08822700	-1.11920500
C	1.18254600	-3.95089900	-2.67500700	C	4.81317100	-0.72961200	-1.27742700
H	1.14622700	-3.92799400	-3.76702000	O	6.01370500	-0.35971600	-1.38331700
C	2.18788300	-4.67353000	-2.02033200	O	4.53871900	-2.08747400	-1.32915000
H	2.94228400	-5.21261400	-2.59796200	C	5.64044200	-2.96396700	-1.45412500
C	2.22369200	-4.69256700	-0.62570100	H	6.22767400	-2.75277000	-2.36203600
H	3.00982900	-5.24496600	-0.10509500	H	6.31823600	-2.89447900	-0.58720200
C	1.26365000	-3.99747300	0.11810000	H	5.22355200	-3.97910800	-1.51196500
H	1.32314900	-4.01597600	1.20517900	C	1.22219000	2.41554400	-0.84454000
P	-2.31176100	1.46036200	0.52679800	H	1.34426500	1.95059700	-1.82922600
P	-0.95500100	-2.20730900	0.36491800	H	0.31174700	3.03148300	-0.83697200
Pd	-0.45594400	0.08599500	0.27464400	Na	5.25779500	1.86930300	-1.22568800
C	2.44190100	-0.38165800	-0.97126100	O	3.64458700	3.38991300	-1.74975700
C	1.82659400	0.17998900	0.30222400	S	2.57316600	3.68367900	-0.75395300
H	2.35724500	-1.47677500	-0.97062800	O	2.99434400	3.84582300	0.65469300
H	1.82919200	-0.04531400	-1.82834100	C	1.79166200	5.20690400	-1.29057500
C	1.26022600	1.47729200	0.31723300	H	0.98096900	5.45015000	-0.59307900
H	1.19532300	2.00603400	1.26919700	H	2.58030700	5.97033500	-1.26614500
C	2.17898800	-0.48402800	1.58966200	H	1.41522500	5.06626400	-2.31179200
C	2.99216700	-1.63665300	1.61450200				
C	1.68215000	-0.02459900	2.83298900				
C	3.26376900	-2.30892700	2.80987600				
H	3.41140300	-2.02435800	0.68871700				
C	1.95288800	-0.69660500	4.02297400				
H	1.03916100	0.85467500	2.86819100				
C	2.74347100	-1.85307400	4.02316800				
H	3.89009300	-3.20500100	2.78537800				
H	1.53407300	-0.31840200	4.95933200				
H	2.95079300	-2.38469700	4.95489600				

**DI**



Energy: -3353.58429891

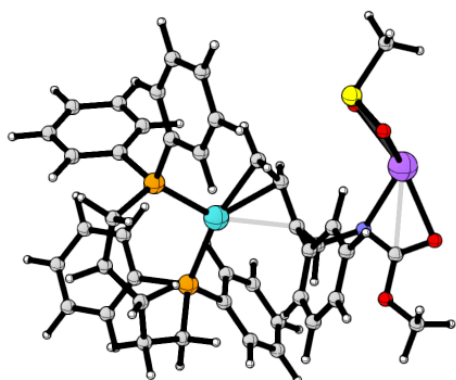
Zero point energy correction: 0.787684

Atom Coordinates:

C	-3.20000500	2.02070300	-0.66772700
C	-4.59385500	2.06185400	-0.52955700
H	-5.06116400	1.95761000	0.44966800
C	-5.41007100	2.22154100	-1.65394700
H	-6.49532600	2.24246500	-1.53295700
C	-4.84326800	2.34515400	-2.92398900
H	-5.48307500	2.46711100	-3.80079800
C	-3.45160300	2.30286200	-3.07083500
H	-3.00024400	2.39279900	-4.06128600
C	-2.63633100	2.13401000	-1.95208800
H	-1.55300900	2.07721100	-2.07650200
C	-1.33051300	3.41698700	1.05680200
C	-0.37560700	3.52006700	2.08376500
H	-0.08886800	2.63219500	2.65442100
C	0.22629200	4.74547800	2.36902100
H	0.96866000	4.81164600	3.16758300
C	-0.11210200	5.88217300	1.62511300
H	0.36489700	6.84055900	1.84221800
C	-1.05874400	5.78517800	0.60270300
H	-1.32779900	6.66883500	0.01932300
C	-1.66935900	4.55844100	0.31849500
H	-2.40724700	4.49590200	-0.48254000
C	-3.22335400	-2.13481800	-0.28628800
C	-4.14497200	-3.10553700	0.13947800
H	-3.88343100	-3.81243000	0.92821600
C	-5.40855000	-3.18043100	-0.45035200
H	-6.12202200	-3.93272400	-0.10608500
C	-5.75797200	-2.30195200	-1.48226200
H	-6.74708300	-2.36437400	-1.94186600
C	-4.83809300	-1.34790800	-1.92443100
H	-5.09861300	-0.65826500	-2.72900800
C	-3.57927100	-1.26128800	-1.32418400
H	-2.86930100	-0.50605100	-1.66172300
C	-0.67914600	-3.32549000	-0.56668200
C	-0.72740000	-3.23363100	-1.96799400
H	-1.27950400	-2.41947700	-2.44229900
C	-0.07013700	-4.17053500	-2.76454600
H	-0.11891200	-4.08461400	-3.85244600
C	0.65838000	-5.20879800	-2.17302100
H	1.18041600	-5.93812100	-2.79636300
C	0.71594900	-5.30482000	-0.78159600
H	1.28523800	-6.10869400	-0.30948100
C	0.04873200	-4.37156900	0.01924000
H	0.11337000	-4.47290400	1.10253200
P	-2.05613200	1.76034900	0.73793400
P	-1.53025900	-2.01560600	0.41468400
Pd	-0.47208600	0.11989500	0.16218600
C	2.25689500	-1.79734000	-1.10967300
C	1.80724100	-0.59861100	-0.28995200
H	2.10197700	-2.73115800	-0.55266400
H	1.65234900	-1.85270400	-2.02656600
C	1.39134200	0.54402700	-0.99417600
C	2.27955800	-0.54735100	1.12376700
C	1.97723700	-1.60441800	2.00043200
C	3.09723700	0.49911500	1.58695800
C	2.42546500	-1.59610200	3.31951000
H	1.39389000	-2.44640300	1.63045200
C	3.55444700	0.50072700	2.90917800
H	3.41969100	1.28776800	0.90060000
C	3.21212900	-0.53475000	3.78322600
H	2.16916100	-2.42380500	3.98517100
H	4.19607100	1.31628200	3.25250100
H	3.57039100	-0.52639200	4.81549100
C	-1.62402900	-2.78820300	2.09848000
H	-0.59393700	-2.72331100	2.48031200
H	-1.84570500	-3.85793000	1.96861600
C	-2.57740100	-2.18027600	3.13534900
H	-2.35059000	-2.67668500	4.09200700
H	-3.61741000	-2.45445800	2.89502700
C	-2.47472400	-0.65867800	3.29295800
H	-1.46282000	-0.32705800	3.00127000
H	-2.58324600	-0.37676900	4.35269700
C	-3.52939400	0.10551500	2.48175000
H	-4.49081000	0.07464400	3.01956600

H	-3.71894500	-0.39726400	1.52077800
C	-3.12198700	1.55693900	2.23473400
H	-3.98033800	2.23565900	2.12660300
H	-2.53432400	1.94533400	3.08010900
N	3.64168100	-1.53390100	-1.44245200
C	4.60290700	-1.96647700	-0.64942900
O	5.79278400	-1.57311700	-0.70944000
O	4.26200500	-2.91028600	0.29871000
C	5.21250000	-3.16948500	1.31362400
H	6.17574200	-3.50052600	0.89610900
H	5.38890600	-2.27384500	1.93230700
H	4.78780400	-3.96233700	1.94525300
Na	4.96177800	0.39841000	-1.76525600
C	0.88863100	1.70563600	-0.36277700
H	0.51257400	2.51694400	-0.98787400
S	3.68456100	2.97667800	-1.64062000
O	3.62545200	1.98998500	-2.83004800
O	4.60966400	2.36479800	-0.55437500
C	4.76921600	4.29285100	-2.32005000
H	4.97509700	5.03328000	-1.53329100
H	5.69866300	3.79934500	-2.64299900
H	4.26519700	4.76907200	-3.17381100
H	1.25984900	2.02026100	0.61145100
H	1.28446300	0.44922500	-2.07759200

#### TS-D1



Energy: -3353.56266120

Zero point energy correction: 0.787127

Atom Coordinates:

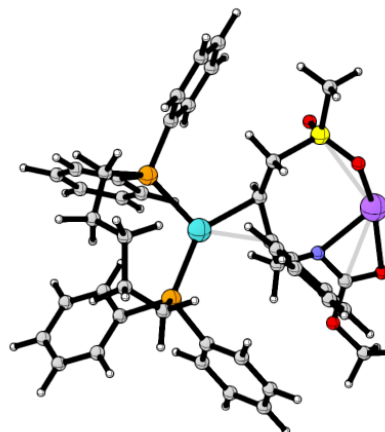
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C	-4.76975500	1.29613800	-1.32026100
H	-5.38133900	1.32281000	-0.41821900

C	-5.39309500	1.06472600	-2.55116000
H	-6.47510400	0.91891500	-2.58796800
C	-4.63872500	1.01369000	-3.72517100
H	-5.12754500	0.82949700	-4.68453000
C	-3.25134300	1.19292800	-3.66597000
H	-2.65238400	1.15067300	-4.57847000
C	-2.62705800	1.41078500	-2.43793400
H	-1.54010000	1.51887000	-2.39445100
C	-2.02364400	3.44728900	0.39851100
C	-1.40829100	3.91806000	1.57328400
H	-1.24378000	3.23937200	2.41477800
C	-0.97072600	5.23874500	1.66658500
H	-0.49267500	5.58776500	2.58490900
C	-1.12950800	6.10924600	0.58122300
H	-0.77775000	7.14118100	0.64912000
C	-1.73941200	5.64956700	-0.58839600
H	-1.86981600	6.32276100	-1.43907000
C	-2.18947600	4.32727900	-0.67994300
H	-2.66385200	3.98367300	-1.60027400
C	-2.74843300	-2.65088600	0.01810700
C	-3.37821600	-3.79246600	0.54121600
H	-2.94597300	-4.31946000	1.39422400
C	-4.55945400	-4.26872600	-0.03084000
H	-5.04638300	-5.15297000	0.38718700
C	-5.11645600	-3.61892400	-1.13896500
H	-6.04085100	-3.99402900	-1.58453900
C	-4.48649800	-2.49273900	-1.67463100
H	-4.91092400	-1.97874900	-2.53929600
C	-3.30890900	-2.00963800	-1.09547100
H	-2.82312300	-1.12437300	-1.50590000
C	0.01419900	-3.28224800	0.17333800
C	-0.09024800	-3.82885600	-1.11717600
H	-0.92286400	-3.54419300	-1.76379900
C	0.86384400	-4.73506300	-1.58170600
H	0.77022900	-5.15071200	-2.58789300
C	1.93781000	-5.10676700	-0.76572400
H	2.68834700	-5.81051100	-1.13254700
C	2.04843500	-4.56689500	0.51707500
H	2.89093600	-4.83836300	1.15723600
C	1.09529400	-3.65928800	0.98609800
H	1.21662300	-3.23546500	1.98239800
P	-2.44874000	1.65773700	0.31954100
P	-1.18344200	-2.00086200	0.72499900
Pd	-0.57235900	0.21410200	0.23074500

C	2.07674600	-0.96067900	-1.28942200
C	1.67152100	-0.08875100	-0.09989400
H	2.11713700	-2.01565400	-0.99177100
H	1.27090000	-0.88079700	-2.04463100
C	1.29727200	1.24259600	-0.47512600
C	2.24397900	-0.43707200	1.23419800
C	3.33879800	-1.32008900	1.32802900
C	1.68660500	0.02631000	2.44722000
C	3.85371500	-1.70971200	2.56633100
H	3.78269600	-1.72823100	0.42377000
C	2.19512700	-0.36897000	3.68454100
H	0.79999100	0.66244600	2.42744300
C	3.28800400	-1.23965800	3.75417000
H	4.70088000	-2.39955800	2.59869500
H	1.72383900	-0.00294200	4.60013700
H	3.68608900	-1.55335200	4.72202300
C	-1.27945900	-2.35938900	2.54836700
H	-0.35515700	-1.91936700	2.95598900
H	-1.19821600	-3.44889300	2.68329800
C	-2.48536800	-1.82120100	3.32791500
H	-2.30814600	-2.07253500	4.38601100
H	-3.39440800	-2.37393100	3.03787100
C	-2.73077700	-0.31150100	3.18523800
H	-1.78395100	0.18084500	2.90380800
H	-3.01326200	0.12120600	4.15897600
C	-3.82041200	0.04959400	2.16617700
H	-4.81117200	-0.10776500	2.62332700
H	-3.78209400	-0.63389700	1.30431800
C	-3.69861000	1.49592700	1.67984400
H	-4.65599100	1.91416600	1.33739700
H	-3.35776800	2.14917900	2.49720900
N	3.32646900	-0.46591300	-1.82927500
C	4.36768000	-1.24468700	-2.00181700
O	5.50526400	-0.83967300	-2.35904200
O	4.20436200	-2.59759100	-1.74612200
C	5.35559700	-3.41272400	-1.84585800
H	5.79348900	-3.37736100	-2.85605300
H	6.13381200	-3.10802600	-1.12685800
H	5.03109000	-4.43837900	-1.62004300
Na	4.83162000	1.33197500	-1.74262000
C	1.25471000	2.39916800	0.32032900
H	0.76943000	3.29053300	-0.07521300
S	3.46771900	3.30017100	-0.15222900
O	3.51000900	3.33072200	-1.67261900

O	4.54174600	2.37385700	0.39601100
C	3.99406200	4.97209700	0.35429000
H	4.03557800	5.00462300	1.45126900
H	4.98904700	5.13458000	-0.08516300
H	3.26554600	5.69636300	-0.03423600
H	1.40262900	2.36811300	1.39815000
H	1.15966200	1.40554500	-1.54832900

#### TS-D2



Energy: -3353.58423474

Zero point energy correction: 0.788846

Atom Coordinates:

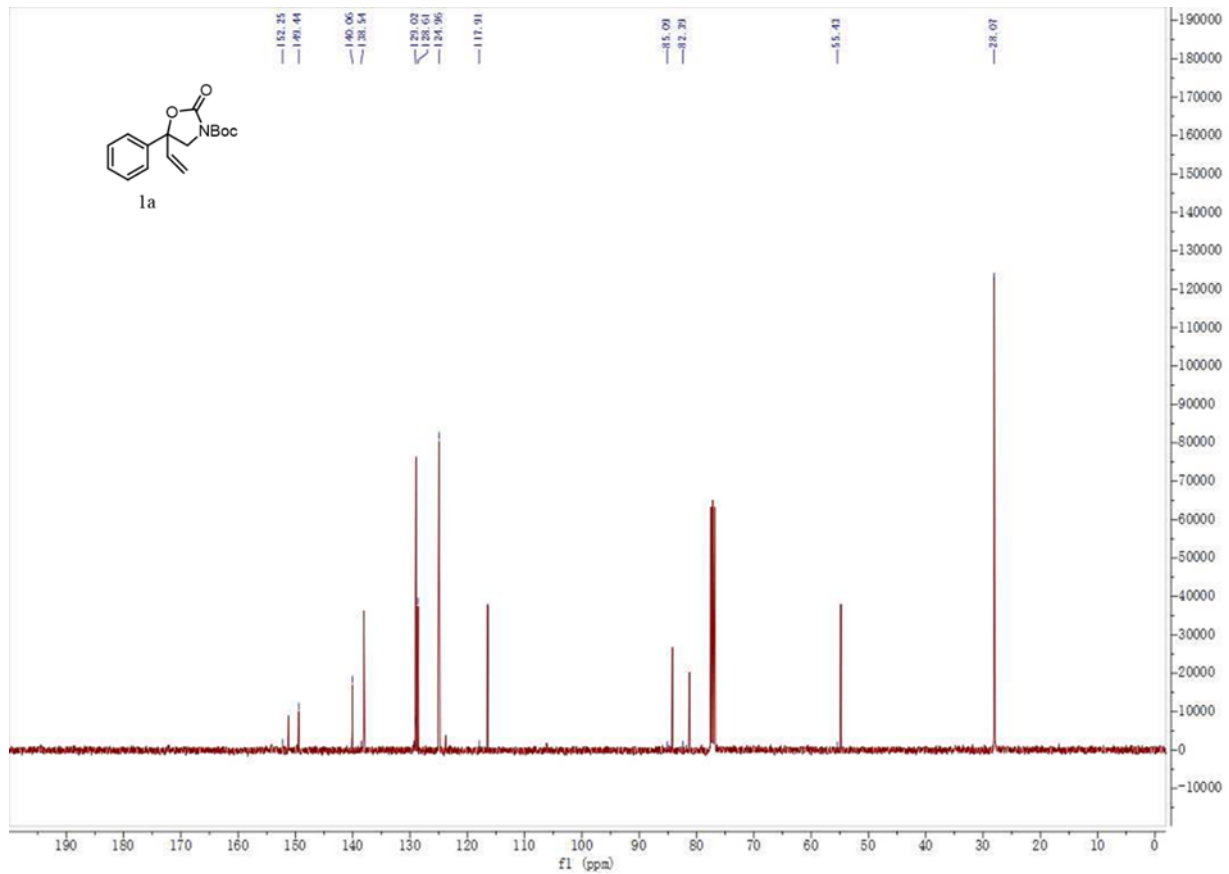
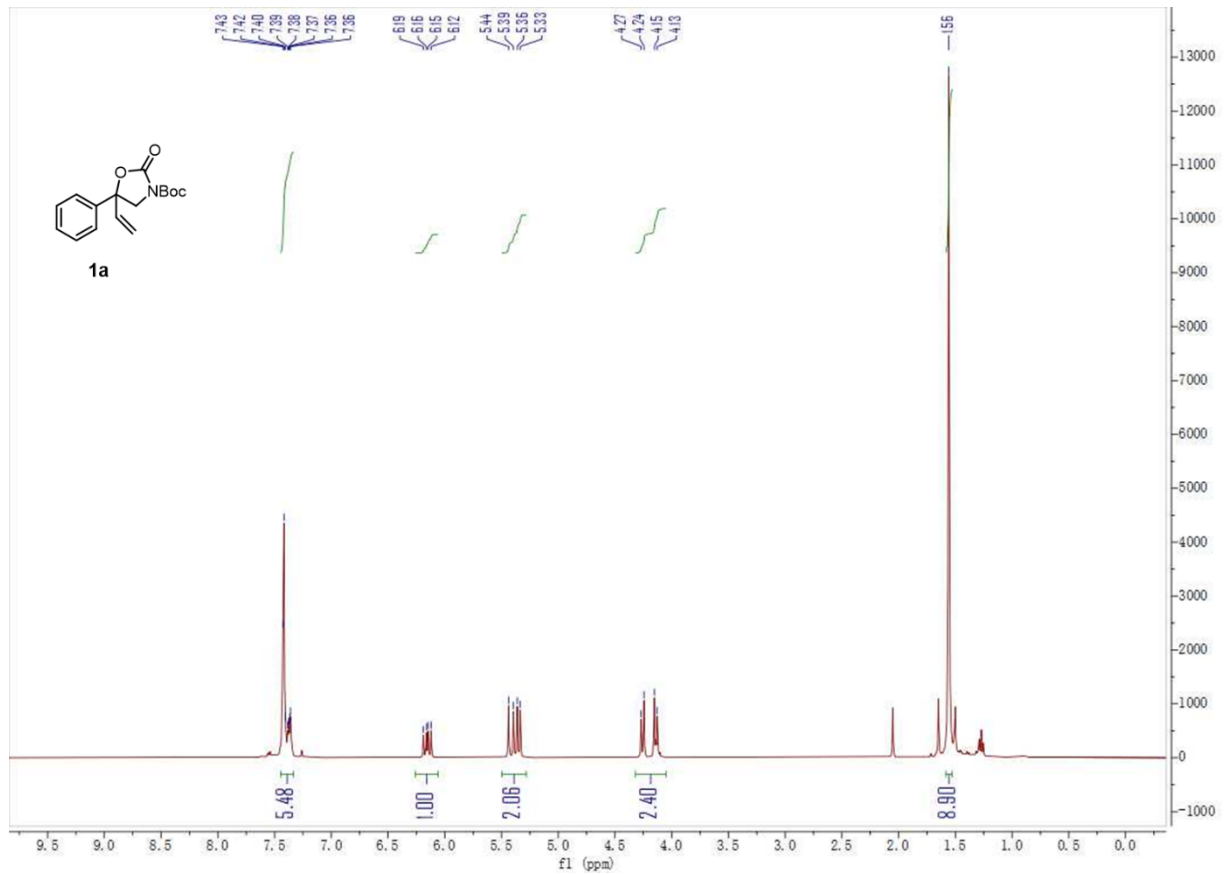
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C	-4.45053500	2.11104400	-1.40109900
H	-5.02213400	2.45404300	-0.53792000
C	-5.10652400	1.96209900	-2.62748000
H	-6.17344900	2.18652800	-2.69909300
C	-4.40460400	1.52821300	-3.75537700
H	-4.92026800	1.41070900	-4.71128400
C	-3.03953200	1.23917100	-3.65192100
H	-2.48269500	0.89321500	-4.52580300
C	-2.38928300	1.37113800	-2.42388800
H	-1.33401000	1.09978300	-2.33118500
C	-1.42591800	3.58431700	0.28828800
C	-1.20279300	4.28821100	1.48508400
H	-1.57404900	3.89908200	2.43441200
C	-0.48009200	5.48542600	1.48742600
H	-0.32192600	6.01695700	2.42888000
C	0.04708300	5.99421300	0.29692900
H	0.61694200	6.92620500	0.29993500
C	-0.15749900	5.29538000	-0.89788600
H	0.26167200	5.67364700	-1.83265600
C	-0.89136200	4.10819600	-0.90297300

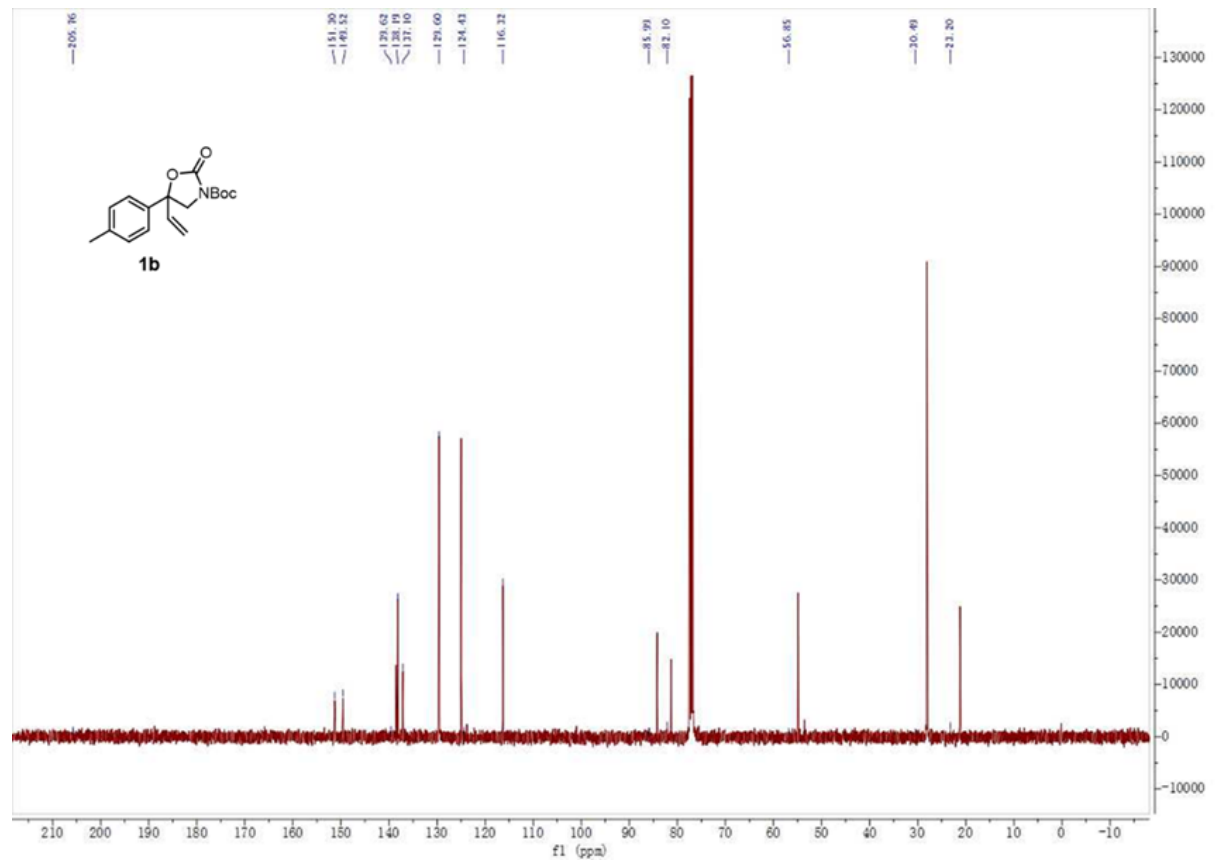
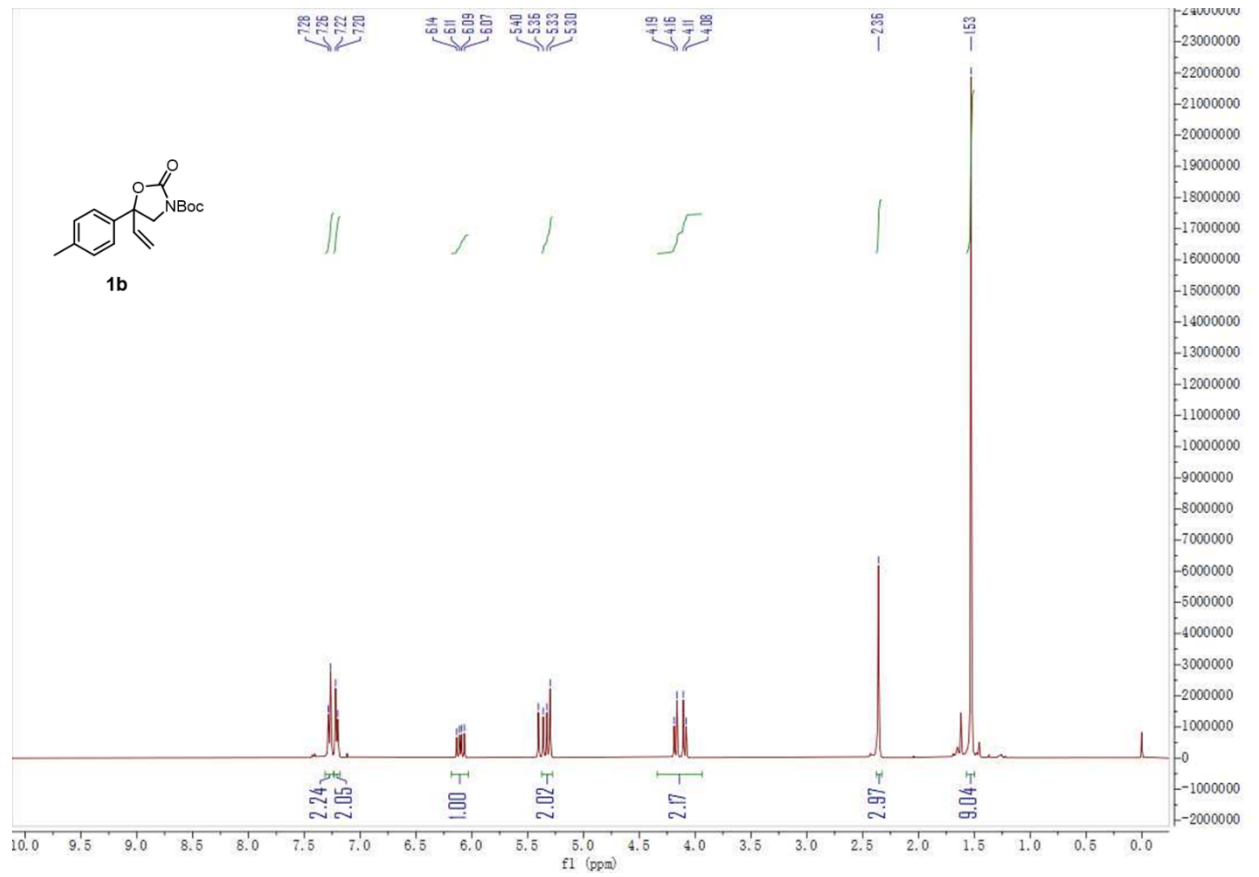
H	-1.03237000	3.57385100	-1.84367800	H	1.93791500	-0.70659100	4.58613100
C	-3.00905200	-2.48508800	0.04823400	H	3.80550400	-2.36767100	4.41724300
C	-3.70357500	-3.61674700	0.50736100	C	-1.62047000	-2.27433000	2.59834700
H	-3.29048100	-4.22613600	1.31431700	H	-0.66823400	-1.95828500	3.05393700
C	-4.92524400	-3.97606900	-0.06631300	H	-1.70077200	-3.36113600	2.75625500
H	-5.46064100	-4.85440800	0.30243100	C	-2.78318300	-1.54949600	3.29089000
C	-5.46341900	-3.21514800	-1.11170200	H	-2.73121600	-1.81769400	4.35866500
H	-6.42019400	-3.49825800	-1.55713700	H	-3.74125800	-1.95856400	2.92815800
C	-4.77247300	-2.09606300	-1.58350400	C	-2.78130300	-0.01746600	3.13876300
H	-5.18028600	-1.49563200	-2.40010900	H	-1.76435800	0.31598700	2.86801500
C	-3.55283300	-1.73399800	-1.00285800	H	-3.00615200	0.45970700	4.10720800
H	-3.01943800	-0.85428800	-1.36124600	C	-3.77889900	0.51598600	2.10024600
C	-0.30321800	-3.34459800	0.28722000	H	-4.79295500	0.50826900	2.53327700
C	-0.45689400	-3.96038100	-0.96751100	H	-3.82119200	-0.15810800	1.23127300
H	-1.28032500	-3.66373100	-1.62082400	C	-3.42910600	1.93483000	1.63324100
C	0.43196100	-4.95158200	-1.38764200	H	-4.31039200	2.49199200	1.28612000
H	0.29737600	-5.41951300	-2.36607200	H	-3.01802200	2.51063500	2.47482700
C	1.48945800	-5.34598900	-0.56023900	N	3.22639400	-0.53397400	-1.91909300
H	2.18570600	-6.12126800	-0.88867000	C	4.11290000	-1.43059300	-2.27730600
C	1.65399900	-4.73278300	0.68427700	O	5.29858700	-1.16123000	-2.61134100
H	2.48577000	-5.01791000	1.33249500	O	3.72627600	-2.76105500	-2.25070200
C	0.76920600	-3.73641200	1.10519300	C	4.72596300	-3.72619100	-2.51481300
H	0.93743000	-3.25452800	2.06880600	H	5.17977600	-3.58321500	-3.50820400
P	-2.14036700	1.88330900	0.29867600	H	5.53305000	-3.69216900	-1.76409700
P	-1.40400700	-1.94921400	0.77611200	H	4.23078700	-4.70677200	-2.47122500
Pd	-0.53505000	0.18275500	0.29627700	Na	4.99330800	0.90165200	-1.50154900
C	1.93131400	-0.89787100	-1.37900200	C	1.75473700	2.31246400	0.74829200
C	1.69415400	-0.15266900	-0.06599600	H	1.01360600	3.11745600	0.82932800
H	1.81218000	-1.98014100	-1.22043300	S	3.23293900	3.14188700	0.07108500
H	1.12750000	-0.59758600	-2.07919700	O	2.94756000	3.61008200	-1.30239400
C	1.34052200	1.21692200	-0.18324700	O	4.41594000	2.24809600	0.24036800
C	2.29896800	-0.72419600	1.17012600	C	3.49188700	4.57515400	1.11554000
C	3.33890300	-1.67279200	1.10012000	H	3.65902500	4.23876300	2.14652900
C	1.81767700	-0.39693800	2.45813800	H	4.38245800	5.07945700	0.71774800
C	3.87630000	-2.25082600	2.25356200	H	2.60573900	5.21692300	1.03644600
H	3.71623000	-1.98577000	0.13014400	H	2.05226000	1.97596300	1.74788400
C	2.35071900	-0.97428300	3.60995900	H	1.19711600	1.57895500	-1.20687900
H	0.96556900	0.28028100	2.55020700				
C	3.39055800	-1.90764900	3.51729600				
H	4.67627000	-2.98961800	2.15707000				

## 8. Reference

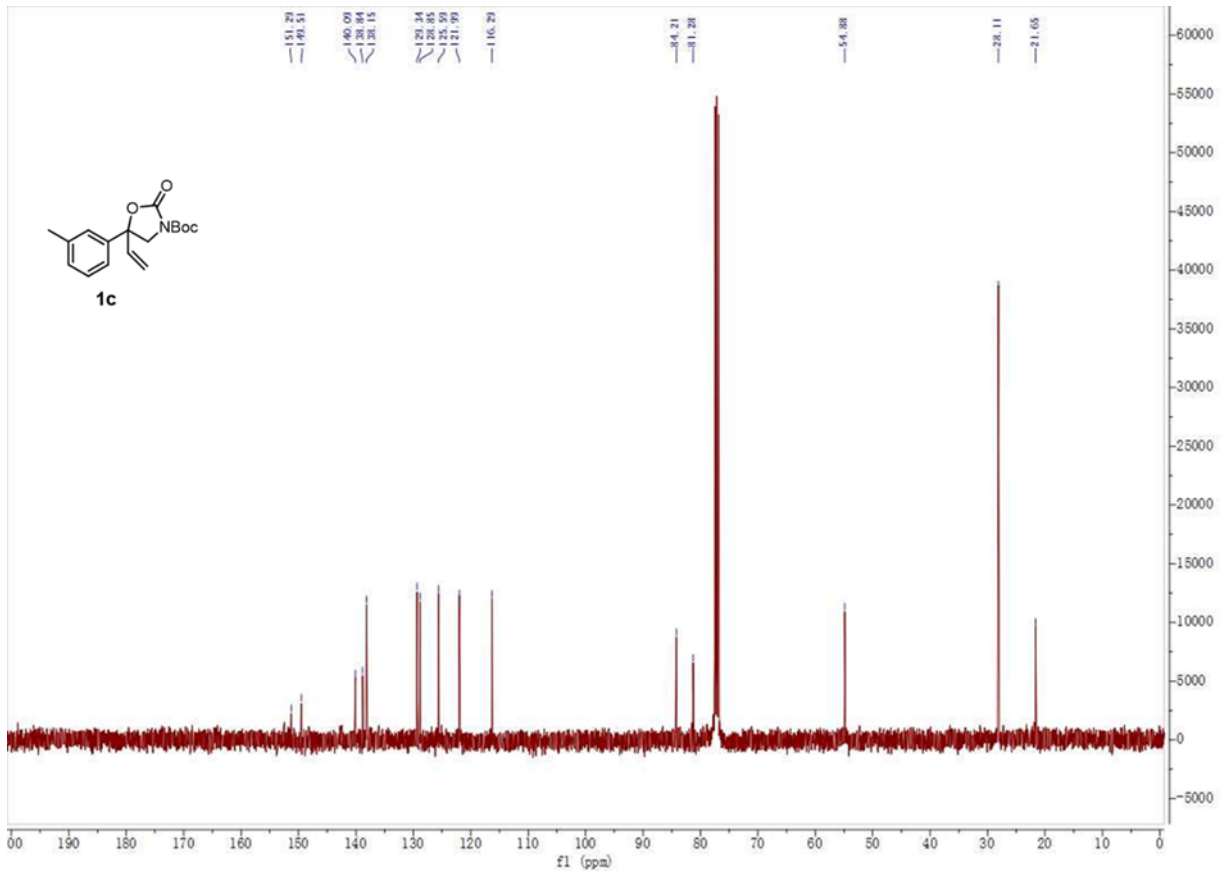
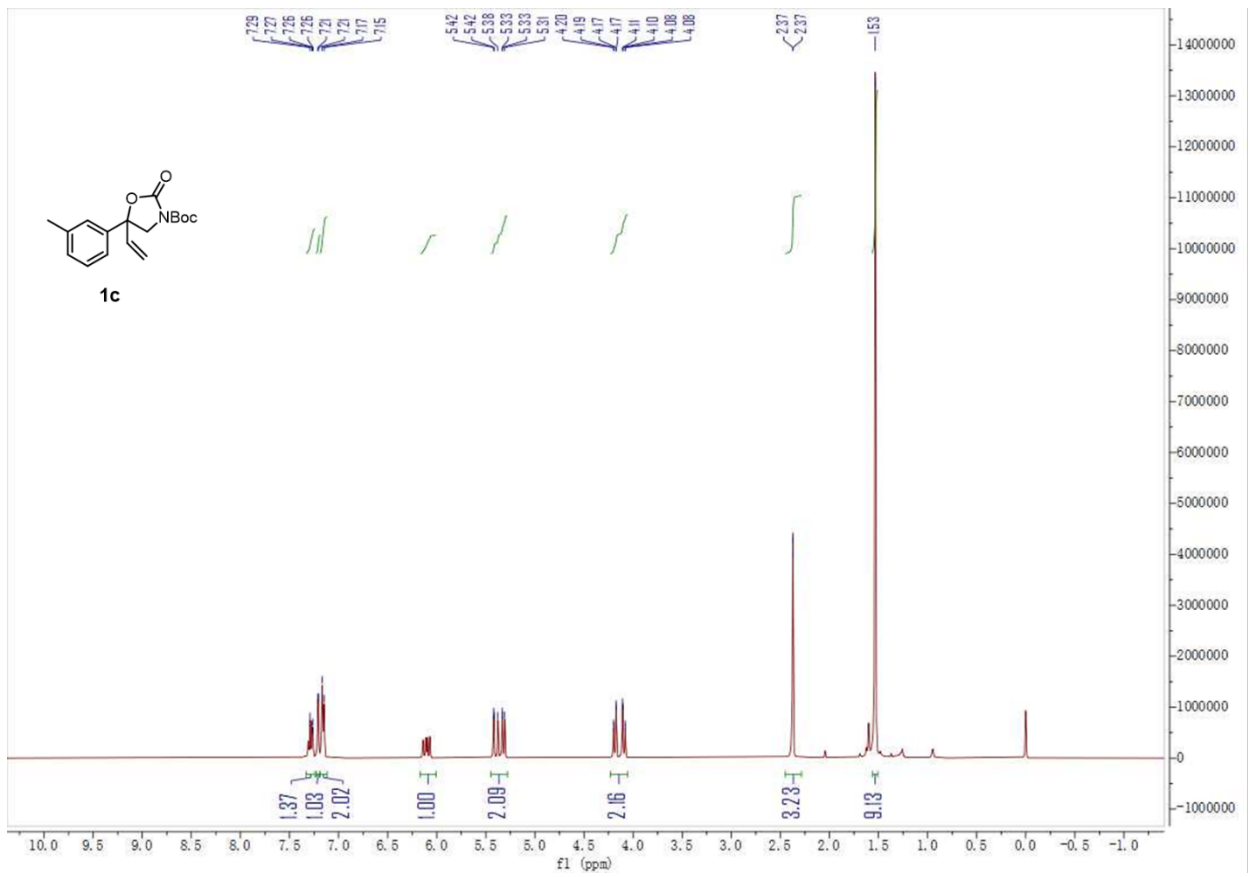
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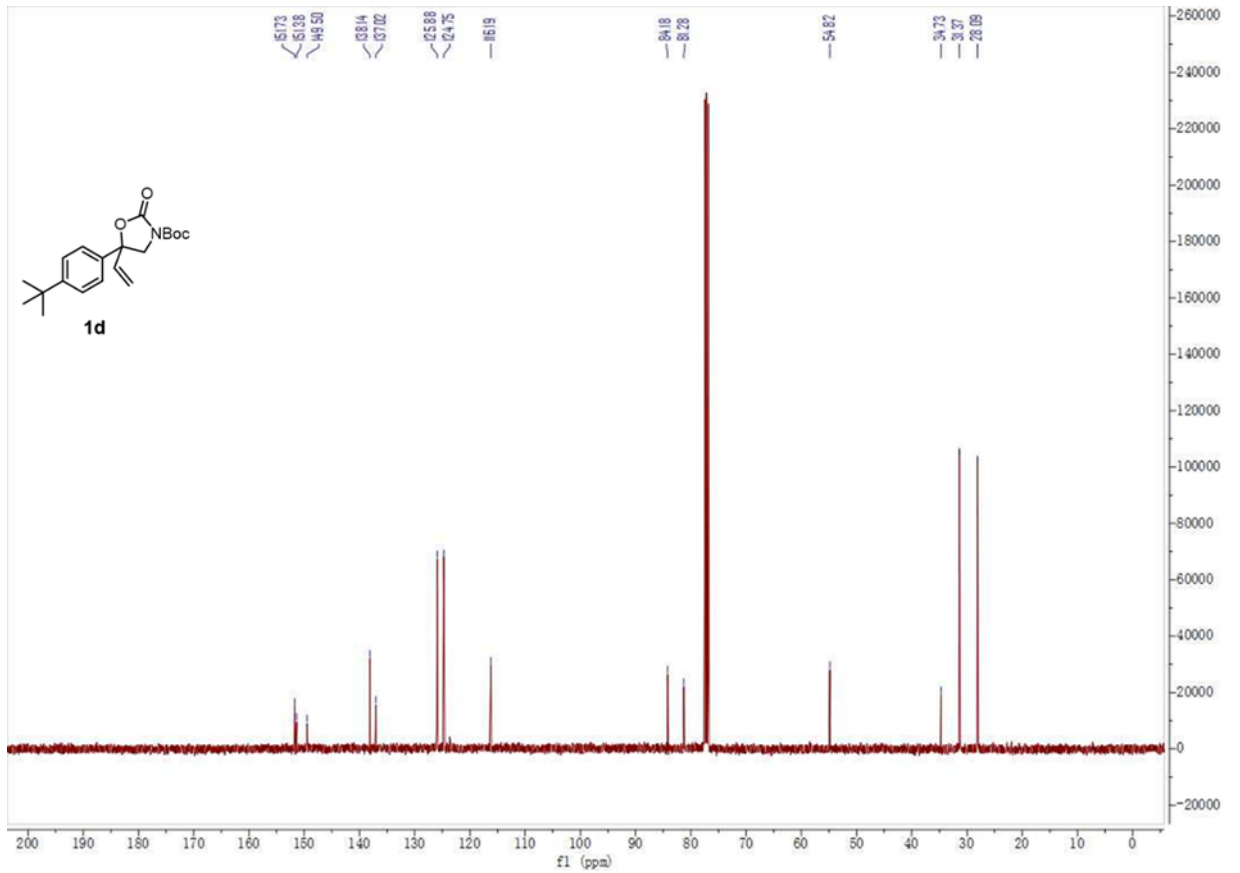
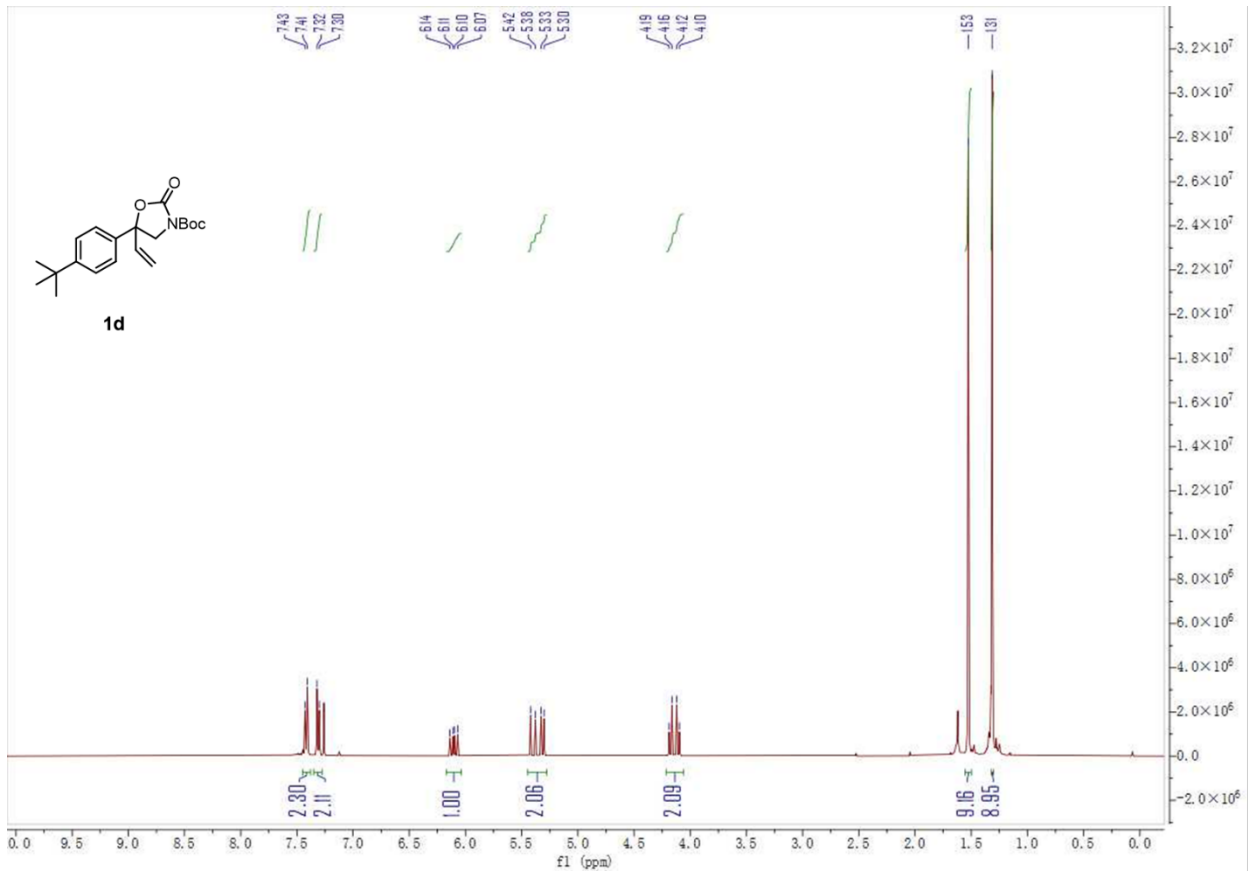
## 9. NMR Spectra.

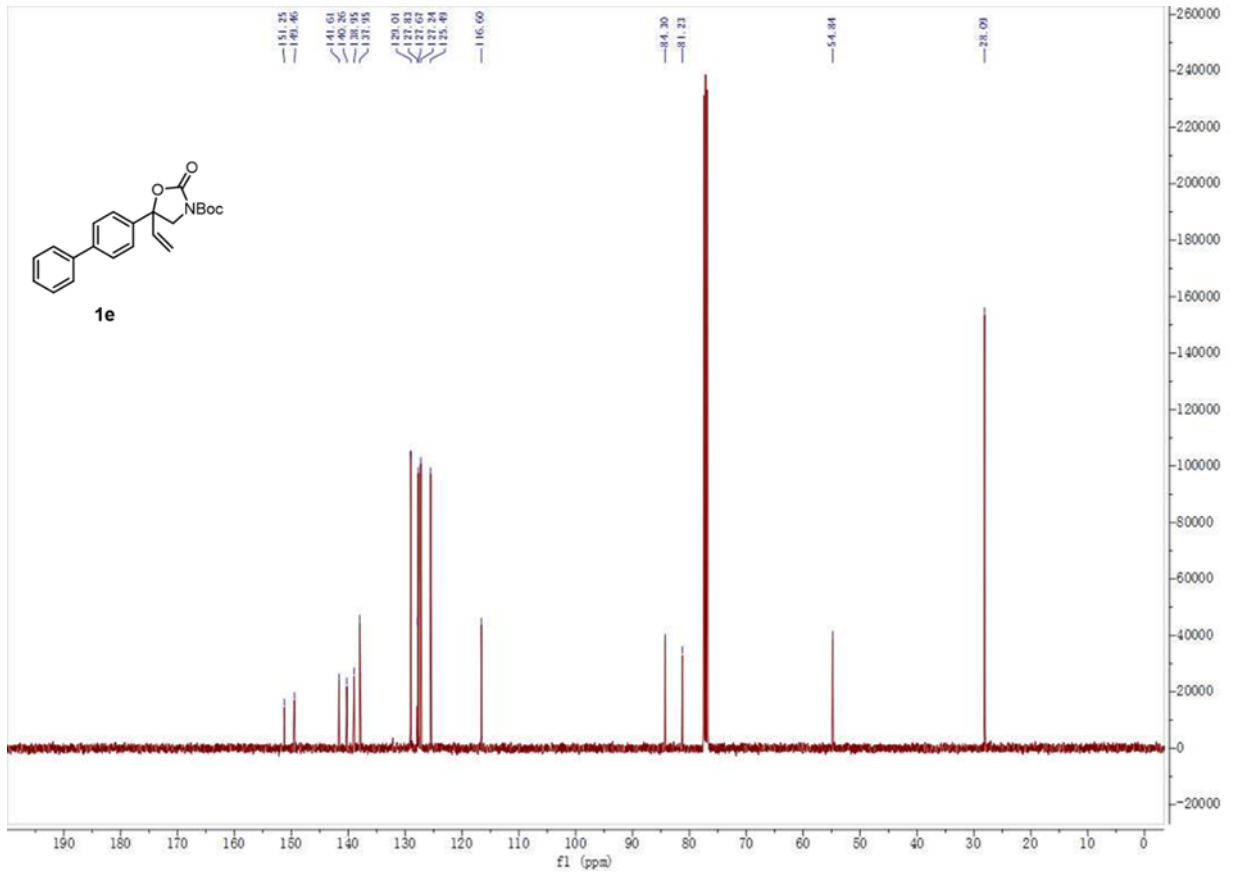
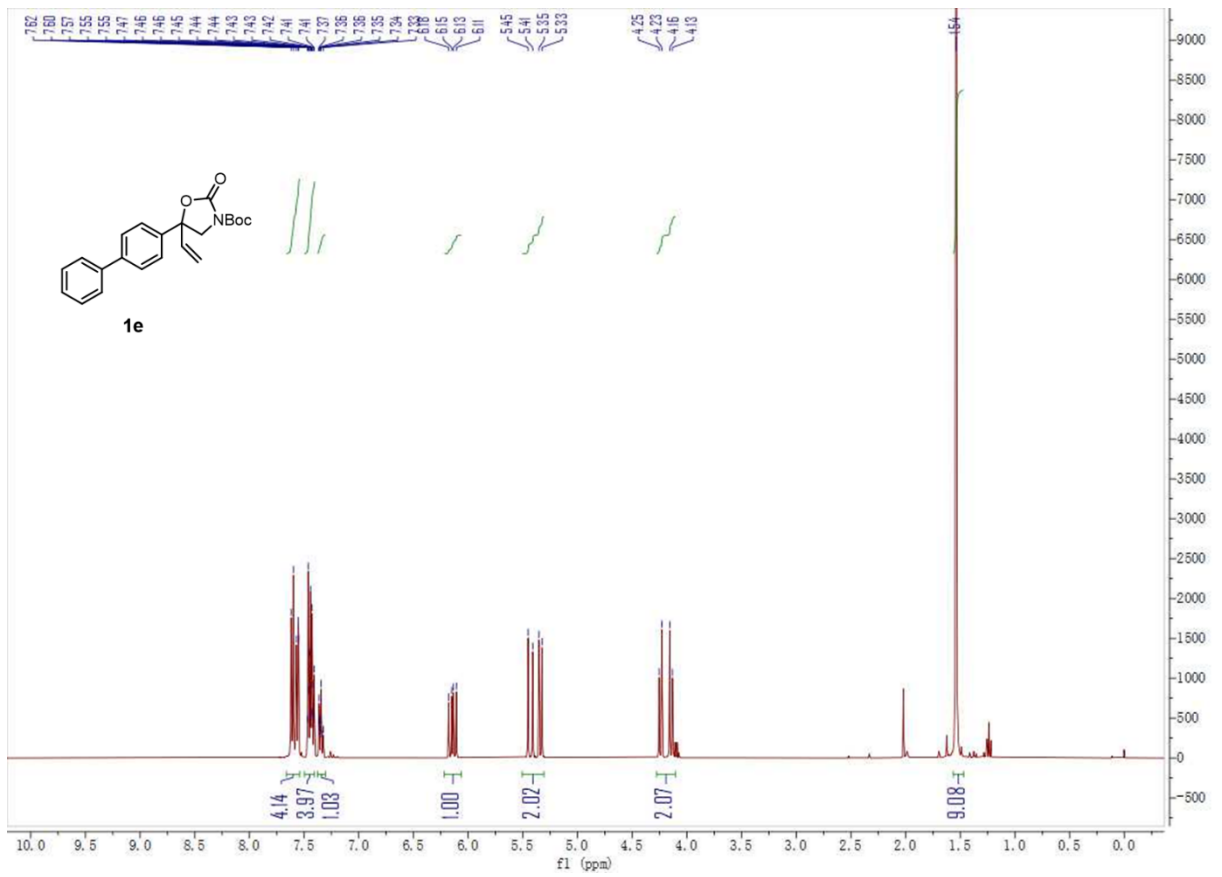


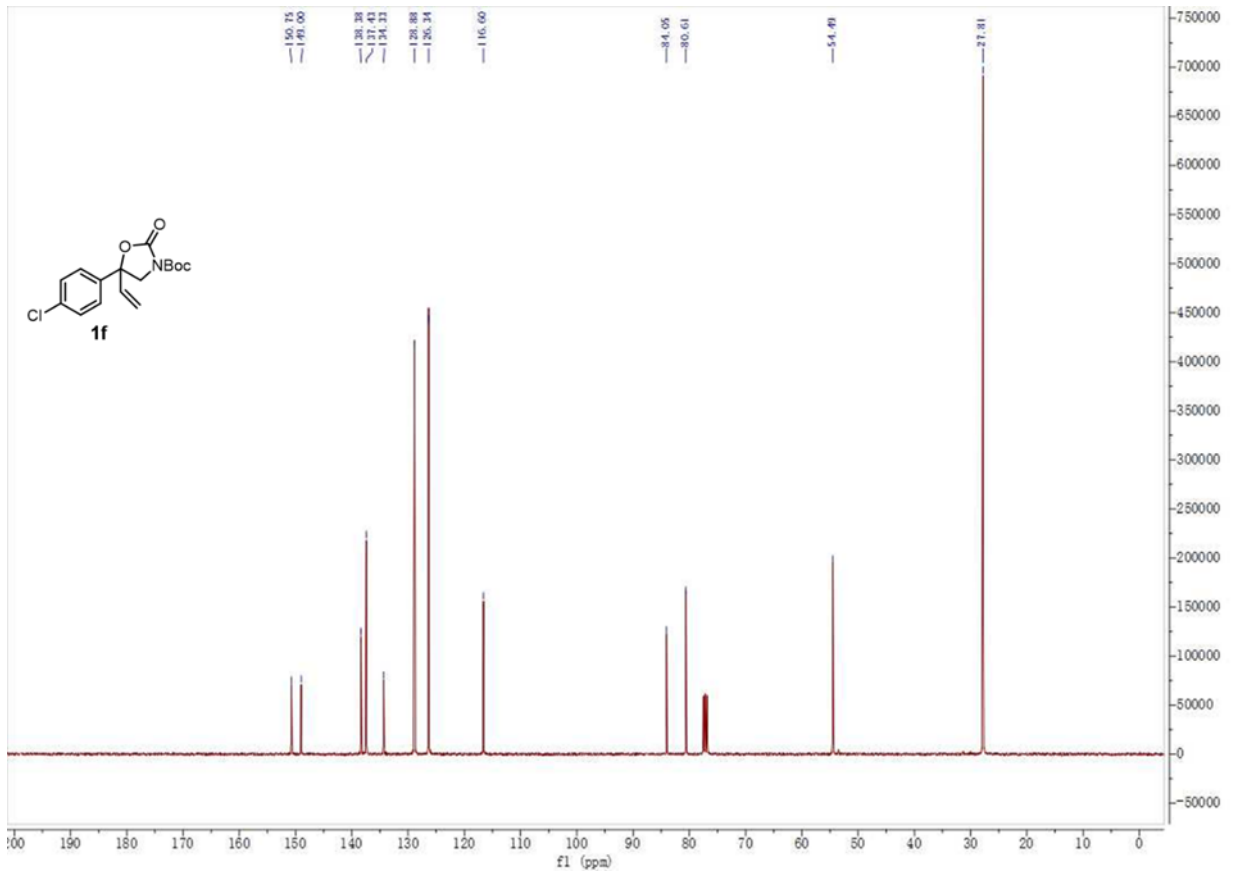
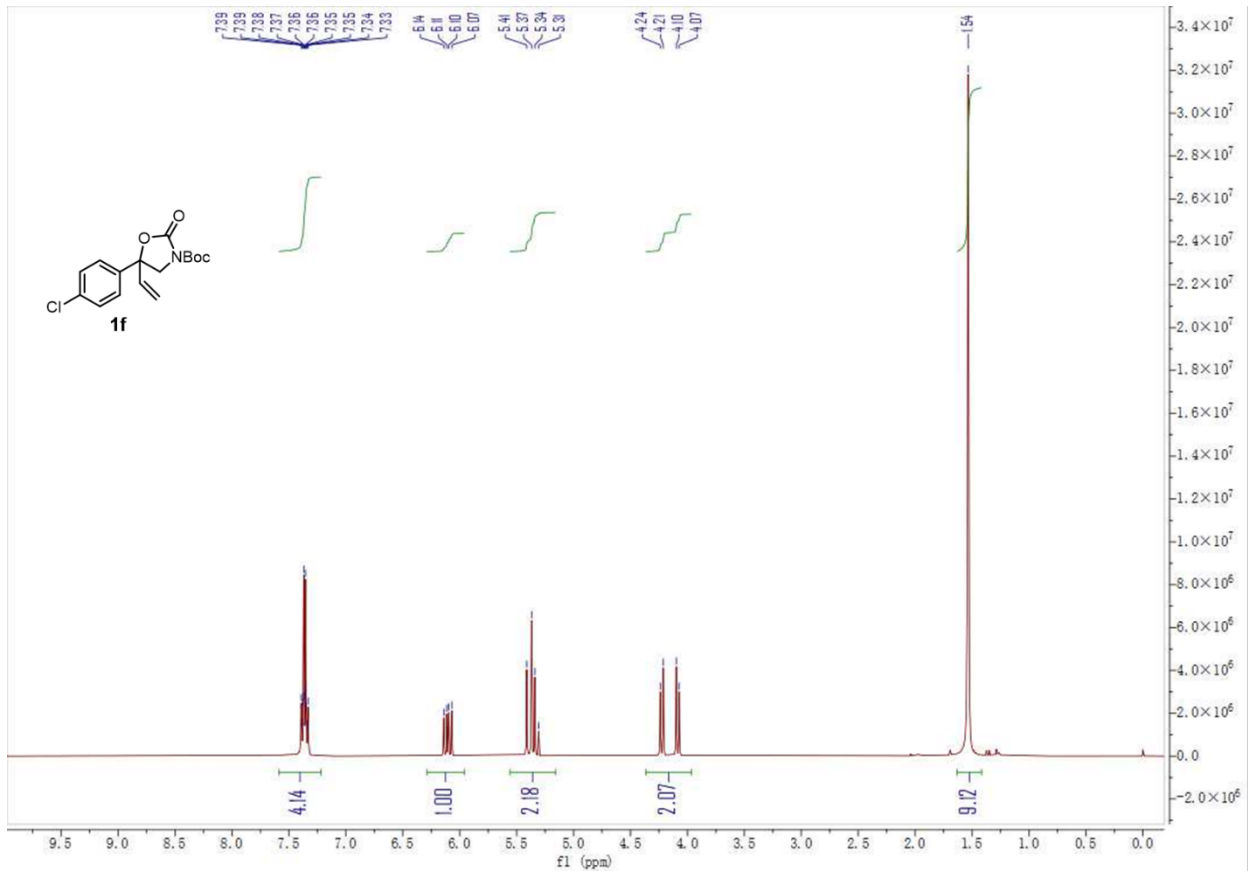


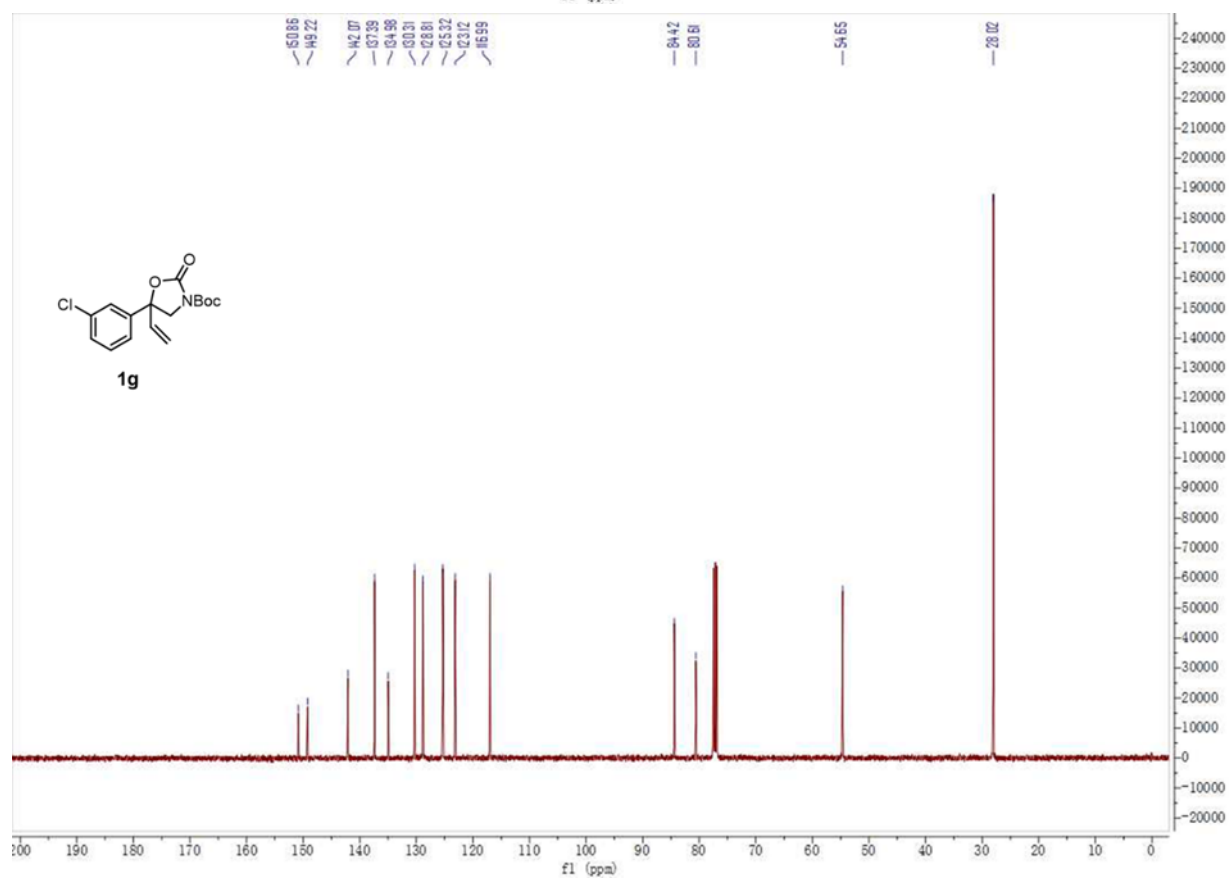
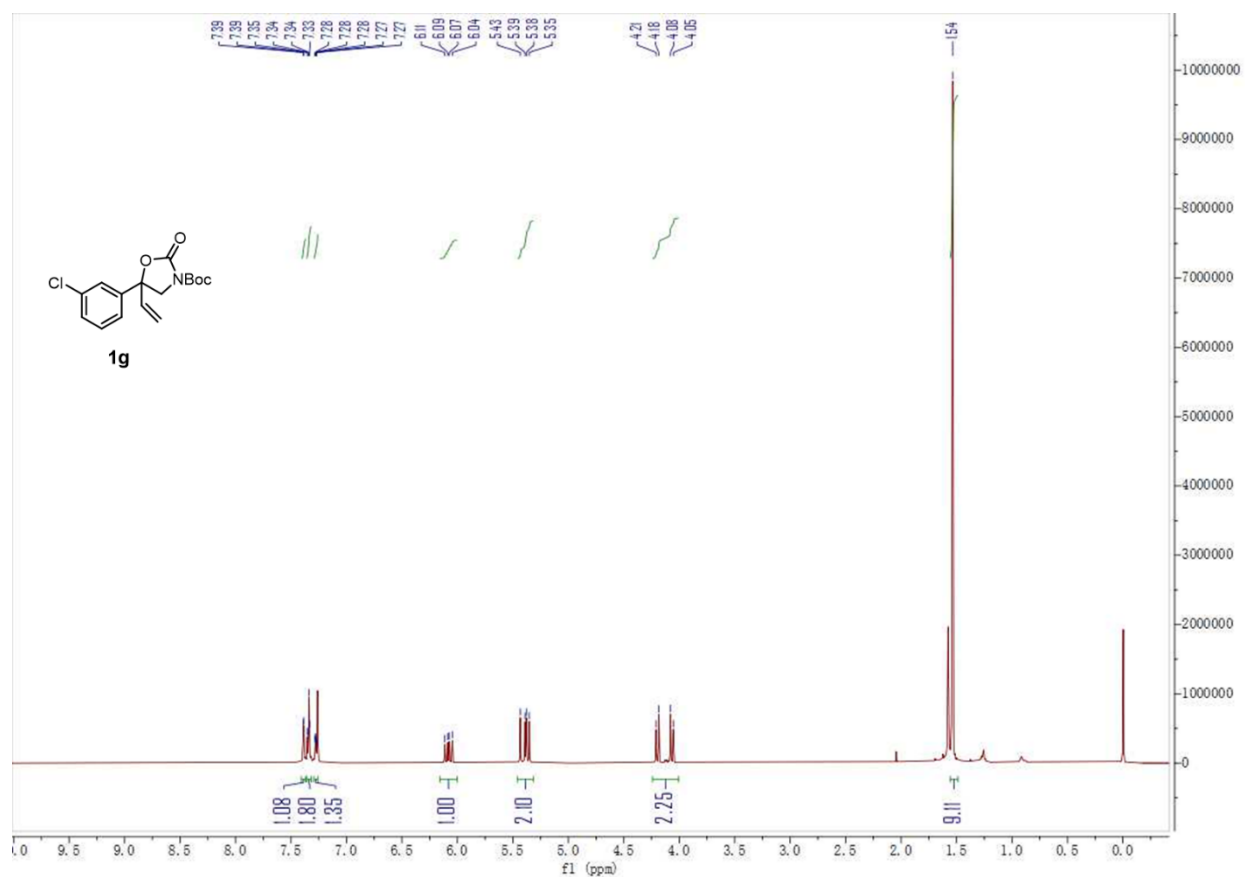


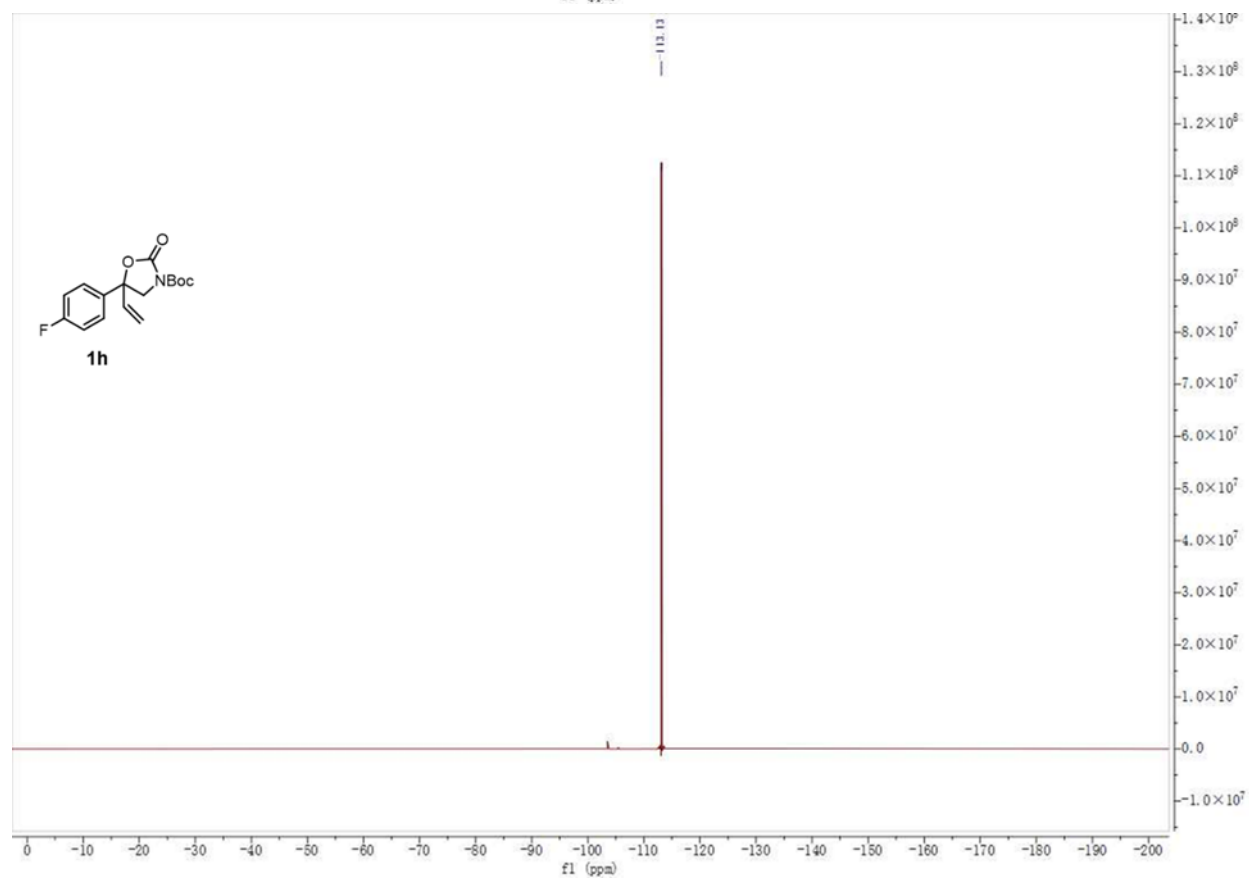
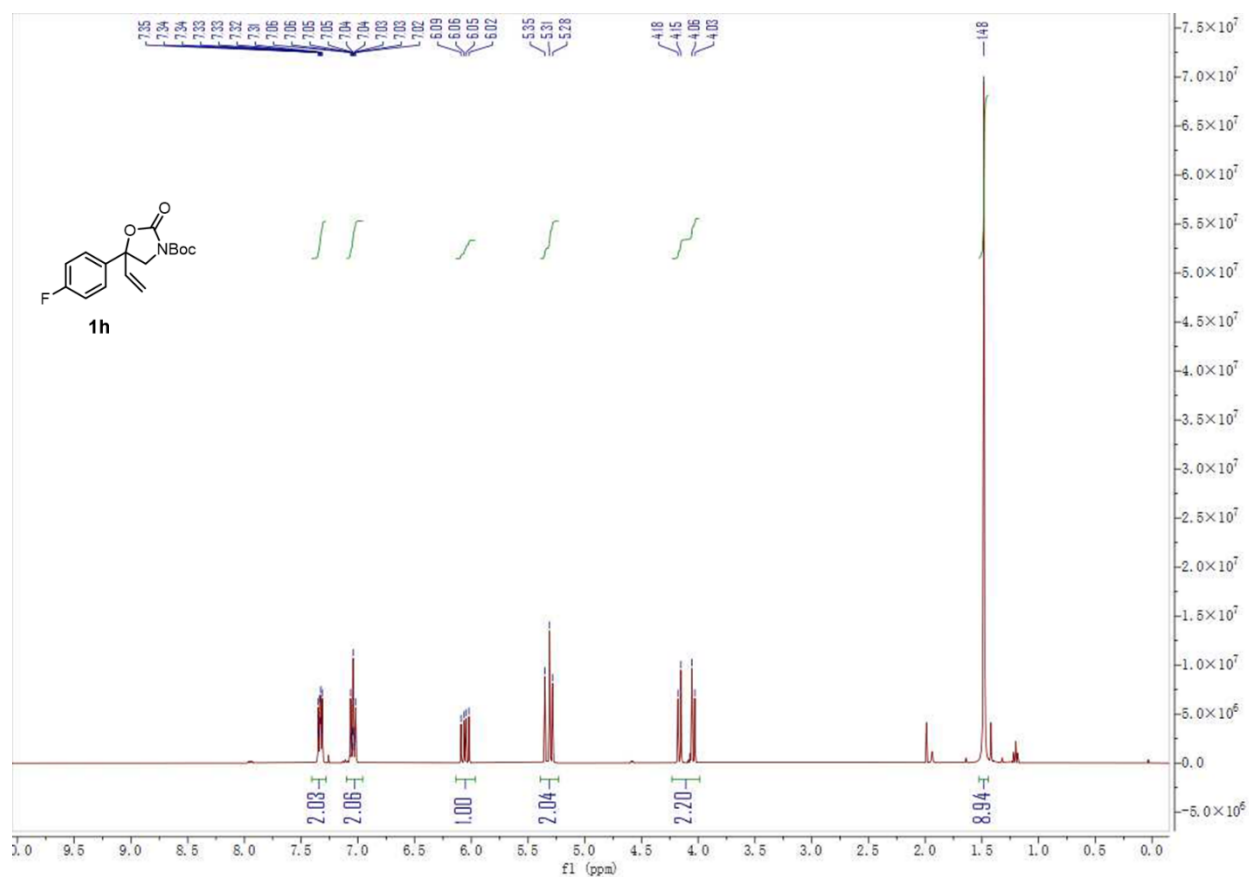


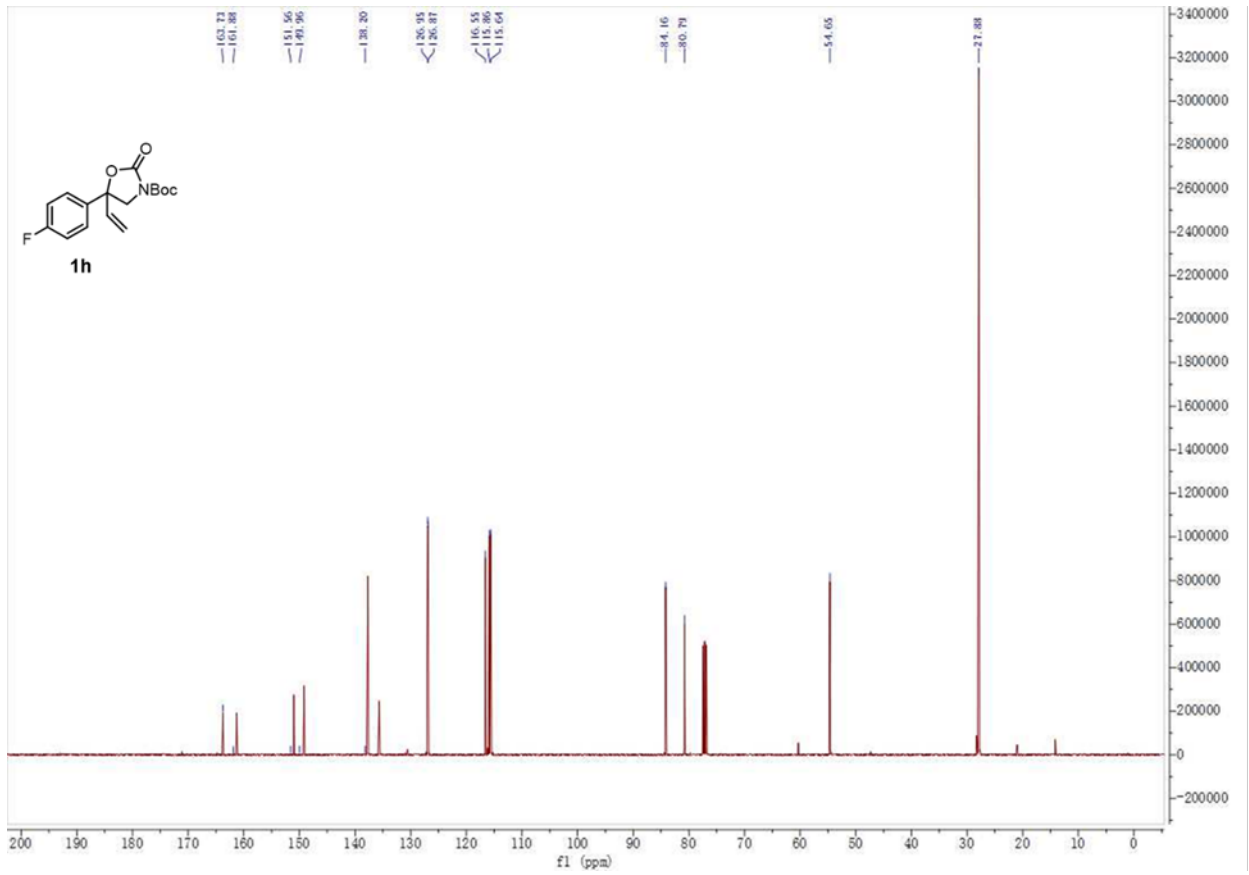




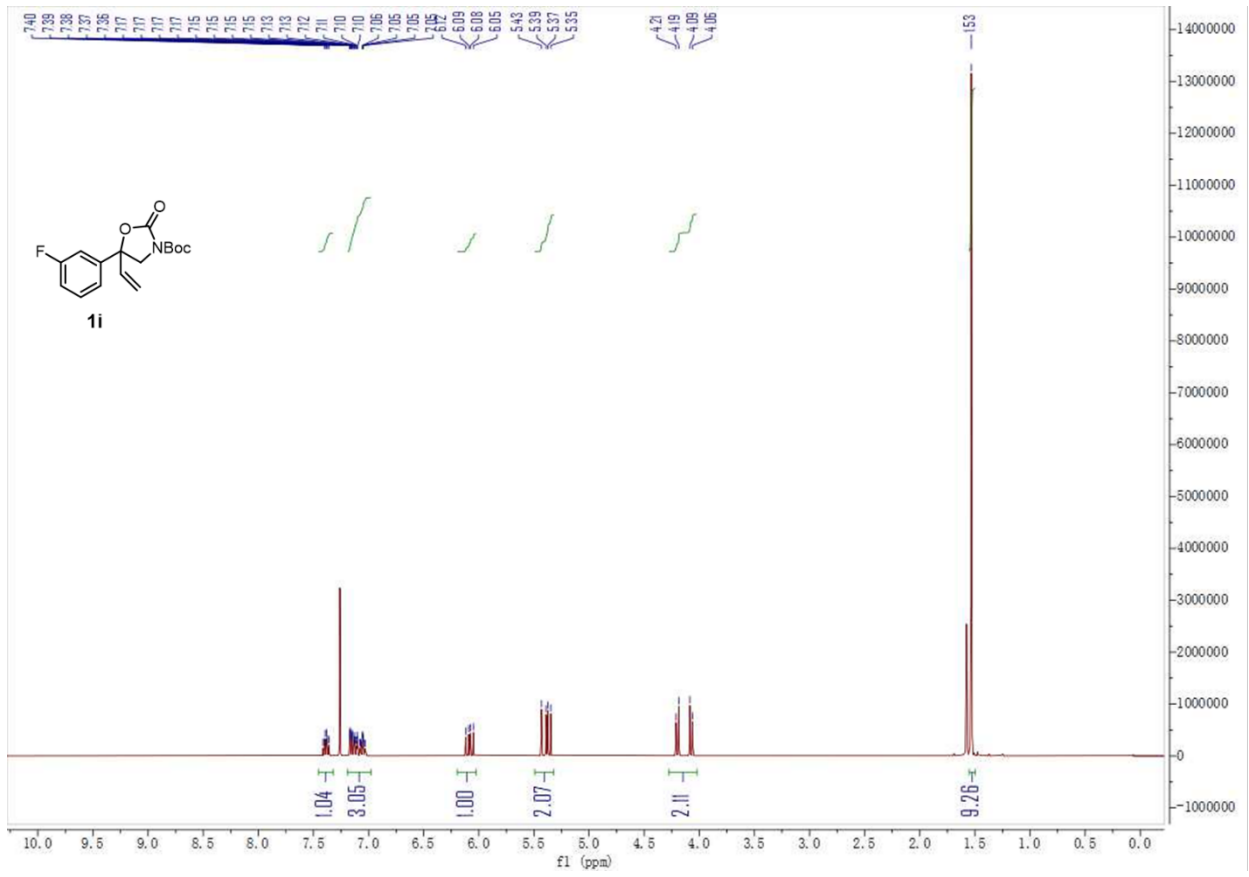




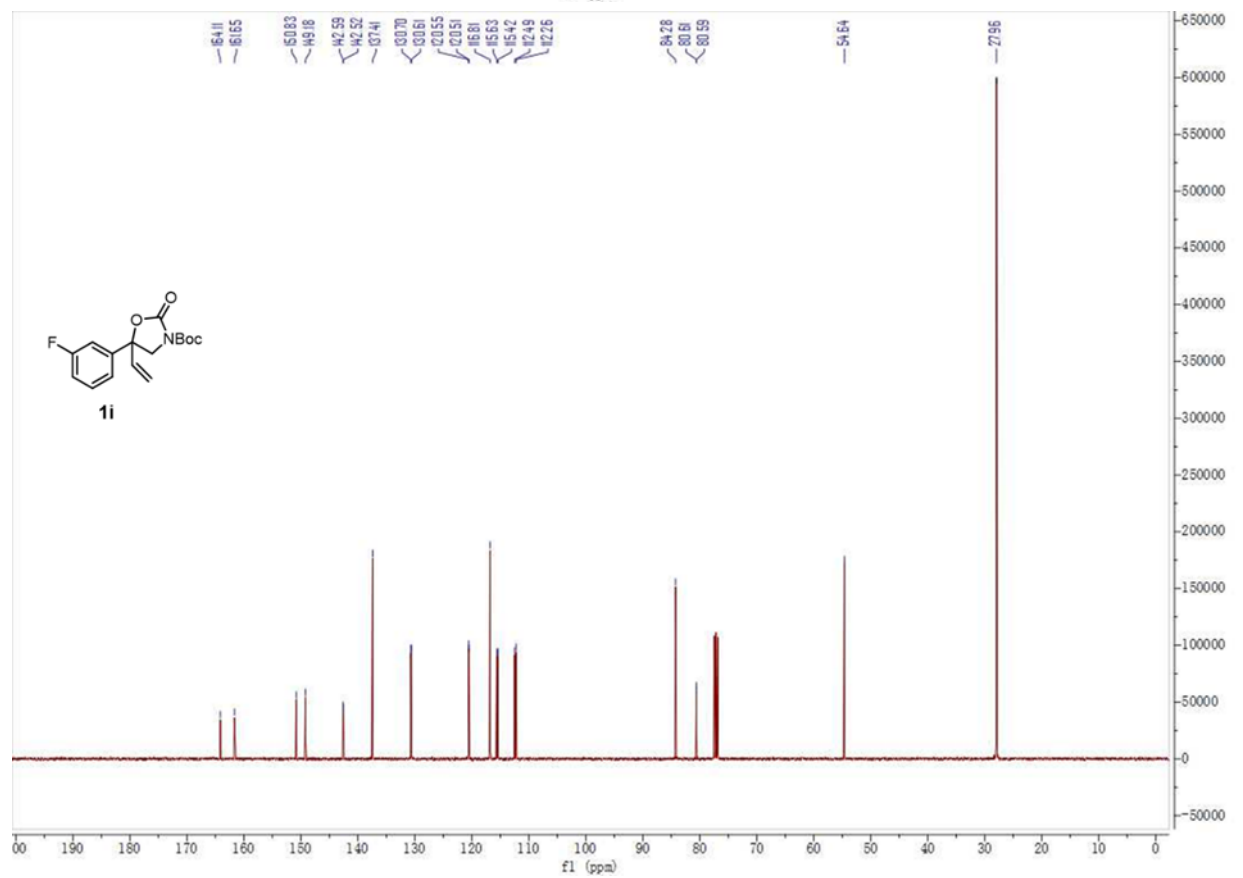
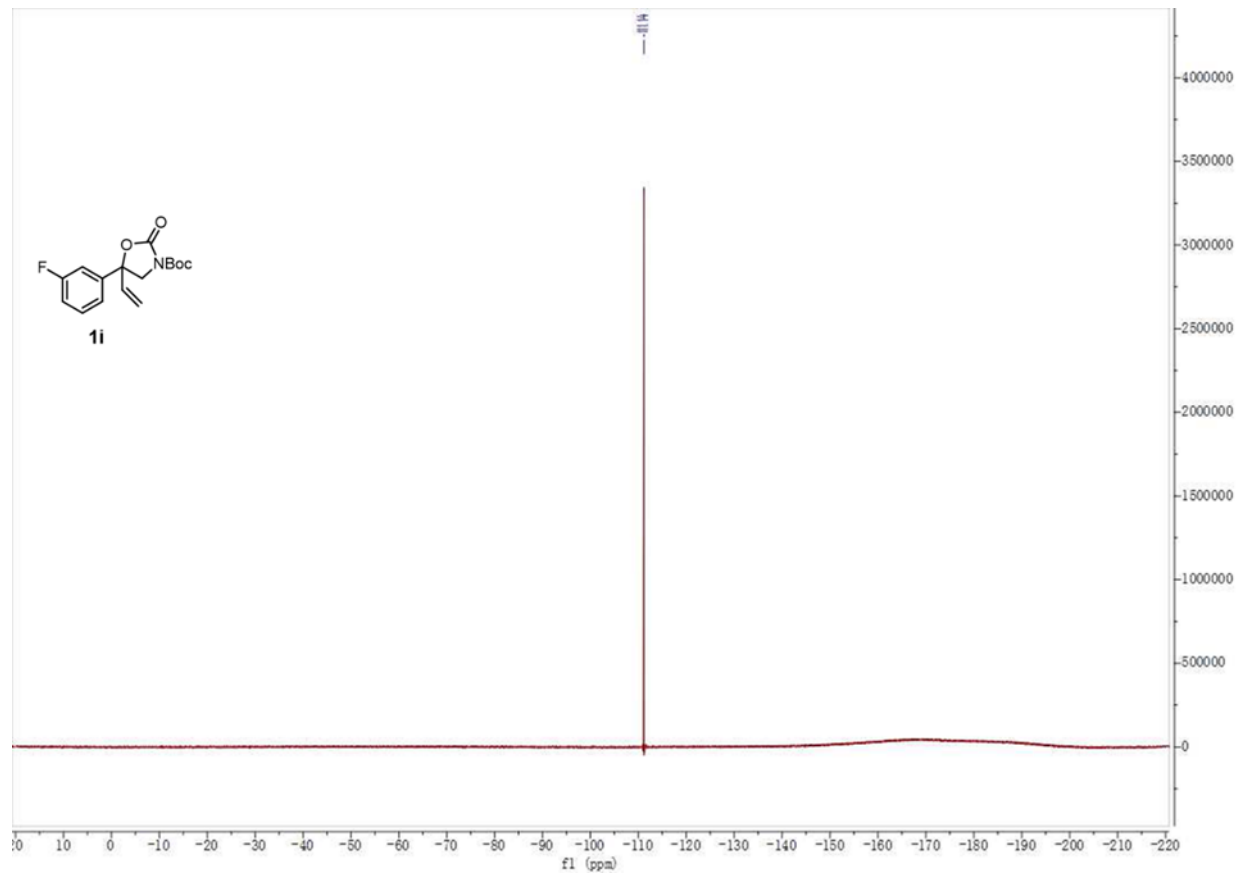




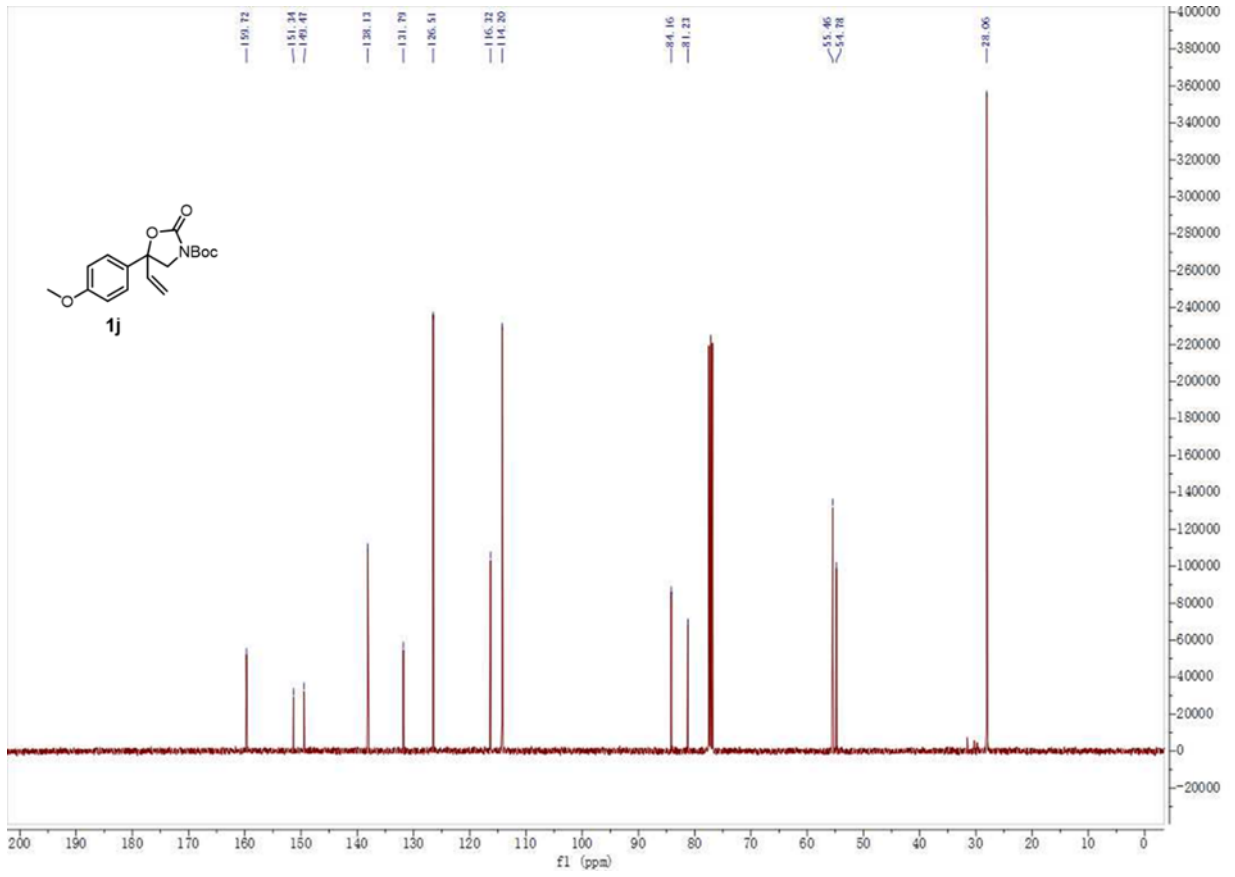
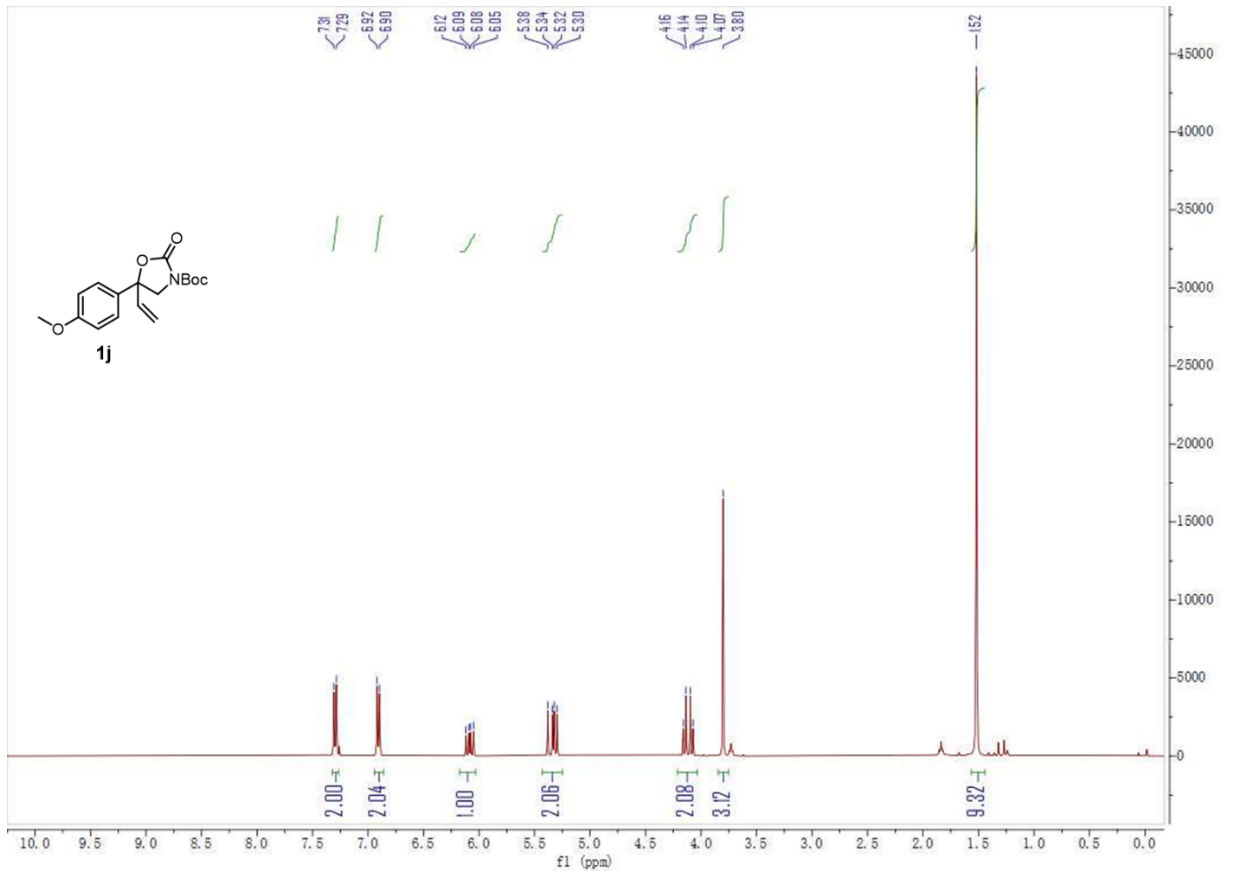
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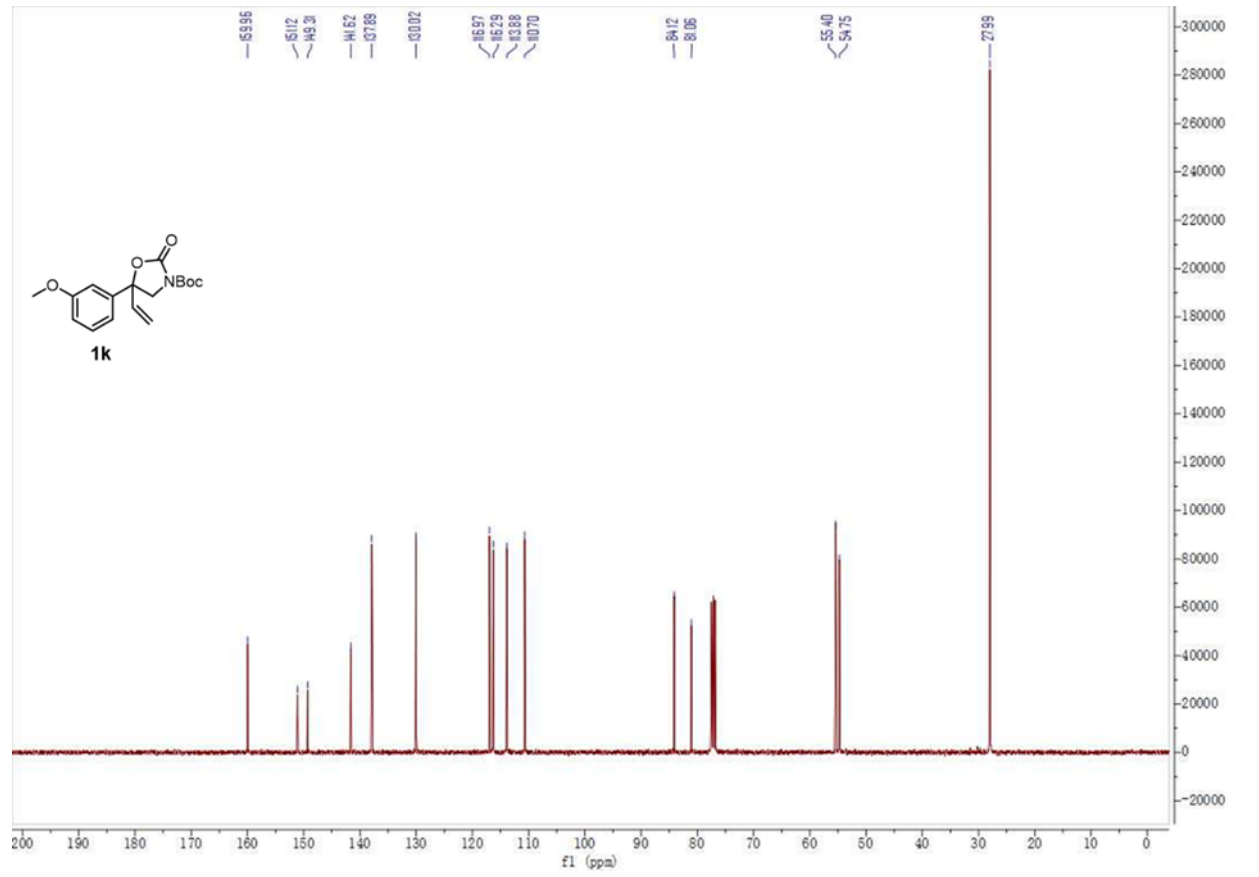
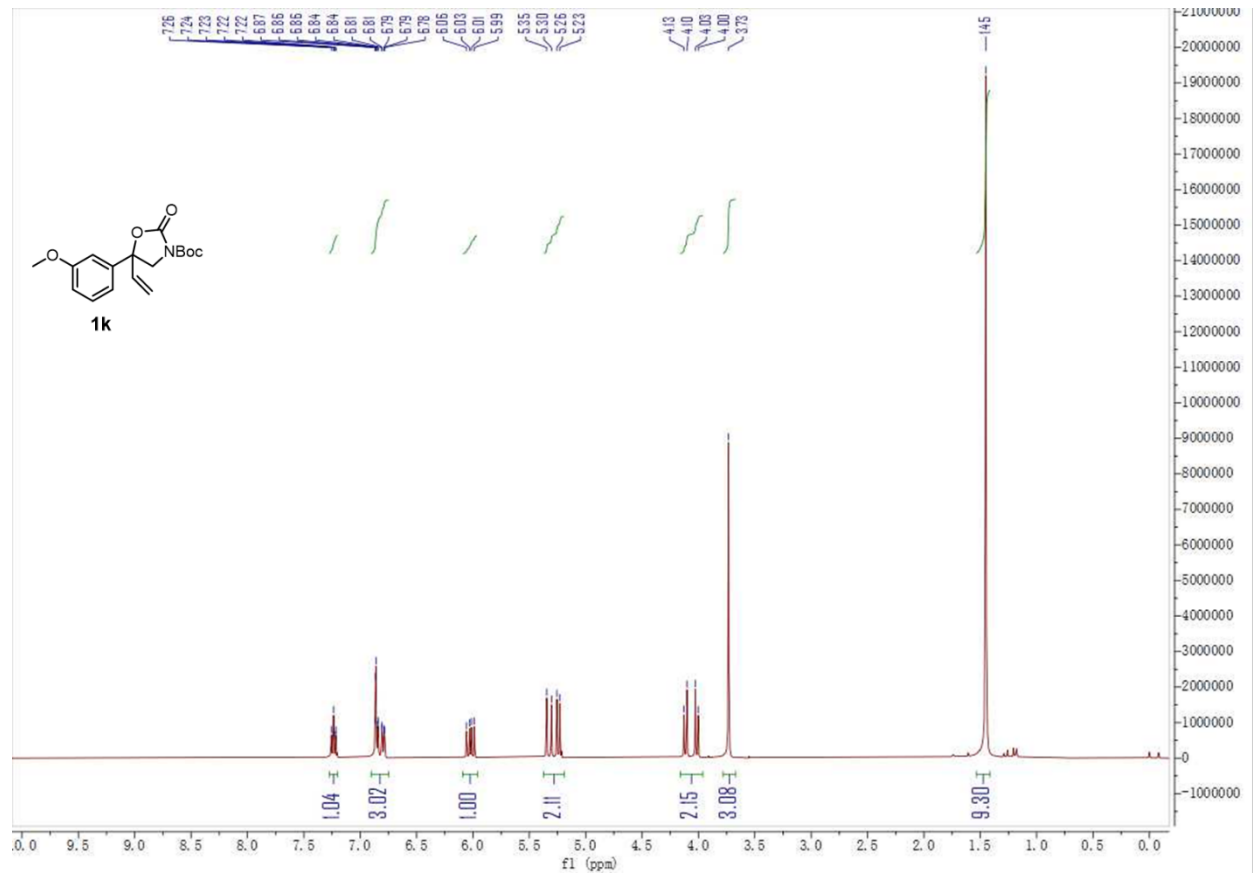


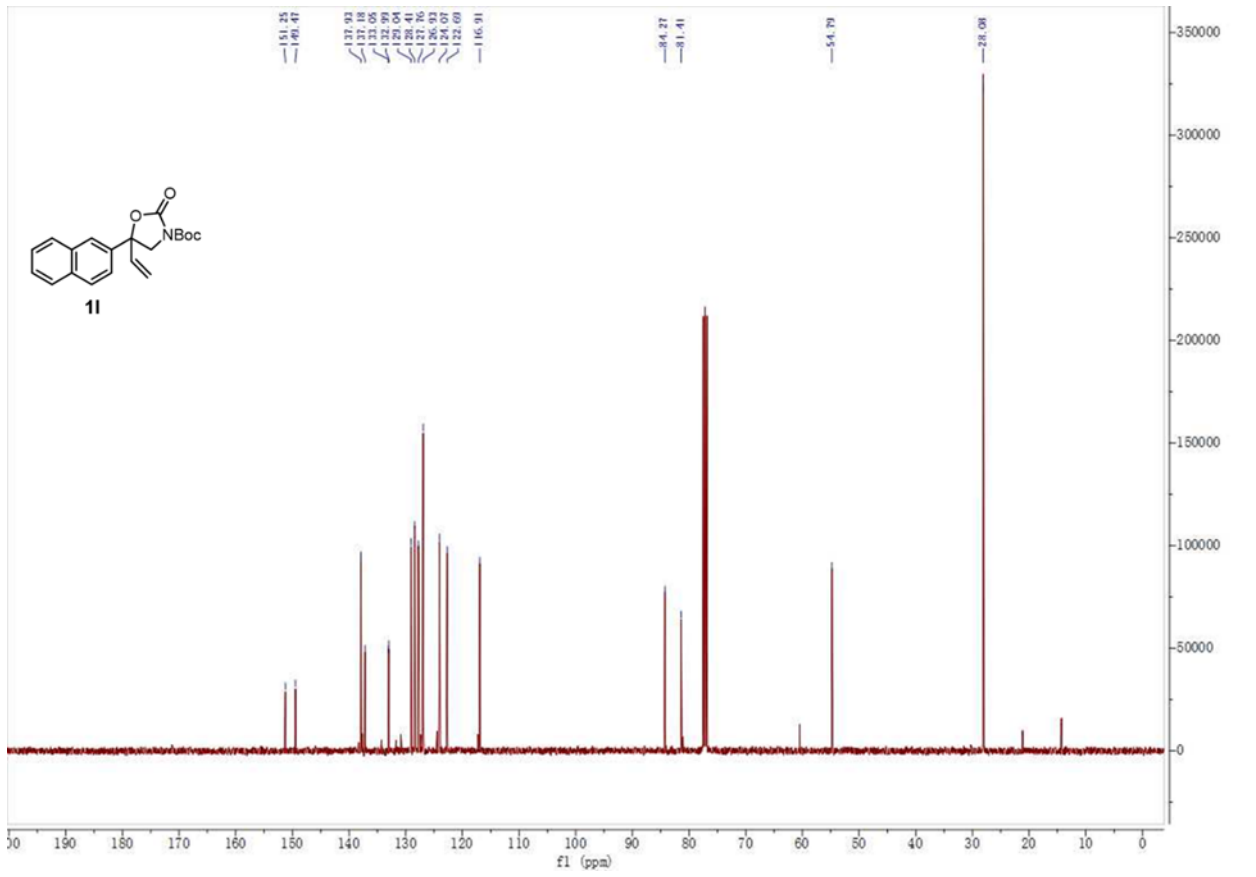
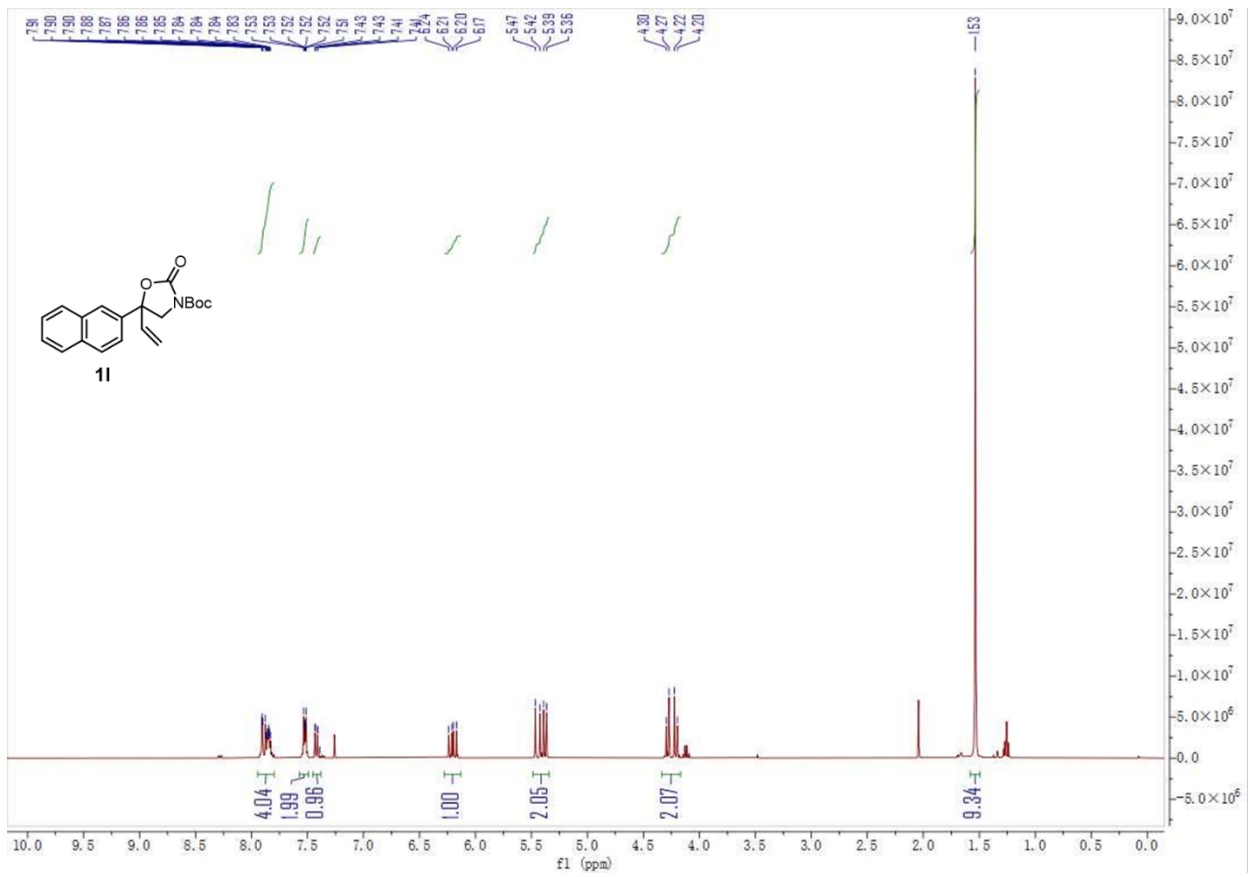
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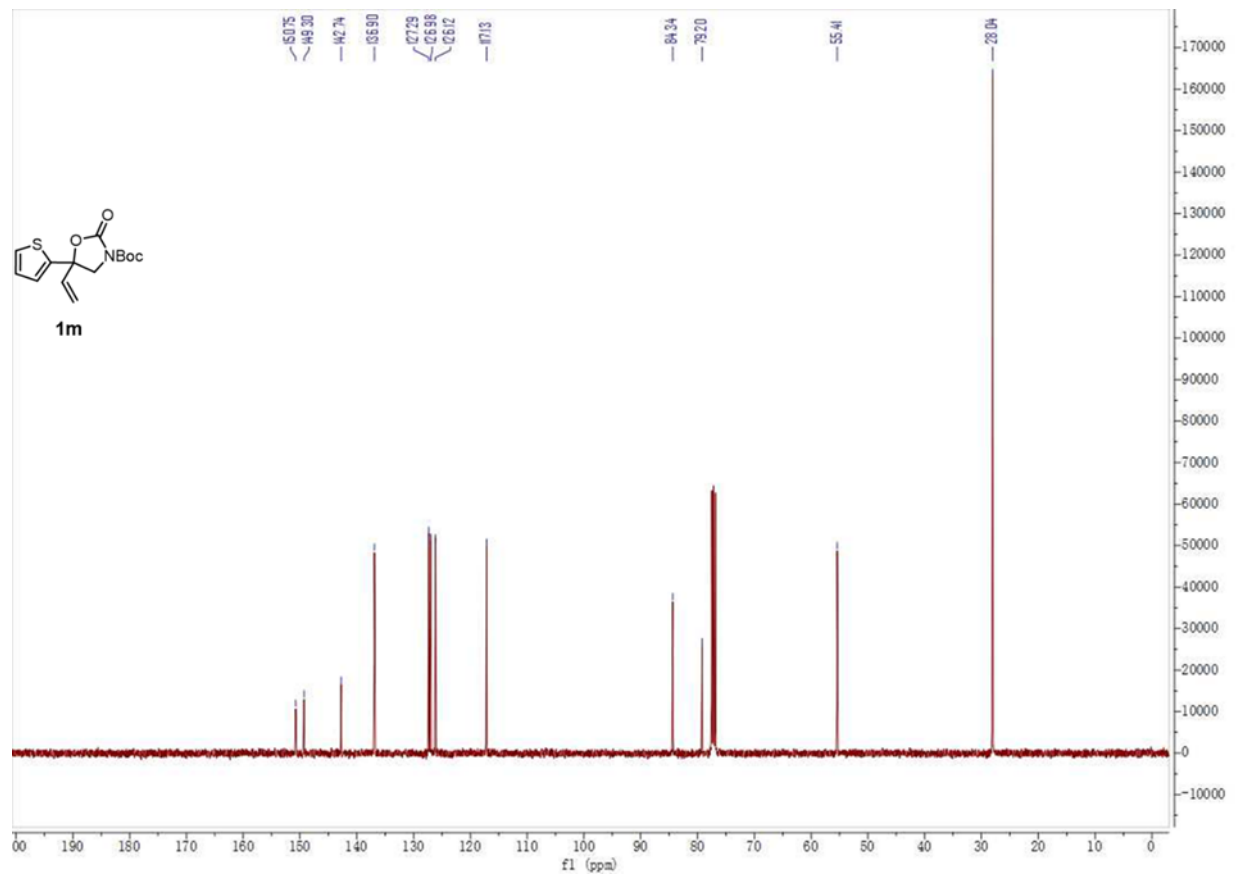
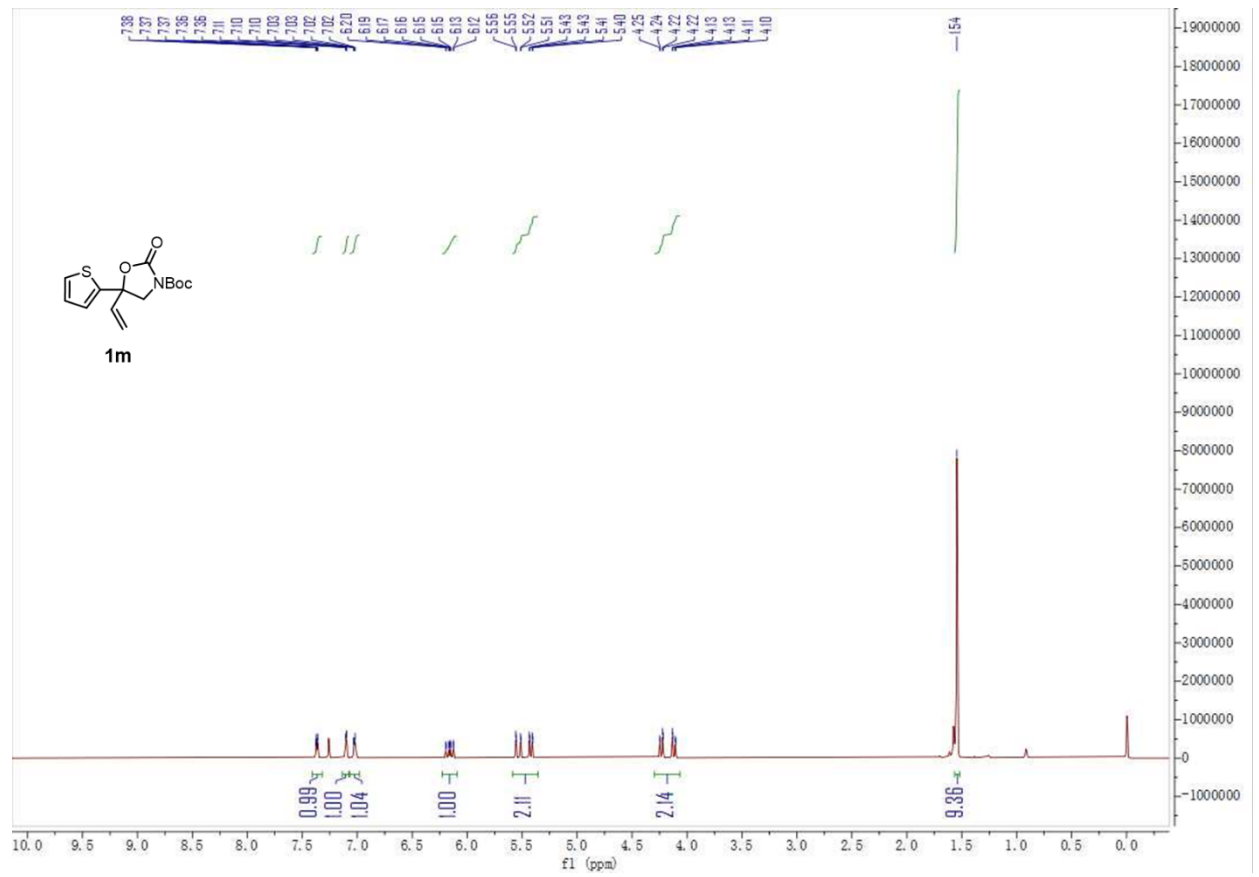


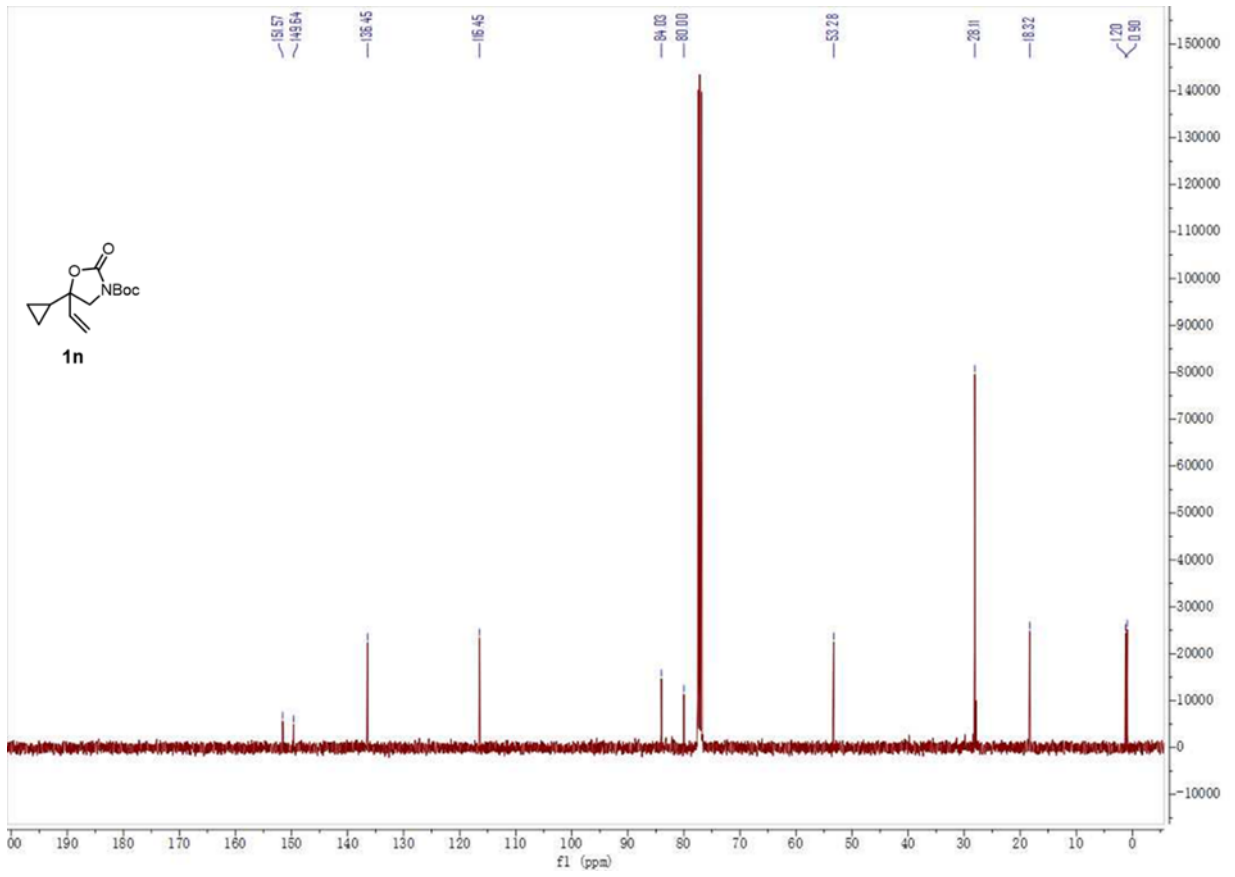
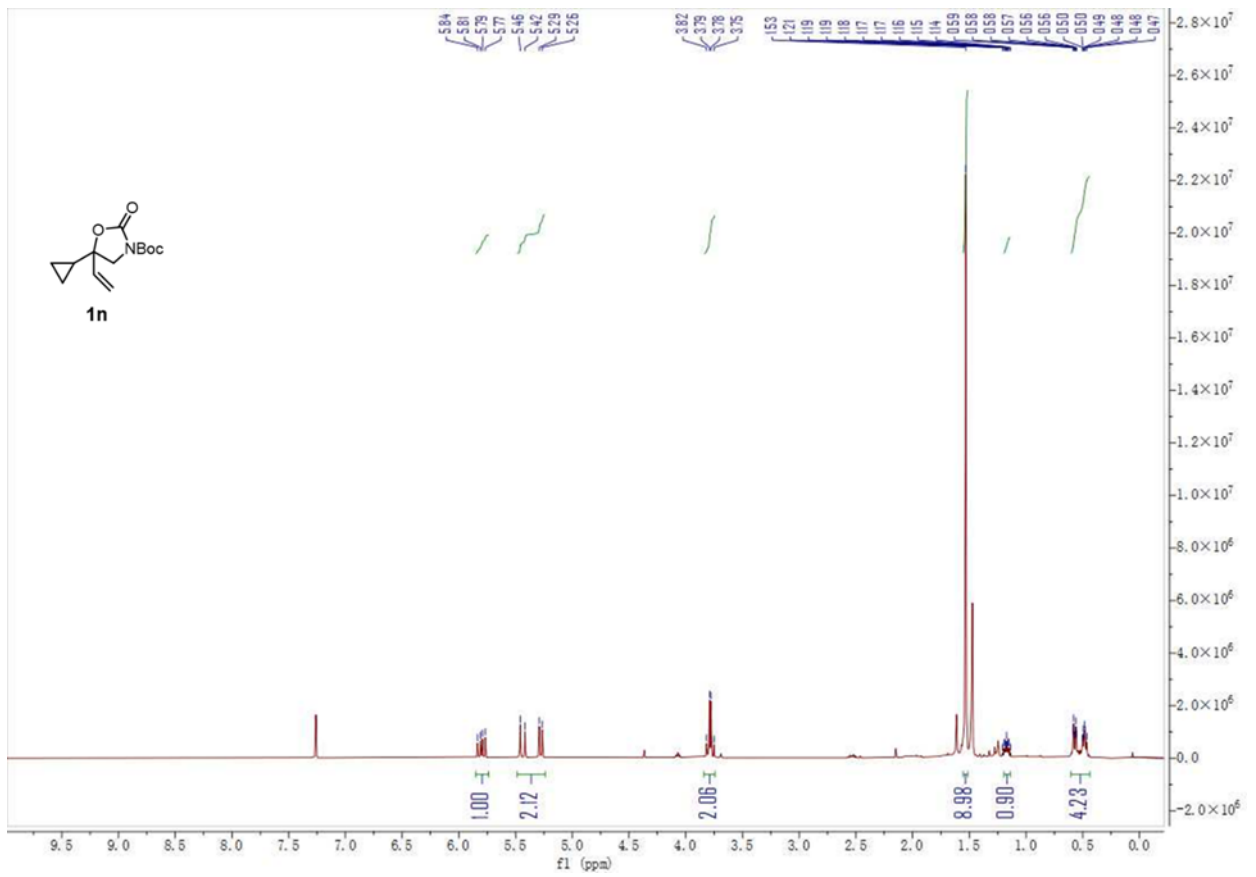


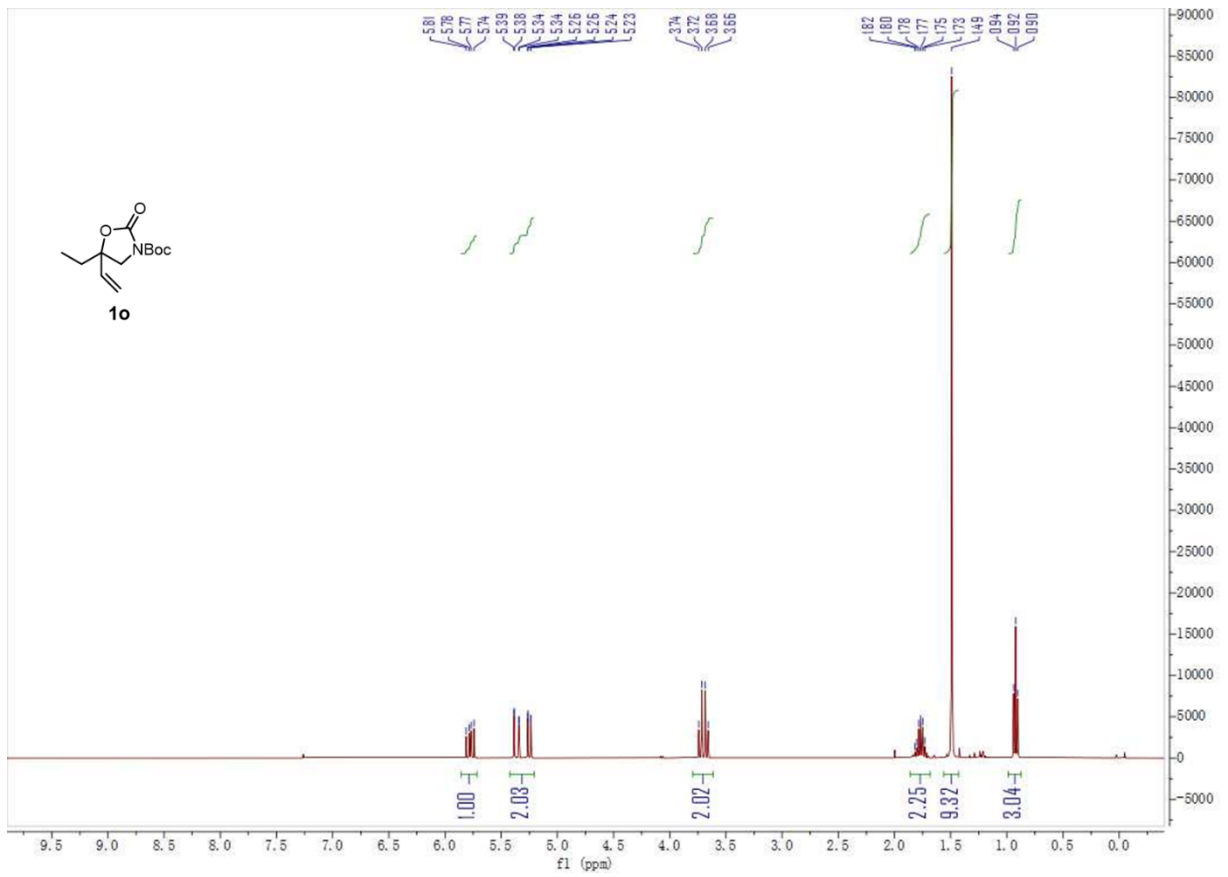




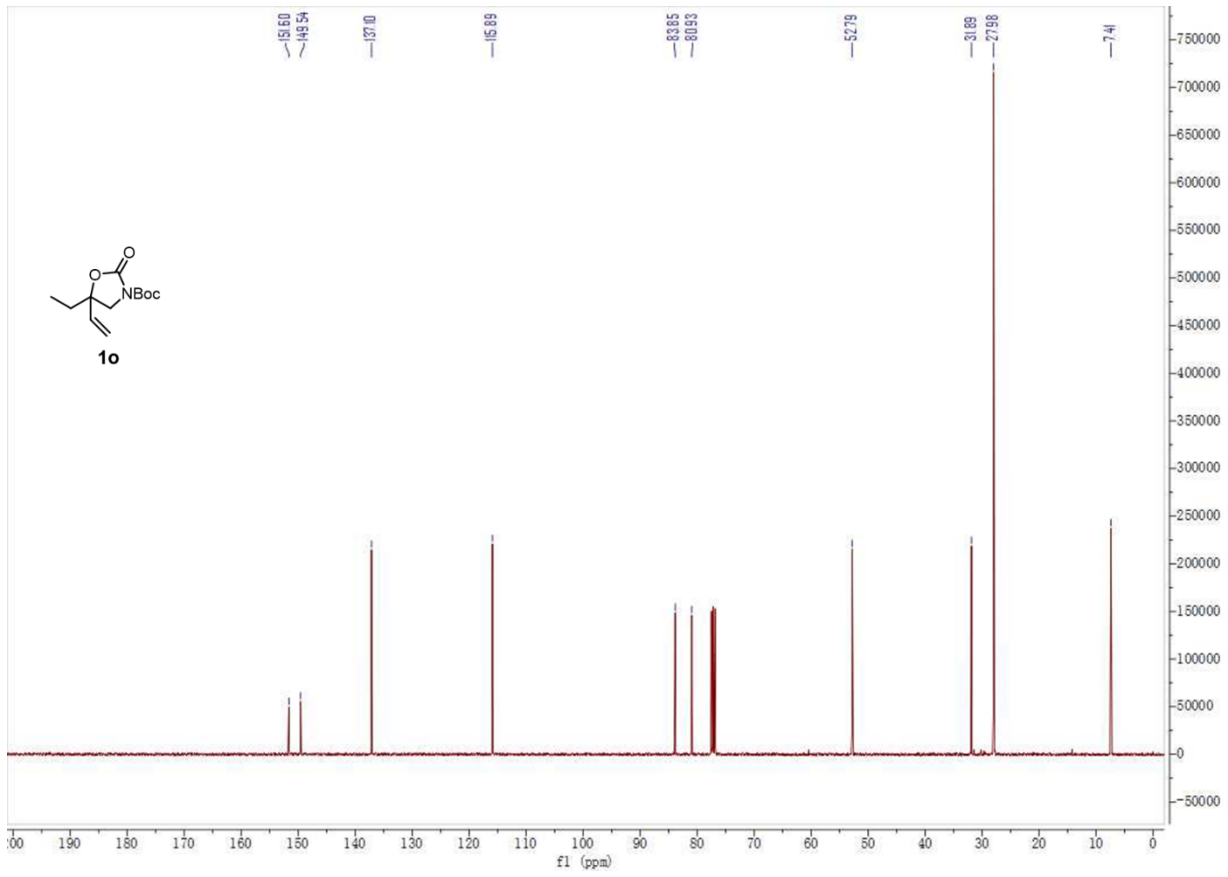








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