

## Supporting Information for the Paper

### **Palladium-Catalyzed Carbocyclization/Cross-Coupling Reactions of Two Different Allenic Moieties: Synthesis of 3-(Buta-1,3-dienyl) Carbazoles and Mechanistic Insights**

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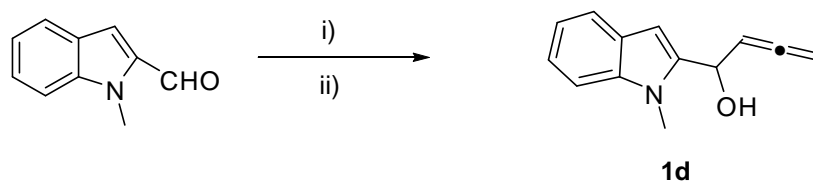
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**General Methods:** <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra were recorded on a Bruker Avance AVIII-700 with cryoprobe, Bruker AMX-500, Bruker Avance-300, Varian VRX-300S or Bruker AC-200. NMR spectra were recorded in CDCl<sub>3</sub> solutions, except otherwise stated. Chemical shifts are given in ppm relative to TMS (<sup>1</sup>H, 0.0 ppm), or CDCl<sub>3</sub> (<sup>13</sup>C, 76.9 ppm). Low and high resolution mass spectra were taken on an AGILENT 6520 Accurate-Mass QTOF LC/MS spectrometer using the electronic impact (EI) or electrospray modes (ES) unless otherwise stated. IR spectra were recorded

on a Bruker Tensor 27 spectrometer. Specific rotation  $[\alpha]_D$  is given in  $10^{-1}$  deg  $\text{cm}^2 \text{g}^{-1}$  at 20 °C, and the concentration ( $c$ ) is expressed in g per 100 mL. All commercially available compounds were used without further purification.

Allenol **1d** was prepared as follow:



- i) Ethynyl magnesium bromide, THF, -60°C, 16h  
ii)  $(\text{CH}_2\text{O})_n$ , CuBr,  $i\text{Pr}_2\text{NH}$ , 1,4-dioxane, reflux, 2h

**Procedure for the preparation of allenol 1d:** i) A solution of ethynyl magnesium bromide (1M THF, 11 mL) was added to a -60°C cooled solution of the commercially available N-methyl indole 2-carboxyaldehyde (300 mg) in dry THF (1 mL). The mixture was stirred for 16 hours (the reaction was monitored by TLC). The crude reaction was quenched with  $\text{NaHCO}_3$  (saturated solution) and extracted with AcOEt (3 x 10 mL). Evaporation of the solvent followed by column chromatography (hexanes/AcOEt 4:1) afforded the corresponding indole alkynol as a yellow oil, which was employed for the next reaction step. ii) To a solution of the above indole alkynol (245 mg) in 1,4-dioxane (6,5 mL) was added  $(\text{CH}_2\text{O})_n$  (99 mg, 2.55 mmol),  $i\text{Pr}_2\text{NH}$  (0,33 mL, 1.8 mmol) and CuBr (93 mg, 0.5 mmol). The mixture was heated at reflux for two hours until completion (TLC). The reaction mixture was quenched with water and extracted with AcOEt (3 x 10 mL). Column chromatography afforded **1d** as a pale thick oil ( 173 mg, 67%).  $^1\text{H}$  RMN (300 MHz,  $\text{CDCl}_3$ , 25°C):  $\delta$  = 1. 99 (d, 1H,  $J$  = 5.4 Hz, OH); 3.73 (s, 3H, Me); 4.92 (m, 2H,  $\text{CH}=\text{C}=\text{CH}_2$ ); 5.41 (m, 1H,  $\text{CHOH}$ ); 5.56 (m, 1H,  $\text{CH}=\text{C}=\text{CH}_2$ ); 6.42 (s, 1H, Ar); 7.02 (m, 1H, Ar); 7.19 (dd,  $J$  = 1.17, 8.19 Hz, 1H, Ar); 7.24 (d, 1H,  $J$  = 8.19 Hz, Ar); 7.56 (d, 1H,  $J$  = 7.74 Hz, Ar).  $^{13}\text{C}$  RMN (75 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 207.5 ( $\text{CH}=\text{C}=\text{CHH}$ ); 140.3 (C); 138.3 (C); 127.0 (C); 122.0 (CH Ar); 120.9 (CH Ar); 119.6 (CH Ar); 109.1 (CH Ar); 100.2 (CH Ar); 93.2 ( $\text{CH}=\text{C}=\text{CHH}$ ); 79.0 ( $\text{CH}=\text{C}=\text{CHH}$ ); 65.3

(CHOH); 30.2 (CH<sub>3</sub>). IR (CHCl<sub>3</sub>):  $\nu = 3490; 1542; 1038 \text{ cm}^{-1}$ . HRMS (ES): calcd for C<sub>13</sub>H<sub>13</sub>NO [M]<sup>+</sup>: 199.0997; found: 199.1003.

*O*-Acetyl allenols **2a–f**, and **2g–i**, were prepared following procedures reported in previous works (Alcaide, B.; Almendros, P.; Martínez del Campo, T.; Carrascosa, R. *Chem. Asian J.* **2008**, 3, 1140; Ma, S.; Jiao, S.; Zhao, S.; Hou, H. *J. Org. Chem.* **2002**, 2837). Data for previously unreported compounds **2**, follows:

Compound **2b**: starting from the corresponding allenol (300 mg, 1.579 mmol), Ac<sub>2</sub>O (0.18 mL, 1.895 mmol), TEA (0.53 mL, 3.780 mmol) and DMAP (cat.) in DCM (15 mL/mmol), compound **2b** was obtained as a yellow oil (301 mg, 82%). <sup>1</sup>H RMN (300 MHz, CDCl<sub>3</sub>, 25°C):  $\delta = 1.52$  (t,  $J = 3.10$  Hz, 3H, Me); 2.02 (s, 3H, Me); 3.73 (s, 3H, MeO); 4.72 (m, 2H, CH<sub>2</sub>=); 6.02 (m, 1H, CHOAc); 6.80 (m, 2H, Ar). <sup>13</sup>C RMN (75 MHz, CDCl<sub>3</sub>):  $\delta = 206.19$  (C); 169.96 (C=O); 159.54 (C); 130.44 (C); 128.57 (CH); 113.77 (CH); 99.30 (CH); 75.63 (CH<sub>2</sub>=); 55.27 (Me); 21.17 (Me); 15.13 (Me). IR (CHCl<sub>3</sub>):  $\nu = 1542, 1038 \text{ cm}^{-1}$ .

Compound **2c**: starting from the corresponding allenol (300 mg, 1.261 mmol), Ac<sub>2</sub>O (0.14 mL, 1.531 mmol), TEA (0.42 mL, 3.026 mmol) and DMAP (cat.) in DCM (15 mL/mmol), compound **2c** was obtained as a yellow oil (330 mg, 93%). <sup>1</sup>H RMN (300 MHz, CDCl<sub>3</sub>, 25°C):  $\delta = 1.53$  (t,  $J = 3.09$  Hz, 3H, Me); 2.04 (s, 3H, Me); 4.72 (m, 2H, CH<sub>2</sub>=); 6.05 (m, 1H, HCOAc); 7.16 (m, 2H, Ar); 7.41 (m, 2H, Ar). <sup>13</sup>C RMN (75 MHz, CDCl<sub>3</sub>):  $\delta = 206.59$  (C); 169.82 (C=O); 137.56 (C); 131.51 (CH); 128.73 (CH); 122.11 (C); 98.77 (CH); 75.47 (CH<sub>2</sub>); 21.09 (Me); 14.85 (Me). IR (CHCl<sub>3</sub>):  $\nu = 1542, 1038 \text{ cm}^{-1}$ .

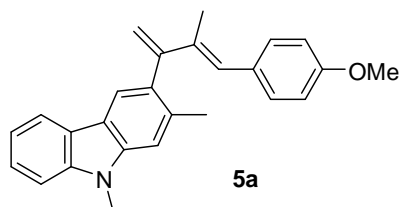
Compound **2e**: starting from the corresponding allenol (420 mg, 2.386 mmol), Ac<sub>2</sub>O (0.27 mL, 2.864 mmol), TEA (0.79 mL, 5.726 mmol) and DMAP (cat.) in DCM (15 mL/mmol), compound **2e** was obtained as a yellow oil (468 mg, 90%). <sup>1</sup>H RMN (300 MHz, CDCl<sub>3</sub>, 25°C):  $\delta = 2.12$  (s, 3H, Me); 3.84 (s, 3H, OMe); 4.90 (m, 2H, CH<sub>2</sub>=); 4.45 (q,  $J = 6.57$  Hz, 1H, CH=); 6.29 (m, 1H, HCOAc); 6.94 (m, 2H, Ar); 7.36 (m, 2H, Ar).

$^{13}\text{C}$  RMN (75 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 208.45 (C); 170.02 (C=O); 159.59 (C); 142.69 (C); 131.32 (CH); 113.87 (C); 91.74 (CH); 73.11 ( $\text{CH}_2$ ); 55.33 (Me); 21.24 (Me). IR ( $\text{CHCl}_3$ ):  $\nu$  = 1542, 1038  $\text{cm}^{-1}$ .

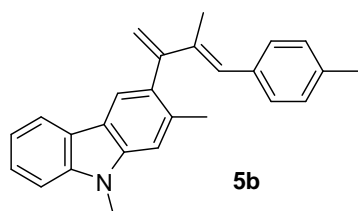
Compound **2g**: starting from the corresponding allenol (3 mmol), prepared in situ from the DIBAL-H reduction of the methyl ester,  $\text{Ac}_2\text{O}$  (0.34 mL, 3.6 mmol), TEA (1 mL, 7.2 mmol) and DMAP (cat.) were added in DCM (25 mL) at  $0^\circ\text{C}$ . Compound **2i** was obtained as a pale orange oil (254 mg, 55%), which was used straightforward to avoid volatilization.  $^1\text{H}$  RMN (300 MHz,  $\text{CDCl}_3$ ,  $25^\circ\text{C}$ ):  $\delta$  = 0.87 (m, 3H, Me); 1.35 (m, 2H,  $\text{CH}_2$ ); 1.91 (m, 2H,  $\text{CH}_2$ ); 1.93 (s, 3H, Me); 4.46 (m, 2H,  $\text{CH}_2\text{O}$ ); 5.51 (m, 2H,  $2\text{CH}=\text{}$ ).  $^{13}\text{C}$  RMN (75 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 205.3 (C); 171.89 (C=O); 92.79 (CH); 88.80 (CH); 62.96 ( $\text{CH}_2$ ); 30.43 ( $\text{CH}_2$ ); 22.23 ( $\text{CH}_2$ ); 21.00 (Me); 13.57 (Me). IR ( $\text{CHCl}_3$ ):  $\nu$  = 1531, 1038  $\text{cm}^{-1}$ .

Compound **2i**: starting from the corresponding allenol (3 mmol), prepared in situ from the DIBAL-H reduction of the methyl ester,  $\text{Ac}_2\text{O}$  (0.34 mL, 3.6 mmol), TEA (1 mL, 7.2 mmol) and DMAP (cat.) were added in DCM (25 mL) at  $0^\circ\text{C}$ . Compound **2i** was obtained as a pale orange oil (252 mg, 50%), which was used straightforward to avoid volatilization.  $^1\text{H}$  RMN (300 MHz,  $\text{CDCl}_3$ ,  $25^\circ\text{C}$ ):  $\delta$  = 0.96 (s, 9H, 3Me); 2.00 (s, 3H, Me); 4.47 (m, 2H,  $\text{CH}_2\text{O}$ ); 5.52 (m, 2H,  $2\text{CH}=\text{}$ ).  $^{13}\text{C}$  RMN (75 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 202.81 (C); 170.80 (C=O); 104.93 (CH); 88.70 (CH); 62.92 ( $\text{CH}_2$ ); 31.79 (C); 30.05 (3Me); 20.98 (Me). IR ( $\text{CHCl}_3$ ):  $\nu$  = 1540, 1026  $\text{cm}^{-1}$ .

**General procedure for the synthesis of carbazoles 5:** A solution of allenol **1b** (1 equiv.) and the corresponding *O*-acetyl allenol **2** (3.5 eq.) in anhydrous DMF (10 mL/mmol) was warmed up to  $80^\circ\text{C}$ . Then,  $\text{PdCl}_2$  was added (5 mmol%), and the mixture was stirred at this temperature. After completion (TLC, typically 30 minutes), the reaction mixture was diluted with plenty of  $\text{AcOEt}$ , and washed several times with water. The organic layers were combined, washed with brine, and dried with  $\text{MgSO}_4$ . The solvent was evaporated under reduced pressure, and the resulting residue was purified by column chromatography (hexanes), yielding analytically pure compounds.

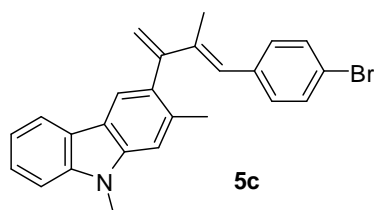


Compound **5a**: Starting from allenol **1b** (114 mg, 0.536 mmol), and *O*-acetyl allenol **2a** (435 mg, 1,876 mmol) in DMF (5.4 mL) with PdCl<sub>2</sub> (4.7 mg), and after purification by column chromatography (hexanes), compound **5a** was obtained as a pale yellow oil (139 mg, 71%). <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>, 25°C): δ = 2.35 (s, 3H, Me); 2.46 (s, 3H, Me); 3.83 (s, 3H, Me); 3.89 (s, 3H, OMe); 5.21 (d, *J* = 0.9 Hz, 1H, CH=); 5.66 (d, *J* = 1.4 Hz, 1H, CH=); 6.17 (s, 1H, CH=); 6.86 (m, 2H, Ar); 7.16 (m, 2H, Ar); 7.25 (m, 2H, Ar); 7.49 (m, 2H, Ar); 7.93 (s, 1H, Ar); 8.09 (d, *J* = 7.6 Hz, 1H, Ar). <sup>13</sup>C RMN (75 MHz, CDCl<sub>3</sub>): δ = 158.19 (C); 152.86 (C); 145.19 (C); 140.73 (C); 136.15 (C); 134.50 (C); 133.54 (C); 130.98 (C); 130.49 (2C, CH); 130.34 (CH); 125.19 (CH); 122.92 (C); 121.36 (CH); 120.56 (C); 120.07 (CH); 118.78 (CH); 114.29 (CHH=); 113.46 (2C, CH); 109.12 (CH); 108.35 (CH); 55.25 (Me); 29.09 (Me); 20.75 (Me); 15.27 (Me). IR (CHCl<sub>3</sub>): ν = 2927, 1504, 1469, 1250, 743 cm<sup>-1</sup>. HRMS (ES): calcd for C<sub>26</sub>H<sub>26</sub>NO [*M* + H]<sup>+</sup>: 368.2014; found: 368.2009.

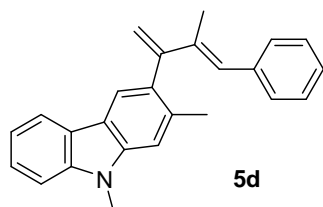


Compound **5b**: Starting from allenol **1b** (100 mg, 0.469 mmol), and *O*-acetyl allenol **2b** (355 mg, 1,643 mmol) in DMF (5.8 mL) with PdCl<sub>2</sub> (4.2 mg), and after purification by column chromatography (hexanes), compound **5b** was obtained as a pale yellow oil (97 mg, 60%). <sup>1</sup>H RMN (300 MHz, CDCl<sub>3</sub>, 25°C): δ = 2.13 (s, 3H, Me); 2.23 (s, 3H, Me); 2.34 (s, 3H, Me); 3.78 (s, 3H, Me); 5.09 (s, 1H, =CH); 5.55 (s, 1H, =CH); 6.07 (s, 1H, =CH); 7.00 (m, 4H, Ar); 7.15 (m, 2H, Ar); 7.34 (m, 2H, Ar); 7.81 (s, 1H, Ar); 7.97 (d, *J* = 7.5 Hz, 1H, Ar). <sup>13</sup>C RMN (75 MHz, CDCl<sub>3</sub>): δ =

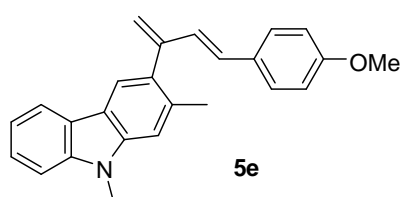
153.21 (C); 141.55 (C); 141.09 (C); 137.23 (C); 136.48 (C); 135.87 (C); 134.89 (C); 133.85 (C); 131.09 (CH, Ar); 129.55 (2C, CH Ar); 129.06 (2C, CH Ar); 125.56 (CH, Ar); 123.27 (C); 121.75 (CH, Ar); 120.92 (C); 120.45 (C); 119.15 (CH); 114.53 (CHH=); 109.51 (CH); 108.73 (CH); 29.48 (Me); 21.54 (Me); 21.13 (Me); 15.67 (Me). IR (CHCl<sub>3</sub>):  $\nu$  = 2921, 1471, 1277, 745 cm<sup>-1</sup>. HRMS (ES): calcd for C<sub>26</sub>H<sub>26</sub>N [M + H]<sup>+</sup>: 352.2065; found: 352.2060.



Compound **5c**: Starting from allenol **1b** (50 mg, 0.235 mmol), and *O*-acetyl allenol **2c** (230 mg, 0.825 mmol) in DMF (2.2 mL) with PdCl<sub>2</sub> (2.4 mg), and after purification by column chromatography (hexanes), compound **5c** was obtained as a pale yellow oil (44 mg, 47%). <sup>1</sup>H RMN (300 MHz, CDCl<sub>3</sub>, 25°C):  $\delta$  = 2.09 (s, 3H, Me); 2.32 (s, 3H, Me); 3.78 (s, 3H, Me); 5.14 (s, 1H, CH=); 5.57 (s, 1H, CH=); 6.01 (s, 1H, CH=); 6.95 (m, 2H, Ar); 7.22 (m, 2H, Ar); 7.35 (m, 4H, Ar); 7.79 (s, 1H, Ar); 7.96 (d, *J* = 7.7 Hz, 1H, Ar). <sup>13</sup>C RMN (300 MHz, CDCl<sub>3</sub>):  $\delta$  = 152.43 (C); 141.19 (C); 140.77 (C); 138.27 (C); 137.32 (C); 134.35 (C); 131.07 (2C, CH); 130.82 (2C, CH); 129.48 (CH); 125.28 (CH); 121.36 (CH); 120.60 (C); 120.26 (C); 120.06 (CH); 118.83 (CH); 115.34 (CHH=); 109.19 (CH); 108.38 (CH); 29.09 (Me); 20.72 (Me); 15.22 (Me). IR (CHCl<sub>3</sub>):  $\nu$  = 2930, 1502, 1465, 745 cm<sup>-1</sup>. HRMS (ES): calcd for C<sub>25</sub>H<sub>23</sub>NBr [M + H]<sup>+</sup>: 416.1014; found: 416.1008.

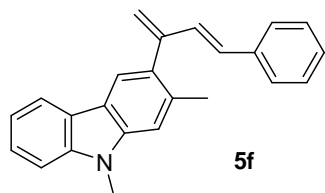


Compound **5d**: Starting from allenol **1b** (60 mg, 0.282 mmol), and *O*-acetyl allenol **5d** (199 mg, 0.987 mmol) in DMF (2.7 mL) with PdCl<sub>2</sub> (2.8 mg), and after purification by column chromatography (hexanes), compound **5d** was obtained as a pale yellow oil (59 mg, 63%). <sup>1</sup>H RMN (300 MHz, CDCl<sub>3</sub>, 25°C): δ = 2.13 (s, 3H, Me); 2.23 (s, 3H, Me); 2.34 (s, 3H, Me); 5.12 (s, 1H, CH=); 5.57 (d, *J* = 1.4 Hz, 1H, CH=); 6.10 (s, 1H, CH=); 7.11 (m, 2H, Ar); 7.18 (m, 5H, Ar); 7.82 (s, 1H, Ar); 7.97 (d, *J* = 8.1 Hz, 1H, Ar). <sup>13</sup>C RMN (75 MHz, CDCl<sub>3</sub>): δ = 157.72 (C); 141.19 (C); 140.75 (C); 138.44 (C); 137.49 (C); 134.46 (C); 133.37 (C); 130.77 (CH); 129.22 (2C, CH); 127.95 (2C, CH); 126.37 (CH); 125.21 (CH); 122.90 (C); 121.38 (CH); 120.57 (C); 120.07 (CH); 118.79 (CH); 114.85 (CHH=); 109.15 (CH); 108.35 (CH); 29.09 (Me); 20.75 (Me); 15.25 (Me). IR (CHCl<sub>3</sub>): ν = 2923, 1475, 1280, 745 cm<sup>-1</sup>. HRMS (ES): calcd for C<sub>25</sub>H<sub>24</sub>N [M + H]<sup>+</sup>: 338.1909; found: 338.1903.

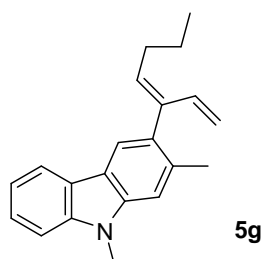


Compound **5e**: Starting from allenol **1b** (60 mg, 0.282 mmol), and *O*-acetyl allenol **2e** (215 mg, 0.987 mmol) in DMF (2.7 mL) with PdCl<sub>2</sub> (2.8 mg), and after purification by column chromatography (hexanes), compound **5e** was obtained as a green oil (62 mg, 63%). <sup>1</sup>H RMN (300 MHz, CDCl<sub>3</sub>, 25°C): δ = 2.37 (s, 3H, Me); 3.71 (s, 3H, Me); 3.79 (s, 3H, Me); 5.07 (s, 1H, CH=); 5.46 (s, 1H, CH=); 5.86 (d, *J* = 15.9 Hz, 1H, CH=); 6.73 (m, 2H, Ar); 6.95 (d, *J* = 15.9 Hz, 1H, CH=); 7.30 (m, 2H, Ar); 7.78 (s, 1H, Ar); 7.96 (d, *J* = 7.8 Hz, 1H, Ar). <sup>13</sup>C RMN (75 MHz, CDCl<sub>3</sub>): δ = 159.22 (C); 149.18 (C); 141.20 (C); 140.82 (C); 134.23 (C); 131.42 (C); 131.35 (CH); 130.15

(C); 129.77 (CH); 127.75 (2C, CH); 125.27 (CH); 122.87 (C); 121.16 (CH); 120.65 (C); 120.10 (CH); 118.84 (CH); 117.86 (CHH=); 114.03 (2C, CH); 109.24 (CH); 108.37 (CH); 55.29 (Me); 29.11 (Me); 20.75 (Me). IR (CHCl<sub>3</sub>):  $\nu = 2922, 1475, 1277, 740 \text{ cm}^{-1}$ . HRMS (ES): calcd for C<sub>25</sub>H<sub>24</sub>NO [M + H]<sup>+</sup>: 354.1858; found: 354.1848.



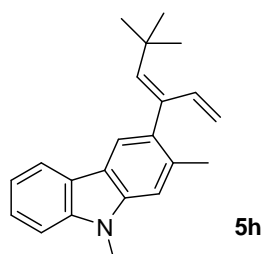
Compound **5f**: Starting from allenol **1b** (75 mg, 0.355 mmol), and *O*-acetyl allenol **2f** (233 mg, 1.241 mmol) in DMF (3.3 mL) with PdCl<sub>2</sub> (3.4 mg), and after purification by column chromatography (hexanes), compound **5f** was obtained as a yellow oil (76 mg, 67%). <sup>1</sup>H RMN (300 MHz, CDCl<sub>3</sub>, 25°C):  $\delta = 2.37$  (s, 3H, Me); 3.79 (s, 3H, Me); 5.12 (s, 1H, CH=); 5.52 (s, 1H, CH=); 5.95 (d,  $J = 15.9$  Hz, 1H, CH=); 7.19 (m, 7H, Ar + CH=); 7.32 (m, 2H, Ar); 7.78 (s, 1H, Ar); 7.96 (d,  $J = 7.7$  Hz, Ar). <sup>13</sup>C RMN (75 MHz, CDCl<sub>3</sub>):  $\delta = 149.05$  (C); 141.22 (C); 140.87 (C); 137.34 (C); 134.19 (C); 131.85 (CH); 131.73 (CH); 131.19 (C); 128.53 (2C, CH); 127.48 (2C, CH); 126.55 (CH); 125.39 (CH); 122.85 (C); 121.17 (CH); 120.69 (C); 120.10 (CH); 118.93 (CHH=); 118.86 (CH); 109.29 (CH); 108.38 (CH); 29.11 (Me); 20.75 (Me). IR (CHCl<sub>3</sub>):  $\nu = 2921, 1475, 1281, 745 \text{ cm}^{-1}$ . HRMS (ES): calcd for C<sub>24</sub>H<sub>22</sub>N [M + H]<sup>+</sup>: 324.1752; found: 324.1754.



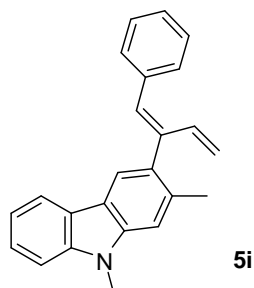
Compound **5g**: Starting from allenol **1b** (84 mg, 0.394 mmol), and *O*-acetyl allenol **2g** (195 mg, 1.266 mmol) in DMF (3.8 mL) with PdCl<sub>2</sub> (3.7 mg), and after purification by column



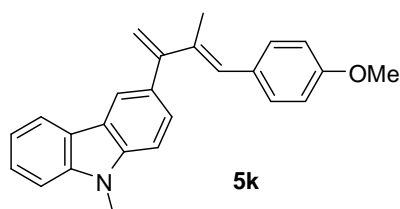
chromatography (hexanes), compound **5g** was obtained as a yellow oil (65 mg, 48%). <sup>1</sup>H RMN (300 MHz, CDCl<sub>3</sub>, 25°C): δ = 0.74 (t, *J* = 7.44 Hz, 3H, Me); 1.30 (sxt, *J* = 7.44 Hz, 2H, CH<sub>2</sub>); 1.74 (m, 2H, CH<sub>2</sub>); 2.26 (s, 3H; Me); 3.78 (s, 3H, Me); 4.40 (d, *J* = 16.95 Hz, 1H, CH=); 4.86 (d, *J* = 10.53 Hz, 1H, CH=); 5.79 (dd, *J* = 7.44, 7.32 Hz, 1H, CH=); 6.58 (dd, *J* = 17.05, 10.48 Hz, 1H, CH=); 7.13 (m, 2H, Ar); 7.32 (m, 2H, Ar); 7.62 (s, 1H, Ar); 7.94 (d, *J* = 7.59 Hz, 1H, Ar). <sup>13</sup>C RMN (75 MHz, CDCl<sub>3</sub>): δ = 142.03 (C); 141.77 (C); 141.09 (C); 140.86 (CH); 140.67 (C); 134.62 (C); 134.15 (C); 128.54 (C); 125.16 (CH); 121.27 (CH); 120.04 (C); 118.69 (CH); 113.73 (CH<sub>2</sub>=); 109.13 (CH); 108.32 (CH); 103.79 (CH); 31.31 (CH<sub>2</sub>); 29.07 (Me); 22.55 (CH<sub>2</sub>); 20.33 (Me); 13.93 (Me). IR (CHCl<sub>3</sub>): ν = 2989, 1475, 1281, 743 cm<sup>-1</sup>. HRMS (ES): calcd for C<sub>21</sub>H<sub>24</sub>N [M + H]<sup>+</sup>: 290.1909; found: 290.1911.



Compound **5h**: Starting from allenol **1b** (40 mg, 0.187 mmol), and *O*-acetyl allenol **2h** (110 mg, 0.655 mmol) in DMF (1.5 mL) with PdCl<sub>2</sub> (2.1 mg), and after purification by column chromatography (hexanes), compound **5h** was obtained as a pale yellow oil (22 mg, 40%). <sup>1</sup>H RMN (300 MHz, CDCl<sub>3</sub>, 25°C): δ = 1.49 (s, 9H, 3Me); 2.29 (s, 3H, Me); 3.77 (s, 3H, Me); 4.29 (d, *J* = 16.1 Hz, 1H, CHH=); 5.52 (d, *J* = 20.0 Hz, 1H, CHH=); 5.74 (s, 1H, CH=); 6.52 (m, 1H, CH=); 7.14 (m, 2H, Ar); 7.35 (m, 2H, Ar); 7.63 (s, 1H, Ar); 7.96 (d, *J* = 7.9 Hz, 1H, Ar). <sup>13</sup>C RMN (75 MHz, CDCl<sub>3</sub>): δ = 157.40 (C); 144.21 (CH); 143.09 (CH); 128.82 (C); 126.71 (C); 125.11 (CH); 122.89 (C); 122.23 (C); 121.78 (CH); 120.37 (C); 120.02 (CH); 118.66 (CH); 113.30 (CH<sub>2</sub>); 108.98 (CH); 108.57 (C); 108.34 (C); 30.95 (Me); 30.66 (3Me); 15.30 (Me). IR (CHCl<sub>3</sub>): ν = 2921, 1473, 1279, 743 cm<sup>-1</sup>. HRMS (ES): calcd for C<sub>22</sub>H<sub>25</sub>N [M]<sup>+</sup>: 303.1987; found: 303.1980.

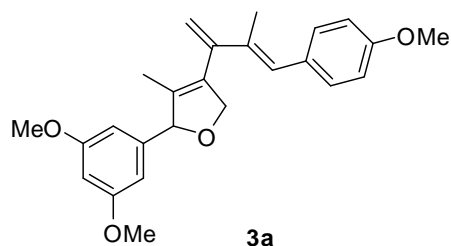


Compound **5i**: Starting from allenol **1b** (50 mg, 0.235 mmol), and *O*-acetyl allenol **2i** (143 mg, 0.823 mmol) in DMF (1.8 mL) with PdCl<sub>2</sub> (2.4 mg), and after purification by column chromatography (hexanes), compound **5i** was obtained as a pale yellow oil (48 mg, 63%). <sup>1</sup>H RMN (300 MHz, CDCl<sub>3</sub>, 25°C): δ = 2.22 (s, 3H, Me); 3.84 (s, 3H, Me); 4.60 (dd, *J* = 16.96, 0.88 Hz, 1H, CH=); 5.05 (d, *J* = 10.96, 1H, CH=); 6.66 (s, 1H, CH=); 6.78 (m, 2H, Ar + CH=); 6.95 (m, 3H, Ar); 7.11 (m, 1H, Ar); 7.26 (s, 1H, Ar); 7.38 (m, 3H, Ar); 7.68 (s, 1H, Ar); 7.92 (d, *J* = 7.75 Hz, 1H, Ar). <sup>13</sup>C RMN (75 MHz, CDCl<sub>3</sub>): δ = 142.54 (CH); 142.15 (C); 141.47 (C); 141.38 (C); 137.47 (C); 134.68 (C); 132.48 (CH); 129.37 (2C, CH); 128.66 (C); 128.53 (2C, CH); 127.31 (CH); 125.67 (CH); 123.23 (C); 121.81 (CH); 121.38 (C); 120.62 (CH); 119.18 (CH); 116.39 (CH<sub>2</sub>=); 110.78 (CH); 108.79 (CH); 29.53 (Me); 20.62 (Me). IR (CHCl<sub>3</sub>): ν = 2922, 1475, 1279, 745 cm<sup>-1</sup>. HRMS (ES): calcd for C<sub>24</sub>H<sub>22</sub>N [M + H]<sup>+</sup>: 324.1752; found: 324.1746.

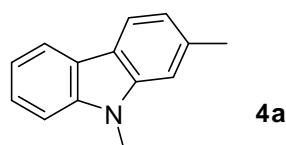


Compound **5k**: Starting from allenol **1d** (50 mg, 0.251 mmol), and *O*-acetyl allenol **2a** (175 mg, 0.755 mmol) in DMF (3.5 mL) with PdCl<sub>2</sub> (2.8 mg), and after purification by column chromatography (hexanes, triethylamine 1%), compound **5k** was obtained as a dark yellow oil (48 mg, 59%). <sup>1</sup>H RMN (300 MHz, CDCl<sub>3</sub>, 25°C): δ = 1.90 (s, 3H, Me); 3.65 (s, 3H, Me); 3.68 (s, 3H, Me); 5.29 (s, 1H, =CHH); 5.35 (s, 1H, =CHH); 6.74 (m, 2H, Ar); 6.96 (s, 1H, =CH); 7.07 (m, 4H, Ar); 7.25 (s, 1H, Ar); 7.31 (m, 1H, Ar); 7.93 (m, 2H, Ar). <sup>13</sup>C RMN (75 MHz, CDCl<sub>3</sub>): δ = 158.7

(C); 142.5 (C); 141.0 (2C); 131.14 (2C); 131.08 (C); 130.76 (2CH); 129.70 (C); 125.67 (2CH); 122.76 (2C); 120.32 (2CH); 118.82 (2CH); 113.67 (2CH); 112.50 (CH<sub>2</sub>); 108.42 (2CH); 55.31 (Me); 29.09 (Me); 15.59 (Me). IR (CHCl<sub>3</sub>):  $\nu$  = 2930, 1471, 1277, 743 cm<sup>-1</sup>. HRMS (ES): calcd for C<sub>25</sub>H<sub>24</sub>NO [M + H]<sup>+</sup>: 354.1858; found: 354.1846.



Compound **3a**: Starting from allenol **1a** (60 mg, 0.273 mmol), and *O*-acetyl allenol **2a** (127 mg, 0.546 mmol) in DMF (2.6 mL) with PdCl<sub>2</sub> (2.4 mg), and after purification by column chromatography (hexanes), compound **3a** was obtained as a yellow oil (65 mg, 61%). <sup>1</sup>H RMN (300 MHz, CDCl<sub>3</sub>, 25°C):  $\delta$  = 1.43 (s, 3H, Me); 1.98 (s, 3H, Me); 3.71 (s, 6H, 2Me); 3.74 (s, 3H, Me); 4.79 (m, 2H, CH<sub>2</sub>); 4.98 (m, 1H, CH=); 5.32 (s, 1H, CH=); 5.51 (s, 1H, HCOCH<sub>2</sub>); 6.33 (s, 1H, Ar); 6.43 (m, 2H, Ar + CH=); 6.83 (s, 1H, Ar); 7.17 (m, 2H, Ar). <sup>13</sup>C RMN (75 MHz, CDCl<sub>3</sub>):  $\delta$  = 161.03 (2C); 158.52 (C); 144.79 (C); 144.36 (C); 134.38 (C); 134.10 (C); 132.97 (C); 130.49 (2C, CH); 104.91 (2C, CH); 94.94 (CH); 92.46 (CH); 78.90 (CH<sub>2</sub>); 55.31 (MeO); 55.27 (2C, MeO); 15.68 (Me); 11.00 (Me). IR (CHCl<sub>3</sub>):  $\nu$  = 2944, 1602, 1462, 1249, 1155, 1032, 835. 1475, 1203, 835 cm<sup>-1</sup>. HRMS (ES): calcd for C<sub>25</sub>H<sub>29</sub>O<sub>4</sub> [M + H]<sup>+</sup>: 393.2066; found: 393.2070.



Compound **4a**: From 60 mg (0.28 mmol) of allenol **1b**, and after chromatography of the residue using hexanes/ethyl acetate (8:1) as eluent gave compound **4a** (37 mg, 69%) as a colorless solid; mp

92–93°C;  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ , 25 °C):  $\delta$  = 7.96 (d,  $J$  = 7.8 Hz, 1H, Ar); 7.88 (d,  $J$  = 8.0 Hz, 1H, Ar); 7.36 (m, 1H, Ar); 7.27 (d,  $J$  = 8.10 Hz, 1H, Ar); 7.13 (m, 2H, Ar); 6.97 (dd,  $J$  = 8.0, 0.8 Hz, 1H, Ar); 3.72 (s, 3H, NMe); 2.49 (s, 3H, Me).  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ , 25 °C):  $\delta$  = 142.0 (C Ar); 141.4 (C Ar); 136.3 (C Ar); 125.5 (CH Ar); 123.8 (C Ar); 120.9 (C Ar); 120.8 (CH Ar); 120.4 (CH Ar, 2C); 119.1 (CH Ar); 109.1 (CH Ar); 108.7 (CH Ar); 29.4 (NMe); 22.7 (Me). IR ( $\text{CHCl}_3$ ):  $\nu$  = 1469, 1249, 701  $\text{cm}^{-1}$ . HRMS (ES): calcd for  $\text{C}_{14}\text{H}_{13}\text{N}$  [ $M$ ] $^+$ : 195.1048; found: 195.1040.

### Computational Details

All the calculations reported in this paper were obtained with the GAUSSIAN 09 suite of programs.<sup>1</sup> Electron correlation was partially taken into account using the hybrid functional usually denoted as B3LYP<sup>2</sup> using the double- $\zeta$  quality plus polarization def2-SVP basis set<sup>3</sup> for all atoms. Zero point vibrational energy (ZPVE) corrections were computed at the B3LYP/def2-SVP level and were not scaled. Reactants and products were characterized by frequency calculations,<sup>4</sup> and have positive definite Hessian matrices. Transition structures (TS's) show only one negative eigenvalue in their diagonalized force constant matrices, and their associated eigenvectors were confirmed to correspond to the motion along the reaction coordinate under consideration using the Intrinsic Reaction Coordinate (IRC) method.<sup>5</sup>

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<sup>1</sup> Gaussian 09, Revision B.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

<sup>2</sup> (a) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648. (b) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1998**, *37*, 785. (c) Vosko, S. H.; Wilk, L.; Nusair, M. *Can. J. Phys.* **1980**, *58*, 1200.

<sup>3</sup> Weigend, F.; Alhrichs, R. *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297.

<sup>4</sup> McIver, J. W.; Komornicki, A. K. *J. Am. Chem. Soc.* **1972**, *94*, 2625.

<sup>5</sup> González, C.; Schlegel, H. B. *J. Phys. Chem.* **1990**, *94*, 5523.

Cartesian coordinates (in Å) and total energies (in a. u., non corrected zero-point vibrational energies included) of all the stationary points discussed in the text. All calculations have been performed at the B3LYP/def2-SVP +  $\Delta$ ZPVE level.

**1b-Pd:** E= -1719.832919

C	1.397821000	-0.555389000	-0.287379000
C	0.473198000	-0.905328000	0.580048000
C	-1.975878000	-0.777478000	0.082733000
C	-4.171140000	-0.284260000	0.020993000
C	-5.574867000	-0.313506000	-0.006861000
C	-6.245960000	0.905867000	-0.029148000
C	-5.544733000	2.132449000	-0.020206000
C	-4.155325000	2.161440000	0.011880000
C	-3.446585000	0.944018000	0.033262000
H	-6.129575000	-1.254157000	-0.004055000
H	-7.338710000	0.913740000	-0.049818000
H	-6.107011000	3.069301000	-0.036300000
H	-3.616746000	3.112494000	0.021113000
C	0.535316000	-0.642007000	2.061858000
H	1.337378000	0.063120000	2.315046000
H	-0.419635000	-0.227099000	2.418316000
H	0.716512000	-1.586149000	2.603243000
C	-0.754792000	-1.658162000	0.050579000
H	-0.897791000	-2.518336000	0.729421000
C	-2.054760000	0.600585000	0.068752000
H	-1.206443000	1.283129000	0.086306000
N	-3.257052000	-1.321154000	0.039791000
Pd	3.156642000	0.522795000	-0.014408000
Cl	2.009141000	2.510077000	-0.154456000
Cl	4.557412000	-1.265172000	0.265611000
C	-3.582703000	-2.732970000	0.009003000
H	-4.526325000	-2.880343000	-0.535079000
H	-2.797732000	-3.282496000	-0.528081000
H	-3.698096000	-3.158438000	1.021451000
C	2.033430000	-0.417831000	-1.515065000
H	1.723591000	0.373185000	-2.208504000
H	2.628344000	-1.245222000	-1.918020000
O	-0.561078000	-2.226537000	-1.236637000
H	-0.814821000	-1.558878000	-1.890028000

**TS1:** E= -2131.430770

C	1.021597000	0.221442000	-0.397460000
C	0.831877000	1.305781000	-1.144967000
C	-1.661038000	0.929285000	-0.785180000
C	-3.507572000	0.058937000	0.168531000
C	-4.704612000	-0.119829000	0.871021000
C	-5.236487000	-1.409178000	0.910151000
C	-4.594157000	-2.487099000	0.268524000
C	-3.398291000	-2.302706000	-0.422557000
C	-2.841192000	-1.014399000	-0.470850000
H	-5.209979000	0.708127000	1.370799000
H	-6.170586000	-1.585178000	1.448845000
H	-5.042456000	-3.482140000	0.317240000
H	-2.902922000	-3.142631000	-0.915577000
C	1.921614000	2.139749000	-1.761764000
H	2.913603000	1.797972000	-1.440670000
H	1.872702000	2.075663000	-2.863195000
H	1.805257000	3.200258000	-1.490903000
C	-0.585830000	1.897244000	-1.234876000
H	-0.796017000	2.181893000	-2.282721000

C	-1.645481000	-0.455442000	-1.053246000
H	-1.037791000	-0.914552000	-1.829807000
N	-2.773372000	1.230010000	-0.047856000
Pd	2.626146000	-0.570297000	0.413795000
Cl	2.811072000	-2.286714000	-1.121379000
Cl	2.635621000	1.066523000	2.049229000
C	-3.237591000	2.518147000	0.456571000
H	-3.198540000	2.535614000	1.557951000
H	-2.608061000	3.317467000	0.061374000
H	-4.281013000	2.671356000	0.142316000
C	0.197311000	-0.722408000	0.264074000
H	0.200446000	-1.762252000	-0.068218000
H	-0.168112000	-0.529966000	1.279326000
O	-0.580059000	3.121008000	-0.509585000
H	-0.079816000	2.969998000	0.309057000

**TS1'**: E= -1719.807532

C	-3.320897000	0.923404000	-0.079212000
C	-4.020132000	-0.319903000	-0.075602000
C	-5.408614000	-0.383647000	-0.282451000
C	-6.084293000	0.812695000	-0.499814000
C	-5.406578000	2.053552000	-0.509848000
C	-4.035227000	2.118498000	-0.301010000
C	-1.942774000	0.625766000	0.168087000
C	-1.844283000	-0.744050000	0.311835000
H	-5.950852000	-1.331446000	-0.269894000
H	-7.164789000	0.792170000	-0.663070000
H	-5.974515000	2.970833000	-0.682400000
H	-3.512243000	3.077972000	-0.306817000
H	-1.113448000	1.329155000	0.232891000
C	-0.621635000	-1.556938000	0.572981000
H	-0.837681000	-2.399961000	1.251500000
C	1.249103000	-1.037864000	-1.221397000
H	1.961065000	-1.788045000	-1.585770000
H	0.738328000	-0.446270000	-1.991287000
C	-3.398400000	-2.739879000	0.236244000
H	-2.645639000	-3.323415000	-0.314686000
H	-3.440389000	-3.102346000	1.278819000
H	-4.371919000	-2.936888000	-0.231068000
C	0.555087000	-0.720397000	1.070303000
C	1.430594000	-0.491707000	0.089475000
C	0.576462000	-0.216109000	2.479839000
H	1.327531000	0.577507000	2.585443000
H	-0.404295000	0.196851000	2.765555000
H	0.813470000	-1.027348000	3.190920000
Pd	3.048898000	0.564599000	-0.144290000
Cl	4.406973000	-1.278363000	-0.503306000
Cl	1.885839000	2.525440000	0.197239000
N	-3.101827000	-1.326422000	0.155987000
H	0.269469000	-3.005381000	-0.513114000
O	-0.197362000	-2.176353000	-0.719374000

**6**: E= -1719.838970

C	0.973987000	0.195308000	-0.174319000
C	0.813508000	1.495201000	-0.496997000
C	-1.657914000	1.103085000	-0.461003000
C	-3.571895000	-0.014368000	-0.029049000
C	-4.875195000	-0.295192000	0.371852000
C	-5.312048000	-1.614894000	0.205963000
C	-4.468644000	-2.594352000	-0.338282000
C	-3.160405000	-2.285599000	-0.734076000
C	-2.712264000	-0.976700000	-0.574800000
H	-5.533479000	0.464289000	0.795985000

H	-6.326840000	-1.883405000	0.507600000
H	-4.838362000	-3.615680000	-0.453255000
H	-2.509006000	-3.055386000	-1.153752000
C	1.950170000	2.473572000	-0.698571000
H	1.644967000	3.303594000	-1.357731000
H	2.296289000	2.919500000	0.250017000
H	2.803993000	1.953434000	-1.154453000
C	-0.572418000	2.136443000	-0.567639000
H	-0.701788000	2.629333000	-1.555039000
C	-1.402982000	-0.304520000	-0.860062000
H	-1.103786000	-0.350005000	-1.922801000
N	-2.875707000	1.235686000	0.022384000
Pd	2.677837000	-0.609753000	0.258728000
Cl	3.459319000	-0.663390000	-1.925875000
Cl	2.095419000	-0.664942000	2.522145000
C	-3.523536000	2.442840000	0.539799000
H	-3.871007000	2.248722000	1.564905000
H	-2.801802000	3.263841000	0.541922000
H	-4.391666000	2.676778000	-0.093797000
C	-0.155010000	-0.786556000	-0.037372000
H	0.136567000	-1.774232000	-0.422584000
H	-0.408175000	-0.925623000	1.027211000
O	-0.707163000	3.171209000	0.399144000
H	-0.171857000	2.910038000	1.165183000

**6'**: E= -1719.811830

C	-3.272313000	0.919519000	-0.147626000
C	-3.986056000	-0.314633000	-0.052374000
C	-5.376016000	-0.375004000	-0.261488000
C	-6.031867000	0.809892000	-0.571491000
C	-5.339241000	2.041178000	-0.672101000
C	-3.970696000	2.106060000	-0.461959000
C	-1.903221000	0.630790000	0.123206000
C	-1.817783000	-0.731541000	0.372048000
H	-5.932151000	-1.311094000	-0.181625000
H	-7.111687000	0.791276000	-0.739155000
H	-5.896757000	2.948083000	-0.916965000
H	-3.433601000	3.054479000	-0.537036000
H	-1.063699000	1.326232000	0.148731000
C	-0.613388000	-1.492178000	0.707234000
H	-0.807297000	-2.382922000	1.325169000
C	1.008758000	-1.243920000	-1.186629000
H	1.810238000	-1.860556000	-1.615303000
H	0.511161000	-0.640461000	-1.958388000
C	-3.395945000	-2.710735000	0.449907000
H	-2.688818000	-3.347000000	-0.104647000
H	-3.377902000	-3.000221000	1.515209000
H	-4.399335000	-2.919465000	0.058195000
C	0.596561000	-0.675114000	1.080385000
C	1.421128000	-0.492902000	0.033008000
C	0.696547000	-0.113899000	2.468794000
H	1.463770000	0.670647000	2.491329000
H	-0.258649000	0.334157000	2.788744000
H	0.958328000	-0.896867000	3.202886000
Pd	3.020311000	0.566796000	-0.143194000
Cl	4.278338000	-1.313231000	-0.697819000
Cl	1.895456000	2.536836000	0.335883000
N	-3.085145000	-1.310621000	0.258479000
H	0.395083000	-3.013928000	-0.408691000
O	-0.070038000	-2.199625000	-0.677930000

**7**: E= -1259.162879

C	0.194071000	-0.930902000	-0.018133000
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C	1.205643000	0.172474000	-0.165495000
C	0.993249000	1.500829000	-0.123837000
C	-0.430919000	2.067991000	-0.032382000
C	-1.457520000	0.980915000	-0.034828000
C	-1.196184000	-0.369679000	-0.015552000
C	-2.465490000	-1.044710000	-0.024914000
C	-3.463001000	-0.023633000	-0.040854000
N	-2.828309000	1.204627000	-0.037638000
C	-2.861820000	-2.395159000	-0.016289000
C	-4.219538000	-2.700249000	-0.027659000
C	-5.192920000	-1.677966000	-0.047201000
C	-4.831697000	-0.332513000	-0.055176000
Pd	3.000335000	-0.419293000	-0.588612000
Cl	3.527132000	-1.468607000	1.357321000
C	2.072486000	2.557897000	-0.134625000
O	-0.560150000	2.932313000	1.101187000
C	-3.489853000	2.493018000	-0.072620000
H	-5.593658000	0.449471000	-0.076679000
H	-6.252246000	-1.946924000	-0.058750000
H	-4.540679000	-3.744740000	-0.022166000
H	-2.114413000	-3.192798000	-0.000477000
H	2.073517000	3.112489000	-1.089669000
H	1.874258000	3.291916000	0.661112000
H	3.076472000	2.132898000	0.020178000
H	-0.580496000	2.748689000	-0.891191000
H	-4.391764000	2.467042000	0.557588000
H	-2.814164000	3.256166000	0.333483000
H	-3.792390000	2.776467000	-1.096312000
H	0.311561000	-1.670867000	-0.830552000
H	0.418122000	-1.484689000	0.911704000
H	-0.510456000	2.377913000	1.894791000

7': E= -1259.138792

O	-0.080077000	1.845301000	-0.642246000
C	0.334728000	1.149286000	0.547082000
C	-0.821853000	0.229069000	0.908193000
C	-1.693631000	0.277166000	-0.113926000
C	-1.289895000	1.293816000	-1.152196000
C	1.653609000	0.455480000	0.330994000
C	1.941387000	-0.890008000	0.236461000
C	3.353101000	-1.012085000	0.014640000
C	3.872846000	0.315343000	-0.022550000
N	2.821121000	1.191555000	0.165481000
C	5.238974000	0.568730000	-0.223051000
C	6.082696000	-0.526253000	-0.391929000
C	5.585630000	-1.847860000	-0.360168000
C	4.232478000	-2.098475000	-0.158135000
C	-0.906851000	-0.466852000	2.229529000
Pd	-3.213431000	-0.878198000	-0.317924000
C	2.926157000	2.637170000	0.155956000
Cl	-4.815631000	0.652251000	0.093532000
H	5.635893000	1.585941000	-0.240458000
H	7.151421000	-0.358898000	-0.548499000
H	6.277845000	-2.682726000	-0.495325000
H	3.854408000	-3.124080000	-0.134209000
H	1.220414000	-1.700704000	0.312626000
H	0.453801000	1.903982000	1.351815000
H	-2.056656000	2.082086000	-1.260809000
H	-1.121042000	0.846097000	-2.149822000
H	1.980155000	3.075372000	-0.187085000
H	3.179102000	3.043109000	1.151464000
H	3.711009000	2.944689000	-0.550331000
H	-1.864414000	-0.994479000	2.347560000
H	-0.085530000	-1.189181000	2.362675000



H -0.816338000 0.267156000 3.049055000

**8:** E= -1182.851201

C 0.069974000 -0.749121000 -0.020089000  
C 1.125259000 0.159574000 -0.119653000  
C 0.954532000 1.567386000 -0.078122000  
C -0.357755000 2.055954000 -0.044449000  
C -1.438452000 1.161660000 -0.010740000  
C -1.239884000 -0.246331000 -0.002039000  
C -2.554132000 -0.853632000 0.051362000  
C -3.488557000 0.220445000 0.069056000  
N -2.797582000 1.427938000 0.046721000  
C -3.018005000 -2.176108000 0.081062000  
C -4.391754000 -2.412691000 0.123803000  
C -5.304011000 -1.340835000 0.133854000  
C -4.869134000 -0.014765000 0.104085000  
Pd 2.813217000 -0.664309000 -0.552513000  
Cl 3.978220000 -0.407007000 1.374808000  
C 2.125624000 2.520868000 -0.086549000  
C -3.404247000 2.738614000 0.030065000  
H -5.589741000 0.805322000 0.104844000  
H -6.376645000 -1.548681000 0.162513000  
H -4.766031000 -3.438756000 0.146948000  
H -2.312841000 -3.011090000 0.069736000  
H 2.634980000 2.528388000 -1.064944000  
H 1.796263000 3.548217000 0.127605000  
H 2.874725000 2.223695000 0.662705000  
H -0.520495000 3.136123000 -0.044196000  
H -4.338291000 2.726317000 0.610066000  
H -2.731912000 3.469533000 0.500856000  
H -3.633284000 3.081978000 -0.994847000  
H 0.251864000 -1.825364000 0.045673000

**10:** E= -1643.533530

C 0.133632000 -0.624189000 -0.250241000  
C -0.910433000 0.271940000 -0.018391000  
C -0.692438000 1.634558000 0.308300000  
C 0.632385000 2.077943000 0.435031000  
C 1.692403000 1.184367000 0.233704000  
C 1.458651000 -0.170826000 -0.118320000  
C 2.758303000 -0.790456000 -0.277597000  
C 3.720664000 0.225749000 -0.010173000  
N 3.061162000 1.405550000 0.313833000  
C 3.189474000 -2.080500000 -0.618801000  
C 4.556965000 -2.342590000 -0.693779000  
C 5.496352000 -1.326733000 -0.434042000  
C 5.095204000 -0.034087000 -0.093360000  
Pd -2.735713000 -0.463737000 -0.088637000  
Cl -3.256708000 0.434214000 -2.103512000  
C -1.834494000 2.603476000 0.498366000  
C 3.691070000 2.675698000 0.585812000  
H 5.837149000 0.744636000 0.093734000  
H 6.563687000 -1.551309000 -0.505030000  
H 4.905187000 -3.342854000 -0.961574000  
H 2.462882000 -2.869714000 -0.828817000  
H -2.482265000 2.306566000 1.340326000  
H -1.463010000 3.619354000 0.698416000  
H -2.470942000 2.626373000 -0.399678000  
H 0.818455000 3.126501000 0.678768000  
H 3.081621000 3.253421000 1.295948000  
H 4.674808000 2.513842000 1.048695000  
H 3.829685000 3.280870000 -0.328382000  
H -0.065096000 -1.655684000 -0.552680000

H	-1.021550000	-1.248083000	2.043504000
C1	-2.283433000	-1.559919000	2.161052000

**11:** E= -1566.318994

C	-6.058123000	1.177169000	-0.219991000
C	-4.675662000	1.009949000	-0.062820000
C	-4.059426000	-0.261439000	-0.247623000
C	-4.847703000	-1.372312000	-0.579177000
C	-6.224577000	-1.208902000	-0.728400000
C	-6.818840000	0.054743000	-0.550975000
N	-3.703396000	1.944924000	0.272588000
C	-2.466584000	1.313743000	0.283216000
C	-2.641678000	-0.060834000	-0.025892000
C	-1.517496000	-0.900940000	-0.067096000
C	-0.267422000	-0.349635000	0.194833000
C	-0.067460000	1.010158000	0.519121000
C	-1.199099000	1.842498000	0.548488000
Pd	1.255997000	-1.650623000	0.152367000
C	2.132015000	-1.166083000	-1.712564000
C	3.292252000	-0.563810000	-1.911084000
C	4.205642000	-0.019663000	-0.851914000
O	4.406913000	1.369006000	-1.119899000
C	5.238547000	2.145521000	-0.365458000
C	5.899936000	1.498130000	0.833491000
C	1.287098000	1.587214000	0.848785000
C	-3.926642000	3.353093000	0.498631000
C1	1.380095000	-1.876990000	2.432587000
C	1.008489000	-1.887128000	-2.003993000
O	5.394221000	3.292136000	-0.680126000
H	-6.534454000	2.151384000	-0.093738000
H	-7.899184000	0.162662000	-0.677228000
H	-6.849543000	-2.066891000	-0.986867000
H	-4.389168000	-2.354745000	-0.718589000
H	1.948300000	1.604531000	-0.032495000
H	1.193364000	2.621849000	1.209049000
H	1.777473000	0.990759000	1.634267000
H	-1.067737000	2.899490000	0.790153000
H	-4.941282000	3.512534000	0.889710000
H	-3.218785000	3.730614000	1.251091000
H	-3.808781000	3.950984000	-0.423306000
H	-1.636614000	-1.961845000	-0.296921000
H	1.074073000	-2.962196000	-2.214053000
H	0.086126000	-1.383962000	-2.311680000
H	3.635888000	-0.452457000	-2.948158000
H	3.775380000	-0.177707000	0.149641000
H	5.170731000	-0.556426000	-0.899567000
H	5.149281000	1.121301000	1.545841000
H	6.528407000	0.644140000	0.536309000
H	6.524128000	2.251024000	1.328310000

**TS2:** E= -1643.530372

C	0.155007000	-0.702335000	0.062996000
C	-0.915040000	0.209153000	0.173525000
C	-0.690843000	1.623554000	0.174314000
C	0.622286000	2.096433000	0.146968000
C	1.688809000	1.185423000	0.081314000
C	1.463073000	-0.223263000	0.035745000
C	2.768200000	-0.853475000	-0.034493000
C	3.717802000	0.203238000	-0.029886000
N	3.046926000	1.423743000	0.052372000
C	3.210693000	-2.180838000	-0.102905000
C	4.581428000	-2.433812000	-0.167614000

C	5.508890000	-1.375925000	-0.167507000
C	5.093251000	-0.044204000	-0.101166000
Pd	-2.771625000	-0.503681000	-0.100068000
Cl	-2.852201000	-0.198330000	-2.346225000
C	-1.847546000	2.587694000	0.202065000
C	3.700285000	2.713349000	0.056267000
H	5.822026000	0.768503000	-0.109258000
H	6.577362000	-1.598520000	-0.223475000
H	4.940561000	-3.464025000	-0.221849000
H	2.494242000	-3.005908000	-0.107521000
H	-2.533800000	2.359675000	1.034107000
H	-1.503337000	3.626555000	0.309856000
H	-2.434047000	2.502838000	-0.727050000
H	0.800469000	3.173592000	0.163496000
H	2.987085000	3.492143000	0.353739000
H	4.529633000	2.719050000	0.780891000
H	4.103612000	2.969467000	-0.938761000
H	-0.041195000	-1.776371000	0.027632000
H	-1.467061000	-0.158755000	1.566435000
Cl	-2.585861000	-0.697852000	2.366845000

**TS3:** E= -1566.301110

C	-6.246531000	-0.489629000	-0.093351000
C	-4.909154000	-0.072982000	-0.097774000
C	-3.839787000	-1.012186000	-0.063266000
C	-4.124364000	-2.384613000	-0.035582000
C	-5.454901000	-2.802433000	-0.039052000
C	-6.501559000	-1.861737000	-0.066692000
N	-4.386040000	1.215721000	-0.132337000
C	-3.003000000	1.134011000	-0.093251000
C	-2.616350000	-0.234518000	-0.061693000
C	-1.254817000	-0.558176000	-0.047231000
C	-0.306829000	0.468970000	-0.035307000
C	-0.683961000	1.840283000	-0.064458000
C	-2.048152000	2.158568000	-0.085257000
C	1.308519000	-0.122003000	-1.326318000
C	1.230487000	0.556196000	-2.464294000
C	0.333688000	2.959207000	0.011750000
C	-5.162030000	2.433752000	-0.130738000
C	1.896995000	-1.271309000	-0.746152000
Pd	1.549862000	0.104091000	0.746359000
Cl	3.087017000	-0.186141000	2.471014000
C	3.341865000	-1.675156000	-0.971577000
O	4.108395000	-0.609528000	-1.484885000
C	5.339537000	-0.230246000	-1.014073000
C	5.913537000	-0.983612000	0.163318000
O	5.885666000	0.684478000	-1.563503000
H	-7.069630000	0.227415000	-0.104655000
H	-7.537323000	-2.210640000	-0.062805000
H	-5.689856000	-3.869035000	-0.015460000
H	-3.314663000	-3.118261000	-0.007790000
H	-0.054061000	3.880350000	-0.449479000
H	0.575353000	3.201628000	1.061734000
H	1.282295000	2.702304000	-0.482043000
H	-2.348737000	3.208994000	-0.082343000
H	-4.600170000	3.236621000	-0.628462000
H	-6.095014000	2.284290000	-0.693201000
H	-5.418935000	2.766561000	0.891019000
H	-0.946974000	-1.606183000	-0.046790000
H	1.251010000	-2.135239000	-0.531752000
H	3.331950000	-2.489797000	-1.724436000
H	3.750764000	-2.092077000	-0.040925000
H	5.269206000	-0.857298000	1.049779000
H	6.012825000	-2.060398000	-0.046373000

H	6.905205000	-0.565950000	0.372645000
H	1.609358000	0.099632000	-3.384160000
H	0.785113000	1.549322000	-2.534800000

**12:** E= -1643.562202

C	0.235706000	-0.592266000	-1.080528000
C	1.265306000	0.394315000	-1.277861000
C	0.962931000	1.809474000	-1.118641000
C	-0.309795000	2.194060000	-0.756934000
C	-1.295784000	1.206739000	-0.508276000
C	-1.032004000	-0.185013000	-0.667416000
C	-2.260872000	-0.884322000	-0.351021000
C	-3.206691000	0.117898000	-0.011975000
N	-2.595579000	1.372678000	-0.112383000
C	-2.640127000	-2.232198000	-0.312536000
C	-3.948625000	-2.552055000	0.053014000
C	-4.875264000	-1.545235000	0.380118000
C	-4.519216000	-0.194714000	0.353240000
Pd	2.108243000	-0.466541000	0.507387000
Cl	1.416835000	1.090594000	2.062740000
C	2.058429000	2.817483000	-1.325503000
C	-3.273311000	2.621054000	0.167606000
H	-5.244362000	0.579704000	0.609845000
H	-5.893391000	-1.823234000	0.662992000
H	-4.259035000	-3.598792000	0.088487000
H	-1.923740000	-3.019095000	-0.559713000
H	2.723398000	2.530343000	-2.154995000
H	1.654925000	3.820341000	-1.527327000
H	2.675371000	2.880120000	-0.413053000
H	-0.540016000	3.254508000	-0.640727000
H	-2.558682000	3.451372000	0.133140000
H	-4.072381000	2.811682000	-0.567967000
H	-3.720560000	2.595234000	1.173740000
H	0.441249000	-1.626258000	-1.363017000
H	2.099857000	0.129205000	-1.935649000
Cl	3.103351000	-2.148495000	-0.728539000

**13:** E= -1566.359080

C	5.448914000	-0.083728000	-0.770724000
C	4.139102000	0.292532000	-0.449201000
C	3.346695000	-0.461441000	0.460999000
C	3.881219000	-1.618493000	1.047747000
C	5.184003000	-1.997385000	0.727938000
C	5.957165000	-1.236498000	-0.170349000
N	3.399453000	1.379223000	-0.905846000
C	2.156096000	1.352482000	-0.303864000
C	2.075068000	0.221095000	0.545885000
C	0.883627000	-0.009959000	1.267765000
C	-0.209904000	0.897077000	1.140163000
C	-0.095852000	2.057695000	0.280116000
C	1.084248000	2.262667000	-0.423787000
C	-1.427641000	0.624856000	1.990359000
C	-1.846595000	1.373141000	3.014787000
C	-1.233493000	3.038099000	0.144539000
C	3.896064000	2.370557000	-1.834079000
C	-2.073522000	-0.630091000	1.456530000
Pd	-0.788475000	-0.920754000	-0.082330000
Cl	-1.889224000	-2.543838000	-1.310546000
C	-3.524510000	-0.538278000	1.021620000
O	-3.712817000	0.594831000	0.182520000
C	-4.433678000	0.604378000	-0.973389000
C	-5.141023000	-0.665102000	-1.385196000
O	-4.456746000	1.626511000	-1.606445000

H	6.057544000	0.498958000	-1.464798000
H	6.976270000	-1.554585000	-0.403825000
H	5.612461000	-2.896380000	1.176951000
H	3.285073000	-2.215881000	1.741909000
H	-1.415729000	3.574753000	1.089342000
H	-1.009151000	3.786158000	-0.629148000
H	-2.176418000	2.536426000	-0.120943000
H	1.167203000	3.137881000	-1.071052000
H	3.075412000	3.021340000	-2.159582000
H	4.679631000	2.998072000	-1.375626000
H	4.317867000	1.883841000	-2.727920000
H	0.864902000	-0.774775000	2.048109000
H	-1.929372000	-1.515763000	2.098457000
H	-4.155717000	-0.403095000	1.923518000
H	-3.816449000	-1.475053000	0.531952000
H	-4.397434000	-1.447163000	-1.612705000
H	-5.805412000	-1.041873000	-0.591989000
H	-5.730557000	-0.447040000	-2.283291000
H	-2.744981000	1.114891000	3.582853000
H	-1.304039000	2.272298000	3.319403000

**14-trans:** E= -1566.356513

C	-5.500585000	-0.835643000	1.081378000
C	-4.351026000	-0.178602000	0.623783000
C	-3.246469000	-0.902281000	0.091878000
C	-3.296506000	-2.301830000	0.033062000
C	-4.437263000	-2.958722000	0.495351000
C	-5.525136000	-2.230149000	1.011622000
N	-4.063506000	1.182677000	0.590462000
C	-2.808919000	1.356683000	0.021784000
C	-2.257736000	0.085684000	-0.292451000
C	-0.983602000	0.013067000	-0.864816000
C	-0.265017000	1.186606000	-1.130335000
C	-0.830579000	2.459715000	-0.829539000
C	-2.104986000	2.535144000	-0.250897000
C	1.098773000	1.065875000	-1.752510000
C	1.272712000	1.220548000	-3.080676000
C	-0.086145000	3.738332000	-1.143967000
C	-4.958413000	2.237246000	1.001238000
C	2.267807000	0.751160000	-0.891077000
Pd	2.345775000	-1.140322000	-0.119088000
Cl	1.740843000	-2.558072000	-1.784713000
C	2.361289000	1.442815000	0.461993000
O	2.861246000	0.402105000	1.368104000
C	3.906997000	0.682349000	2.221911000
C	4.328499000	-0.543509000	2.982267000
O	4.369044000	1.783649000	2.308004000
H	-6.356710000	-0.284854000	1.476208000
H	-2.453709000	-2.867638000	-0.372070000
H	-4.490698000	-4.049157000	0.453411000
H	-6.411629000	-2.764802000	1.362647000
H	-0.541051000	-0.952616000	-1.120616000
H	-2.536771000	3.513833000	-0.030104000
H	2.257932000	1.111725000	-3.543847000
H	0.428785000	1.438505000	-3.740072000
H	0.057036000	3.869014000	-2.228787000
H	-0.630883000	4.616582000	-0.767636000
H	0.922245000	3.755216000	-0.698126000
H	-4.380195000	3.113167000	1.328687000
H	-5.640525000	2.552274000	0.190453000
H	-5.566046000	1.903197000	1.855032000
H	3.214287000	0.793759000	-1.450480000
H	3.058287000	2.293155000	0.488690000
H	1.379890000	1.748432000	0.848024000

H	3.460107000	-1.000567000	3.480029000
H	4.738974000	-1.290373000	2.284124000
H	5.090738000	-0.268498000	3.720487000

**14-cis:** E= -1566.355242

C	-6.345256000	0.621795000	-0.514741000
C	-5.053682000	0.240424000	-0.129131000
C	-3.983564000	1.179915000	-0.090546000
C	-4.226607000	2.517869000	-0.429887000
C	-5.514125000	2.902353000	-0.805695000
C	-6.559052000	1.960876000	-0.847754000
N	-4.579743000	-1.007512000	0.259542000
C	-3.220599000	-0.903457000	0.522790000
C	-2.808118000	0.440384000	0.325918000
C	-1.468216000	0.773440000	0.545019000
C	-0.547274000	-0.197215000	0.962358000
C	-0.968446000	-1.548127000	1.145479000
C	-2.307770000	-1.887434000	0.917566000
C	0.863260000	0.245763000	1.215078000
C	1.405749000	0.179430000	2.451450000
C	0.003634000	-2.640399000	1.527507000
C	-5.355753000	-2.223833000	0.295804000
C	1.611217000	0.818557000	0.060388000
Pd	2.822686000	-0.608853000	-0.744351000
Cl	1.444225000	-1.963955000	-1.921851000
C	2.733500000	1.813245000	0.332675000
O	3.939873000	0.976918000	0.335644000
C	5.164778000	1.603316000	0.341266000
C	6.290675000	0.614379000	0.220266000
O	5.248479000	2.794354000	0.437506000
H	-7.164294000	-0.098578000	-0.561745000
H	-7.559220000	2.281056000	-1.151035000
H	-5.714628000	3.942302000	-1.074132000
H	-3.416592000	3.251391000	-0.402924000
H	0.443160000	-2.485028000	2.524797000
H	-0.497280000	-3.619405000	1.533795000
H	0.830979000	-2.690956000	0.802267000
H	-2.620501000	-2.927033000	1.035323000
H	-4.936798000	-2.912568000	1.043093000
H	-6.390923000	-2.000774000	0.593171000
H	-5.376186000	-2.739329000	-0.681535000
H	-1.137897000	1.806722000	0.405532000
H	0.952153000	1.124827000	-0.760653000
H	2.839083000	2.557664000	-0.467848000
H	2.661138000	2.335012000	1.298154000
H	6.178043000	-0.191223000	0.960953000
H	6.269298000	0.149985000	-0.778671000
H	7.245679000	1.133624000	0.362150000
H	2.433501000	0.491992000	2.655192000
H	0.831188000	-0.200498000	3.298853000

**TS4-trans:** E= -1566.325247

C	-5.403449000	-1.397676000	-0.102152000
C	-4.296186000	-0.542673000	-0.029440000
C	-3.081310000	-0.842648000	-0.708115000
C	-2.979379000	-2.023885000	-1.456032000
C	-4.077559000	-2.881412000	-1.523410000
C	-5.274852000	-2.567530000	-0.853418000
N	-4.154085000	0.661697000	0.652030000
C	-2.882149000	1.161035000	0.409107000
C	-2.175062000	0.252751000	-0.424684000
C	-0.856755000	0.546246000	-0.787786000
C	-0.246075000	1.724206000	-0.339758000

C	-0.963834000	2.633874000	0.489542000
C	-2.284280000	2.344607000	0.857419000
C	1.170571000	2.007434000	-0.749834000
C	1.455898000	2.796025000	-1.803295000
C	-0.325551000	3.919580000	0.964379000
C	-5.189661000	1.312195000	1.418631000
C	2.279717000	1.405423000	0.035675000
Pd	2.613658000	-0.639561000	-0.443436000
Cl	3.503626000	-0.324907000	-2.509944000
C	2.090572000	0.961690000	1.376532000
O	1.805075000	-1.076878000	1.421860000
C	2.556334000	-1.601928000	2.403093000
C	1.978037000	-2.913878000	2.899838000
O	3.552840000	-1.087661000	2.858451000
H	-6.341882000	-1.163683000	0.404442000
H	-2.052159000	-2.268195000	-1.980542000
H	-4.011460000	-3.804200000	-2.104479000
H	-6.125166000	-3.250647000	-0.924637000
H	-0.293250000	-0.138467000	-1.427125000
H	-2.832951000	3.051091000	1.484087000
H	2.487023000	2.972410000	-2.121791000
H	0.659777000	3.260829000	-2.389961000
H	-0.111808000	4.600808000	0.124898000
H	-0.979817000	4.450051000	1.671495000
H	0.639013000	3.741758000	1.468622000
H	-4.738434000	1.969292000	2.175059000
H	-5.863671000	1.918091000	0.786249000
H	-5.793775000	0.561423000	1.949568000
H	3.283988000	1.770638000	-0.212365000
H	2.943743000	0.889356000	2.053599000
H	1.094882000	1.016966000	1.818476000
H	0.922703000	-2.780121000	3.180517000
H	2.006301000	-3.659030000	2.089573000
H	2.562112000	-3.271348000	3.756953000

**TS4-cis:** E= -1566.322874

C	-6.442186000	0.835601000	-0.541513000
C	-5.179367000	0.339263000	-0.193199000
C	-4.076764000	1.212123000	0.033487000
C	-4.257121000	2.597492000	-0.079811000
C	-5.515685000	3.094754000	-0.418915000
C	-6.593573000	2.219523000	-0.647770000
N	-4.764791000	-0.976054000	-0.011245000
C	-3.413169000	-0.975644000	0.301069000
C	-2.944299000	0.363674000	0.349047000
C	-1.601181000	0.596050000	0.657693000
C	-0.732155000	-0.471368000	0.926122000
C	-1.207681000	-1.815397000	0.856378000
C	-2.551096000	-2.051752000	0.539557000
C	0.686477000	-0.142364000	1.275969000
C	1.231024000	-0.474880000	2.463337000
C	-0.288027000	-2.997632000	1.061045000
C	-5.583420000	-2.150443000	-0.196960000
C	1.447654000	0.643037000	0.258291000
Pd	3.070819000	-0.429617000	-0.578806000
Cl	1.847717000	-1.791218000	-1.924460000
C	2.412238000	1.623799000	0.622625000
O	4.288399000	0.732728000	0.648278000
C	5.179201000	1.593760000	0.130633000
C	6.572322000	1.346029000	0.679340000
O	4.909501000	2.474488000	-0.653901000
H	-7.286252000	0.169624000	-0.731478000
H	-7.570185000	2.629028000	-0.918439000
H	-5.667633000	4.172674000	-0.511950000

H	-3.421366000	3.280510000	0.093177000
H	0.079342000	-3.071265000	2.096597000
H	-0.810170000	-3.937273000	0.828722000
H	0.591254000	-2.927461000	0.401671000
H	-2.906644000	-3.081501000	0.464905000
H	-5.250330000	-2.950830000	0.479592000
H	-6.629411000	-1.920120000	0.050758000
H	-5.544700000	-2.530794000	-1.233790000
H	-1.226516000	1.622469000	0.705793000
H	0.913507000	0.831455000	-0.680983000
H	2.716224000	2.388939000	-0.094677000
H	2.603668000	1.829846000	1.676290000
H	6.553933000	1.362767000	1.779419000
H	6.916927000	0.345247000	0.375781000
H	7.259331000	2.110708000	0.296187000
H	2.275936000	-0.257417000	2.702767000
H	0.645393000	-0.992593000	3.225727000

**15-trans:** E= -1566.383632

C	-2.273941000	-2.553950000	-0.362672000
C	-2.984391000	-1.354963000	-0.228619000
C	-2.398210000	-0.222535000	0.395902000
C	-1.083604000	-0.305990000	0.865823000
C	-0.355630000	-1.492881000	0.719344000
C	-0.957199000	-2.632799000	0.105600000
C	-3.401932000	0.823342000	0.383746000
C	-4.551003000	0.269105000	-0.248895000
N	-4.276112000	-1.041381000	-0.626335000
C	-3.435489000	2.147974000	0.840876000
C	-4.599406000	2.897622000	0.669093000
C	-5.729536000	2.333854000	0.048120000
C	-5.723856000	1.016893000	-0.415497000
C	-5.205985000	-1.945621000	-1.259532000
C	1.039074000	-1.567020000	1.264320000
C	2.199187000	-1.654189000	0.350824000
C	2.162728000	-1.500511000	-1.033881000
Pd	2.906650000	0.375292000	-0.282491000
O	3.180535000	2.491197000	-0.160412000
C	1.923323000	2.649318000	-0.219509000
C	1.314077000	4.019086000	-0.225440000
C	-0.209219000	-3.940841000	-0.013204000
C	1.271413000	-1.575005000	2.594299000
Cl	5.047111000	-0.452762000	-0.296066000
O	1.192656000	1.604594000	-0.291452000
H	-6.612048000	0.591729000	-0.887108000
H	-2.560570000	2.585618000	1.328310000
H	-4.638384000	3.930786000	1.022327000
H	-6.633587000	2.936426000	-0.071570000
H	-0.605028000	0.559941000	1.324518000
H	-2.736712000	-3.435783000	-0.811158000
H	2.290060000	-1.612328000	2.992501000
H	0.449001000	-1.533359000	3.312516000
H	0.231820000	-4.244424000	0.949768000
H	-0.875425000	-4.748248000	-0.350019000
H	0.622309000	-3.878146000	-0.735173000
H	-4.660932000	-2.664912000	-1.887613000
H	-5.810873000	-2.509650000	-0.526449000
H	-5.888064000	-1.384418000	-1.914411000
H	3.122448000	-2.041943000	0.791036000
H	2.991151000	-1.871555000	-1.640725000
H	1.216924000	-1.285347000	-1.540395000
H	1.557281000	4.512897000	-1.179765000
H	0.223814000	3.959640000	-0.113909000
H	1.754909000	4.624597000	0.580105000



**15-cis:** E= -1566.382137

C	6.818864000	0.310599000	0.119949000
C	5.420308000	0.346596000	0.192843000
C	4.631745000	-0.800389000	-0.108103000
C	5.263743000	-1.997177000	-0.473080000
C	6.656629000	-2.038252000	-0.538804000
C	7.422159000	-0.894224000	-0.245803000
N	4.581015000	1.400432000	0.537625000
C	3.265483000	0.969034000	0.440934000
C	3.248765000	-0.396846000	0.052990000
C	2.018030000	-1.043876000	-0.097150000
C	0.817976000	-0.354250000	0.125095000
C	0.844287000	1.018253000	0.516765000
C	2.074537000	1.668108000	0.670198000
C	-0.465569000	-1.107098000	-0.060865000
C	-0.749018000	-2.188441000	0.695382000
C	-0.428680000	1.779471000	0.806809000
C	5.013235000	2.739139000	0.861919000
C	-1.336193000	-0.664798000	-1.176582000
Pd	-3.366177000	-0.010100000	-0.479627000
Cl	-3.305398000	1.645041000	-2.069492000
C	-2.375968000	-1.381858000	-1.773973000
O	-3.786947000	-1.266719000	1.153988000
C	-4.658888000	-0.441420000	1.595600000
C	-5.453132000	-0.755408000	2.827641000
O	-4.845302000	0.628583000	0.943494000
H	7.425731000	1.192278000	0.335252000
H	8.512124000	-0.946394000	-0.308979000
H	7.160312000	-2.964994000	-0.823589000
H	4.672628000	-2.886707000	-0.705677000
H	-1.110986000	1.195221000	1.445046000
H	-0.211173000	2.724705000	1.325022000
H	-0.989800000	2.031850000	-0.108461000
H	2.087802000	2.716307000	0.976632000
H	4.264552000	3.230019000	1.499134000
H	5.957205000	2.703572000	1.425676000
H	5.167428000	3.360853000	-0.038577000
H	1.981923000	-2.091644000	-0.405356000
H	-0.980057000	0.212094000	-1.723579000
H	-2.706116000	-1.100366000	-2.776473000
H	-2.645926000	-2.384991000	-1.431482000
H	-6.361682000	-1.305317000	2.531858000
H	-4.870781000	-1.392564000	3.506941000
H	-5.761006000	0.172944000	3.327213000
H	-1.659279000	-2.775800000	0.559562000
H	-0.075994000	-2.493079000	1.500241000

