

# Supporting Information

## S1: Synthetic details

## S2: UV-Vis spectral studies

## S3: Kinetic and thermodynamic studies

## S4: X-Ray diffraction studies

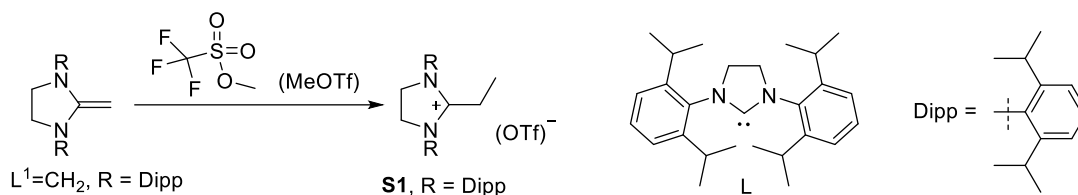
## S5: Theoretical details

## S6: References

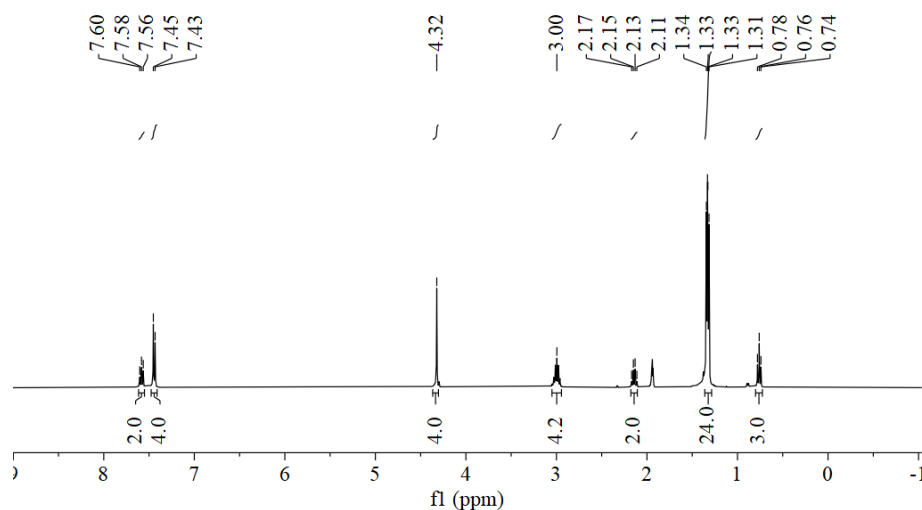
### S1: Synthetic details

**General:** All manipulations were performed under an inert atmosphere of dry nitrogen, using standard Schlenk techniques. Dry, oxygen-free solvents were employed unless otherwise mentioned. The compounds  $L=CH_2$  ( $L = 1,3$ -Bis(2,6-diisopropylphenyl)imidazolidin-2-ylidene),  $[(LCH_2)TMS](OTf)$  (**S4**), was prepared following reported procedure,<sup>[1]</sup> while all other starting materials were purchased from commercial sources. NMR spectra were recorded on Bruker Avance 400 MHz spectrometers ( $^1H$ , 400.1 MHz;  $^{13}C$ , 100.5 MHz;  $^{31}P$ , 161.9 MHz) or Bruker Avance 600 MHz spectrometers ( $^1H$ , 600.2 MHz;  $^{13}C$ , 150.8 MHz;  $^{31}P$ , 242.9 MHz). The chemical shifts ( $\delta$ ) were measured according to IUPAC and expressed in ppm relative to  $SiMe_4$  ( $^1H$ ,  $^{13}C$ ), and 85%  $H_3PO_4$  ( $^{31}P$ ). Coupling constants  $J$  are reported in Hertz [Hz] as absolute values. The high purity of these isolated compounds has been proved mainly by NMR. ESI-MS spectra were measured on Bruker ESI-Q-TOF maxis 4G. UV/vis spectra were measured on Shimadzu UV/vis/NIR UV-3600-spectrometer. Melting point (M. P.) were measured on Jiahang JH30 apparatus.

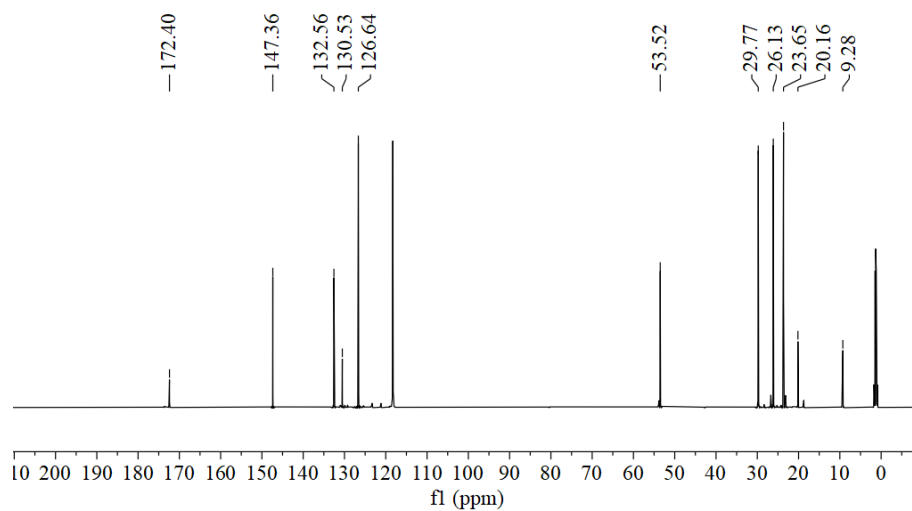
### Synthesis of $[\text{LCH}_2(\text{CH}_3)](\text{OTf})$ (**S1**):



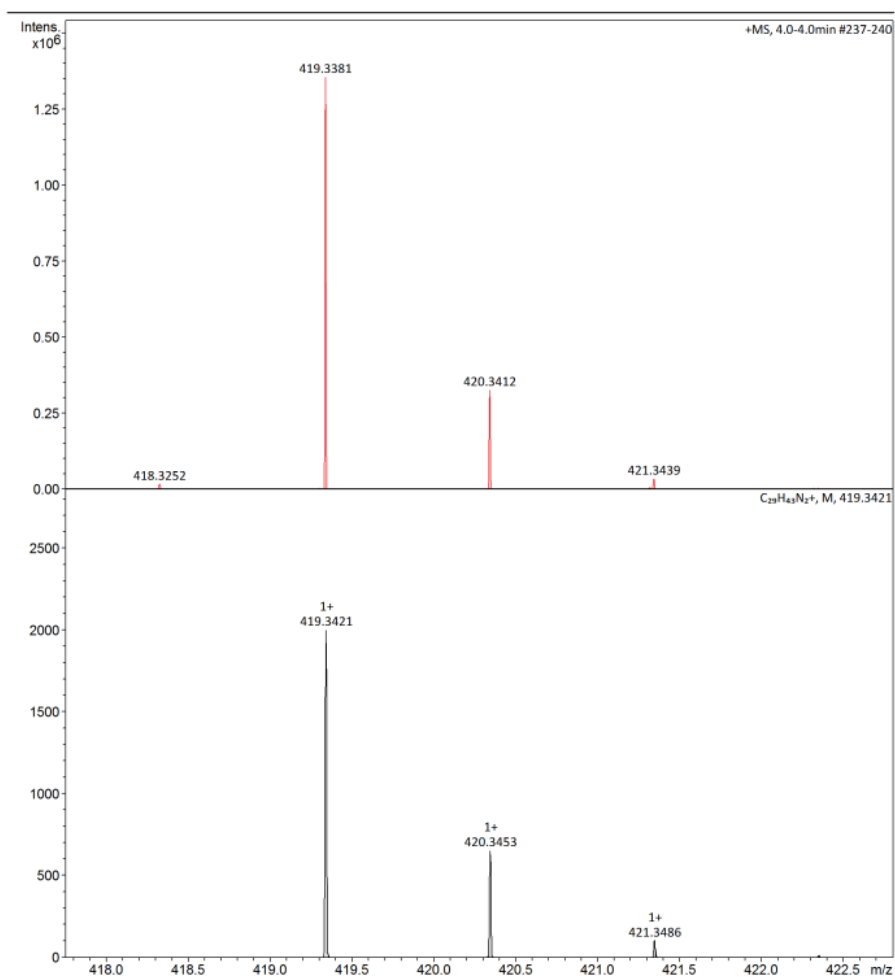
Methyl trifluoromethanesulfonate (MeOTf) (1.81 mg, 11 mmol) in toluene (10 mL) was added dropwise to a stirred solution of  $\text{L}=\text{CH}_2$  (4.04 g, 10 mmol) in toluene (60 mL) at room temperature. After stirring for 1.0 hour, the resulting precipitates were collected via filtration, washed with hexane ( $3 \times 4.0$  mL) and then dried *in vacuo* affording  $[\text{LCH}_2(\text{CH}_3)](\text{OTf})$  (**S1**) as a white solid (5.45 g, 96 %). M. P.  $> 250$  °C.  $^1\text{H}$  NMR (400.1 MHz,  $\text{CD}_3\text{CN}$ ):  $\delta = 7.58$  (t,  $J = 7.8$  Hz, 2 H,  $\text{C}_{\text{ar}}\text{H}$ ), 7.44 (d,  $J = 7.8$  Hz, 4 H,  $\text{C}_{\text{ar}}\text{H}$ ), 4.32 (s, 4 H, NCH), 3.00 (m, 4 H,  $\text{CH}(\text{CH}_3)_2$ ), 2.14 (m,  $J = 7.64$  Hz, 2 H,  $\text{CH}_2\text{CH}_3$ ), 1.33 (d,  $J = 4.76$  Hz, 12 H,  $\text{CH}(\text{CH}_3)_2$ ), 1.32 (d,  $J = 4.8$  Hz, 12 H,  $\text{CH}(\text{CH}_3)_2$ ), 0.76 (t,  $J = 7.64$  Hz, 3 H,  $\text{CH}_2\text{CH}_3$ ).  $^{13}\text{C}\{^1\text{H}\}$  NMR (150.8 MHz,  $\text{CD}_3\text{CN}$ ):  $\delta = 172.40$  (NCN), 147.36 ( $\text{C}_{\text{Ar}}$ ), 132.56 ( $\text{C}_{\text{Ar}}$ ), 130.63 ( $\text{C}_{\text{Ar}}$ ), 126.64 ( $\text{CF}_3$ ), 53.52 (NCH), 29.77, 26.13, 23.65, 20.16, 9.28. HRMS (ESI,  $m/z$ ): calc. for:  $\text{C}_{29}\text{H}_{43}\text{N}_2^+$ : 419.3421 ( $\text{M}^+$ ), found: 419.3381.



**Figure S1.**  $^1\text{H}$  NMR of **S1** in  $\text{CD}_3\text{CN}$ .

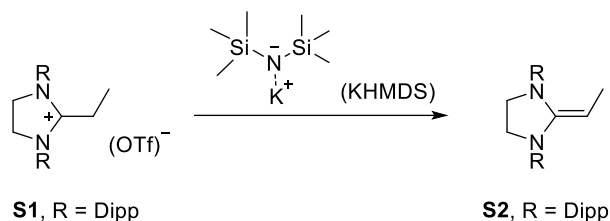


**Figure S2.**  $^{13}\text{C}\{^1\text{H}\}$  NMR of **S1** in  $\text{CD}_3\text{CN}$ .

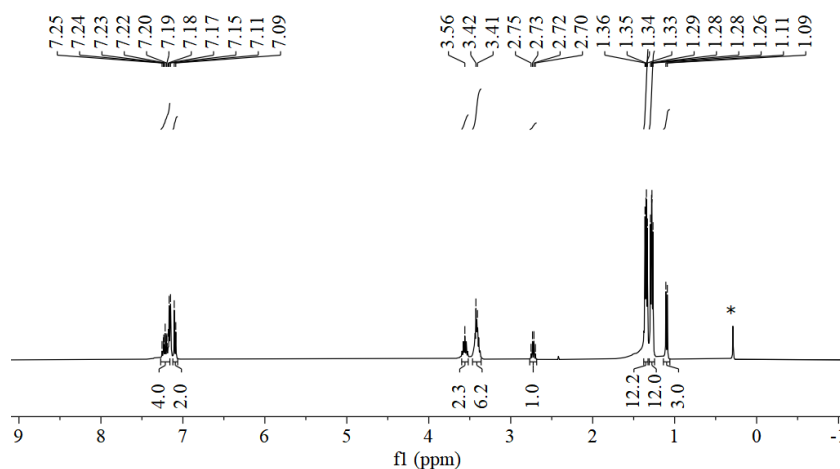


**Figure S3.** HRMS of **S1**.

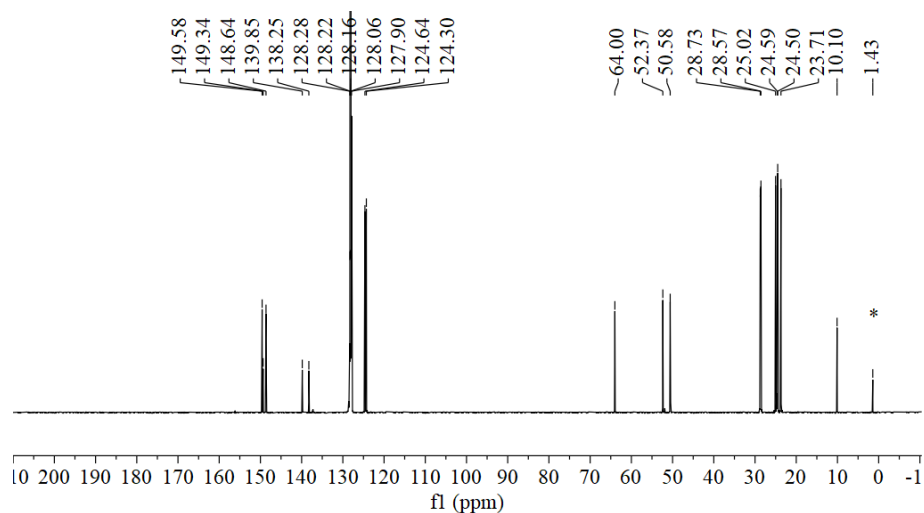
### Synthesis of $L=CH(CH_3)$ (**S2**):



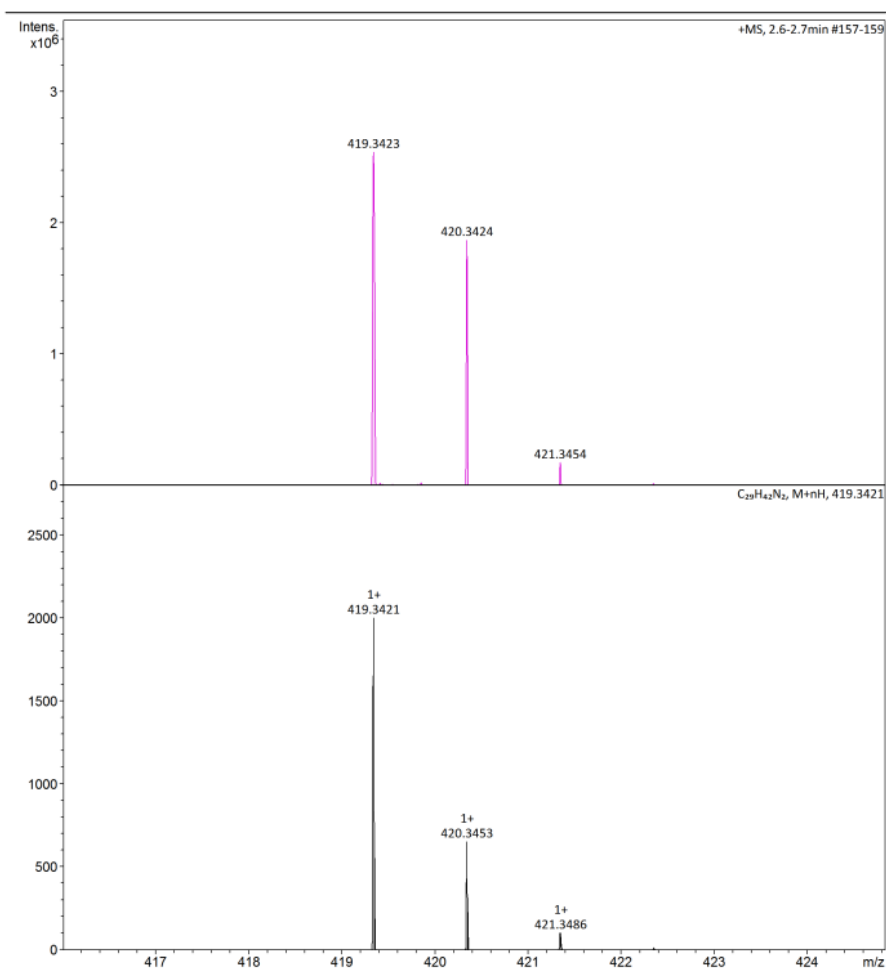
Potassium bis(trimethylsilyl)amide (KHMDS) (20 mL, 0.5 M in toluene) was added dropwise to a solution of **S1** (5.68 g, 10 mmol) in toluene (30 mL) at  $-80\text{ }^\circ\text{C}$ . The mixture was allowed to slowly warm to room temperature and stirred for another 24 h. Then, the volatiles were removed under reduced pressure, and the residue was dissolved in hexane (30 mL). After filtered through a plug of Celite, followed by solvent removing under reduced pressure, the remaining solid was washed with acetonitrile and dried in *vacuo* to afford  $L=CH(CH_3)$  (**S2**) (2.61 g, 62 %) as a white solid. M. P. =  $109.9\text{ }^\circ\text{C}$ .  $^1\text{H}$  NMR (400.1 MHz,  $\text{C}_6\text{D}_6$ ):  $\delta$  = 7.21 (m, 4 H,  $C_{Ar}H$ ), 7.10 (d,  $J$  = 7.7 Hz, 2 H,  $C_{Ar}H$ ), 3.56 (m, 4 H,  $CH(CH_3)_2$ ), 3.42 (s, 4 H, NCH), 3.42 (m, 4 H,  $CH(CH_3)_2$ ), 2.73 (q,  $J$  = 7.1 Hz, 1 H,  $CH-CH_3$ ), 1.34 (dd,  $J$  = 4.8 Hz, 12 H,  $CH(CH_3)_2$ ), 1.28 (dd,  $J$  = 5.2 Hz, 12 H,  $CH(CH_3)_2$ ), 1.10 (d,  $J$  = 7.1 Hz, 3 H,  $CH-CH_3$ ).  $^{13}\text{C}\{^1\text{H}\}$  NMR (150.8 MHz,  $\text{C}_6\text{D}_6$ ):  $\delta$  = 149.58 ( $C_{Ar}$ ), 149.34 (NCN), 148.64 ( $C_{Ar}$ ), 139.85 ( $C_{Ar}$ ), 138.25 ( $C_{Ar}$ ), 128.28 ( $C_{Ar}$ ), 128.16 ( $C_{Ar}$ ), 124.64 ( $C_{Ar}$ ), 124.30 ( $C_{Ar}$ ), 64.00 (NCH), 52.37, 50.58, 28.73, 28.57, 25.02, 24.59, 24.50, 23.71, 10.10. HRMS (ESI,  $m/z$ ): calc. for:  $\text{C}_{29}\text{H}_{43}\text{N}_2$ : 419.3421 [(M + H) $^+$ ]; found: 419.3423.



**Figure S4.**  $^1\text{H}$  NMR of **S2** in  $\text{C}_6\text{D}_6$ . \* silicone grease.

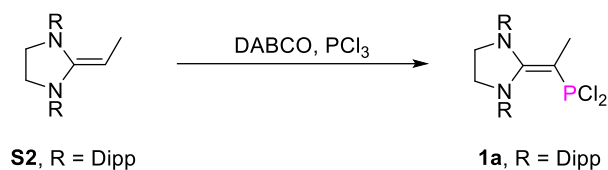


**Figure S5.**  $^{13}\text{C}\{^1\text{H}\}$  NMR of **S2** in  $\text{C}_6\text{D}_6$ . \* silicone grease.

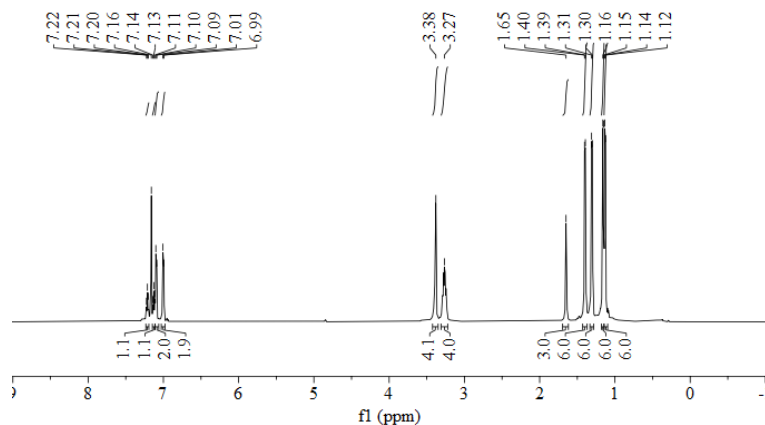


**Figure S6.** HRMS of **S2**.

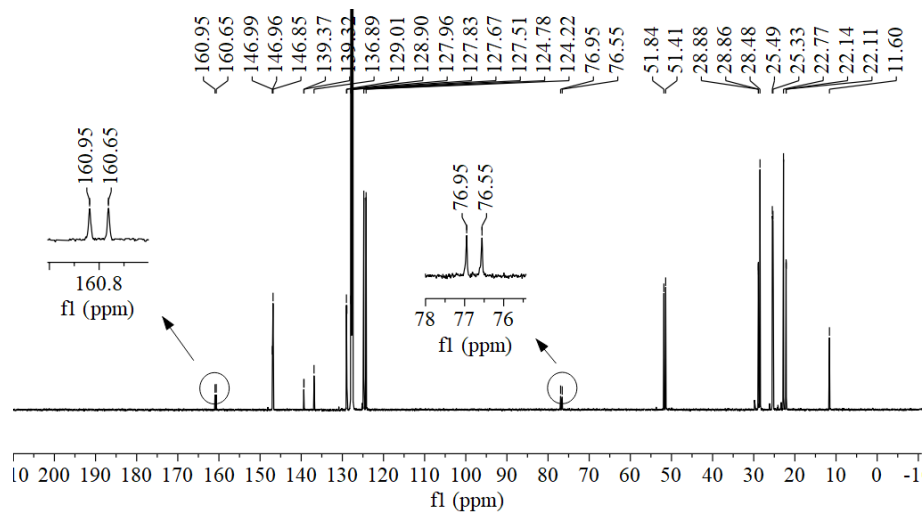
### Synthesis of $[L=C(CH_3)]PCl_2$ (**1a**):



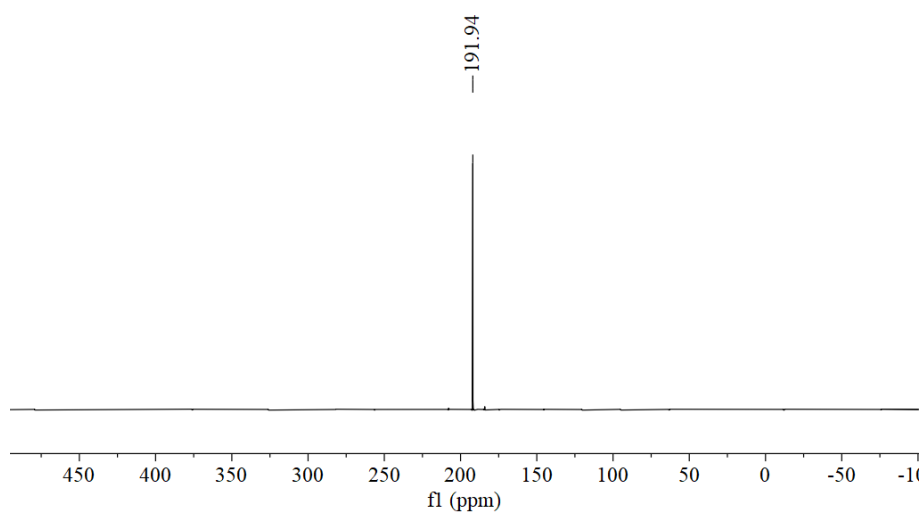
$PCl_3$  (1.6 g, 12 mmol) in toluene (3 mL) was added to a mixture of **S2** (4.18 g, 10.0 mmol) and DABCO (1.2 g, 11 mmol) in toluene (30 mL) at room temperature. After stirring for 2 hours, the resulting suspension was filtered and the filtrate was dried under reduced pressure. The remaining solid was washed with hexane and dried *in vacuo* to afford  $[L=C(CH_3)]PCl_2$  (**1a**) (4.21 g, 81 %) as a white solid. M. P. = 150.1 °C (Decomposition).  $^1H$  NMR (400.1 MHz,  $C_6D_6$ ):  $\delta$  = 7.21 (t,  $J$  = 5.1 Hz, 1 H,  $C_{Ar}H$ ), 7.14 (t,  $J$  = 5.1 Hz, 1 H,  $C_{Ar}H$ ), 7.09 (d,  $J$  = 5.1 Hz, 2 H,  $C_{Ar}H$ ), 7.00 (d,  $J$  = 5.1 Hz, 2 H,  $C_{Ar}H$ ), 3.38 (s, 4 H,  $NCH_2$ ), 3.27 (m, 4 H,  $CH(CH_3)_2$ ), 1.65 (s, 3 H,  $CH-PCl_2$ ), 1.40 (d,  $J$  = 4.6 Hz, 6 H,  $CH(CH_3)_2$ ), 1.30 (d,  $J$  = 4.6 Hz, 6 H,  $CH(CH_3)_2$ ), 1.15 (d,  $J$  = 4.6 Hz, 6 H,  $CH(CH_3)_2$ ), 1.13 (d,  $J$  = 4.6 Hz, 6 H,  $CH(CH_3)_2$ ).  $^{13}C\{^1H\}$  NMR (150.8 MHz,  $C_6D_6$ ):  $\delta$  = 160.80 (d,  $^2J_{PC}$  = 38 Hz, NCN), 146.99 ( $C_{Ar}$ ), 146.96 ( $C_{Ar}$ ), 146.85 ( $C_{Ar}$ ), 139.37 ( $C_{Ar}$ ), 139.32 ( $C_{Ar}$ ), 136.89 ( $C_{Ar}$ ), 129.01 ( $C_{Ar}$ ), 128.90 ( $C_{Ar}$ ), 127.96 ( $C_{Ar}$ ), 124.96 ( $C_{Ar}$ ), 124.78 ( $C_{Ar}$ ), 124.22 ( $C_{Ar}$ ), 76.75 (d,  $^1J_{PC}$  = 48.5 Hz, C- $PCl_2$ ), 51.84 ( $NCH_2$ ), 51.41 ( $NCH_2$ ), 28.88, 28.86, 28.48, 25.49, 25.33, 22.77, 22.14, 22.11, 11.60.  $^{31}P\{^1H\}$  NMR (242.9 MHz,  $C_6D_6$ ):  $\delta$  = 191.94. HRMS (ESI, m/z) calc. for:  $C_{29}H_{43}N_2$ : 419.3421 [(M + H) $^+$ ]; found: 419.3825.



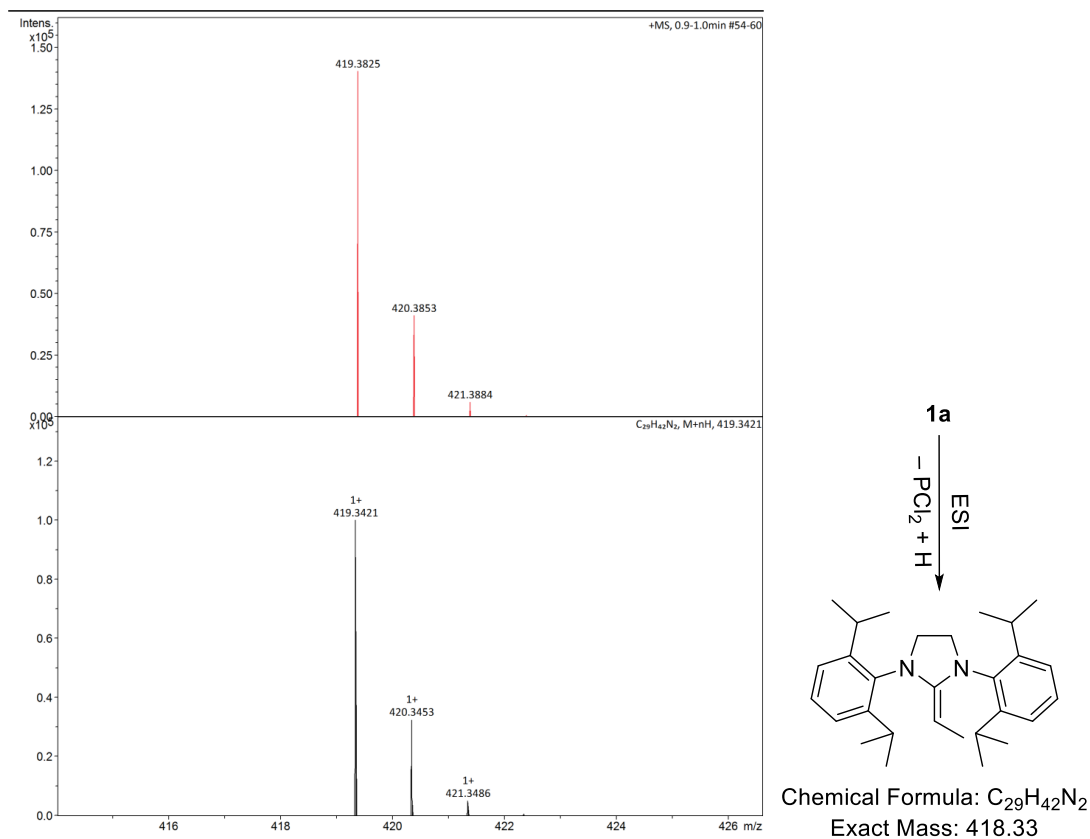
**Figure S7.**  $^1H$  NMR of **1a** in  $C_6D_6$ .



**Figure S8.**  $^{13}\text{C}\{^1\text{H}\}$  NMR of **1a** in  $\text{C}_6\text{D}_6$ .

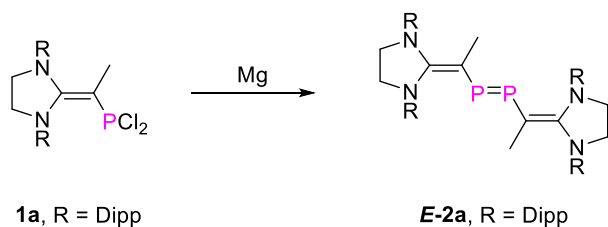


**Figure S9.**  $^{31}\text{P}\{^1\text{H}\}$  NMR of **1a** in  $\text{C}_6\text{D}_6$ .



**Figure S10:** HRMS of **1a**.

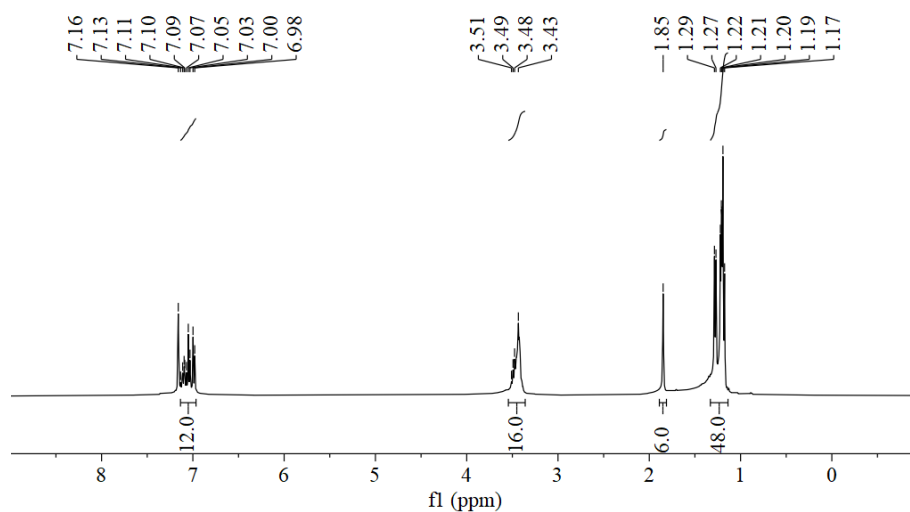
### Synthesis of *E*-2a:



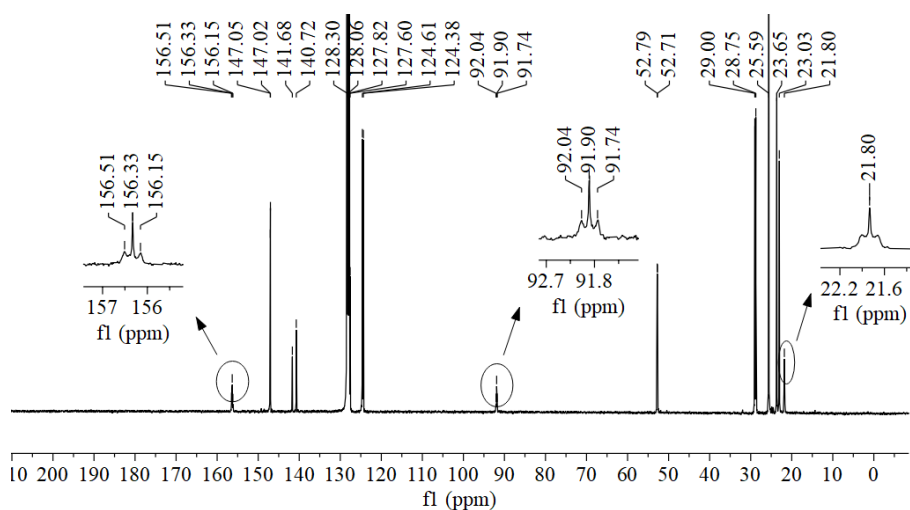
Mg powder (2.4 g, 100 mmol) was added to a solution of **1a** (5.2 g, 10 mmol) in 40 mL THF at room temperature. The resulting suspension was stirred overnight, and the solvent was removed under reduced pressure. The residue was extracted with toluene and washed with a minimum amount of *n*-pentane to afford *E*-**2a** (3.5 g, 78 %) as a red powder. Red crystals of *E*-**2a** were obtained from a saturated *n*-pentane solution stored at -30 °C for 4 days. M.P. = 250.3 °C. <sup>1</sup>H NMR (400.1 MHz, C<sub>6</sub>D<sub>6</sub>): δ = 7.13 ~ 6.98 (m, 12 H, C<sub>Ar</sub>H), 3.51 ~ 3.38 (m, 12 H, NCH<sub>2</sub> & CH(CH<sub>3</sub>)<sub>2</sub>), 1.85 (s, 6 H, PC(CH<sub>3</sub>)<sub>3</sub>), 1.29 ~ 1.17 (m, 48 H, CH(CH<sub>3</sub>)<sub>2</sub>). <sup>13</sup>C{<sup>1</sup>H} NMR (100.5 MHz, C<sub>6</sub>D<sub>6</sub>): δ = 156.33 (t, <sup>2</sup>J<sub>PC</sub> = 18.0 Hz, NCN), 147.05 (C<sub>Ar</sub>), 147.02 (C<sub>Ar</sub>), 141.68 (C<sub>Ar</sub>), 140.72 (C<sub>Ar</sub>), 127.60



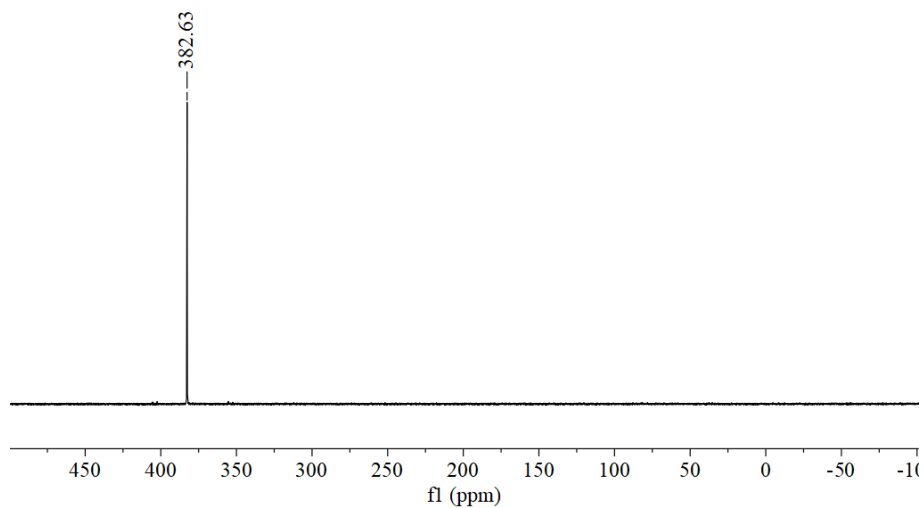
( $C_{Ar}$ ), 124.61 ( $C_{Ar}$ ), 124.38 ( $C_{Ar}$ ), 91.90 (t,  $^1J_{PC} = 16.53$  Hz, CP), 52.79, 52.71 (NCH<sub>2</sub>), 29.00, 28.75, 25.59, 23.65, 21.80 (t,  $^2J_{PC} = 11.0$  Hz, CH<sub>3</sub>CP).  $^{31}P\{^1H\}$  NMR (161.9 MHz, C<sub>6</sub>D<sub>6</sub>):  $\delta = 382.63$ . UV/Vis (Tol,  $\lambda$  (nm)  $\epsilon$  (M<sup>-1</sup>cm<sup>-1</sup>)): 518 (17539.8); 416 (2483.4). HRMS (ESI, m/z) calc. for: C<sub>58</sub>H<sub>83</sub>N<sub>4</sub>P<sub>2</sub>: 897.6087 [(M + H)<sup>+</sup>]; found: 897.6063.



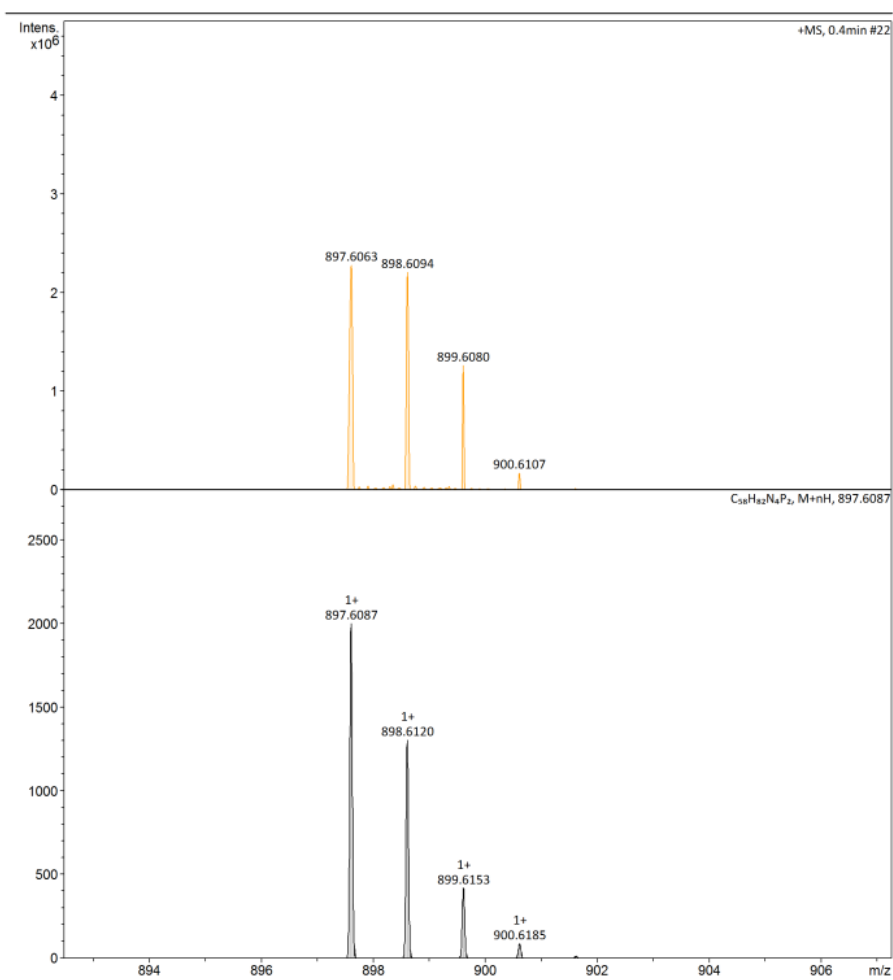
**Figure S11.**  $^1H$  NMR of *E-2a* in C<sub>6</sub>D<sub>6</sub>.



**Figure S12.**  $^{13}C\{^1H\}$  NMR of *E-2a* in C<sub>6</sub>D<sub>6</sub>.

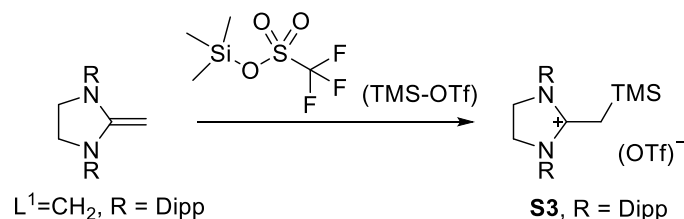


**Figure S13.**  $^{31}\text{P}\{^1\text{H}\}$  NMR of *E-2a* in  $\text{C}_6\text{D}_6$ .

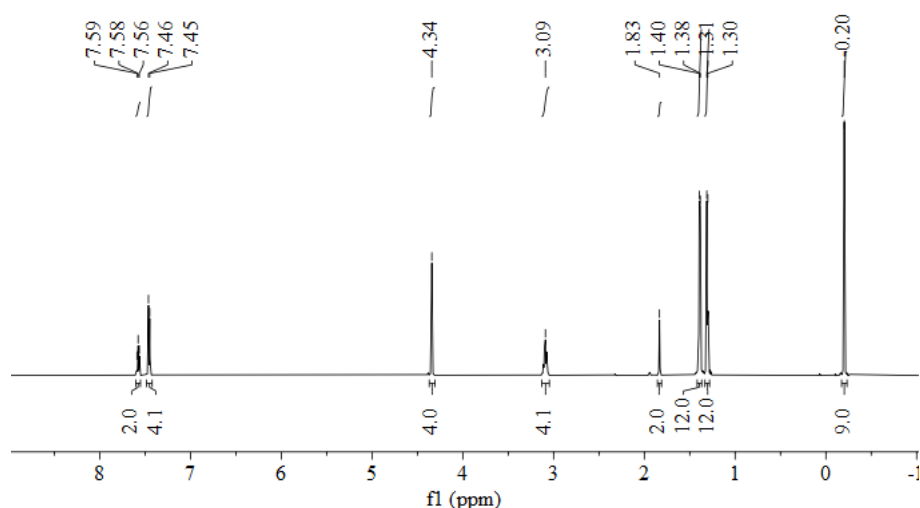


**Figure S14.** HRMS of *E-2a*.

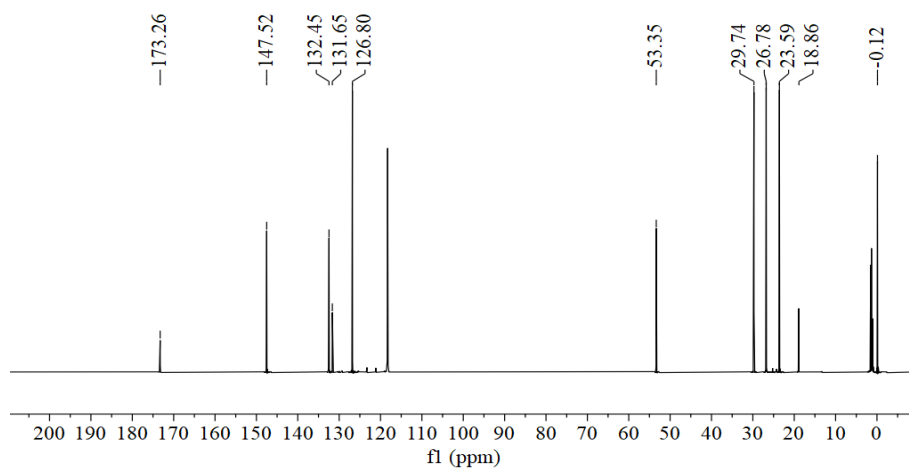
### Synthesis of [(LCH<sub>2</sub>)TMS](OTf) (S3):



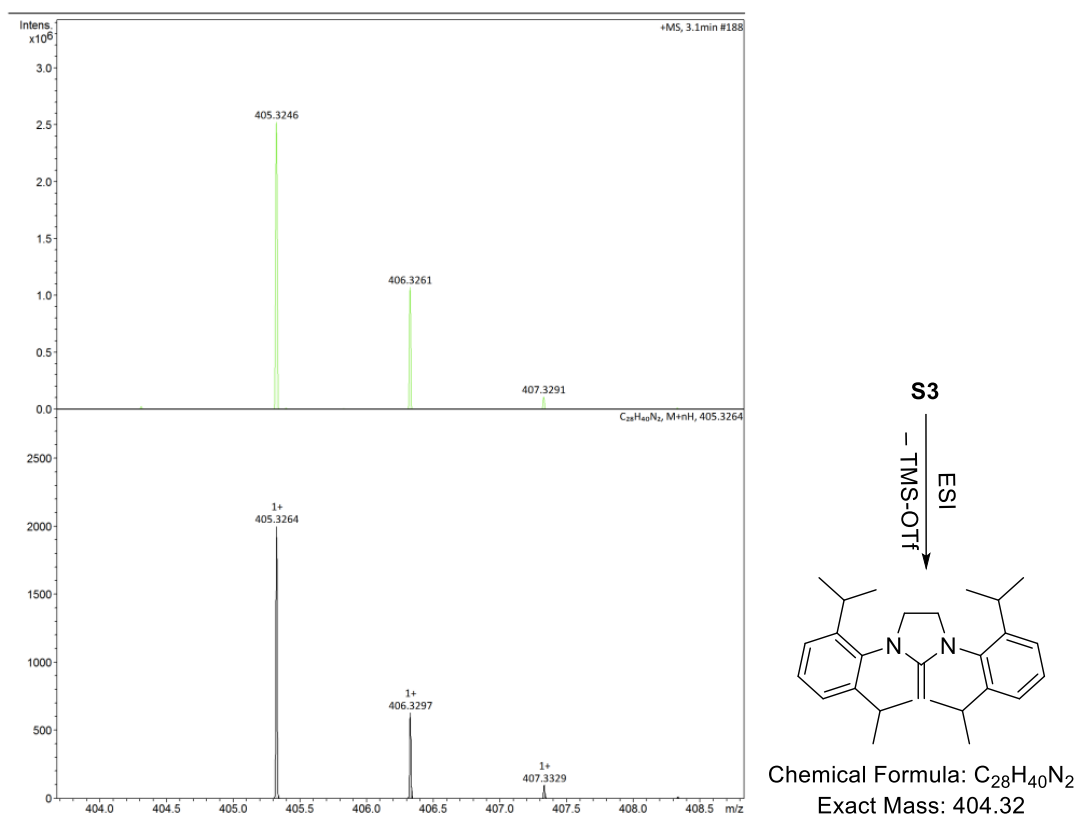
Trimethylsilyl trifluoromethanesulfonate [(TMS)(OTf)] (2.22 g, 10 mmol) in toluene (10 mL) was added dropwise to a solution of L=CH<sub>2</sub> (4.04 g, 10 mmol) in toluene (30 mL). After stirring for 1 h, the precipitate was collected via filtration, washed with hexane and dried *in vacuo* to afford [(LCH<sub>2</sub>)TMS](OTf) (**S3**) (6.00 g, 95.7 %) as white powder. M. P. = 201.7 °C. <sup>1</sup>H NMR (600.2 MHz, C<sub>6</sub>D<sub>6</sub>): δ = 7.58 (t, *J* = 7.9 Hz, 2 H, C<sub>Ar</sub>H), 7.46 (d, *J* = 7.9 Hz, 4 H, C<sub>Ar</sub>H), 4.34 (s, 4 H, NCH<sub>2</sub>), 3.09 (m, 4 H, CH(CH<sub>3</sub>)<sub>2</sub>), 1.83 (s, 2 H, C-CH<sub>2</sub>), 1.39 (d, *J* = 6.8 Hz, 12 H, CH(CH<sub>3</sub>)<sub>2</sub>), 1.31 (d, *J* = 6.8 Hz, 12 H, CH(CH<sub>3</sub>)<sub>2</sub>), -0.20 (s, 9 H, Si(CH<sub>3</sub>)<sub>3</sub>). <sup>13</sup>C{<sup>1</sup>H} NMR (150.8 MHz, C<sub>6</sub>D<sub>6</sub>): δ = 173.26 (NCN), 147.52 (C<sub>Ar</sub>), 132.45 (C<sub>Ar</sub>), 131.65 (C<sub>Ar</sub>), 126.80 (CF<sub>3</sub>), 53.35 (NCH), 29.74, 26.78, 23.59, 18.86, -0.12 (SiC). HRMS (ESI, *m/z*) calc. for: C<sub>28</sub>H<sub>41</sub>N<sub>2</sub>: 405.3264 [(M + H)]<sup>+</sup>; found: 405.3246.



**Figure S15.** <sup>1</sup>H NMR spectrum of **S3** in CD<sub>3</sub>CN.

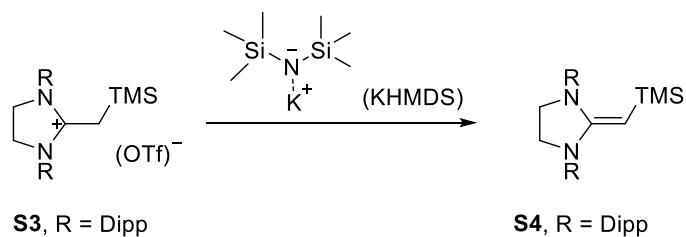


**Figure S16.**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **S3** in  $\text{CD}_3\text{CN}$ .

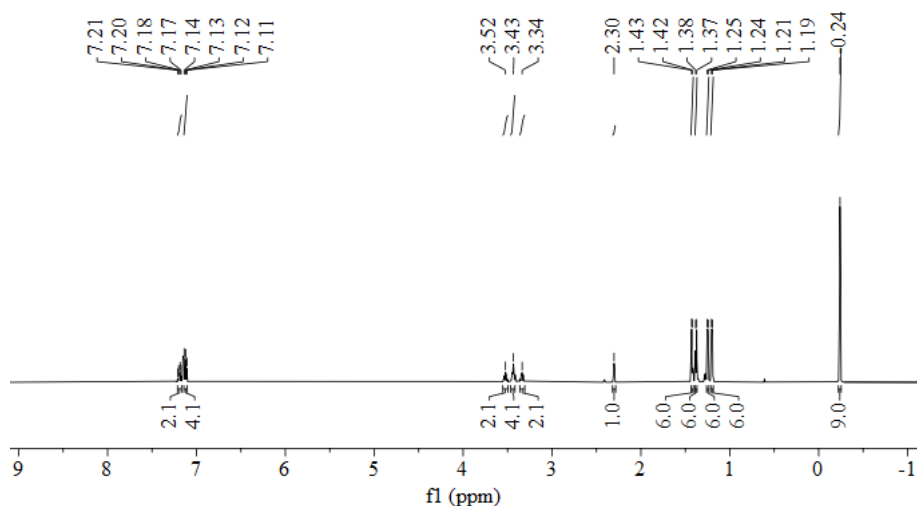


**Figure S17.** HRMS of **S3**.

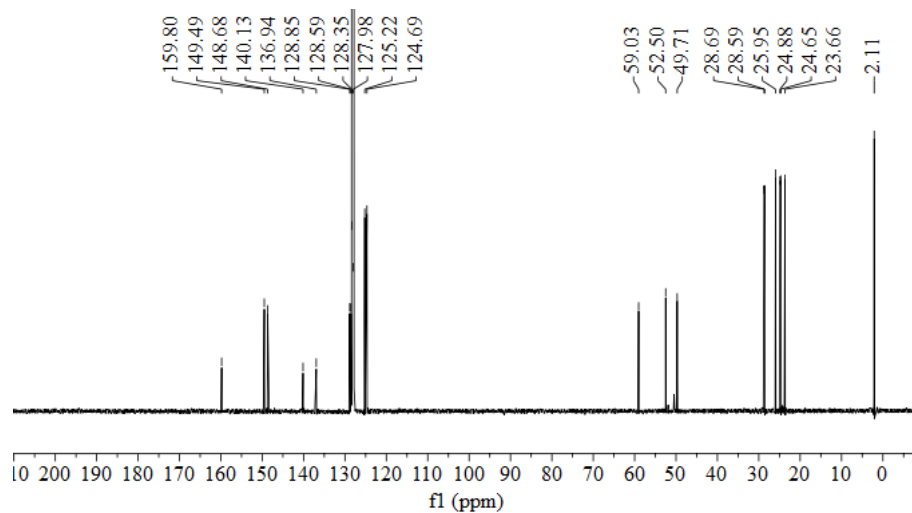
**Synthesis of (L=CH)TMS (S4):**



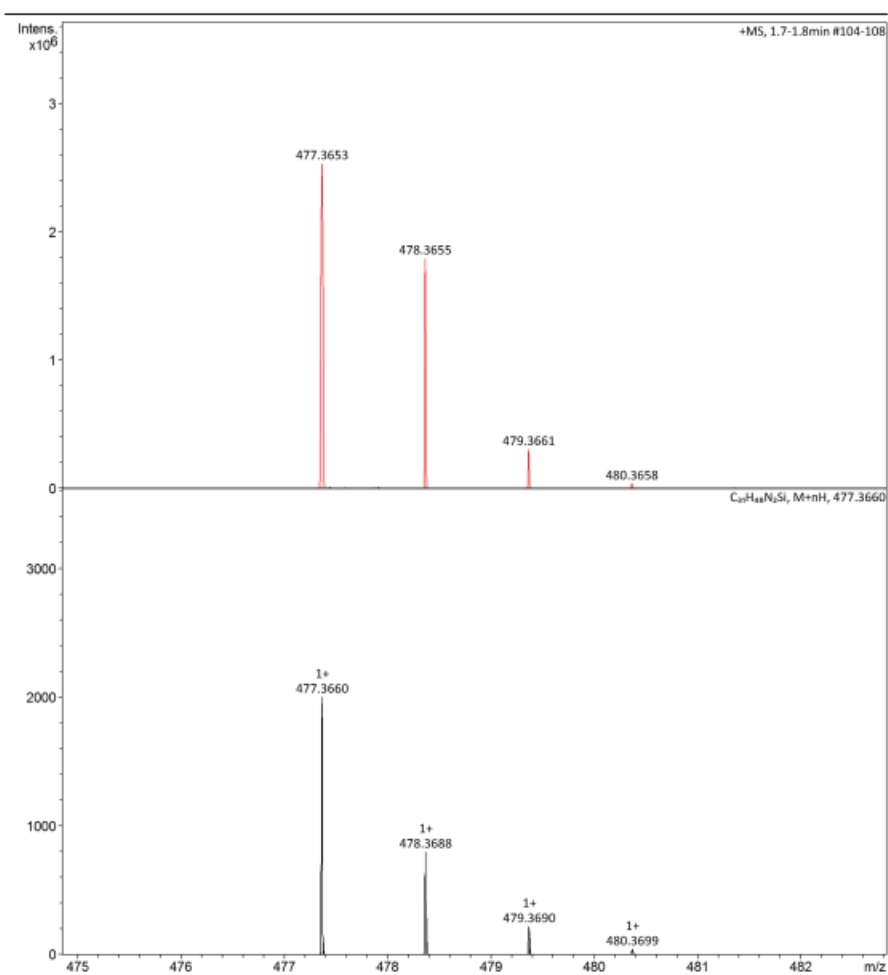
KHMDS (20 mL, 0.5 M in toluene) was added dropwise to a white slurry solution of **S3** (6.26 g, 10 mmol) in toluene (30 mL) at  $-80\text{ }^{\circ}\text{C}$ . The reaction mixture was allowed to warm slowly to room temperature and stirred overnight. The solvent was removed under reduced pressure and the residue was extracted with hexane (20 mL  $\times$  2). The remaining solid was washed with small amount of acetonitrile and dried *in vacuo* to afford **(L=CH)TMS (S4)** (2.64 g, yield = 55.5 %) as white powder. M. P. =  $135.0\text{ }^{\circ}\text{C}$  (Decomposition).  $^1\text{H}$  NMR (600.2 MHz,  $\text{C}_6\text{D}_6$ ):  $\delta$  = 7.21 ~ 7.17(m, 2 H,  $\text{C}_{\text{Ar}}\text{H}$ ), 7.14 ~ 7.11 (m, 4 H,  $\text{C}_{\text{Ar}}\text{H}$ ), 3.52 (m, 2 H,  $\text{NCH}_2$ ), 3.43 (m, 4 H,  $\text{CH}(\text{CH}_3)_2$ ), 3.34 (m, 2 H,  $\text{NCH}_2$ ), 2.30(s, 1 H,  $\text{CH}=\text{Si}$ ), 1.43 (d,  $J$  = 6.72 Hz, 6 H,  $\text{CH}(\text{CH}_3)_2$ ), 1.38 (d,  $J$  = 6.78 Hz, 6 H,  $\text{CH}(\text{CH}_3)_2$ ), 1.25 (d,  $J$  = 6.96 Hz, 6 H,  $\text{CH}(\text{CH}_3)_2$ ), 1.20 (d,  $J$  = 6.90 Hz, 6 H,  $\text{CH}(\text{CH}_3)_2$ ), -0.24 (s, 9 H,  $\text{Si}(\text{CH}_3)_3$ ).  $^{13}\text{C}\{^1\text{H}\}$  NMR (150.8 MHz,  $\text{C}_6\text{D}_6$ ):  $\delta$  = 159.80 (NCN), 149.49 ( $\text{C}_{\text{Ar}}$ ), 148.68 ( $\text{C}_{\text{Ar}}$ ), 140.13 ( $\text{C}_{\text{Ar}}$ ), 136.94 ( $\text{C}_{\text{Ar}}$ ), 128.85 ( $\text{C}_{\text{Ar}}$ ), 128.59 ( $\text{C}_{\text{Ar}}$ ), 128.35 ( $\text{C}_{\text{Ar}}$ ), 127.98 ( $\text{C}_{\text{Ar}}$ ), 125.22 ( $\text{C}_{\text{Ar}}$ ), 124.69 ( $\text{C}_{\text{Ar}}$ ), 59.03 (C=CH), 52.50 ( $\text{NCH}_2$ ), 49.71( $\text{NCH}_2$ ), 28.69, 28.59, 25.95, 24.88, 24.65, 23.66, 2.11 ( $\text{SiCH}_3$ )<sub>3</sub>. HRMS (ESI,  $m/z$ ) calc. for:  $\text{C}_{31}\text{H}_{49}\text{N}_2\text{Si}$ : 477.3660 [(M + H)]<sup>+</sup>; found: 477.3653.



**Figure S18.**  $^1\text{H}$  NMR spectrum of **S4** in  $\text{C}_6\text{D}_6$ .

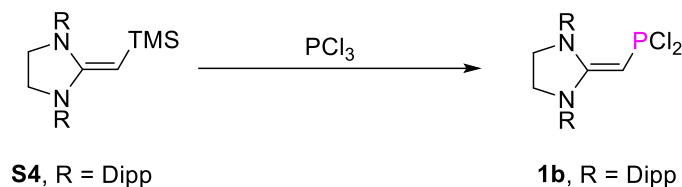


**Figure S19.**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of S4 in  $\text{C}_6\text{D}_6$ .

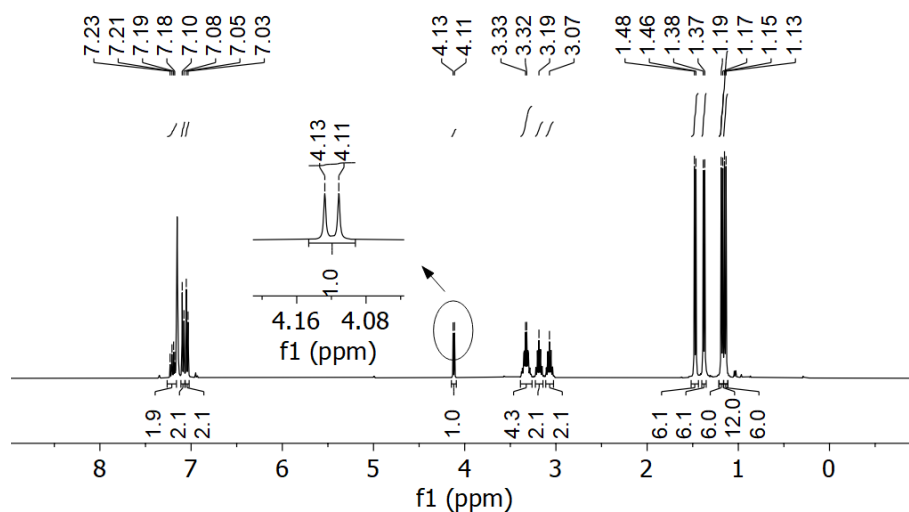


**Figure S20.** HRMS of S4.

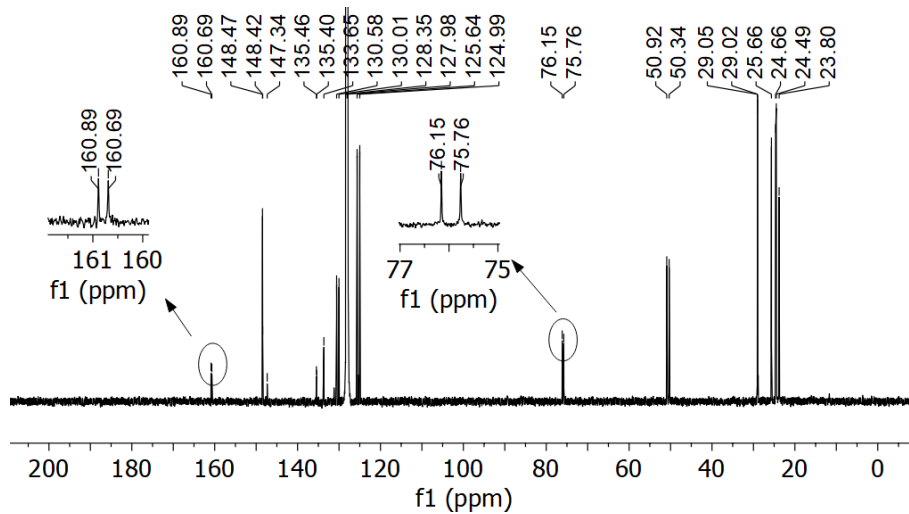
### Synthesis of (L=CH)PCl<sub>2</sub> (**1b**):



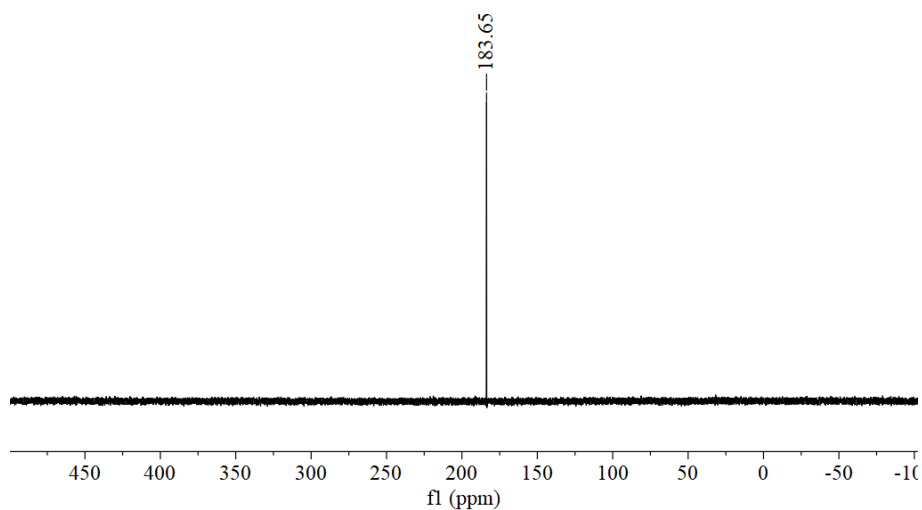
PCl<sub>3</sub> (1.51 g, 11 mmol) in THF (5 mL) was added dropwise to the solution of **S4** (4.77 g, 10 mmol) in THF (30 mL) at room temperature. After stirring for 2 hours, the solvent was removed under reduced pressure. The remaining solid was washed with hexane and dried *in vacuo* to afford (L=CH)PCl<sub>2</sub> (**1b**) (4.55 g, yield = 89.9 %) as white powder. M. P. = 139.0 °C (Decomposition). <sup>1</sup>H NMR (400.1 MHz, C<sub>6</sub>D<sub>6</sub>): δ = 7.22 (m, 2 H, C<sub>Ar</sub>H), 7.09 (d, *J* = 7.8 Hz, 2 H, C<sub>Ar</sub>H), 7.04 (d, *J* = 7.8 Hz, 2 H, C<sub>Ar</sub>H), 4.12 (d, <sup>2</sup>*J*<sub>PH</sub> = 6.5 Hz, CHPCl<sub>2</sub>), 3.32 (m, 4 H, NCH<sub>2</sub>), 3.19 (m, 2 H, CH(CH<sub>3</sub>)<sub>2</sub>), 3.07 (m, 2 H, CH(CH<sub>3</sub>)<sub>2</sub>), 1.47 (d, *J* = 6.8 Hz, 6 H, CH(CH<sub>3</sub>)<sub>2</sub>), 1.38 (d, *J* = 6.8 Hz, 6 H, CH(CH<sub>3</sub>)<sub>2</sub>), 1.18 (d, *J* = 7.0 Hz, 6 H, CH(CH<sub>3</sub>)<sub>2</sub>), 1.14 (d, *J* = 7.0 Hz, 12 H, CH(CH<sub>3</sub>)<sub>2</sub>). <sup>13</sup>C{<sup>1</sup>H} NMR (150.8 MHz, C<sub>6</sub>D<sub>6</sub>): δ = 160.79 (d, <sup>2</sup>*J*<sub>PC</sub> = 29.6 Hz, NCN), 148.48 (C<sub>Ar</sub>), 148.42 (C<sub>Ar</sub>), 135.46 (C<sub>Ar</sub>), 135.40 (C<sub>Ar</sub>), 133.65 (C<sub>Ar</sub>), 130.58 (C<sub>Ar</sub>), 130.01 (C<sub>Ar</sub>), 128.35 (C<sub>Ar</sub>), 128.15 (C<sub>Ar</sub>), 127.98 (C<sub>Ar</sub>), 125.64 (C<sub>Ar</sub>), 124.99 (C<sub>Ar</sub>), 75.96 (d, <sup>1</sup>*J*<sub>PC</sub> = 59.22 Hz, C-P), 50.92 (NCH), 50.34 (NCH), 29.05, 29.02, 25.66, 24.66, 24.49, 23.80. <sup>31</sup>P{<sup>1</sup>H} NMR (161.9 MHz, C<sub>6</sub>D<sub>6</sub>): δ = 183.65. HRMS (ESI, *m/z*) calc. for: C<sub>28</sub>H<sub>40</sub>Cl<sub>2</sub>N<sub>2</sub>P: 505.2301 [(M + H)<sup>+</sup>]; found: 505.2903.



**Figure S21.**  $^1\text{H}$  NMR spectrum of **1b** in  $\text{C}_6\text{D}_6$ .



**Figure S22.**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **1b** in  $\text{C}_6\text{D}_6$ .



**Figure S23.**  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum of **1b** in  $\text{C}_6\text{D}_6$ .



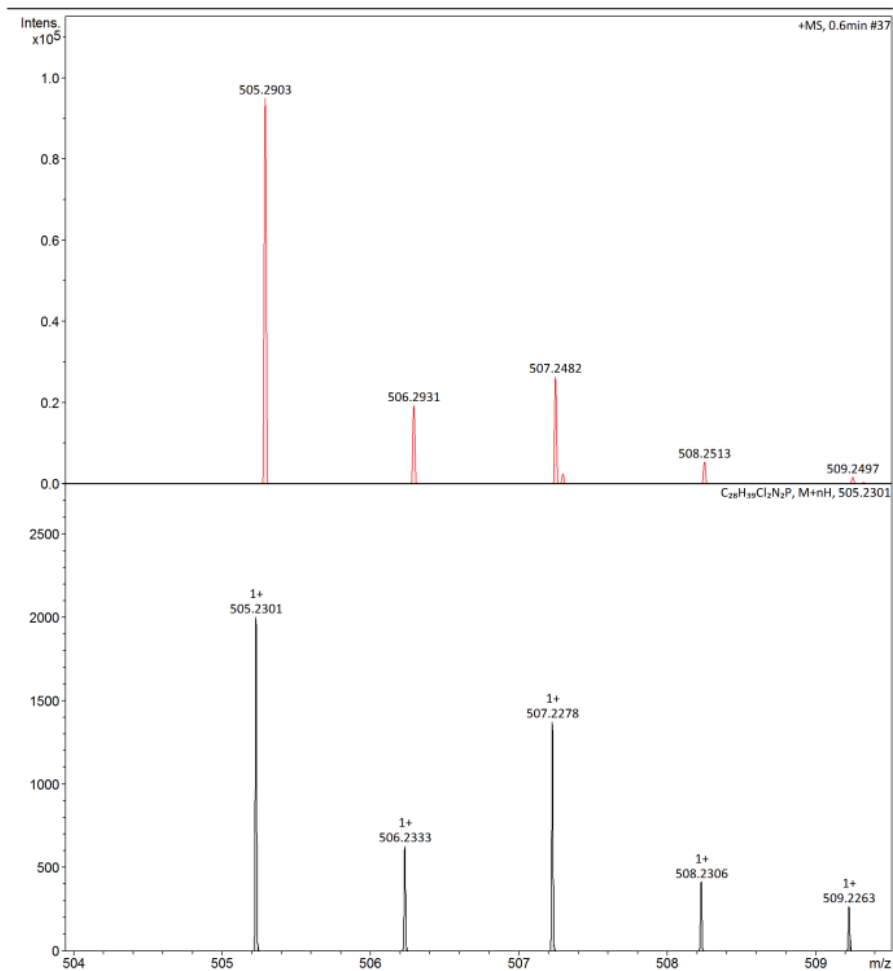
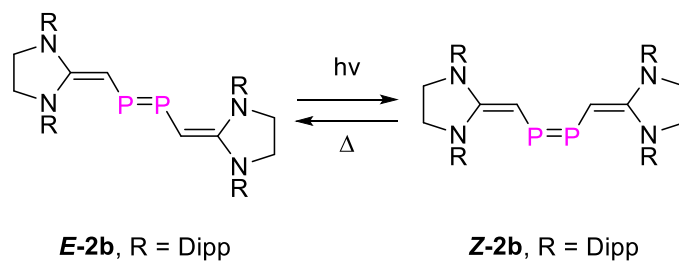
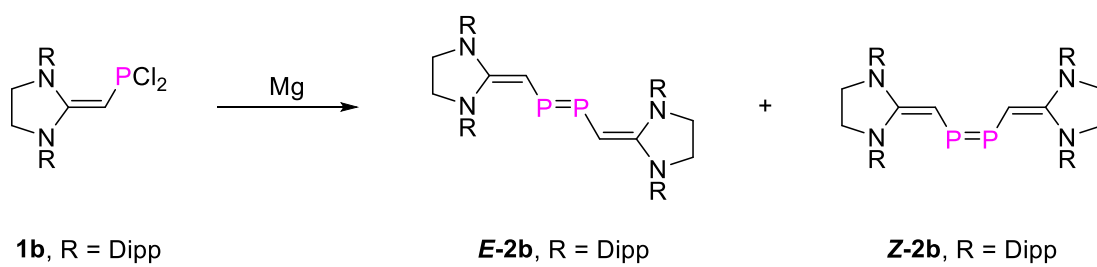
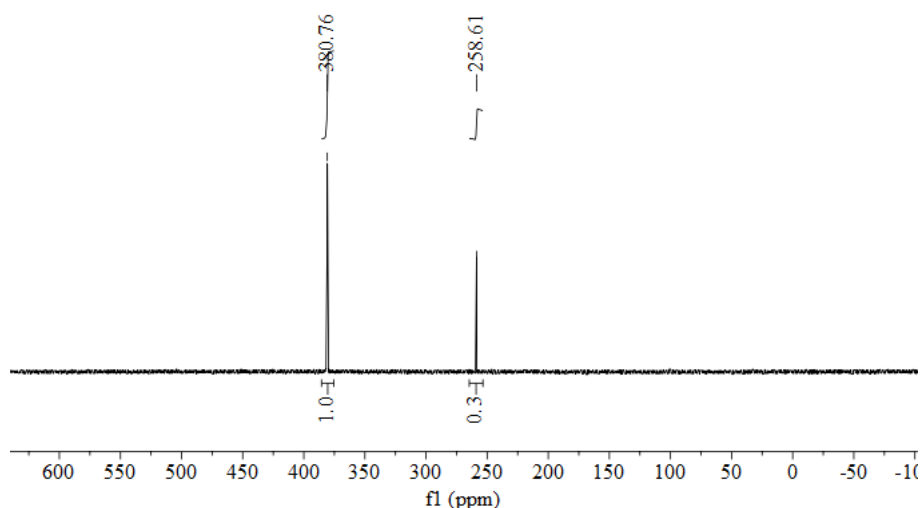


Figure S24. HRMS of 1b.

### Synthesis of *E*-2b and *Z*-2b:



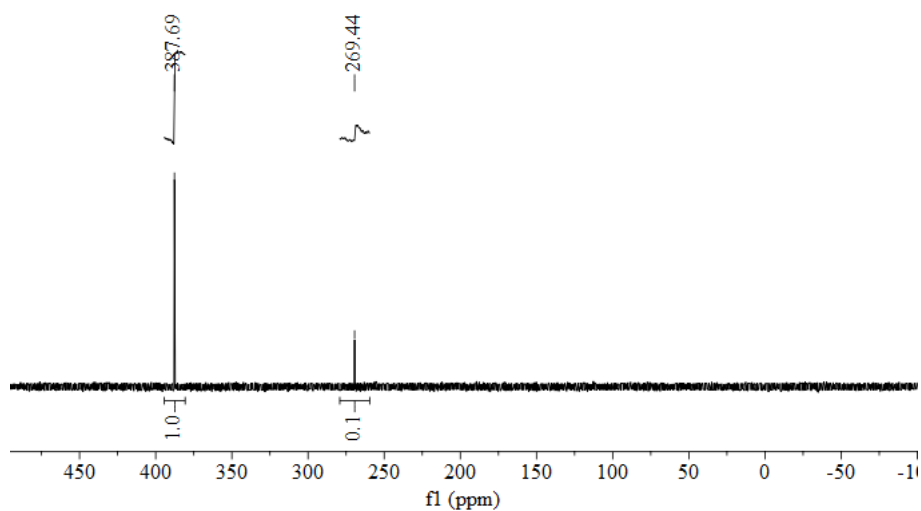
Mg powder (10 eq.) was added to a solution of **1b** (0.51 g, 10 mmol) in THF (20 mL) at room temperature. After stirring overnight in dark, two new species were formed as monitored via  $^{31}\text{P}$  NMR spectra as: *E*-**2b** ( $\delta = 380.76$  ppm):*Z*-**2b** ( $\delta = 380.76$  ppm) = 1.0:0.3. Then, the solvent was removed under reduced pressure and the residue was extracted with toluene to afford purple filtrate.



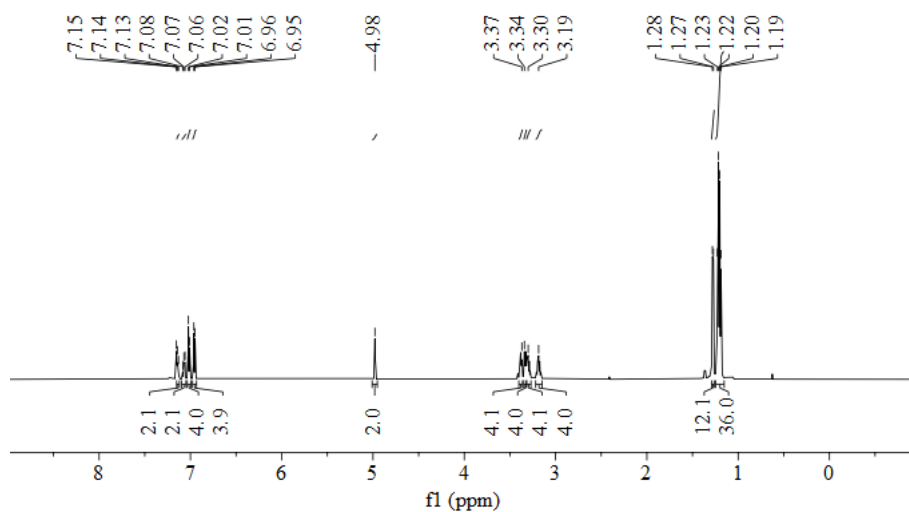
**Figure S25.**  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum of the reaction mixture in THF.

***E*-2b:** The filtrate was heated to 110 °C in the dark for 20 min to enrich the *E*-**2b** (*E*-**2b**:*Z*-**2b** = 1.0:0.1) and then the solvent was removed under reduced pressure. The residue was recrystallized from cold pentane at -30 °C and dried *in vacuo* to afford *E*-**2b** (269.46 mg, yield: 62.0 %) as red powder. Red crystals of *E*-**2b** were obtained from a saturated *n*-pentane solution stored at -30 °C for 1 day. M. P. > 250 °C.  $^1\text{H}$  NMR (600.2 MHz,  $\text{C}_6\text{D}_6$ ):  $\delta = 7.14$  (t, 2 H,  $J = 7.5$  Hz,  $\text{C}_{\text{Ar}}\text{H}$ ), 7.07 (t, 2 H,  $J = 7.5$  Hz,  $\text{C}_{\text{Ar}}\text{H}$ ), 7.02 (d, 4 H,  $J = 7.5$  Hz,  $\text{C}_{\text{Ar}}\text{H}$ ), 6.96 (d, 4 H,  $J = 7.5$  Hz,  $\text{C}_{\text{Ar}}\text{H}$ ), 4.98 (s, 2 H,  $\text{CH-P}$ ), 3.38 (m, 4 H,  $\text{NCH}_2$ ), 3.33 (m, 4 H,  $\text{NCH}_2$ ), 3.30 (m, 4 H,  $\text{CH}(\text{CH}_3)_2$ ), 3.19 (m, 4 H,  $\text{CH}(\text{CH}_3)_2$ ), 1.28 (d, 12 H,  $J = 6.8$  Hz,  $\text{CH}(\text{CH}_3)_2$ ), 1.22 (d, 12 H,  $J = 7.3$  Hz,  $\text{CH}(\text{CH}_3)_2$ ), 1.21 (d, 12 H,  $J = 7.9$  Hz,  $\text{CH}(\text{CH}_3)_2$ ), 1.20 (d, 12 H,  $J = 7.8$  Hz,  $\text{CH}(\text{CH}_3)_2$ ).  $^{13}\text{C}\{^1\text{H}\}$  NMR (150.8 MHz,  $\text{C}_6\text{D}_6$ ):  $\delta = 155.13$  (t,  $\text{NCN}$ ), 149.56 ( $\text{C}_{\text{Ar}}$ ), 148.86 ( $\text{C}_{\text{Ar}}$ ), 148.27 ( $\text{C}_{\text{Ar}}$ ), 137.70 ( $\text{C}_{\text{Ar}}$ ), 136.05 ( $\text{C}_{\text{Ar}}$ ), 128.84 ( $\text{C}_{\text{Ar}}$ ), 128.74 ( $\text{C}_{\text{Ar}}$ ), 128.35 ( $\text{C}_{\text{Ar}}$ ), 128.14 ( $\text{C}_{\text{Ar}}$ ), 127.98 ( $\text{C}_{\text{Ar}}$ ), 124.51 ( $\text{C}_{\text{Ar}}$ ), 124.47 ( $\text{C}_{\text{Ar}}$ ), 79.81 ( $\text{C-P}$ ), 51.80 ( $\text{NCH}$ ), 50.53 ( $\text{NCH}$ ), 28.91, 28.82, 25.31, 24.83, 24.43, 23.84.  $^{31}\text{P}\{^1\text{H}\}$  NMR (161.9 MHz,  $\text{C}_6\text{D}_6$ ):  $\delta = 379.58$ .

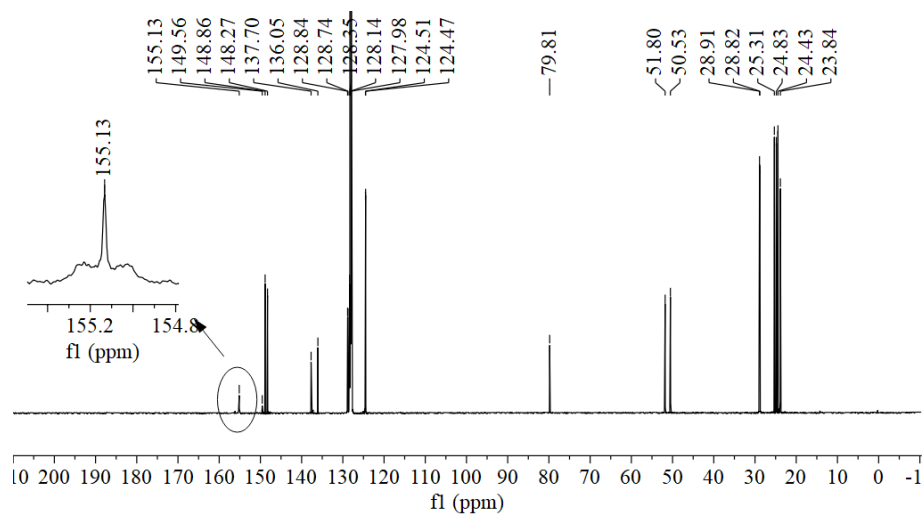
UV/Vis (Tol,  $\lambda$  (nm)  $\epsilon$  ( $M^{-1}cm^{-1}$ )): 534 (17798.9); 401 (2972.8). HRMS (ESI,  $m/z$ ) calc. for:  $C_{56}H_{78}N_4P_2$ : 868.57 [(M + H) $^+$ ]; found: 869.5774.



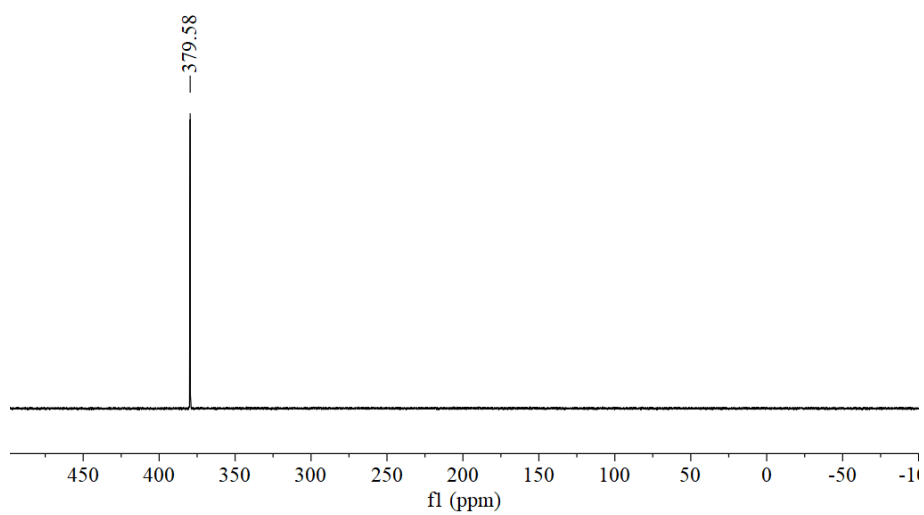
**Figure S26.**  $^{31}P\{^1H\}$  NMR spectrum of the reaction mixture in toluene after heated to  $110^\circ C$  in the dark for 20 min.



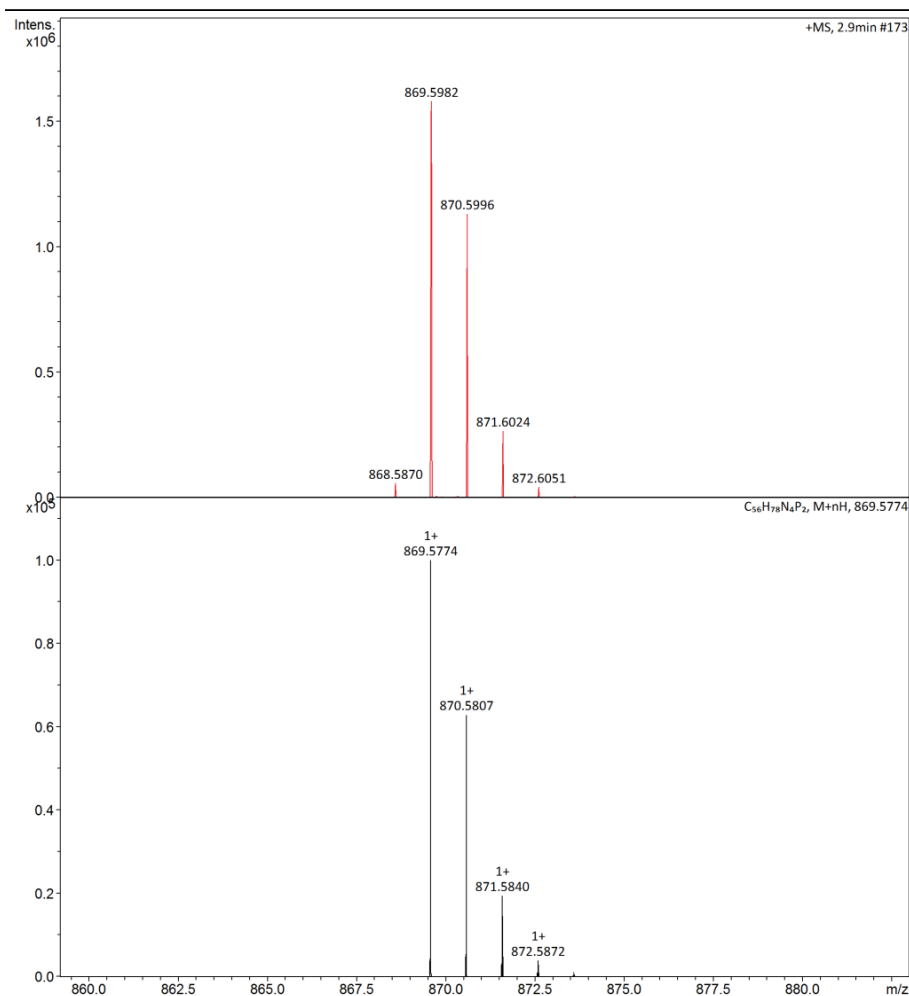
**Figure S27.**  $^1H$  NMR of *E*-**2b** in  $C_6D_6$ .



**Figure S28.**  $^{13}\text{C}\{^1\text{H}\}$  NMR of *E-2b* in  $\text{C}_6\text{D}_6$ .



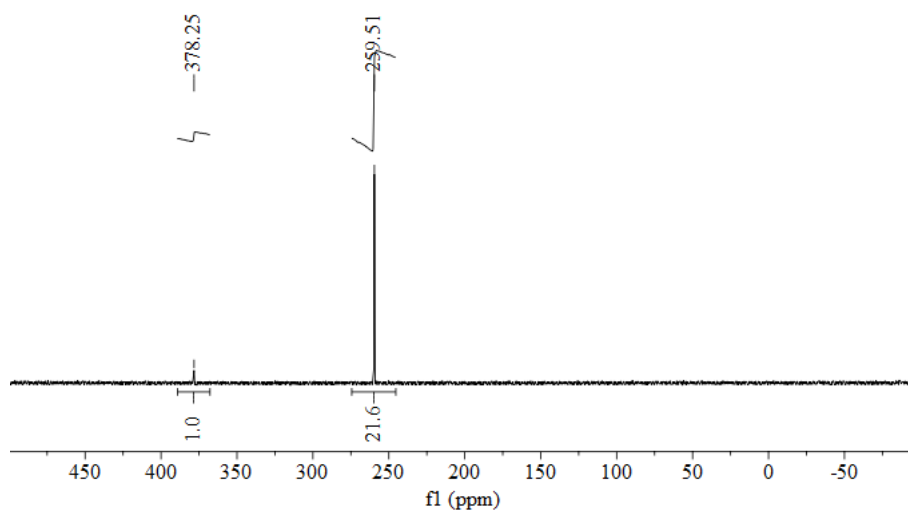
**Figure S29.**  $^{31}\text{P}\{^1\text{H}\}$  NMR of *E-2b* in  $\text{C}_6\text{D}_6$ .



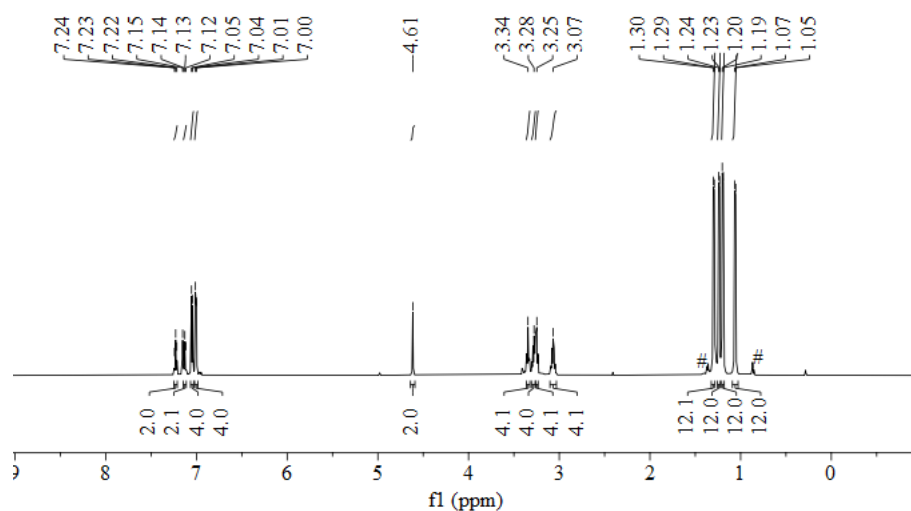
**Figure S30.** HRMS of **E-2b**.

**Z-2b:** The filtrate was irradiated with UV light (Hg lamp) for 30 min at 0 °C leading to predominantly **Z-2b** (**E-2b**:**Z-2b** = 1.0:21.6), then the solvent was removed under reduced pressure. The residue was recrystallized from cold pentane at -30 °C and dried *in vacuo* to afford **Z-2b** (290.32 mg, yield: 66.8 %) as orange powder. Orange crystals of **Z-2b** were obtained from a saturated *n*-pentane solution stored at -30 °C for 3 days. M. P. > 250 °C.  $^1H$  NMR(600.2 MHz,  $C_6D_6$ ):  $\delta$  = 7.23 (t, 2 H,  $J$  = 7.5 Hz,  $C_{Ar}H$ ), 7.13 (t, 2 H,  $J$  = 7.5 Hz,  $C_{Ar}H$ ), 7.05 (d, 4 H,  $J$  = 7.5 Hz,  $C_{Ar}H$ ), 7.01 (d, 4 H,  $J$  = 7.5 Hz,  $C_{Ar}H$ ), 4.61 (s, 2 H,  $CH-P$ ), 3.34 (t, 4 H,  $J$  = 7.3 Hz,  $NCH_2$ ), 3.28 (m, 4 H,  $CH(CH_3)_2$ ), 3.25 (t, 4 H,  $J$  = 7.3 Hz,  $NCH_2$ ), 3.07 (m, 4 H,  $CH(CH_3)_2$ ), 1.30 (d, 12 H,  $J$  = 6.7 Hz,  $CH(CH_3)_2$ ), 1.24 (d, 12 H,  $J$  = 6.9 Hz,  $CH(CH_3)_2$ ), 1.20 (d, 12 H,  $J$  = 6.9 Hz,  $CH(CH_3)_2$ ), 1.06 (d, 12 H,  $J$  = 6.7 Hz,  $CH(CH_3)_2$ ).  $^{13}C\{^1H\}$  NMR (150.8 MHz,  $C_6D_6$ ):  $\delta$  = 155.43 (t,  $NCN$ ), 148.86 ( $C_{Ar}$ ), 148.29 ( $C_{Ar}$ ), 147.66 ( $C_{Ar}$ ), 138.60 ( $C_{Ar}$ ), 136.26 ( $C_{Ar}$ ), 128.94

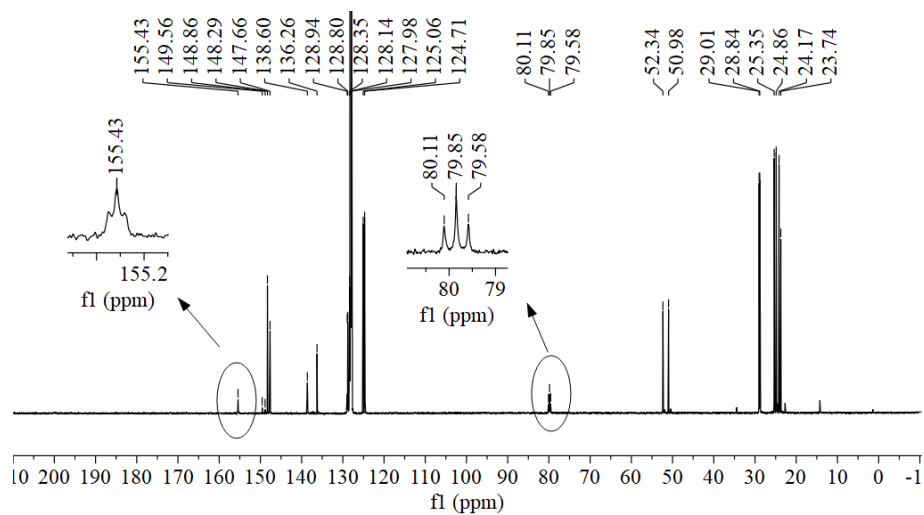
(C<sub>Ar</sub>), 128.80 (C<sub>Ar</sub>), 128.35 (C<sub>Ar</sub>), 128.14 (C<sub>Ar</sub>), 127.98 (C<sub>Ar</sub>), 125.06 (C<sub>Ar</sub>), 124.71 (C<sub>Ar</sub>), 79.85 (t, <sup>1</sup>J<sub>PC</sub> = 39.24 Hz, CP), 52.34 (NCH), 50.98 (NCH), 29.01, 28.84, 25.35, 24.86, 24.17, 23.74. <sup>31</sup>P{<sup>1</sup>H} NMR (242.9 MHz, C<sub>6</sub>D<sub>6</sub>): δ = 259.46. UV/Vis (Tol, λ (nm) ε (M<sup>-1</sup>cm<sup>-1</sup>)): 482 nm (23376.2); 359 (2762.8). HRMS (ESI, m/z) calc. for: C<sub>56</sub>H<sub>79</sub>N<sub>4</sub>P<sub>2</sub>: 868.5774 [(M + H)<sup>+</sup>]; found: 869.5577.



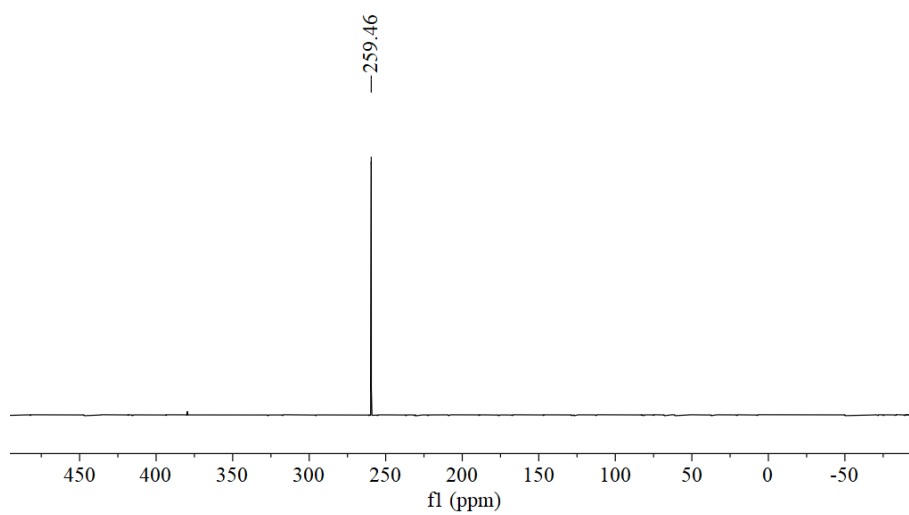
**Figure S31.** <sup>31</sup>P{<sup>1</sup>H} NMR spectrum of the reaction mixture in toluene after irradiated with UV light (Hg lamp) for 30 min at 0 °C.



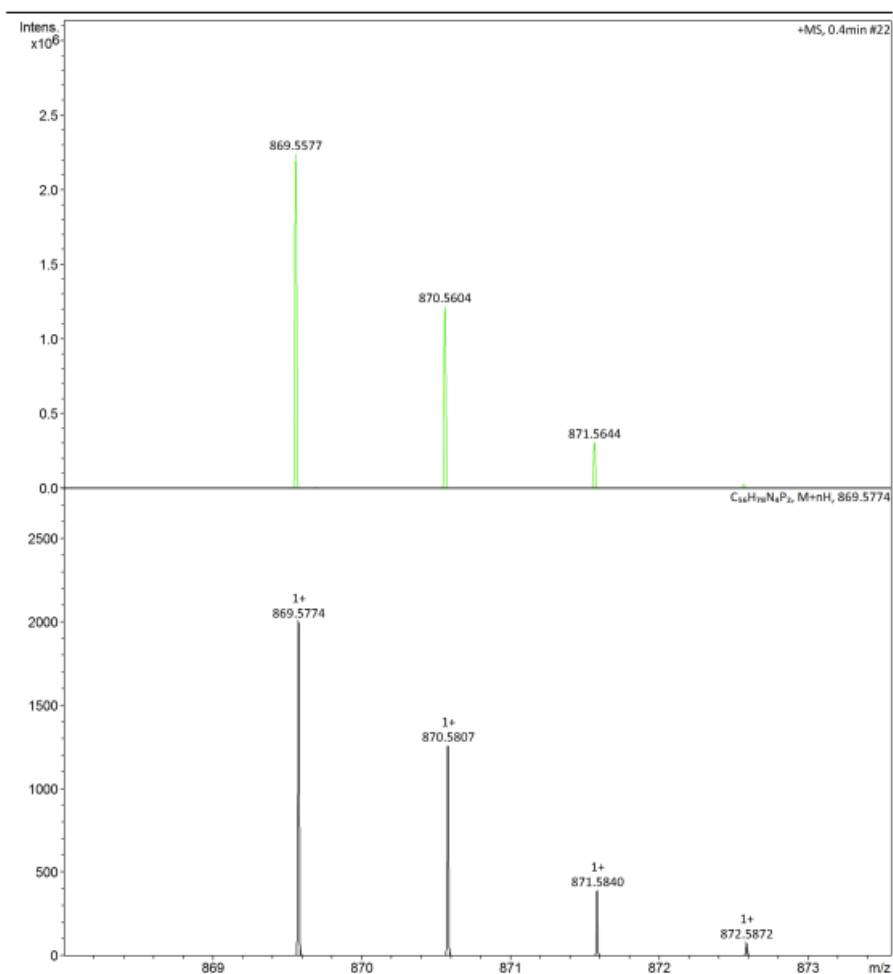
**Figure S32.** <sup>1</sup>H NMR of Z-2b in C<sub>6</sub>D<sub>6</sub>. # n-pentane.



**Figure S33.**  $^{13}\text{C}\{^1\text{H}\}$  NMR of **Z-2b** in  $\text{C}_6\text{D}_6$ .

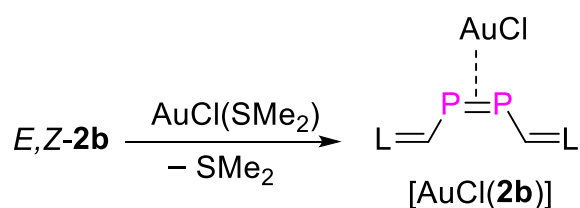


**Figure S34.**  $^{31}\text{P}\{^1\text{H}\}$  NMR of **Z-2b** in  $\text{C}_6\text{D}_6$ .



**Figure S35:** HRMS of **Z-2b**.

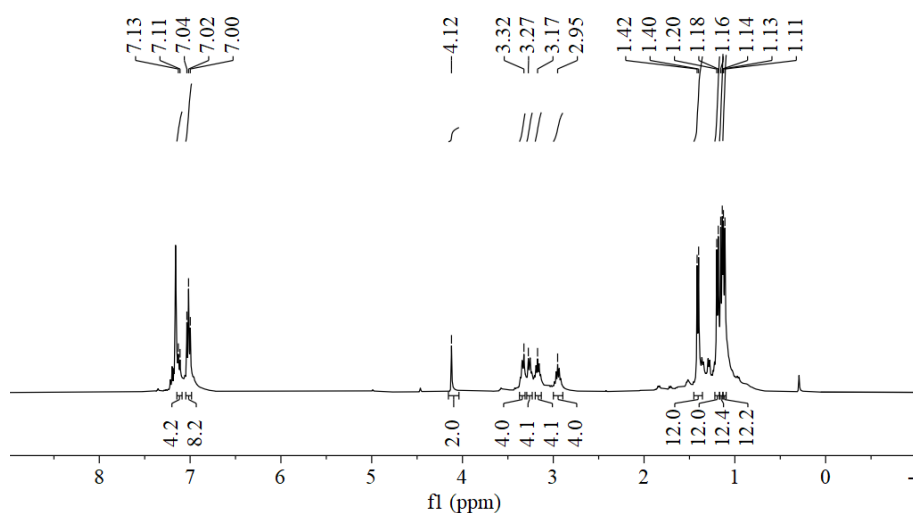
### Synthesis of [AuCl(**2b**)]:



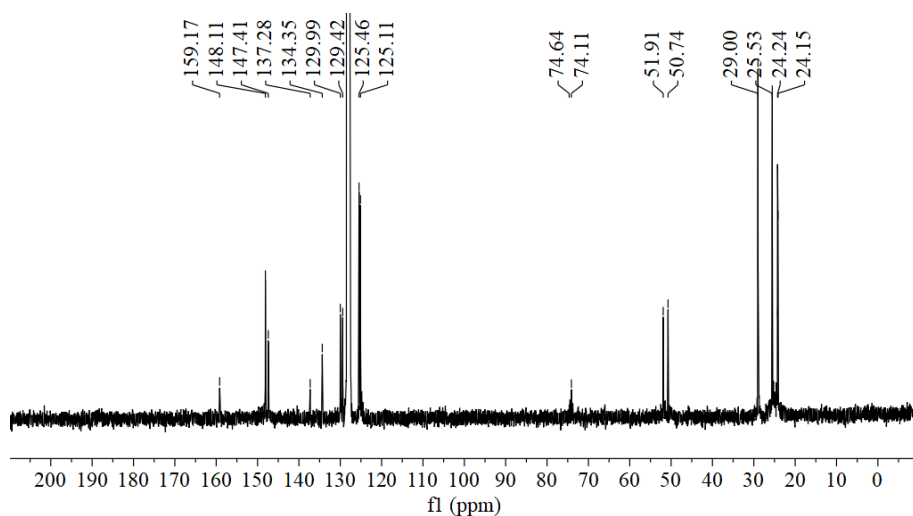
Chloro(dimethylsulfide)gold(I) (75 mg, 0.26 mmol) was added to the solution of **Z-2b** or **E-2b** (250 mg, 0.29 mmol) in THF (20 mL) at room temperature and stirred for 1 hour. Then, the solvent was removed under reduced pressure. The remaining solid was wash with hexanes and dried *in vacuo* to afford [AuCl(**2b**)] (257 mg, yield = 91.5 %) as dark red powder. Red crystals of [AuCl(**2b**)] were obtained from a saturated fluorobenzene solution via laying hexane at -30 °C. M. P. = 129.0 °C (Decomposition). <sup>1</sup>H NMR (400.1 MHz, C<sub>6</sub>D<sub>6</sub>): δ = 7.12 (d, *J* = 7.44 Hz, 4 H, C<sub>Ar</sub>H), 7.02 (t, *J* = 7.44 Hz,



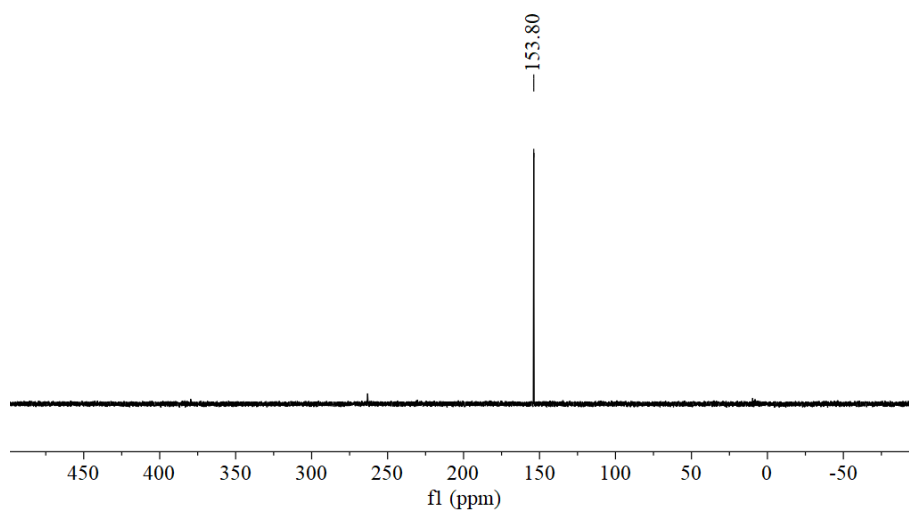
8 H,  $C_{Ar}H$ ), 4.12 (s, 2 H,  $C=CH-P$ ), 3.32 (m, 4 H,  $NCH_2$ ), 3.27 (m, 4 H,  $NCH_2$ ), 3.17 (m, 4 H,  $CH(CH_3)_2$ ), 2.95 (m, 4 H,  $CH(CH_3)_2$ ), 1.41 (d,  $J = 6.84$  Hz, 12 H,  $CH(CH_3)_2$ ), 1.19 (d,  $J = 6.84$  Hz, 12 H,  $CH(CH_3)_2$ ), 1.15 (d,  $J = 6.96$  Hz, 12 H,  $CH(CH_3)_2$ ), 1.12 (d,  $J = 6.88$  Hz, 12 H,  $CH(CH_3)_2$ ).  $^{13}C\{^1H\}$  NMR (100.5 MHz,  $C_6D_6$ ):  $\delta = 159.17$  (NCN), 148.11 ( $C_{Ar}$ ), 147.41 ( $C_{Ar}$ ), 137.28 ( $C_{Ar}$ ), 134.35 ( $C_{Ar}$ ), 129.99 ( $C_{Ar}$ ), 129.42 ( $C_{Ar}$ ), 125.46 ( $C_{Ar}$ ), 125.11 ( $C_{Ar}$ ), 74.64 (NC=CH), 51.91 (NCH), 50.74 (NCH), 29.00, 25.53, 24.24, 24.15, 1.95.  $^{31}P\{^1H\}$  NMR (161.9 MHz,  $C_6D_6$ ):  $\delta = 153.80$ . UV/Vis (THF,  $\lambda$  (nm)  $\epsilon$  ( $M^{-1}cm^{-1}$ )): 480 (8215). HRMS (ESI,  $m/z$ ) calc. for:  $C_{56}H_{79}AuClN_4P_2$ : 1101.5129 [(M + H) $^+$ ]; found: 1101.5251.



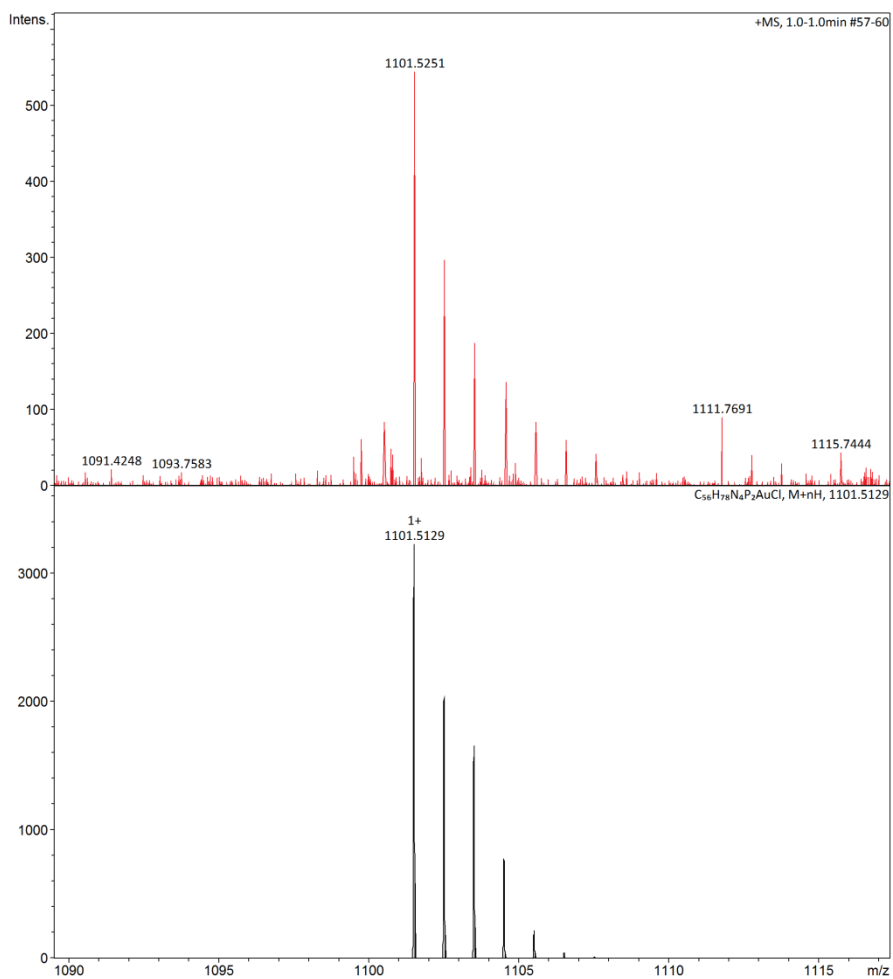
**Figure S36.**  $^1H$  NMR spectrum of  $[AuCl(2b)]$  in  $C_6D_6$ .



**Figure S37.**  $^{13}C\{^1H\}$  NMR spectrum of  $[AuCl(2b)]$  in  $C_6D_6$ .

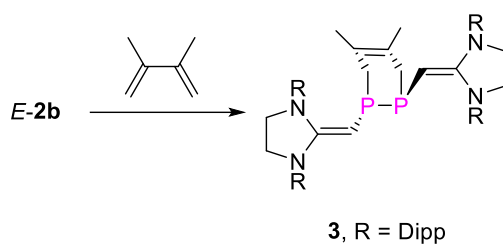


**Figure S38.**  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum of  $[\text{AuCl}(\mathbf{2b})]$  in  $\text{C}_6\text{D}_6$ .

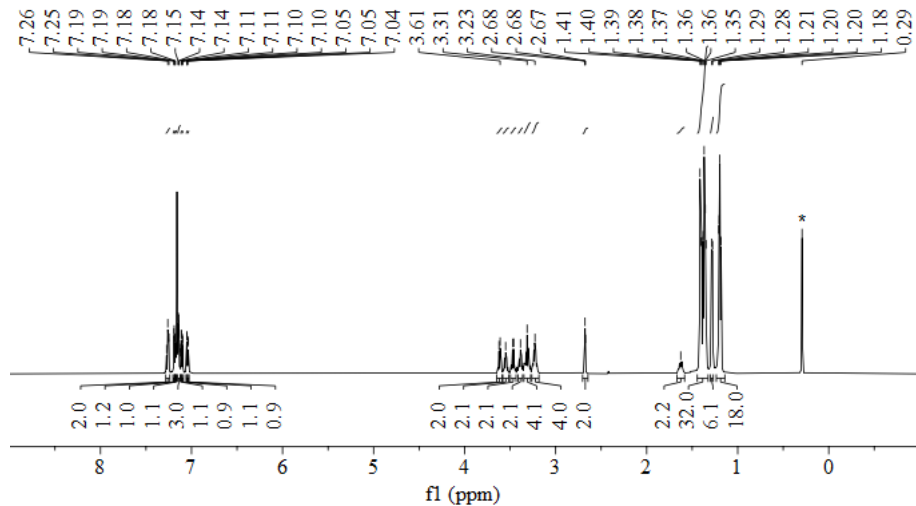


**Figure S39.** HRMS of  $[\text{AuCl}(\mathbf{2b})]$

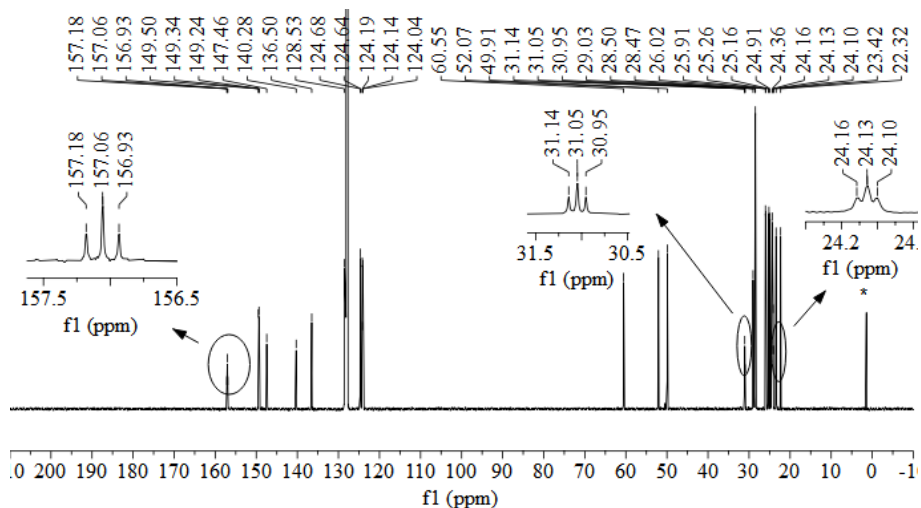
### Synthesis of **3**:



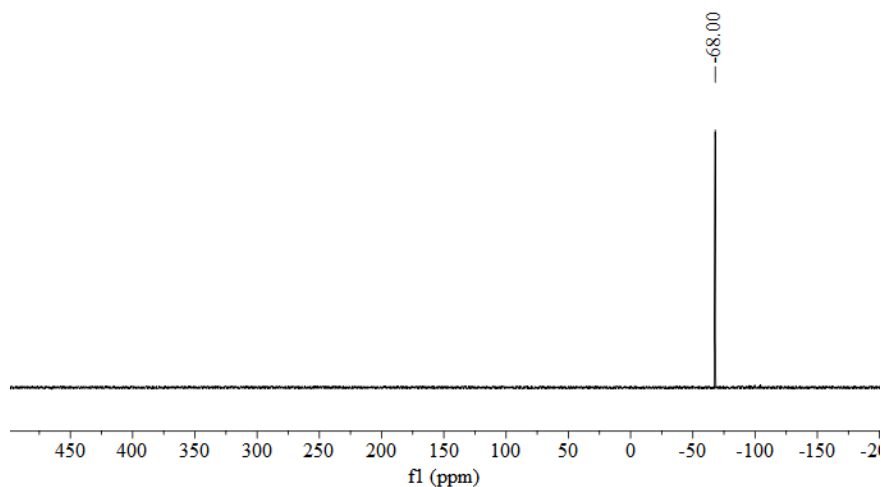
2,3-Dimethyl-1,3-butadiene (72 mg, 0.88 mmol) in toluene (3 mL) was added to the solution of *E*-**2b** (750 mg, 0.86 mmol) in toluene (10 mL) at room temperature. After stirring for 15 min in the dark, the solvent was removed under reduced pressure, and the residue was washed with acetonitrile and dry *in vacuo* to afford **3** (360 mg, yield = 43.8 %) as light orange powder. Light orange crystals of **3** were obtained from a saturated hexane solution stored at -30 °C for 3 days. M. P. = 170.0 °C (Decomposition). <sup>1</sup>H NMR (600.2 MHz, C<sub>6</sub>D<sub>6</sub>): δ = 7.27 ~ 7.04 (12 H, C<sub>Ar</sub>H), 3.61 (m, 2 H, CH(CH<sub>3</sub>)<sub>2</sub>), 3.55 (m, 2 H, CH(CH<sub>3</sub>)<sub>2</sub>), 3.46 (m, 2 H, CH(CH<sub>3</sub>)<sub>2</sub>), 3.39 (m, 2 H, CH(CH<sub>3</sub>)<sub>2</sub>), 3.31 (m, 4 H, NCH<sub>2</sub>), 3.23 (m, 4 H, NCH<sub>2</sub>), 2.68 (t, 2 H, *J* = 2.7 Hz, C=CH-P), 1.63 (m, 2 H, PCH<sub>2</sub>), 1.41~1.35 (32 H, PCH<sub>2</sub> & CH<sub>3</sub> & CH(CH<sub>3</sub>)<sub>2</sub>), 1.29 (d, 6 H, *J* = 6.90 Hz, CH(CH<sub>3</sub>)<sub>2</sub>), 1.21~1.18 (18 H, CH(CH<sub>3</sub>)<sub>2</sub>). <sup>13</sup>C {<sup>1</sup>H} NMR (150.8 MHz, C<sub>6</sub>D<sub>6</sub>): δ = 157.06 (t, <sup>2</sup>*J*<sub>PC</sub> = 19.26 Hz, NCN), 149.50 (-(CH<sub>3</sub>)CH=CH(CH<sub>3</sub>)-), 149.34 (C<sub>Ar</sub>), 149.24 (C<sub>Ar</sub>), 147.46 (C<sub>Ar</sub>), 140.28 (C<sub>Ar</sub>), 136.50 (C<sub>Ar</sub>), 128.53 (C<sub>Ar</sub>), 128.35 (C<sub>Ar</sub>), 124.68 (C<sub>Ar</sub>), 124.64 (C<sub>Ar</sub>), 124.14 (C<sub>Ar</sub>), 124.04 (C<sub>Ar</sub>), 60.55 (-(CH<sub>3</sub>)CH=CH(CH<sub>3</sub>)-), 52.07 (NCH<sub>2</sub>), 49.91 (NCH<sub>2</sub>), 31.05 (t, PCH=C), 29.03, 28.50, 28.47, 26.02, 25.91, 25.26, 25.16, 24.91, 24.36, 24.13 (t, <sup>1</sup>*J*<sub>PC</sub> = 14.45 Hz, PCH<sub>2</sub>), 23.42, 22.32. <sup>31</sup>P {<sup>1</sup>H} NMR (242.9 MHz, C<sub>6</sub>D<sub>6</sub>): δ = -68.00. UV/Vis (THF, λ (nm) ε (M<sup>-1</sup>cm<sup>-1</sup>)): 253 (42129.3). HRMS (ESI, m/z) calc. for: C<sub>62</sub>H<sub>89</sub>N<sub>4</sub>P<sub>2</sub>: 951.6557 [M + H]<sup>+</sup>; found: 951.6703.



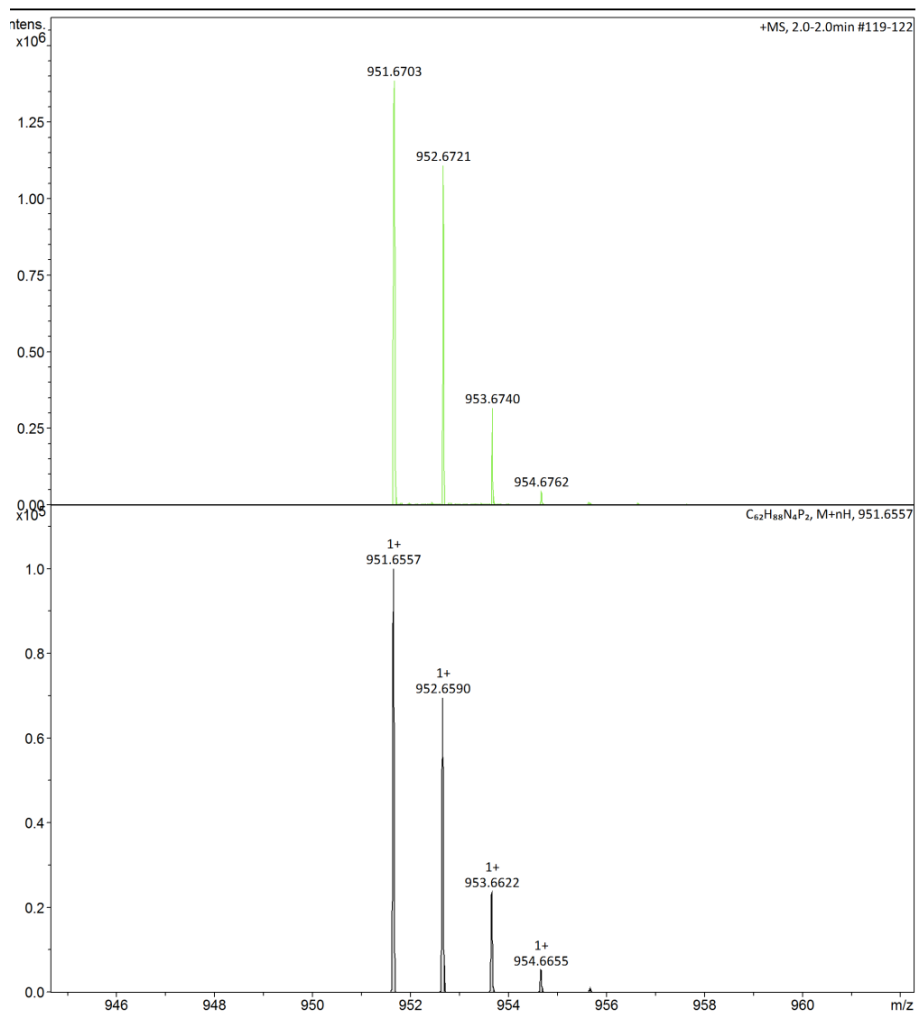
**Figure S40.**  $^1\text{H}$  NMR spectrum of **3** in  $\text{C}_6\text{D}_6$ . \*Silicon grease.



**Figure S41.**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **3** in  $\text{C}_6\text{D}_6$ . \*Silicone grease.

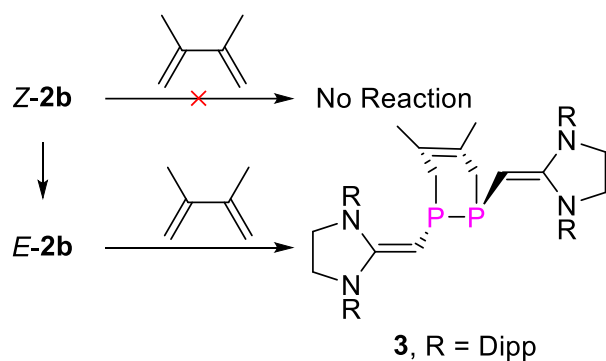


**Figure S42.**  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum of **3** in  $\text{C}_6\text{D}_6$ .

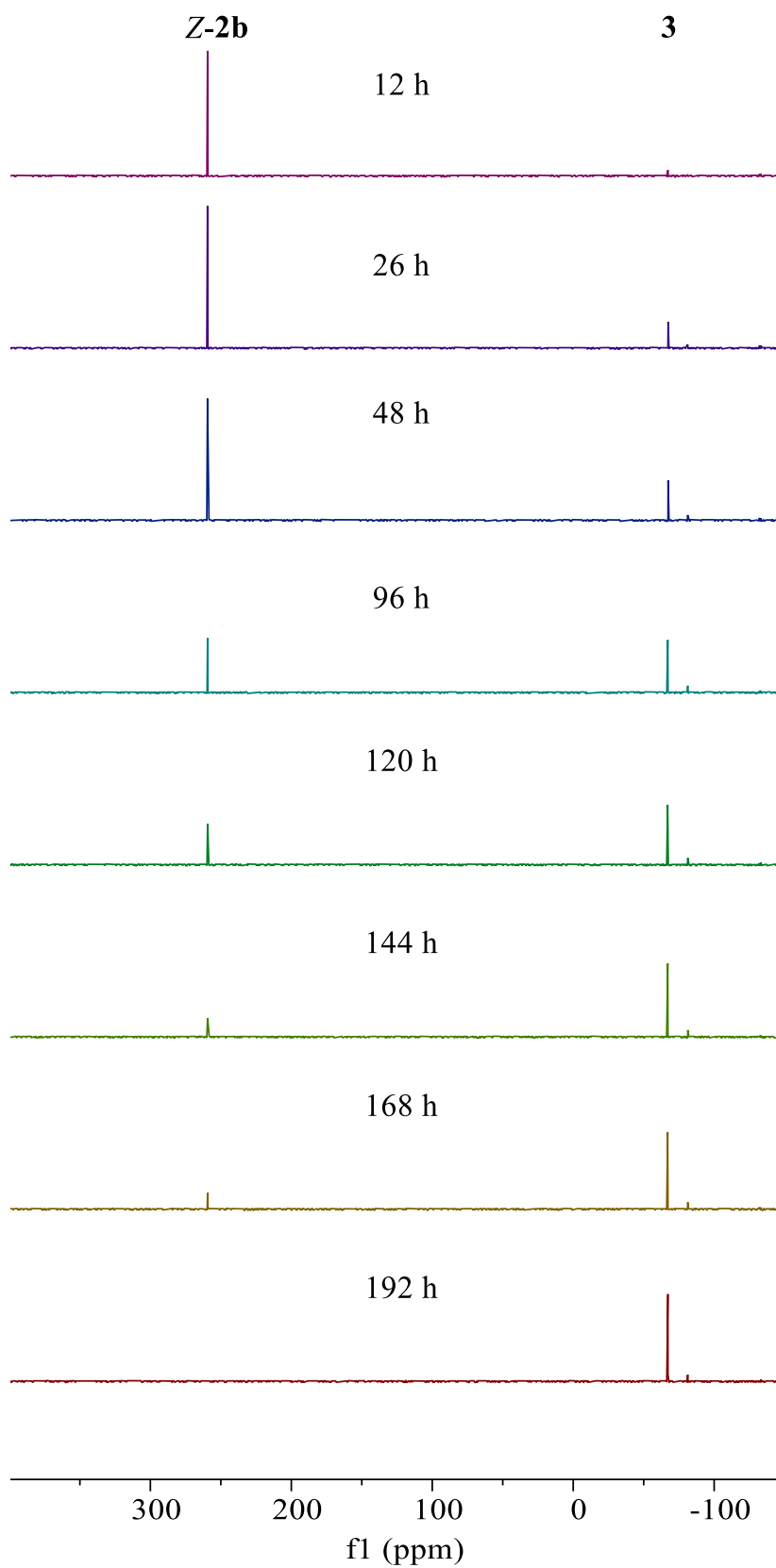


**Figure S43.** HRMS of **3**.

The reaction of **Z-2b** with 2,3-Dimethyl-1,3-butadiene:

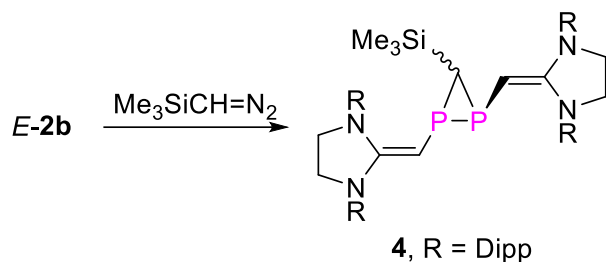


A drop of 2,3-Dimethyl-1,3-butadiene was added to a solution of **Z-2b** (10 mg) in  $\text{C}_6\text{D}_6$  (0.4 mL). The  $^{31}\text{P}$  NMR monitoring shows below:



**Figure S44.**  $^{31}\text{P}$  NMR spectra monitoring of the reaction of **Z-2b** ( $\delta = 259.4$  ppm) with 2,3-Dimethyl-1,3-butadiene to afford **3** ( $\delta = 67.0$  ppm) in  $\text{C}_6\text{D}_6$ .

## Synthesis of 4:



(Trimethylsilyl)diazomethane (2M in hexane, 0.5 mL) was added to the solution of *E*-**2b** (400 mg, 0.46 mmol) in toluene (10 mL). After stirring for 15 min in the dark, the solvent was removed under reduced pressure, and the residue was washed with acetonitrile and dry in vacuo to afford **4** (389 mg, yield = 86.0 %) as light-yellow powder. Light yellow crystals of **4** were obtained from a saturated hexane solution via slow evaporation at room temperature. M. P. = 103.0 °C (Decomposition). <sup>1</sup>H NMR (600.2 MHz, C<sub>6</sub>D<sub>6</sub>): δ = 7.29 (t, 1 H, *J* = 7.62 Hz, C<sub>Ar</sub>H), 7.24~7.19 (3 H, C<sub>Ar</sub>H), 7.15~7.10 (3 H, C<sub>Ar</sub>H), 7.08 (d, 1 H, *J* = 7.74 Hz, C<sub>Ar</sub>H), 7.04~7.01 (3 H, C<sub>Ar</sub>H), 6.90 (d, 1 H, *J* = 7.50 Hz, C<sub>Ar</sub>H), 3.54 (m, 2 H, NCH<sub>2</sub>), 3.49~3.26 (12 H, NCH<sub>2</sub> & CH(CH<sub>3</sub>)<sub>2</sub> & PCH), 3.19 (m, 1 H, CH(CH<sub>3</sub>)<sub>2</sub>), 3.04 (m, 1 H, NCH<sub>2</sub>), 2.08 (s, 1 H, PCH), 1.64 (d, 3 H, *J* = 6.90 Hz, CH(CH<sub>3</sub>)<sub>2</sub>), 1.60 (d, 3 H, *J* = 7.02 Hz, CH(CH<sub>3</sub>)<sub>2</sub>), 1.51 (d, 3 H, *J* = 6.90 Hz, CH(CH<sub>3</sub>)<sub>2</sub>), 1.41 (d, 3 H, *J* = 6.78 Hz, CH(CH<sub>3</sub>)<sub>2</sub>), 1.38 (d, 3 H, *J* = 6.90 Hz, CH(CH<sub>3</sub>)<sub>2</sub>), 1.37 (d, 3 H, *J* = 6.78 Hz, CH(CH<sub>3</sub>)<sub>2</sub>), 1.34 (d, 3 H, *J* = 6.84 Hz, CH(CH<sub>3</sub>)<sub>2</sub>), 1.30~1.28 (m, 6 H, CH(CH<sub>3</sub>)<sub>2</sub>), 1.27 (d, 6 H, *J* = 6.84 Hz, CH(CH<sub>3</sub>)<sub>2</sub>), 1.22 (t, 6 H, *J* = 7.08 Hz, CH(CH<sub>3</sub>)<sub>2</sub>), 1.15~1.12(m, 9 H, CH(CH<sub>3</sub>)<sub>2</sub>), 0.63, -0.11(s, 9 H, Si(CH<sub>3</sub>)<sub>3</sub>), -0.57(d, 1 H, <sup>2</sup>*J*<sub>PH</sub> = 27.97 Hz, P-CH-Si(CH<sub>3</sub>)<sub>3</sub>). <sup>13</sup>C NMR (151 MHz, C<sub>6</sub>D<sub>6</sub>): δ = 158.46 (NCN), 157.51 (NCN), 149.62 (C<sub>Ar</sub>), 149.31 (C<sub>Ar</sub>), 148.77 (C<sub>Ar</sub>), 148.70 (C<sub>Ar</sub>), 148.61 (C<sub>Ar</sub>), 148.05 (C<sub>Ar</sub>), 148.02 (C<sub>Ar</sub>), 138.65 (C<sub>Ar</sub>), 136.39 (C<sub>Ar</sub>), 128.72 (C<sub>Ar</sub>), 128.59 (C<sub>Ar</sub>), 128.55 (C<sub>Ar</sub>), 128.35 (C<sub>Ar</sub>), 128.14 (C<sub>Ar</sub>), 127.98 (C<sub>Ar</sub>), 125.06 (C<sub>Ar</sub>), 124.93 (C<sub>Ar</sub>), 124.83 (C<sub>Ar</sub>), 124.63 (C<sub>Ar</sub>), 124.28 (C<sub>Ar</sub>), 124.25 (C<sub>Ar</sub>), 124.22 (C<sub>Ar</sub>), 123.81 (C<sub>Ar</sub>), 115.80 (C<sub>Ar</sub>), 67.83 (dd, P-CH-C<sub>carbene</sub>), 61.33(dd, P-CH-C<sub>carbene</sub>), 51.93 (NCH<sub>2</sub>), 51.74 (NCH<sub>2</sub>), 50.54 (NCH<sub>2</sub>), 50.22 (NCH<sub>2</sub>), 29.28, 29.02, 28.89, 28.62, 28.59, 28.45, 28.40, 28.33, 25.96, 25.92, 25.72, 25.49, 25.46, 25.36, 25.32, 25.26, 25.00, 24.89, 24.78, 24.75, 24.43, 24.31, 24.18, 17.61, 1.89 (Si(CH<sub>3</sub>)<sub>3</sub>), 0.13 (CHSi(CH<sub>3</sub>)<sub>3</sub>). <sup>31</sup>P NMR (242.9 MHz,

$C_6D_6$ :  $\delta = -161.30$  (dd,  $^1J_{PP} = 158.32$  Hz,  $^2J_{PH} = 29.36$  Hz),  $-181.87$  (d,  $^1J_{PP} = 158.32$  Hz). UV/Vis (THF,  $\lambda$  (nm)  $\epsilon$  ( $M^{-1}cm^{-1}$ )): 332 (23783.2). HRMS (ESI,  $m/z$ ) calc. for:  $C_{60}H_{89}N_4P_2Si$ : 955.6326.  $[M + H]^+$ ; found: 955.6585.

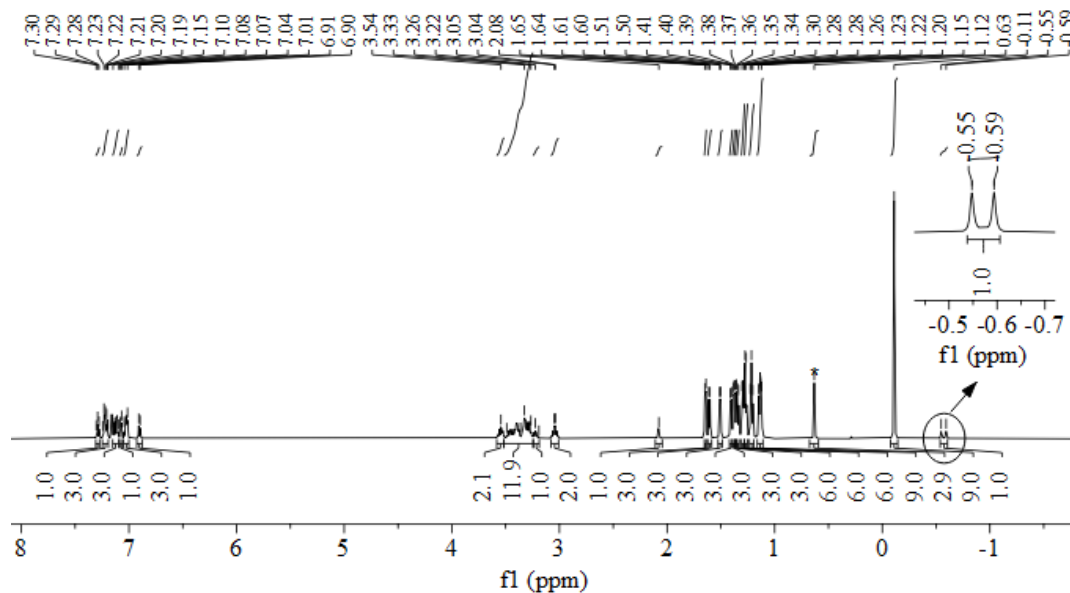


Figure S45.  $^1H$  NMR spectrum of **4** in  $C_6D_6$ .

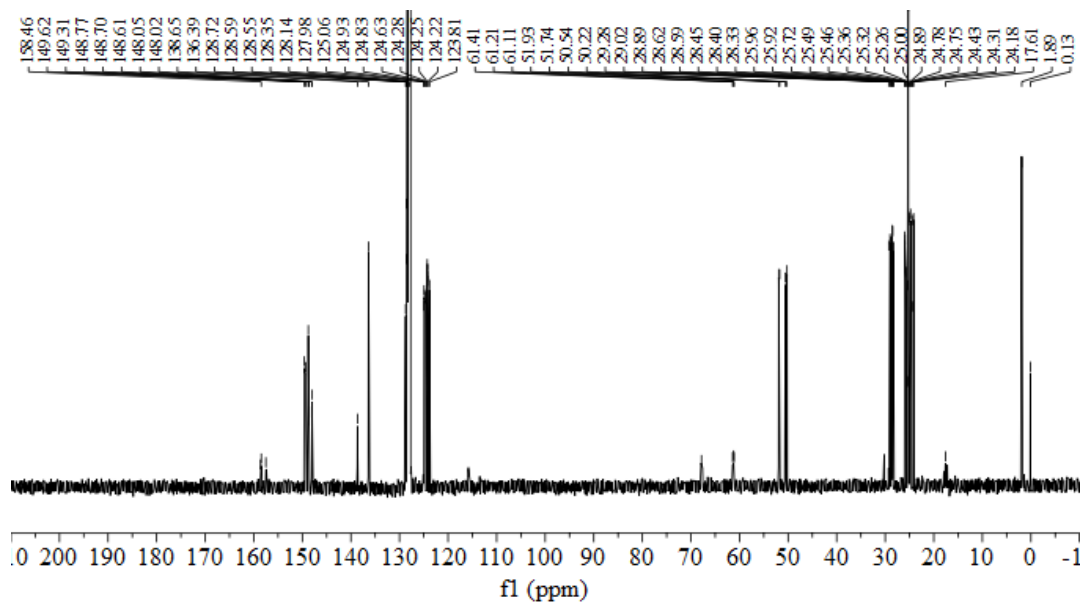
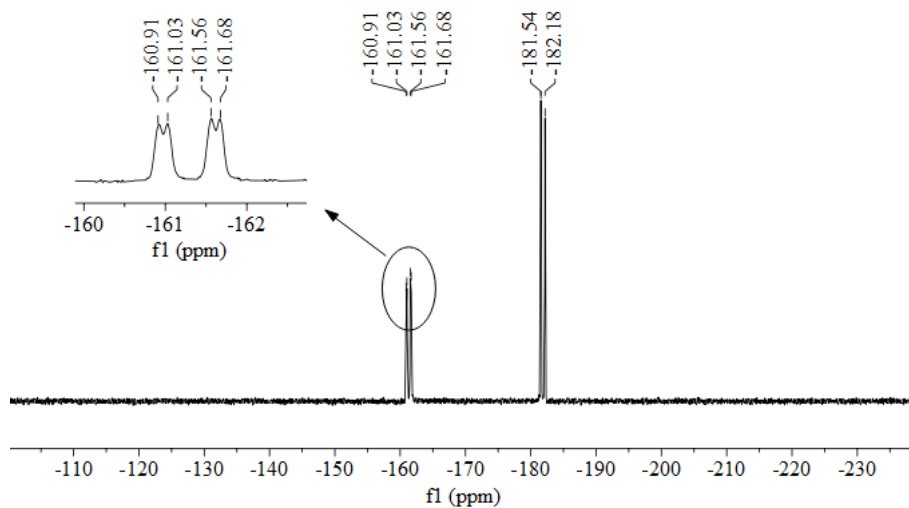
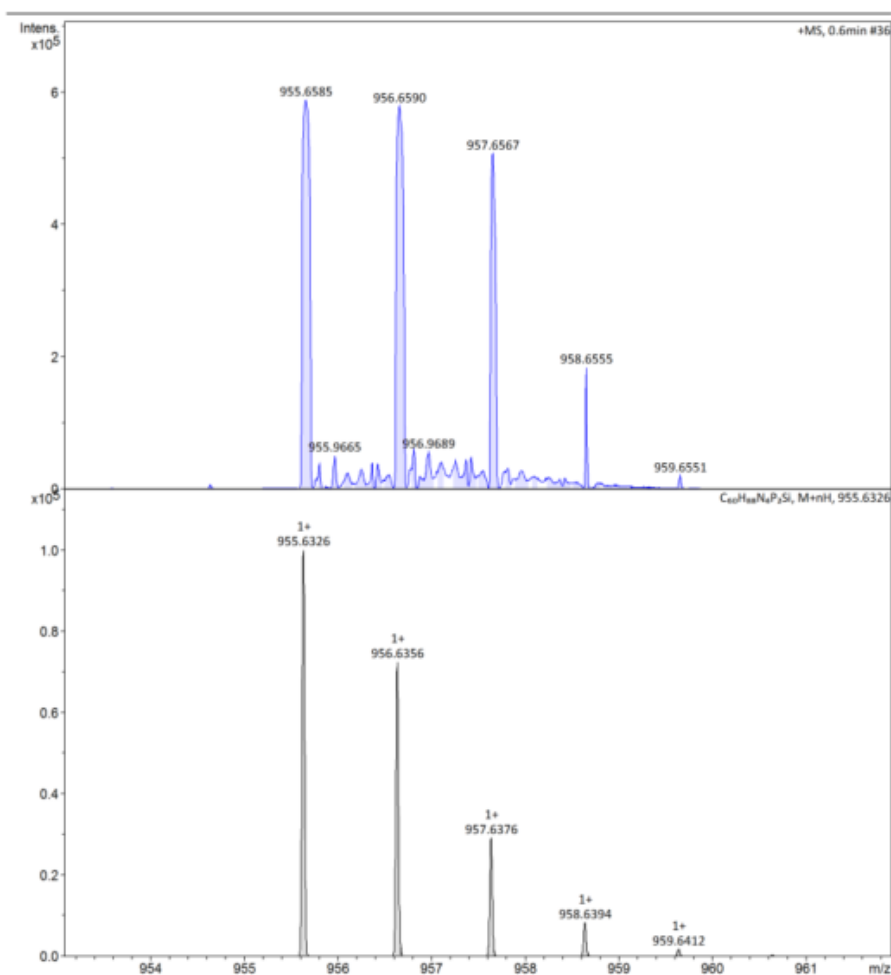


Figure S46.  $^{13}C$   $\{^1H\}$  NMR spectrum of **4** in  $C_6D_6$ .



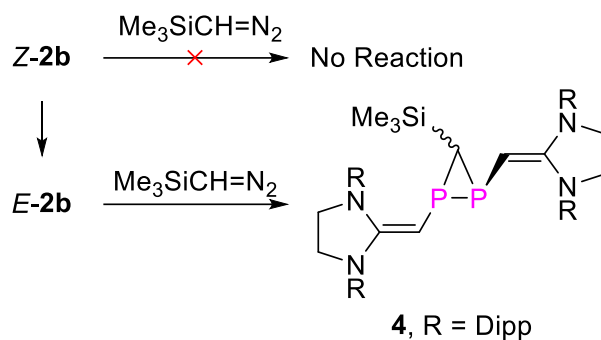


**Figure S47.**  $^{31}\text{P}$  NMR spectrum of **4** in  $\text{C}_6\text{D}_6$ .

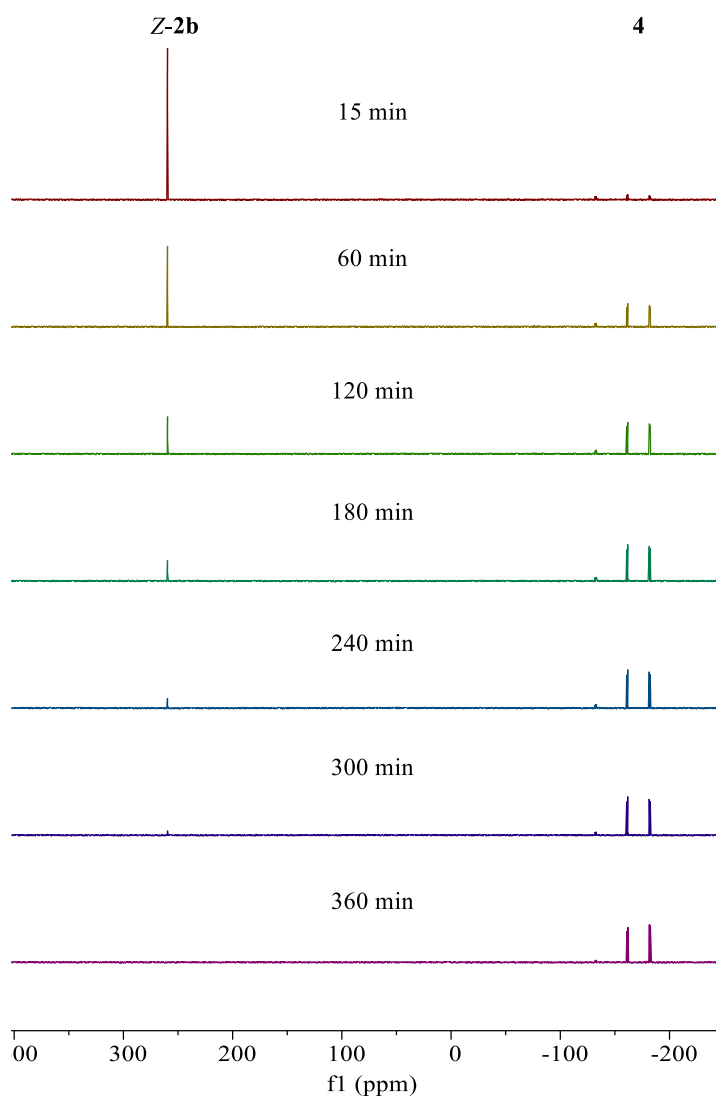


**Figure S48.** HRMS of **4**.

**The reaction of Z-2b with (Trimethylsilyl)diazomethane:**

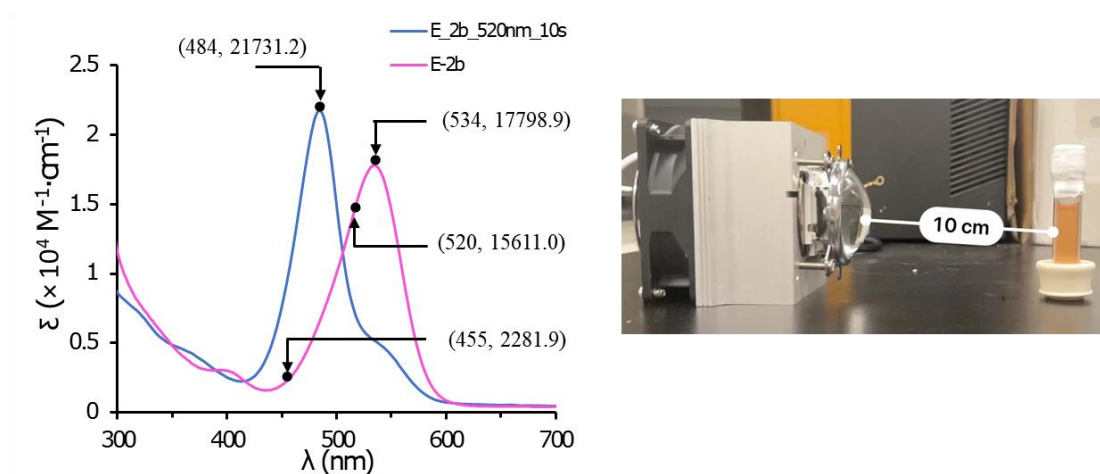


A drop of (Trimethylsilyl)diazomethane (2M in hexane) was added in the solution of Z-2b (10 mg) in C<sub>6</sub>D<sub>6</sub> (0.4 mL). The <sup>31</sup>P NMR monitoring shows below:

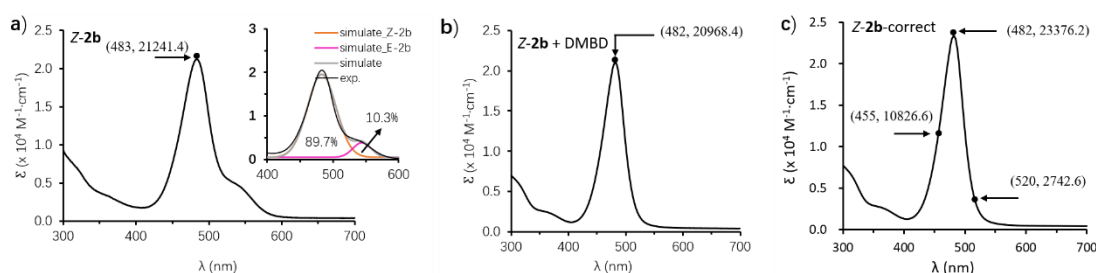


**Figure S49.** <sup>31</sup>P{<sup>1</sup>H} NMR spectra monitoring of the reaction of Z-2b with (Trimethylsilyl)diazomethane in C<sub>6</sub>D<sub>6</sub>.

## S2: UV-Vis spectral studies.



**Figure S50.** The UV-Vis spectra the toluene solution of *E-2b* (red), and after irradiated with LED light (520nm) for 10s. No apparent changes were observed after elongated irradiation.



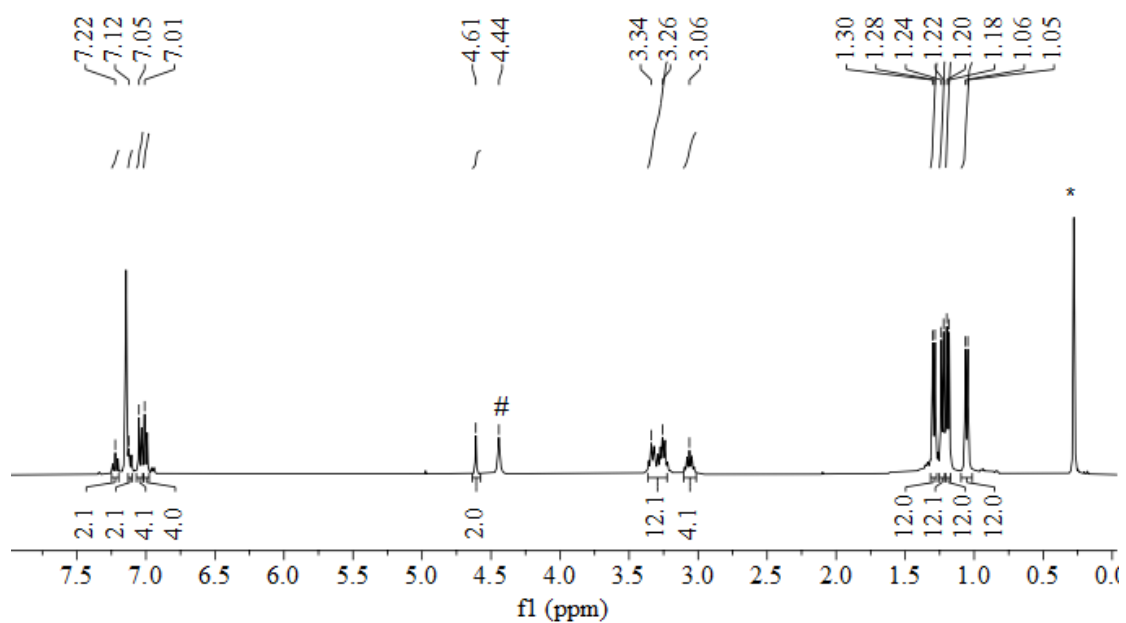
**Figure S51.** The UV-Vis spectra of a) the toluene solution of *Z-2b*, which always contain about 10% *E-2b*; b) this contamination of *E-2b* can be removed via add 0.24 equivalent of DMBD which is known to react with *E-2b* but not with *Z-2b*. Indeed, no apparent decrease of the absorption intensity was observed; c) thus the genuine absorption intensity of *Z-2b* could be obtained via the absorption intensity of [*Z-2b* + DMBD]/0.897.

## S3: Kinetic and thermodynamic studies.

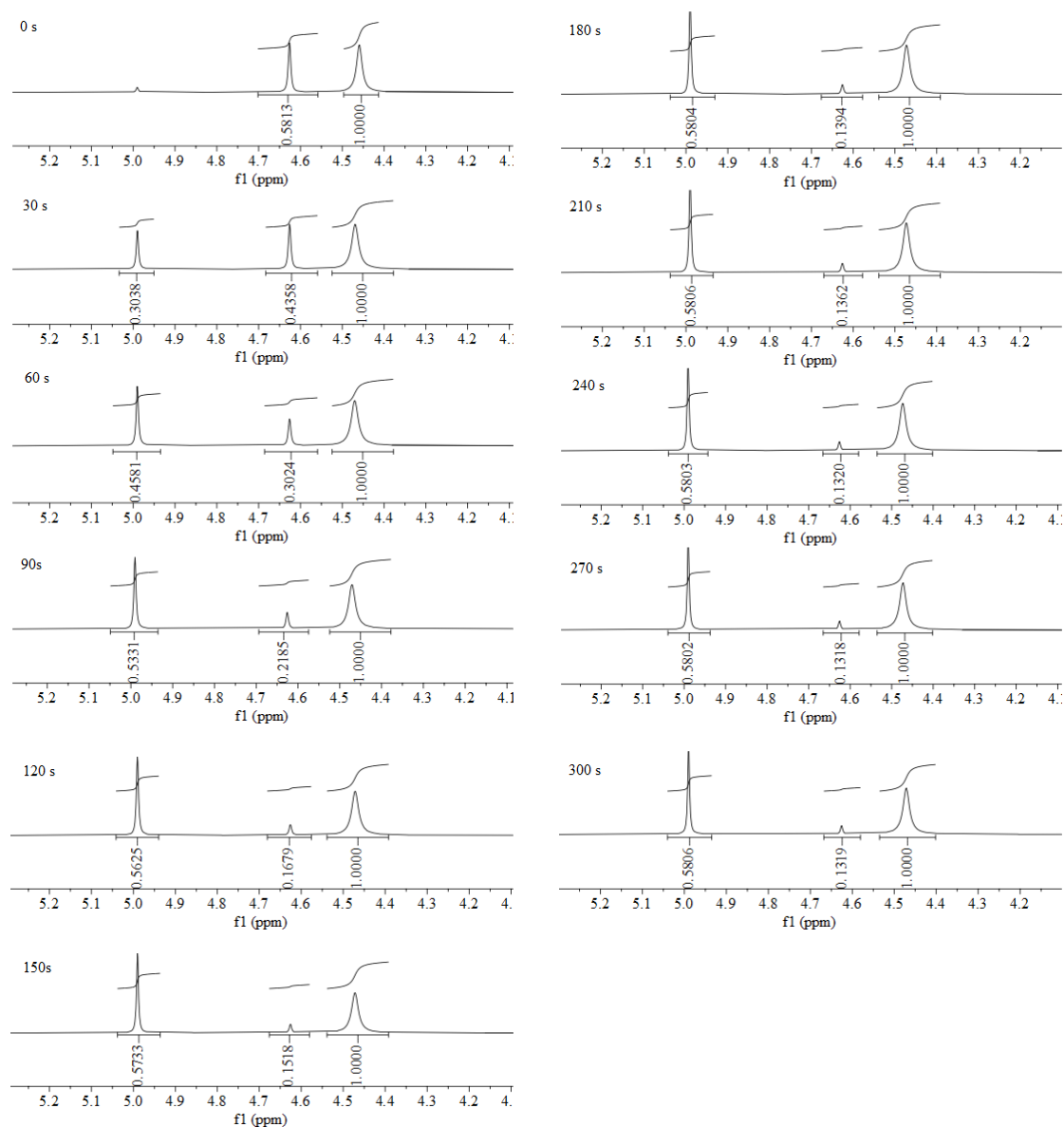
**General method for Determination of Rate Orders:** The order of dependence of each component of the reaction was determined by the method of initial rates. The reaction

was examined by plots of rate constant  $k$  against varying concentrations of *E-2b* or *Z-2b*.

**The *Z-2b* to *E-2b* isomerization irradiated at 455 nm:** *Z-2b* and internal standard hexamethylenetetramine were dissolved in  $C_6D_6$  and loaded in a dried J-Young NMR tube under nitrogen atmosphere at room temperature in dark. The reaction was monitored by NMR spectroscopy every 0.5 minutes under irradiation at 455 nm. According to the integration of reactant *Z-2b*, the concentration of *Z-2b* was plotted against time to determine  $k$  value. Based on results below, the reaction is determined to be first order.



**Figure S52.**  $^1H$  NMR of *Z-2b* and hexamethylenetetramine in  $C_6D_6$ .  
#hexamethylenetetramine. \*Silicon grease.



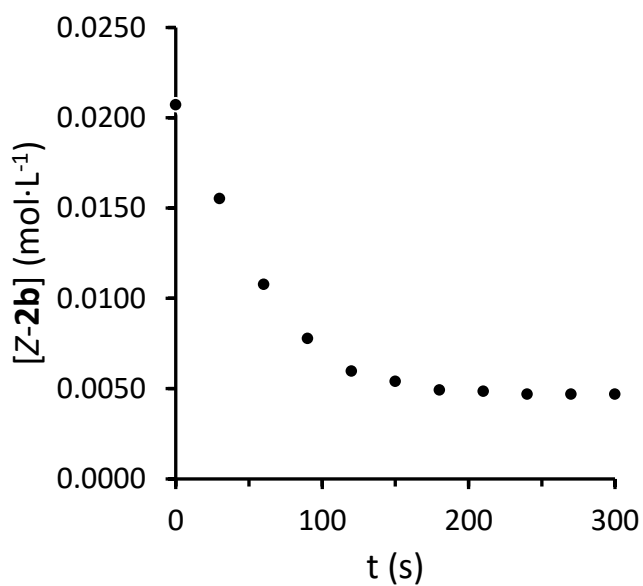
**Figure S53.**  $^1\text{H}$  NMR spectroscopic monitoring of the **Z-2b** to **E-2b** isomerization irradiated at 455 nm in  $\text{C}_6\text{D}_6$ .

**Table S1.** The **Z-2b** to **E-2b** isomerization irradiated at 455 nm in  $\text{C}_6\text{D}_6$ .

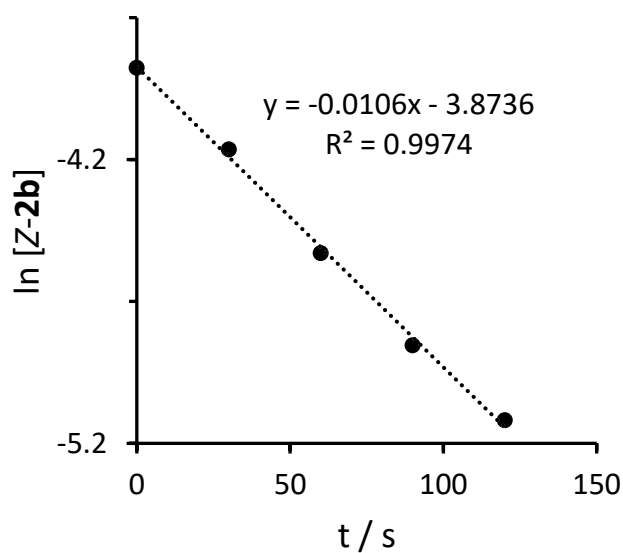
t (s)	integration $\int_{E-2b}$	integration $\int_{Z-2b}$	[ <b>E-2b</b> ] ( $\text{mol}\cdot\text{L}^{-1}$ )	[ <b>Z-2b</b> ] ( $\text{mol}\cdot\text{L}^{-1}$ )	$\ln[\text{E-2b}]$	$\ln[\text{Z-2b}]$
0	0.0000	0.5813	0.000000	0.020733	-	-3.876049
30	0.3038	0.4358	0.010835	0.015543	-4.524946	-4.164133
60	0.4581	0.3024	0.016339	0.010785	-4.114229	-4.529565
90	0.5331	0.2185	0.019013	0.007793	-3.962607	-4.854530
120	0.5625	0.1679	0.020062	0.005988	-3.908925	-5.117947

150	0.5733	0.1518	0.020447	0.005414	-3.889907	-5.218752
180	0.5804	0.1384	0.020700	0.004936	-3.877598	-5.311168
210	0.5806	0.1362	0.020708	0.004858	-3.877254	-5.327192
240	0.5803	0.1320	0.020697	0.004708	-3.877771	-5.358514
270	0.5802	0.1318	0.020693	0.004701	-3.877943	-5.360030
300	0.5806	0.1319	0.020708	0.004704	-3.877254	-5.359272

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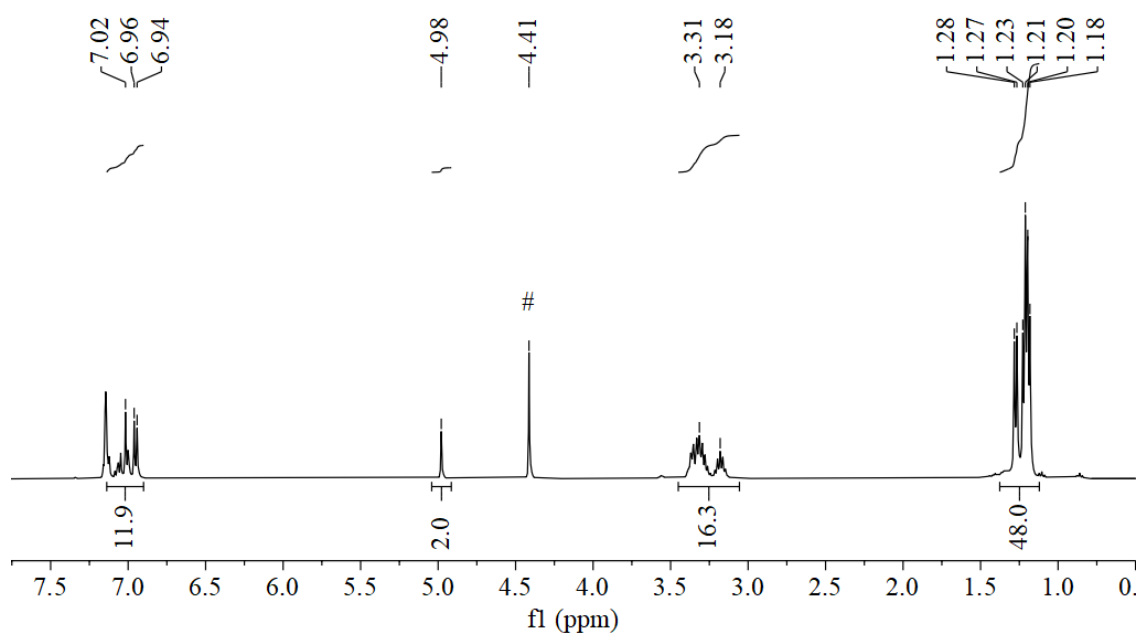


*Figure S54.* Kinetic curve.

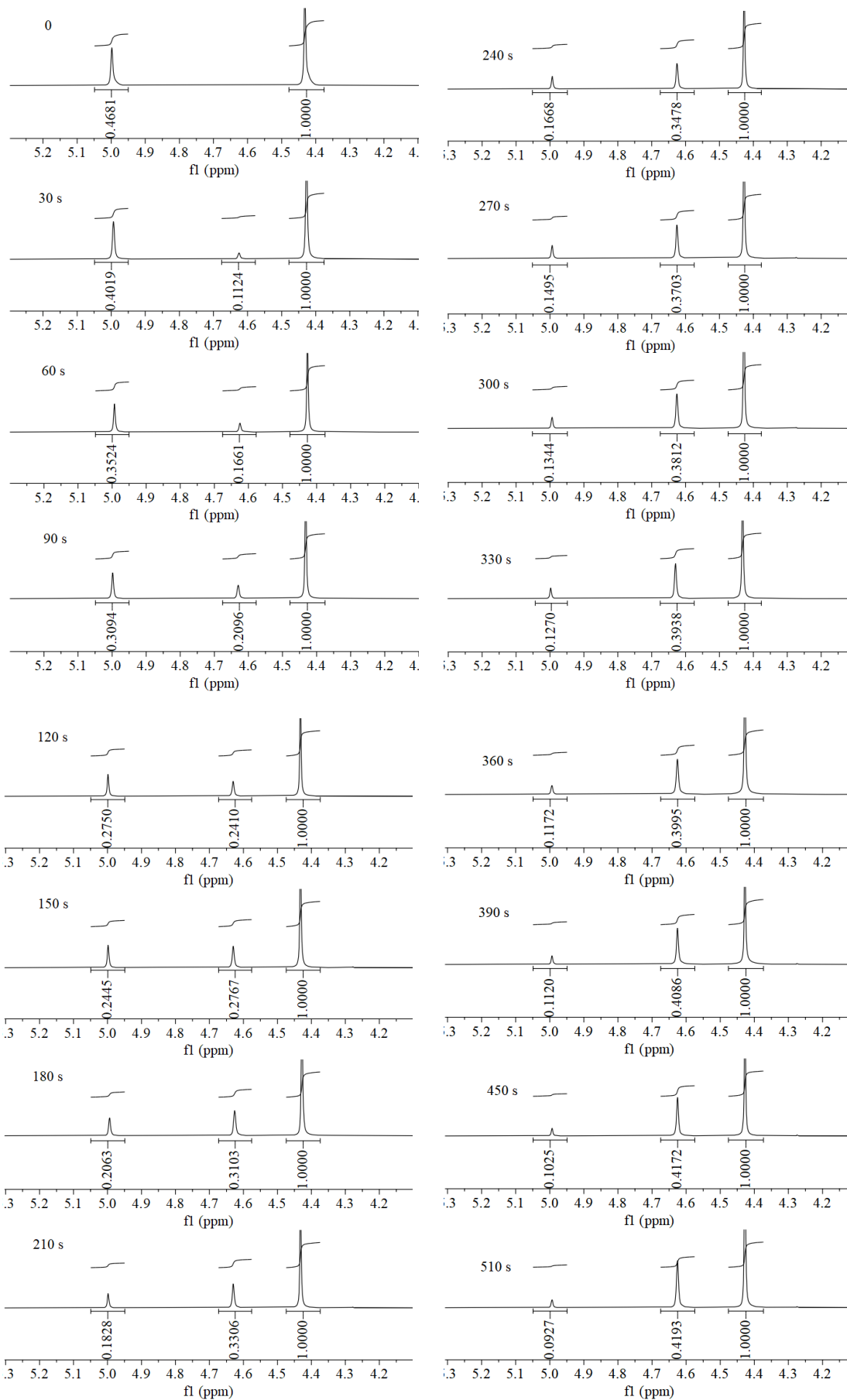


*Figure S55.* First order treatment of the kinetic curve.

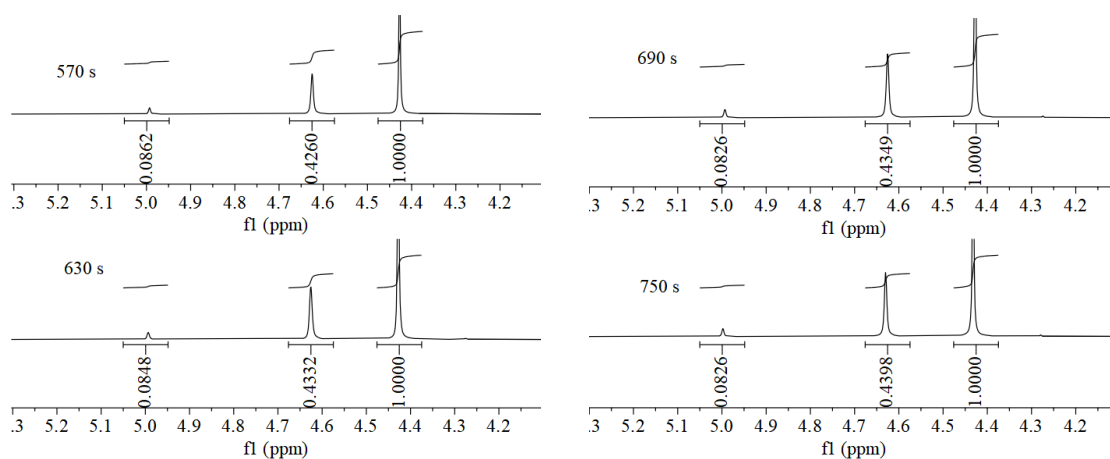
**The *E-2b* to *Z-2b* isomerization irradiated at 520 nm:** *E-2b* and internal standard hexamethylenetetramine were dissolved in C<sub>6</sub>D<sub>6</sub> and loaded in a dried J-Young NMR tube under nitrogen atmosphere at room temperature in dark. The reaction was monitored by NMR spectroscopy every 0.5 minutes to every 1 minutes under irradiation at 520nm. According to the integration of reactant *E-2b*, the concentration of *E-2b* was plotted against time to determine k value. Based on results below, the reaction is determined to be first order.



**Figure S56.** <sup>1</sup>H NMR of *E-2b* and hexamethylenetetramine in C<sub>6</sub>D<sub>6</sub>.  
#hexamethylenetetramine.







**Figure S57.**  $^1\text{H}$  NMR spectroscopic monitoring of the *E-2b* to *Z-2b* isomerization irradiated at 520 nm in  $\text{C}_6\text{D}_6$ .

**Table S2.** The *E-2b* to *Z-2b* isomerization irradiated at 520 nm in  $\text{C}_6\text{D}_6$ .

t (s)	integration $\int_{E-2b}$	integration $\int_{Z-2b}$	[ <i>E-2b</i> ] (mol·L <sup>-1</sup> )	[ <i>Z-2b</i> ] (mol·L <sup>-1</sup> )	ln[ <i>E-2b</i> ]	ln[ <i>Z-2b</i> ]
0	0.4681	0.0000	0.020034	0.000000	-3.910313	-
30	0.4019	0.1124	0.017201	0.004811	-4.062791	-5.336931
60	0.3524	0.1661	0.015082	0.007109	-4.194228	-4.946404
90	0.3094	0.2096	0.013242	0.008971	-4.324360	-4.713794
120	0.2750	0.2410	0.011770	0.010315	-4.442223	-4.574198
150	0.2445	0.2767	0.010464	0.011842	-4.559779	-4.436061
180	0.2063	0.3103	0.008829	0.013281	-4.729663	-4.321455
210	0.1828	0.3306	0.007824	0.014149	-4.850602	-4.258085
240	0.1668	0.3478	0.007139	0.014886	-4.942199	-4.207367
270	0.1495	0.3703	0.006398	0.015848	-5.051698	-4.144681
300	0.1344	0.3812	0.005752	0.016315	-5.158174	-4.115670
330	0.1270	0.3938	0.005435	0.016854	-5.214807	-4.083151
360	0.1172	0.3995	0.005016	0.017098	-5.295113	-4.068781
390	0.1120	0.4086	0.004793	0.017488	-5.340496	-4.046258
450	0.1025	0.4172	0.004387	0.017856	-5.429132	-4.025429
510	0.0927	0.4193	0.003967	0.017946	-5.529626	-4.020408
570	0.0862	0.4260	0.003689	0.018232	-5.602324	-4.004555
630	0.0848	0.4332	0.003629	0.018541	-5.618699	-3.987795
690	0.0826	0.4349	0.003535	0.018613	-5.644985	-3.983878

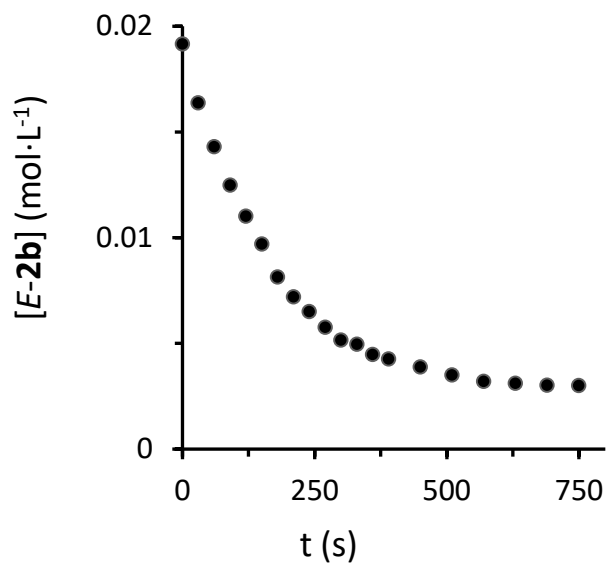


Figure S58. Kinetic curve.

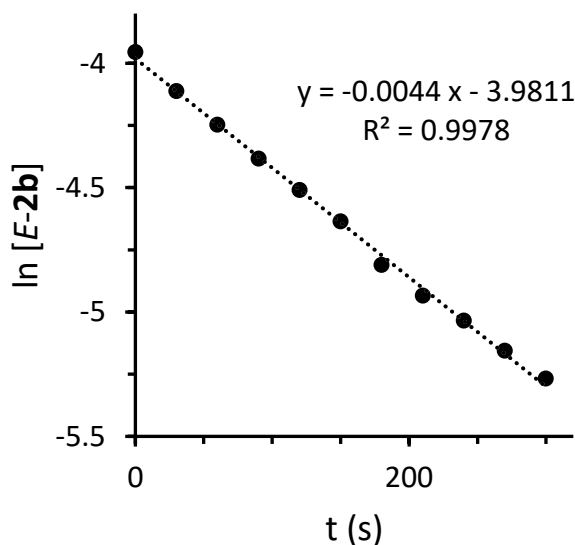
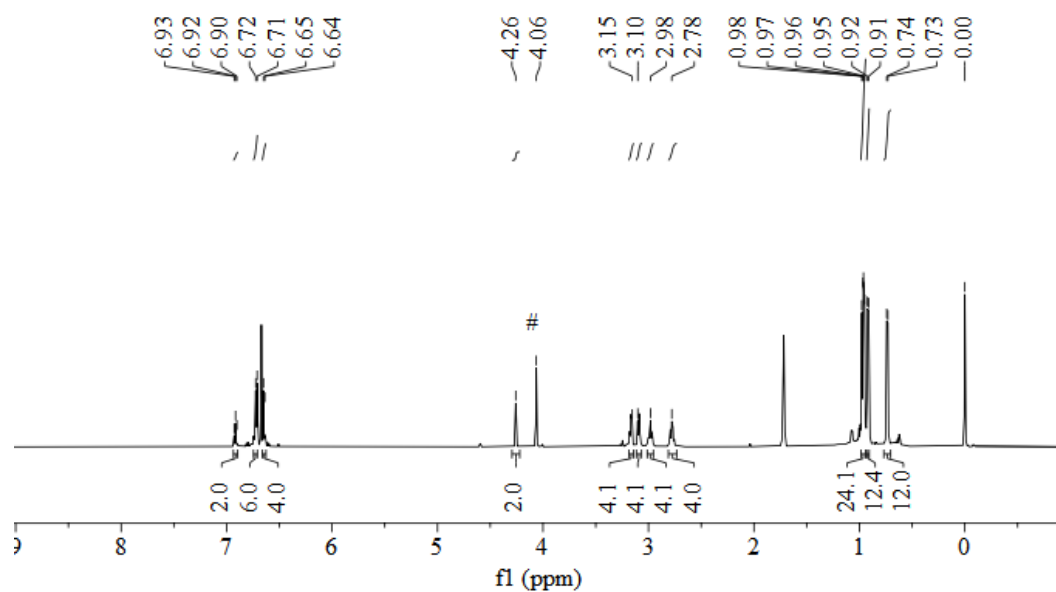


Figure S59. First order treatment of the kinetic curve.

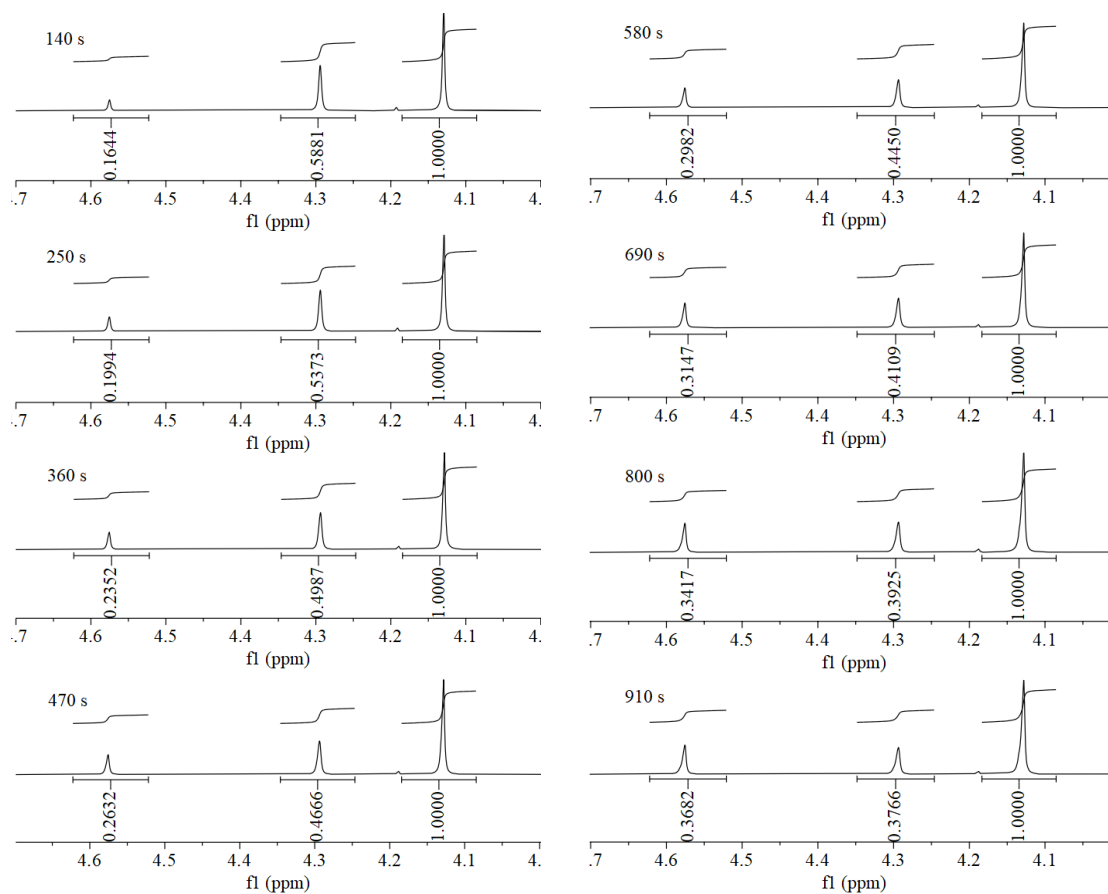
**The Z-2b to E-2b isomerization at 348.15 K:** Z-2b and internal standard hexamethylenetetramine were dissolved in *p*-Xylene-d<sub>10</sub> and loaded in a dried J-Young NMR tube under nitrogen atmosphere at room temperature. The reaction was monitored by NMR spectroscopy every 50 seconds to every 110 seconds at 348.15 K. According to the integration of reactant Z-2b, the concentration of Z-2b was plotted against time

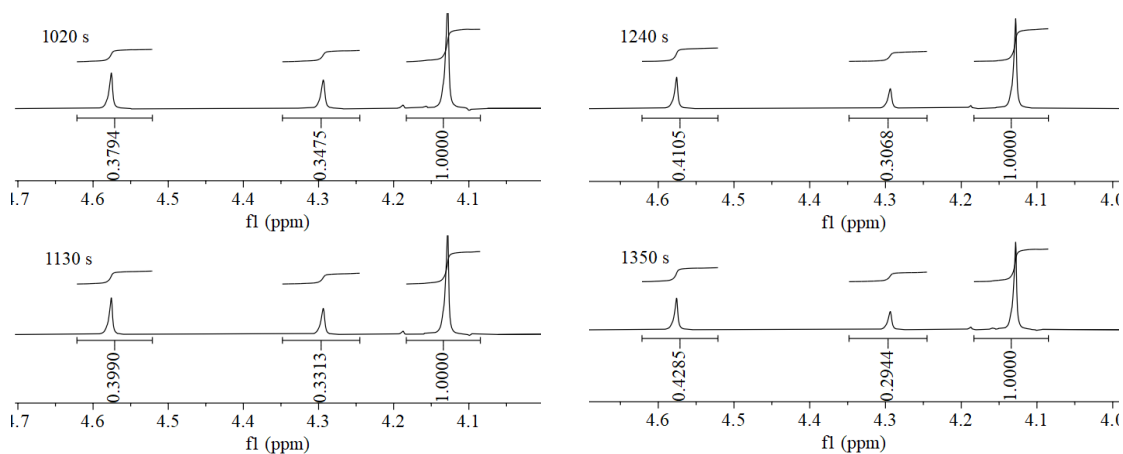
to determine k value. Based on results below, the reactions are determined to be first order.



**Figure S60.**  $^1\text{H}$  NMR spectrum of **Z-2b** and hexamethylenetetramine in *p*-Xylene- $d_{10}$ .

#hexamethylenetetramine.

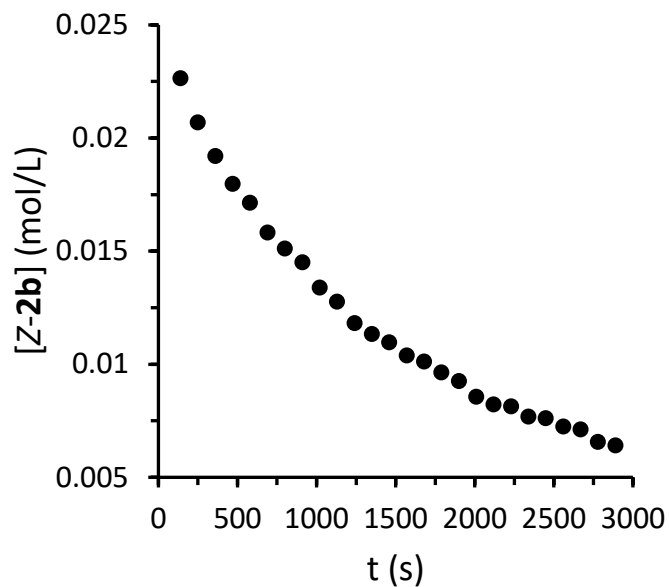




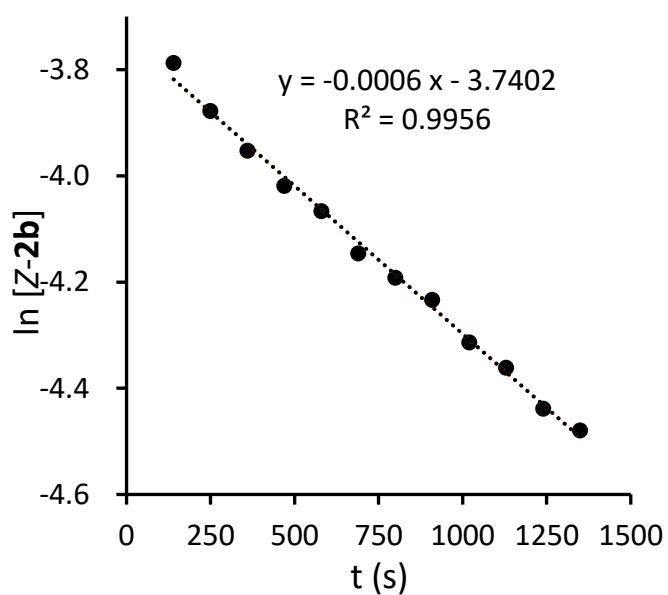
**Figure S61.**  $^1\text{H}$  NMR spectroscopic monitoring of the **Z-2b** to **E-2b** isomerization at 348.15 K in *p*-Xylene- $d_{10}$ .

**Table S4.** The **Z-2b** to **E-2b** isomerization at 348.15 K in *p*-Xylene- $d_{10}$ .

T (s)	integration $\int_{E-2b}$	integration $\int_{Z-2b}$	[ <b>E-2b</b> ] ( $\text{mol}\cdot\text{L}^{-1}$ )	[ <b>Z-2b</b> ] ( $\text{mol}\cdot\text{L}^{-1}$ )	$\ln[\text{E-2b}]$	$\ln[\text{Z-2b}]$
140	0.1643	0.5881	0.006329	0.022653	-5.062661	-3.787458
250	0.1994	0.5373	0.007681	0.020696	-4.869042	-3.877798
360	0.2352	0.4987	0.009060	0.019210	-4.703919	-3.952350
470	0.2632	0.4666	0.010138	0.017973	-4.591441	-4.018883
580	0.2982	0.4450	0.011486	0.017141	-4.466591	-4.066281
690	0.3147	0.4109	0.012122	0.015828	-4.412735	-4.146005
800	0.3417	0.3925	0.013162	0.015119	-4.330422	-4.191818
910	0.3682	0.3766	0.014183	0.014506	-4.255729	-4.233171
1020	0.3794	0.3475	0.014614	0.013385	-4.225764	-4.313590
1130	0.3990	0.3313	0.015369	0.012761	-4.175394	-4.361331
1240	0.4105	0.3068	0.015812	0.011818	-4.146979	-4.438159
1350	0.4285	0.2944	0.016505	0.011340	-4.104064	-4.479416



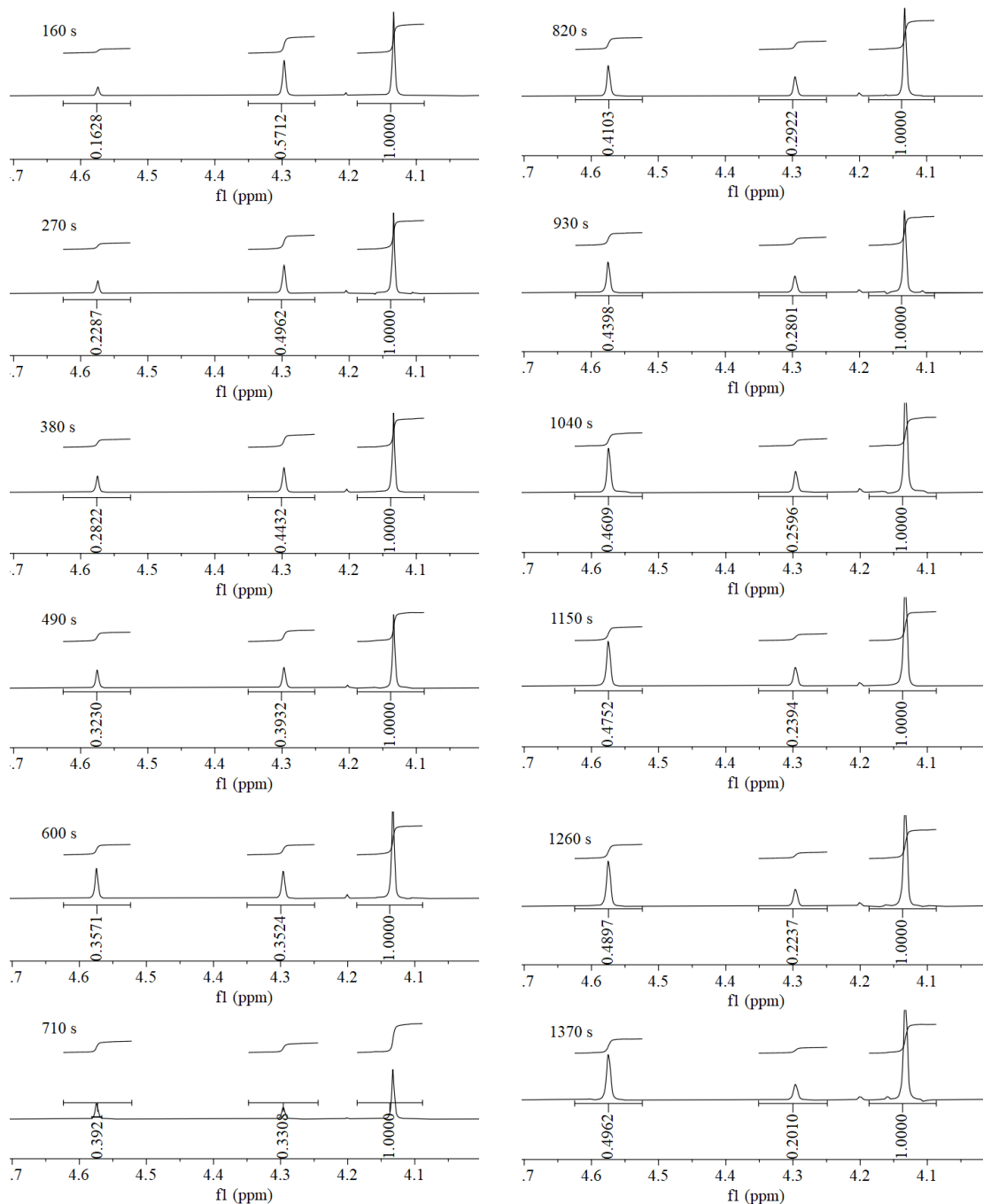
**Figure S62.** Kinetic curve.



**Figure S63.** First order treatment of the kinetic curve.

**General method for Eyring Plot:** Compound **Z-2b** (0.020 g, 0.0297 mmol) and internal standard hexamethylenetetramine (2mg) were dissolved in *p*-Xylene- $d_{10}$  (5 mL), the mixture was loaded into a dried J-Young NMR tube and sealed. The reaction was monitored from every 50 seconds to every 110 seconds over a range of temperature from 348.15 K to 373.15 K. Based on the integration of **Z-2b**, the concentration of **Z-2b** was plotted against time, which follows a pseudo-first order kinetic. The data of

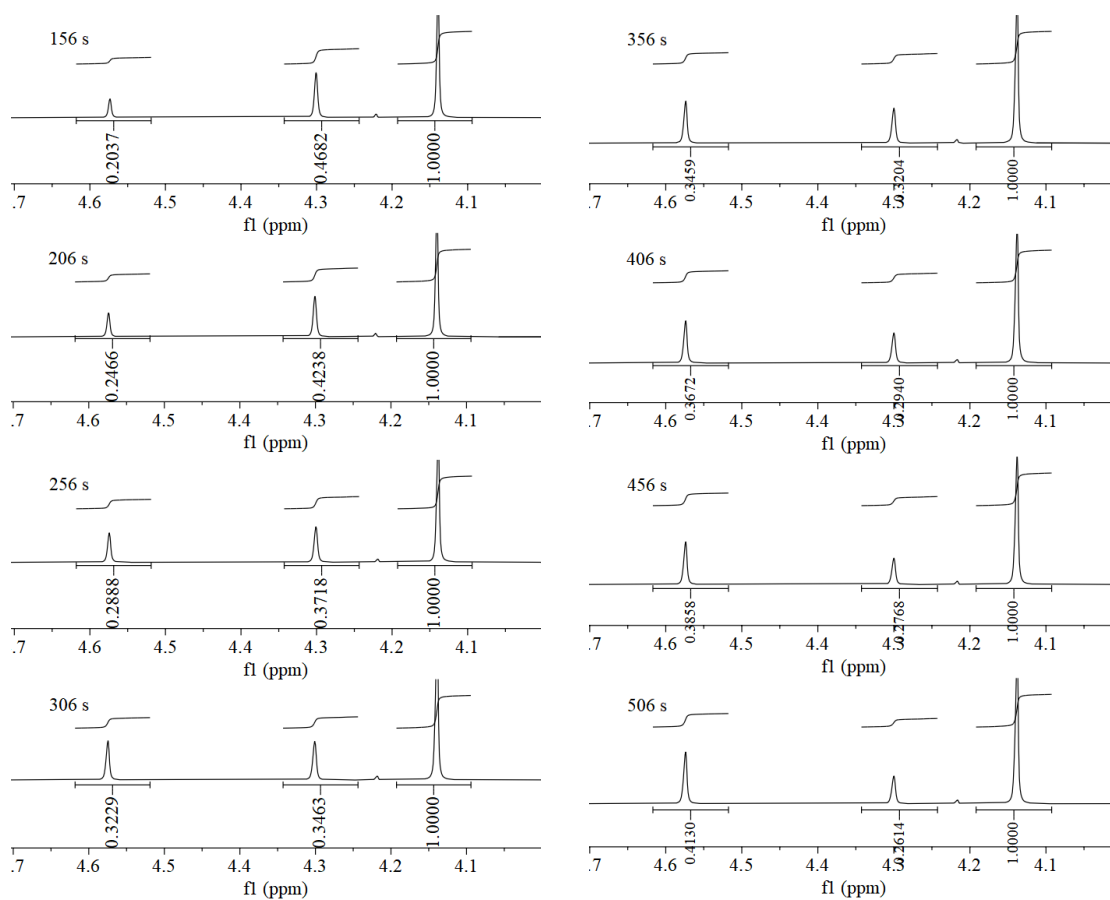
$\ln[E-2b]$  was plotted against time to determine  $k$  value. The Eyring Plot was also obtained based on the rate at each temperature and plotted against inverse of temperature.

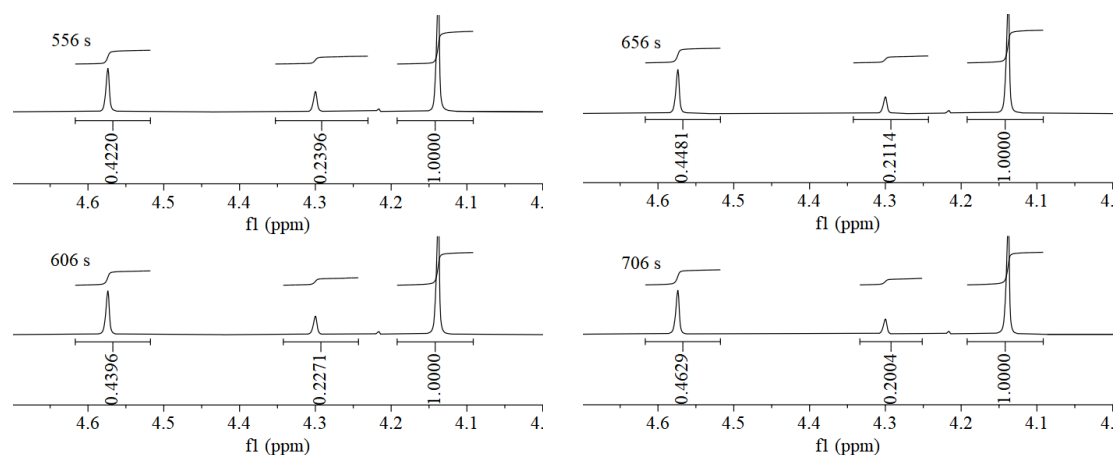


**Figure S64.**  $^1\text{H}$  NMR of the *Z-2b* to *E-2b* isomerization at 353.15 K in *p*-Xylene- $d_{10}$ .

**Table S5.** The table of the *Z-2b* to *E-2b* isomerization at 353.15 K in *p*-Xylene-*d*<sub>10</sub>.

t (s)	integration $\int_{E-2b}$	integration $\int_{Z-2b}$	[ <i>E-2b</i> ] (mol·L <sup>-1</sup> )	[ <i>Z-2b</i> ] (mol·L <sup>-1</sup> )	ln[ <i>E-2b</i> ]	ln[ <i>Z-2b</i> ]
160	0.1628	0.5712	0.006271	0.022002	-5.071832	-3.816616
270	0.2287	0.4962	0.008809	0.019113	-4.731944	-3.957376
380	0.2822	0.4432	0.010870	0.017072	-4.521739	-4.070334
490	0.3230	0.3932	0.012442	0.015146	-4.386703	-4.190037
600	0.3571	0.3524	0.013755	0.013574	-4.286339	-4.299588
710	0.3921	0.3308	0.015103	0.012742	-4.192838	-4.362841
820	0.4103	0.2922	0.015804	0.011255	-4.147466	-4.486916
930	0.4398	0.2801	0.016941	0.010789	-4.078035	-4.529208
1040	0.4609	0.2596	0.017753	0.010000	-4.031174	-4.605213
1150	0.4752	0.2394	0.018304	0.009221	-4.000619	-4.686219
1260	0.4897	0.2237	0.018863	0.008617	-3.970562	-4.754049
1370	0.4962	0.2010	0.019113	0.007742	-3.957376	-4.861050



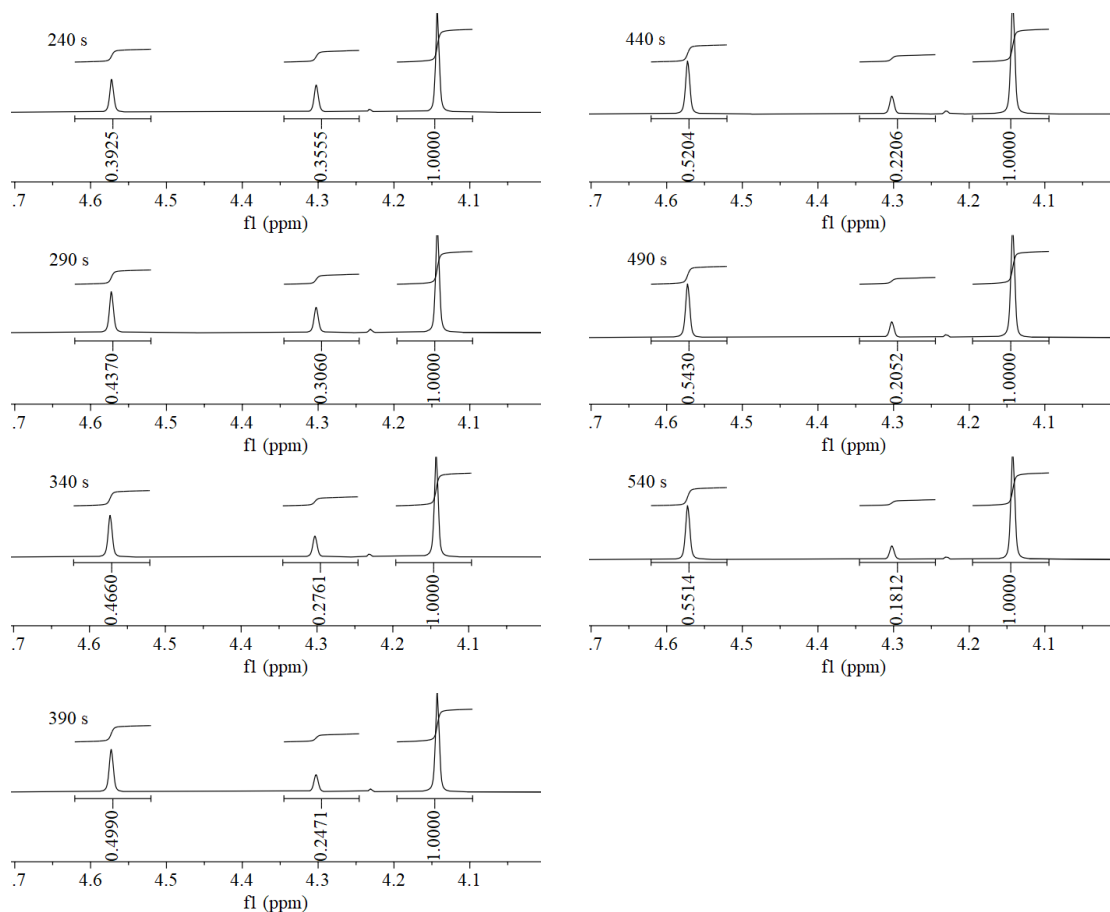


**Figure S65.**  $^1\text{H}$  NMR spectroscopic monitoring of the *Z-2b* to *E-2b* isomerization at 358.15 K in *p*-Xylene- $d_{10}$ .

**Table S6.** The table of the *Z-2b* to *E-2b* isomerization at 358.15 K in *p*-Xylene- $d_{10}$ .

t (s)	integration $\int_{E-2b}$	integration $\int_{Z-2b}$	[ <i>E-2b</i> ] ( $\text{mol}\cdot\text{L}^{-1}$ )	[ <i>Z-2b</i> ] ( $\text{mol}\cdot\text{L}^{-1}$ )	$\ln[E-2b]$	$\ln[Z-2b]$
156	0.2037	0.4682	0.007846	0.018035	-4.847707	-4.015459
206	0.2466	0.4238	0.009499	0.016324	-4.656587	-4.115093
256	0.2888	0.3718	0.011124	0.014321	-4.498621	-4.245999
306	0.3229	0.3464	0.012438	0.013343	-4.387012	-4.316761
356	0.3459	0.3204	0.013324	0.012342	-4.318205	-4.394785
406	0.3672	0.2940	0.014144	0.011325	-4.258448	-4.480775
456	0.3858	0.2768	0.014861	0.010662	-4.209036	-4.541060
506	0.4130	0.2614	0.015908	0.010069	-4.140907	-4.598303
556	0.4220	0.2396	0.016255	0.009229	-4.119350	-4.685384
606	0.4396	0.2271	0.016933	0.008748	-4.078490	-4.738964
656	0.4484	0.2114	0.017272	0.008143	-4.058669	-4.810603
706	0.4629	0.2004	0.017831	0.007719	-4.026844	-4.864040

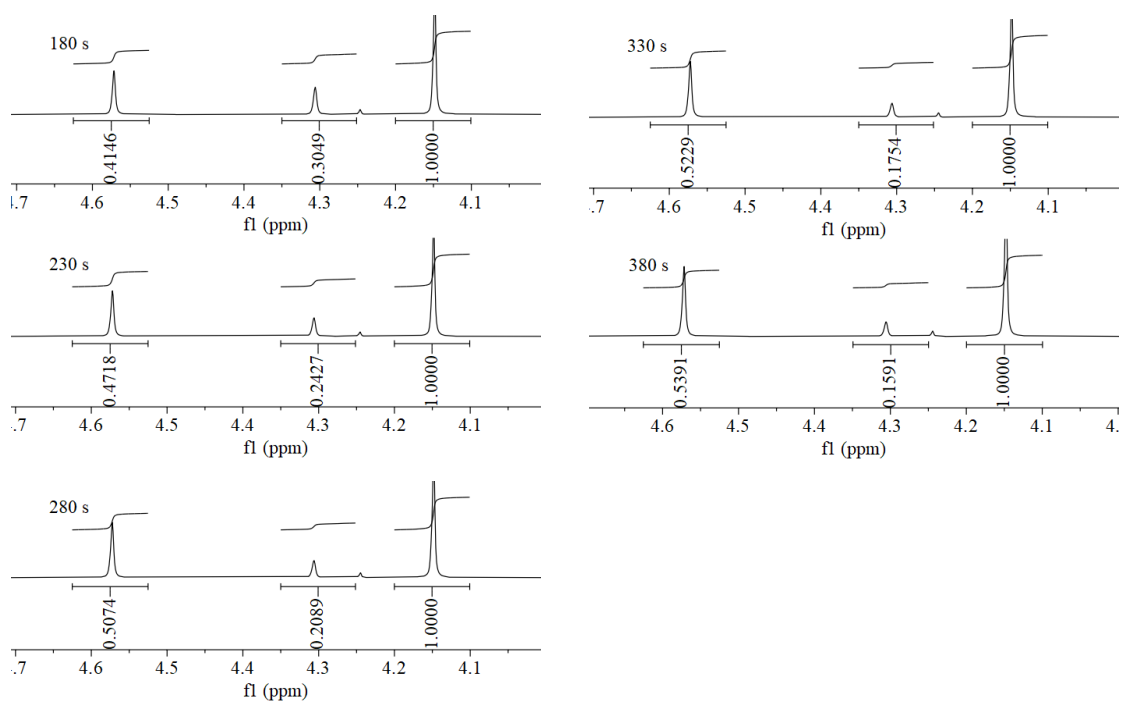




**Figure S66.** The  $^1\text{H}$  NMR spectroscopic monitoring the **Z-2b** to **E-2b** isomerization at 363.15 K in *p*-Xylene- $d_{10}$ .

**Table S7.** The table of the **Z-2b** to **E-2b** isomerization at 363.15 K in *p*-Xylene- $d_{10}$ .

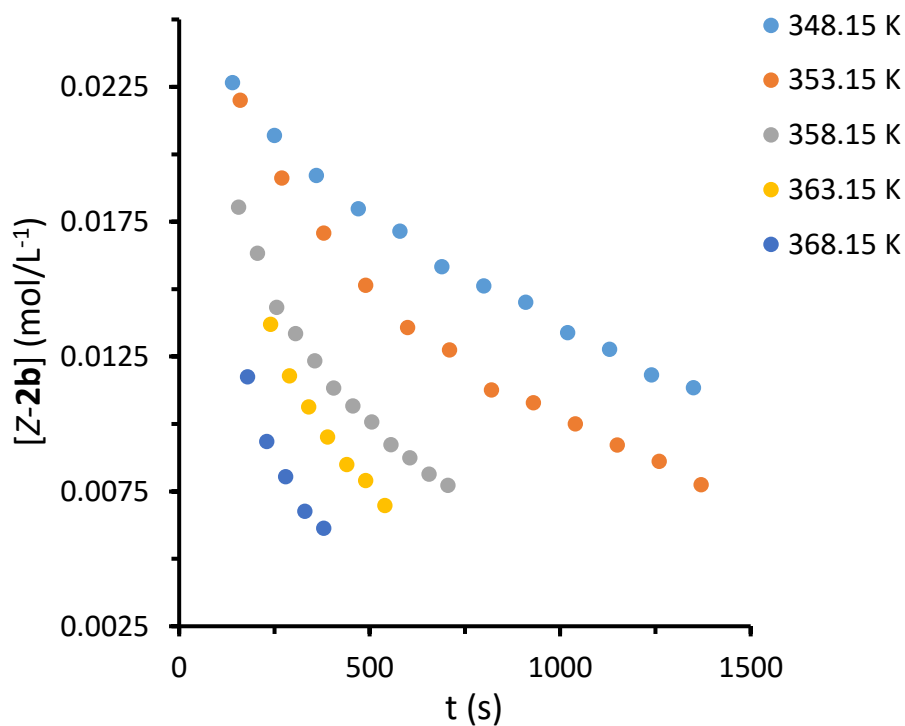
t (s)	integration $\int_{E-2b}$	integration $\int_{Z-2b}$	[ <b>E-2b</b> ] (mol·L $^{-1}$ )	[ <b>Z-2b</b> ] (mol·L $^{-1}$ )	ln[ <b>E-2b</b> ]	ln[ <b>Z-2b</b> ]
240	0.3925	0.3555	0.015119	0.013694	-4.191818	-4.290830
290	0.4370	0.3060	0.016833	0.011787	-4.084422	-4.440770
340	0.4660	0.2761	0.017950	0.010635	-4.020169	-4.543592
390	0.4990	0.2471	0.019221	0.009518	-3.951749	-4.654562
440	0.5204	0.2206	0.020045	0.008497	-3.909757	-4.768004
490	0.5430	0.2052	0.020916	0.007904	-3.867246	-4.840370
540	0.5514	0.1812	0.021239	0.006980	-3.851894	-4.964754



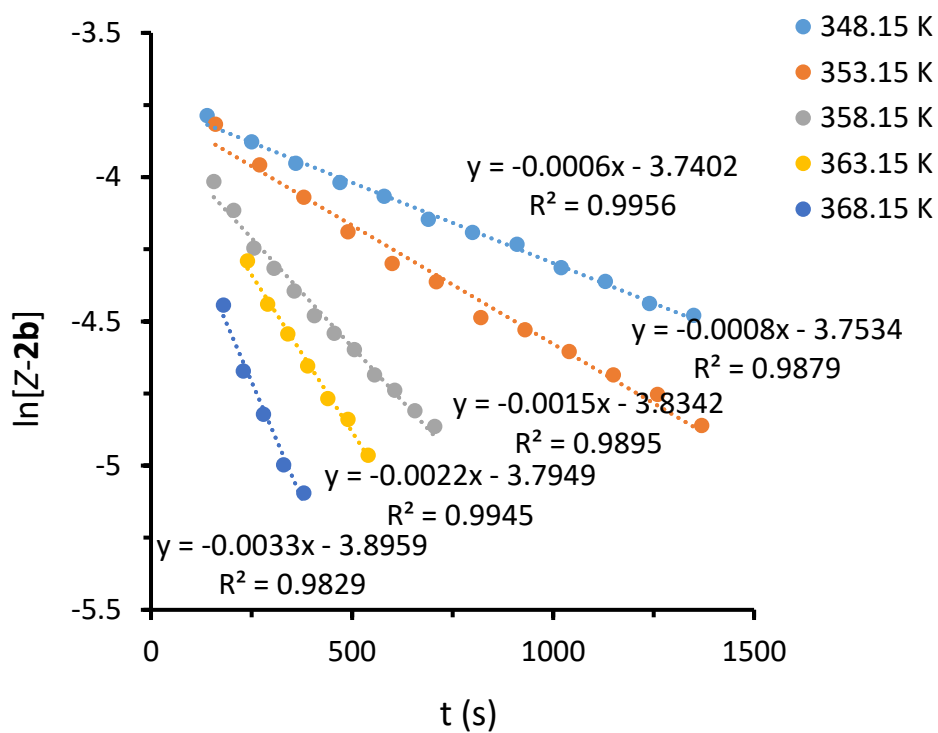
**Figure S67.**  $^1\text{H}$  NMR spectroscopic monitoring of the *Z-2b* to *E-2b* isomerization at 368.15 K in *p*-Xylene- $d_{10}$ .

**Table S8.** The table of the *Z-2b* to *E-2b* isomerization at 368.15 K in *p*-Xylene- $d_{10}$ .

t (s)	integration $\int_{E-2b}$	integration $\int_{Z-2b}$	[ <i>E-2b</i> ] (mol·L <sup>-1</sup> )	[ <i>Z-2b</i> ] (mol·L <sup>-1</sup> )	ln[ <i>E-2b</i> ]	ln[ <i>Z-2b</i> ]
180	0.4146	0.3049	0.015970	0.011744	-4.137041	-4.444371
230	0.4718	0.2427	0.018173	0.009349	-4.007800	-4.672529
280	0.5074	0.2089	0.019545	0.008047	-3.935055	-4.822499
330	0.5229	0.1754	0.020142	0.006756	-3.904965	-4.997286
380	0.5391	0.1591	0.020766	0.006128	-3.874454	-5.094822



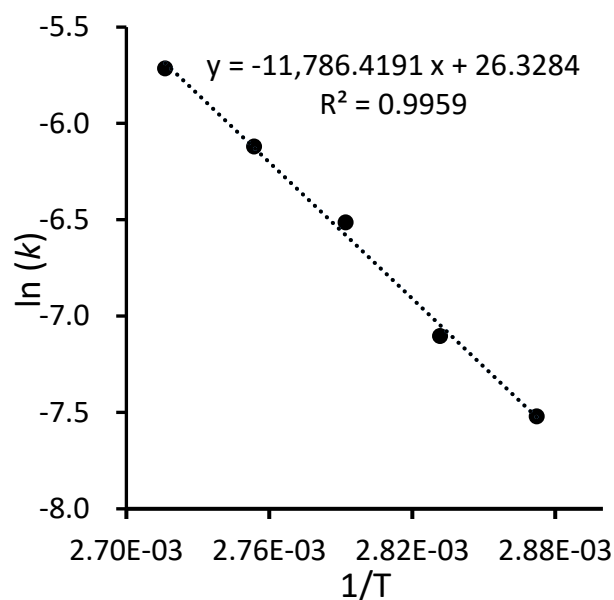
**Figure S68.** Plot of concentration of **Z-2b** against time at different temperatures.



**Figure S69.** Plot of concentration of  $\text{Ln}[Z-2b]$  against time at different temperatures.

**Table S9.** The summary of Eyring plot of the **Z-2b** to **E-2b** isomerization.

T (K)	1 / T (K <sup>-1</sup> )	k (s <sup>-1</sup> )	k / T (K * s <sup>-1</sup> )	ln (k / T)	lnk
348.15	0.002872325	0.0005422	1.55737E-06	-13.3725090	-7.519876
353.15	0.002831658	0.0008228	2.32989E-06	-12.9696903	-7.102797
358.15	0.002792126	0.001485	4.14659E-06	-12.3932250	-6.512273
363.15	0.002753683	0.002200	6.0581E-06	-12.0141138	-6.119298
368.15	0.002716284	0.003300	8.96374E-06	-11.6223232	-5.713833

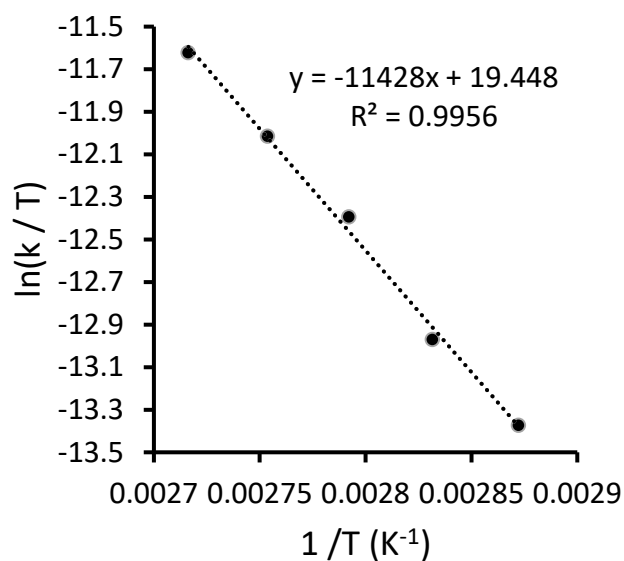


$$A = 2.72 \times 10^{11}$$

$$E_a = 23.4 \pm 0.9 \text{ kcal/mol}$$

$$k = (2.72 \times 10^{11}) \exp[(-2.34 \times 10^4)/RT]$$

**Figure S70.** Arrhenius equation of the **Z-2b** to **E-2b** isomerization



$$\Delta H^\ddagger = 22.7 \pm 0.9 \text{ kcal/mol}$$

$$\Delta S^\ddagger = -8.6 \pm 2.4 \text{ e.u.}$$

$$\Delta G^\ddagger (298) = 25.3 \pm 1.6 \text{ kcal/mol}$$

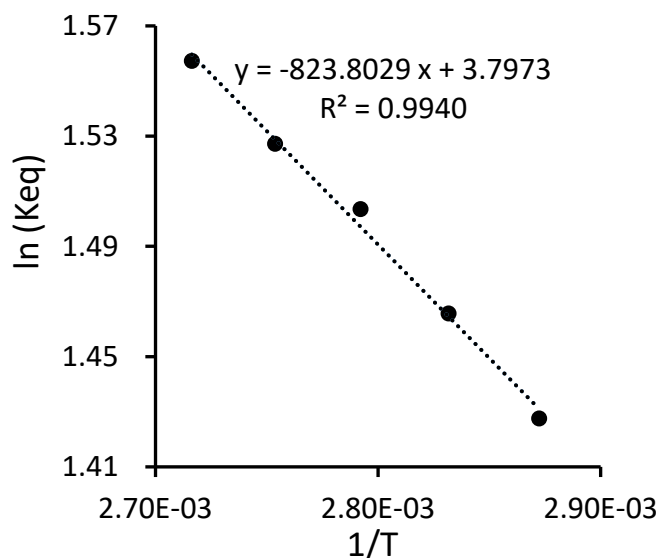
**Figure S71.** Eyring plot of the **Z-2b** to **E-2b** isomerization.

**Van't Hoff Analysis :** Compound **Z-2b** (0.020 g, 0.0297 mmol) and internal standard hexamethylenetetramine (2 mg) were dissolved in *p*-Xylene- $d_{10}$  (5 mL), the mixture was loaded into a dried J-Young NMR tube and sealed. The reaction was monitored by  $^1\text{H}$  NMR spectra over a range of temperature from 348.15 K to 368.15 K.

**Table S10.** The summary of Van't Hoff Analysis of the **Z-2b** to **E-2b** isomerization.

T (K)	1/T (K <sup>-1</sup> )	K <sub>eq</sub>	lnK <sub>eq</sub>
348.15	0.002872325	4.168331	1.427515716
353.15	0.002831658	4.330515	1.465686473
358.15	0.002792126	4.497394	1.503498118
363.15	0.002753683	4.605240	1.527194786
368.15	0.002716284	4.745790	1.557257909

$\Delta H$  and  $\Delta S$  were determined by use of the Van't Hoff equation from the slope and the intercept of the plot of  $\ln(K_{eq})$  versus  $1/T$ .  $\Delta G$  was calculated according to Gibb's Free Energy equation.



$$\Delta G = -0.61 \pm 0.13 \text{ kcal/mol}$$

$$\Delta H = 1.64 \pm 0.07 \text{ kcal/mol}$$

$$\Delta S = 7.55 \pm 0.20 \text{ e.u.}$$

**Figure S72.** Van't Hoff Analysis of the **Z-2b** to **E-2b** isomerization.

## S4. X-Ray diffraction studies

These data can be obtained free of charge via <http://www.ccdc.cam.ac.uk/cgi-bin/catreq.cgi>, or by emailing [data\\_request@ccdc.cam.ac.uk](mailto:data_request@ccdc.cam.ac.uk). The CCDC reference numbers are 2245822-2245824 and 2270969-2270971.

**Table S11.** The summary of crystal data and structure refinement

Compounds	<i>E-2a</i>	<i>E-2b</i>	<i>Z-2b</i>
CCDC	2245822	2245823	2245824
Empirical formula	C <sub>12</sub> H <sub>17</sub> N <sub>8</sub> P <sub>4</sub>	C <sub>5</sub> H <sub>7</sub> N <sub>4</sub> P <sub>2</sub>	C <sub>5</sub> H <sub>7</sub> N <sub>4</sub> P <sub>2</sub>
Formula weight	1866.57	869.16	869.16
Temperature/K	150.00(10)	149.99(10)	151(1)
Crystal system	triclinic	triclinic	monoclinic

Space group	P-1	P-1	P2 <sub>1</sub> /c
a/Å	10.8467(3)	10.9009(6)	10.7687(5)
b/Å	15.6202(4)	20.4655(12)	13.0866(5)
c/Å	18.4959(4)	26.2304(11)	36.6199(17)
α/°	65.623(2)	108.695(5)	90
β/°	86.626(2)	90.684(4)	94.360(4)
γ/°	86.202(2)	97.490(5)	90
Volume/Å <sup>3</sup>	2846.36(13)	5486.8(5)	5145.7(4)
Z	1	4	4
ρ <sub>calc</sub> /cm <sup>3</sup>	1.089	1.052	1.122
μ/mm <sup>-1</sup>	0.116	0.116	0.124
F(000)	1018.0	1888.0	1888.0
Crystal size/mm <sup>3</sup>	0.15 × 0.15 × 0.05	0.12 × 0.09 × 0.08	0.02 × 0.02 × 0.01
Radiation	Mo Kα (λ = 0.71073)	Mo Kα (λ = 0.71073)	Mo Kα (λ = 0.71073)
2θ range for data collection/°	5.732 to 59.926	5.512 to 59.716	5.096 to 59.854
Index ranges	-15 ≤ h ≤ 15, -20 ≤ k ≤ 21, -25 ≤ l ≤ 25	-14 ≤ h ≤ 15, -28 ≤ k ≤ 28, -35 ≤ l ≤ 36	-13 ≤ h ≤ 15, -18 ≤ k ≤ 18, -50 ≤ l ≤ 48
Reflections collected	61291	124812	65194
Independent reflections	14866 [R <sub>int</sub> = 0.0538, R <sub>sigma</sub> = 0.0439]	28328 [R <sub>int</sub> = 0.1663, R <sub>sigma</sub> = 0.1573]	13404 [R <sub>int</sub> = 0.0691, R <sub>sigma</sub> = 0.0585]
Data/restraints/parameters	14866/0/633	28328/0/1149	13404/0/575
Goodness-of-fit on F <sup>2</sup>	1.030	0.949	1.014
Final R indexes [I ≥ 2σ (I)]	R <sub>1</sub> = 0.0488, wR <sub>2</sub> = 0.1201	R <sub>1</sub> = 0.0728, wR <sub>2</sub> = 0.1639	R <sub>1</sub> = 0.0519, wR <sub>2</sub> = 0.1109
Final R indexes [all data]	R <sub>1</sub> = 0.0702, wR <sub>2</sub> = 0.1307	R <sub>1</sub> = 0.1833, wR <sub>2</sub> = 0.2030	R <sub>1</sub> = 0.0792, wR <sub>2</sub> = 0.1186
Largest diff. peak/hole / e Å <sup>-3</sup>	0.46/-0.28	1.14/-0.46	0.34/-0.33
<hr/>			
Compounds	AuCl( <b>2b</b> )	<b>3</b>	<b>4</b>
CCDC	2270969	2270970	2270971
Empirical formula	C <sub>68</sub> H <sub>87</sub> AuClF <sub>2</sub> N <sub>4</sub> P <sub>2</sub>	C <sub>62</sub> H <sub>88</sub> N <sub>4</sub> P <sub>2</sub>	C <sub>129</sub> H <sub>197</sub> N <sub>8</sub> P <sub>4</sub> Si <sub>2</sub>
Formula weight	1292.77	951.30	2039.99
Temperature/K	149.99(10)	150.00(10)	150.00
Crystal system	monoclinic	monoclinic	monoclinic
Space group	P2 <sub>1</sub> /c	P2 <sub>1</sub> /c	P2 <sub>1</sub> /c
a/Å	13.8709(9)	12.9163(17)	12.1506(7)
b/Å	20.0194(14)	14.6645(10)	26.0299(16)
c/Å	23.2162(14)	31.890(3)	21.3810(14)

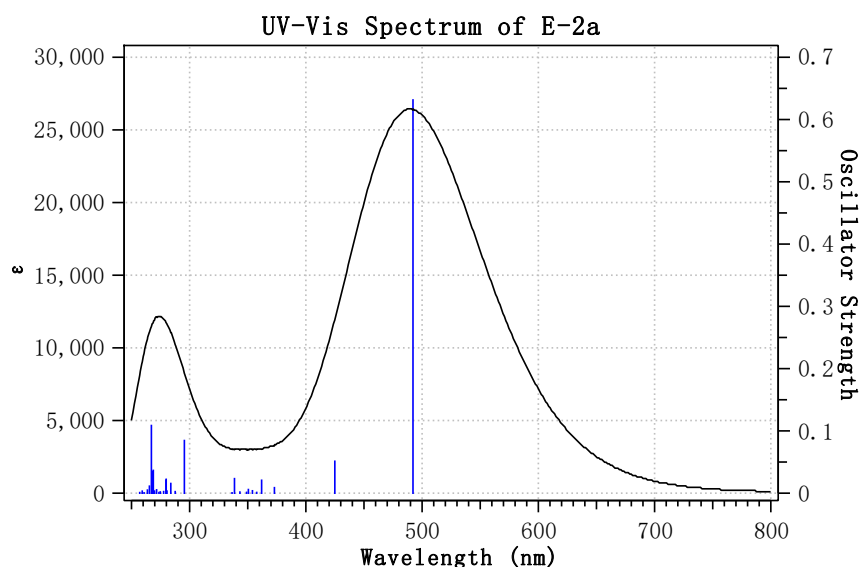
$\alpha/^\circ$	90	90	90
$\beta/^\circ$	98.502(6)	100.295(13)	93.965(3)
$\gamma/^\circ$	90	90	90
Volume/ $\text{\AA}^3$	6376.0(7)	5943.0(11)	6746.2(7)
Z	4	4	2
$\rho_{\text{calc}}/\text{cm}^3$	1.347	1.063	1.004
$\mu/\text{mm}^{-1}$	2.448	0.112	0.119
F(000)	2668.0	2072.0	2230.0
Crystal size/ $\text{mm}^3$	$0.12 \times 0.1 \times 0.05$	$0.5 \times 0.5 \times 0.4$	$0.12 \times 0.08 \times 0.05$
Radiation	Mo K $\alpha$ ( $\lambda = 0.71073$ )	Mo K $\alpha$ ( $\lambda = 0.71073$ )	MoK $\alpha$ ( $\lambda = 0.71073$ )
2 $\theta$ range for data collection/ $^\circ$	5.354 to 59.636	4.784 to 59.724	2.468 to 54.33
Index ranges	$-19 \leq h \leq 18, -27 \leq k \leq 27, -32 \leq l \leq 31$	$-17 \leq h \leq 17, -20 \leq k \leq 20, -43 \leq l \leq 42$	$-15 \leq h \leq 14, -33 \leq k \leq 33, -27 \leq l \leq 27$
Reflections collected	93106	50772	73462
Independent reflections	16888 [ $R_{\text{int}} = 0.0908, R_{\text{sigma}} = 0.0698$ ]	14724 [ $R_{\text{int}} = 0.0793, R_{\text{sigma}} = 0.0691$ ]	14514 [ $R_{\text{int}} = 0.0746, R_{\text{sigma}} = 0.0588$ ]
Data/restraints/parameters	16888/24/690	14724/0/631	14514/6/692
Goodness-of-fit on $F^2$	1.007	1.041	1.059
Final R indexes [ $I \geq 2\sigma(I)$ ]	$R_1 = 0.0447, wR_2 = 0.0984$	$R_1 = 0.0550, wR_2 = 0.1400$	$R_1 = 0.0985, wR_2 = 0.2662$
Final R indexes [all data]	$R_1 = 0.0885, wR_2 = 0.1146$	$R_1 = 0.0870, wR_2 = 0.1557$	$R_1 = 0.1343, wR_2 = 0.2909$
Largest diff. peak/hole / $e \text{\AA}^{-3}$	1.76/-0.64	0.35/-0.26	1.08/-0.48

## S5: Theoretical details

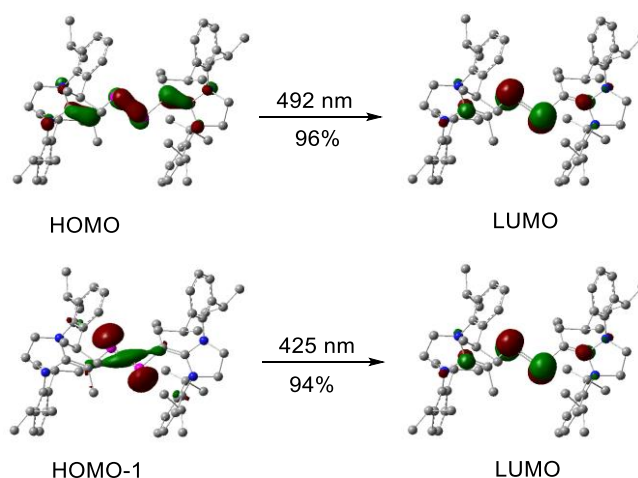
Geometry optimizations were performed using the Gaussian09 optimizer.<sup>[2]</sup> All geometry optimizations were computed using the functional M06-2X or BP86 functional. The Def2-SVP basis set was used for all the atoms. Frequency calculations at the same level of theory were performed to identify the number of imaginary frequencies (zero for local minimum and one for transition states) and provide the thermal corrections of Gibbs free energy. Transition states were submitted to intrinsic reaction coordinate (IRC) calculations to determine two corresponding minima. The single-point energy calculations were performed at the M06-2X/Def2-TZVP level of



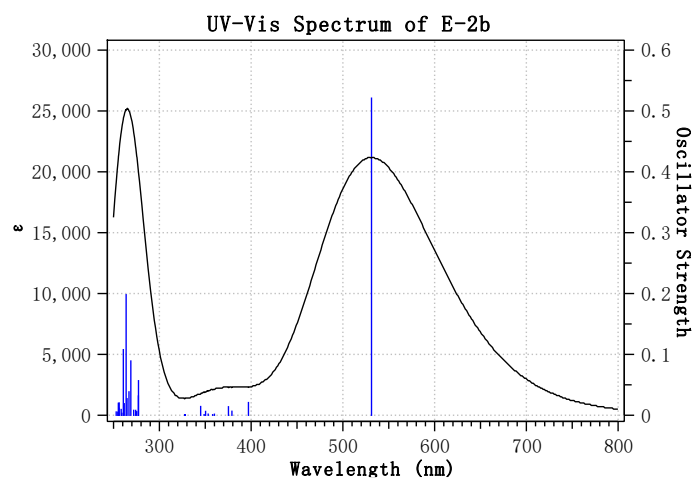
theory for solution-phase (toluene) for organic compounds, and at BP86/Def2-TZVP level of theory for solution-phase (THF) for metal complexes, respectively. The gas-phase geometry was used for all the solution phase calculations. The SMD method was used with the corresponding solvent, while the Bondi radii were chosen as the atomic radii to define the molecular cavity.<sup>[3]</sup> The Gibbs energy corrections from frequency calculations were added to the single-point energies to obtain the Gibbs free energies in solution, respectively. All the solution-phase free energies reported in the paper correspond to the reference state of 1 mol/L, 298K. TD-DFT calculations were performed at the PBE0/def2tzvp level of theory.



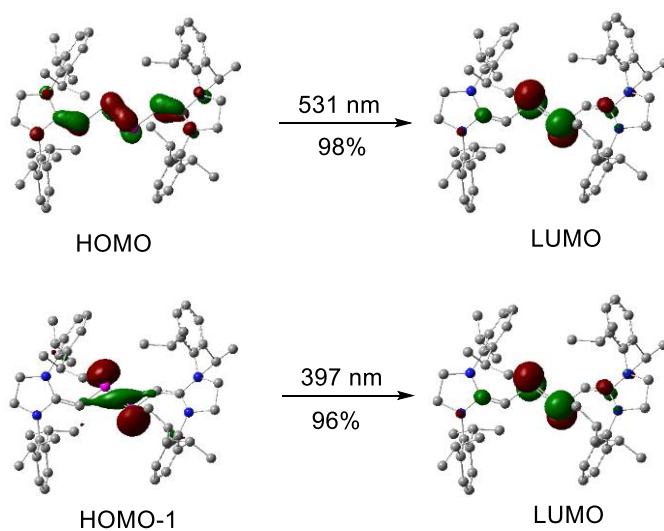
**Figure S73.** Electronic transitions of *E-2a* as modeled by TD-DFT.



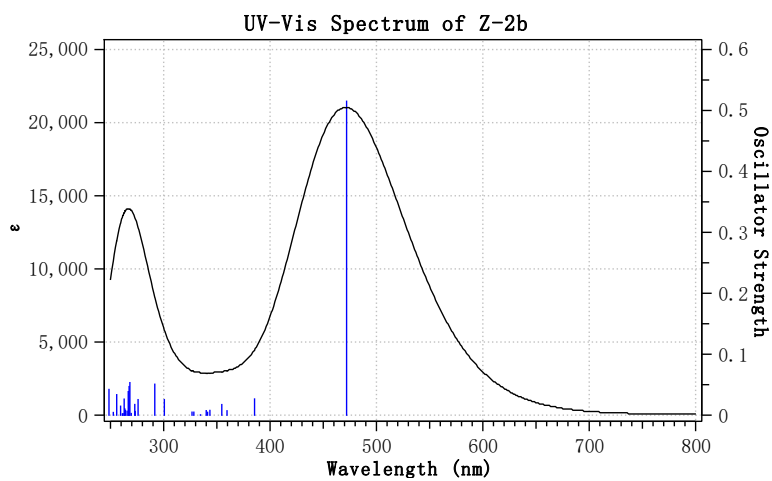
**Figure S74.** Major transition orbitals of *E-2a* for transitions at 492 and 425 nm from TD-DFT calculations.



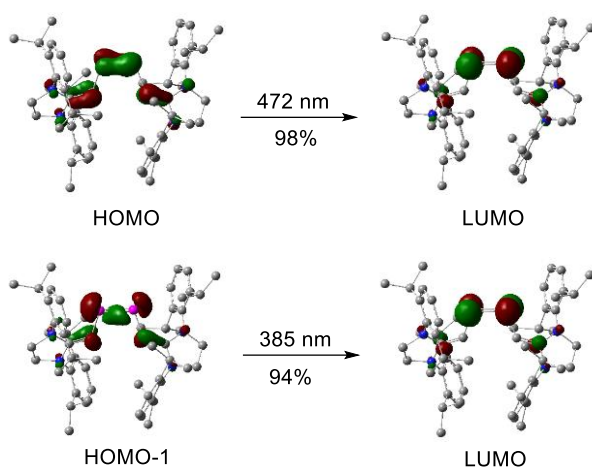
**Figure S75.** Electronic transitions of *E-2b* as modeled by TD-DFT.



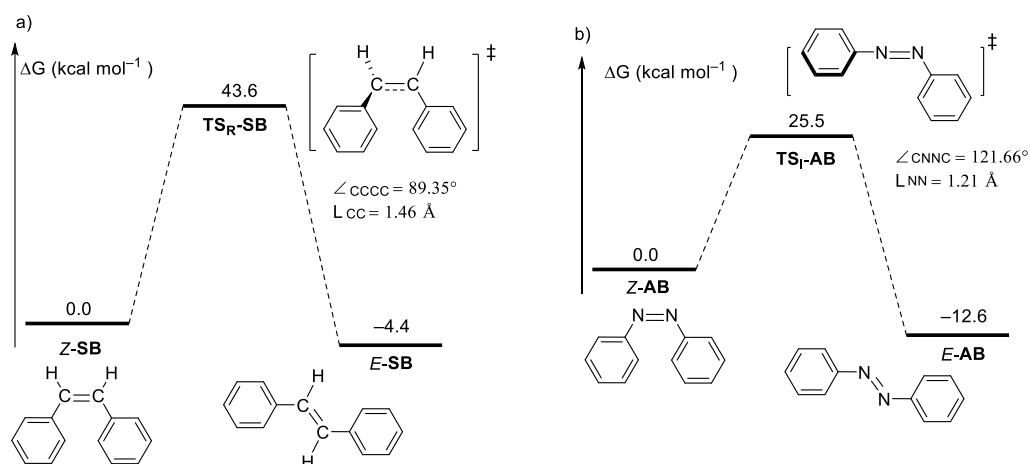
**Figure S76.** Major transition Orbitals of *E-2b* for transitions at 531 and 397 nm from TD-DFT calculations.



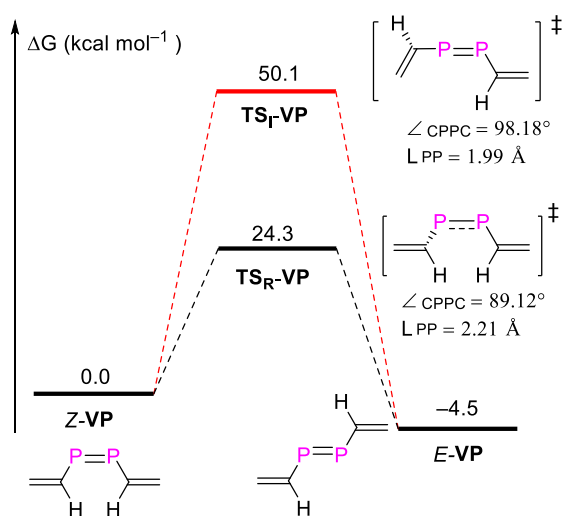
**Figure S77.** Electronic transitions of *Z-2b* as modeled by TD-DFT.



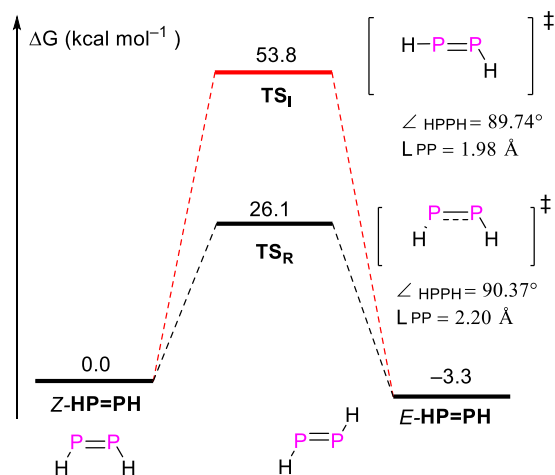
**Figure S78.** Major transition Orbitals of **Z-2b** for transitions at 472 and 385 nm from TD-DFT calculations.



**Figure S79.** Calculated **Z**→**E** isomerization of a) stilbene (**SB**) and b) azobenzene (**AB**).



**Figure S80.** Calculated **Z**→**E** isomerization of 1,2-divinyldiphosphene (**VP**).



**Figure S81.** Calculated Z → E isomerization of HP=PH.

Cartesian Coordinates:

<b>E-2a</b>	H	-8.28581200	-1.79115300	1.79405100			
P	-0.64198800	0.66707100	-0.46446200	H	-7.61793800	-1.34845500	3.38575700
N	-4.71396700	0.42756200	-0.06343600	H	-7.17224100	-2.89236300	2.64305000
N	-3.36504600	2.21026500	-0.14475400	C	-4.22437800	-0.34131700	-2.88001100
C	-3.36687100	0.80941000	-0.09252100	H	-3.98435500	0.61473500	-2.39479300
C	-5.57671600	1.57370600	-0.32976500	C	-2.90333600	-0.95220100	-3.35845900
H	-6.52072700	1.50396000	0.22902200	H	-2.21095400	-1.11645500	-2.52124300
H	-5.81774200	1.63461300	-1.40780000	H	-2.41176800	-0.27743400	-4.07559400
C	-4.70269300	2.73091700	0.10877100	H	-3.07552400	-1.91477500	-3.86510000
H	-4.88750500	3.65420800	-0.45801700	C	-5.14361600	-0.02966000	-4.06705000
H	-4.83595100	2.95407100	1.18429800	H	-5.38320200	-0.94063400	-4.63636800
C	-5.18709200	-0.83048000	-0.54555100	H	-4.65172500	0.67503100	-4.75401000
C	-5.93590300	-1.62794700	0.34521200	H	-6.09281800	0.41574400	-3.73413500
C	-6.38093400	-2.87301300	-0.10142400	C	-2.27569900	3.01449000	0.31561600
H	-6.95664200	-3.51610200	0.56446200	C	-1.68902600	3.91038300	-0.60052600
C	-6.09180700	-3.31256300	-1.39301700	C	-0.56910100	4.63177700	-0.18655300
H	-6.43413100	-4.29503800	-1.72172600	H	-0.07771500	5.31701300	-0.87756300
C	-5.38530800	-2.49566600	-2.26630400	C	-0.05565300	4.47769200	1.10058400
H	-5.18420200	-2.83944900	-3.28344800	H	0.83767900	5.02967700	1.39847600
C	-4.93504300	-1.23030900	-1.86968100	C	-0.69194200	3.64224700	2.01036900
C	-6.19419700	-1.14660100	1.76757700	H	-0.30049100	3.55144100	3.02643300
H	-6.42188200	-0.07095400	1.70719700	C	-1.82612100	2.90938800	1.64485200
C	-4.94522400	-1.28976100	2.64791500	C	-2.24315000	4.04016000	-2.01343600
H	-4.63912200	-2.34556200	2.71344100	H	-3.33991600	3.97633600	-1.93498800
H	-5.15657200	-0.93102300	3.66700200	C	-1.79098200	2.88613500	-2.91609900
H	-4.09931600	-0.71351800	2.24917800	H	-0.69271300	2.85598800	-2.98365300
C	-7.38791800	-1.83491300	2.42724800	H	-2.20171900	3.01657700	-3.92968100

H	-2.12155600	1.91460500	-2.52541300	H	7.90331200	0.70768500	-3.46103000
C	-1.90697200	5.38195000	-2.66365400	H	7.21284000	2.32945000	-3.29645300
H	-2.16544800	6.22852200	-2.01110200	C	3.75679800	1.16444200	2.39722400
H	-2.46128900	5.49031800	-3.60684300	H	3.66060400	0.08738400	2.20265500
H	-0.83607100	5.45167800	-2.90722200	C	2.34070200	1.72356700	2.56741500
C	-2.51292600	2.03481200	2.68319200	H	1.71175700	1.52866300	1.68656700
H	-3.34949600	1.51121200	2.20019300	H	1.85356600	1.25491900	3.43649900
C	-1.57240900	0.96548800	3.24918000	H	2.36505000	2.81128100	2.74145900
H	-1.11585400	0.36818500	2.44669500	C	4.56170500	1.32176500	3.69351100
H	-2.12377600	0.29063600	3.92185900	H	4.64591800	2.38031600	3.98335800
H	-0.76031800	1.42726100	3.83278800	H	4.06515300	0.78681800	4.51680600
C	-3.09934400	2.89535600	3.80862100	H	5.58131800	0.92323300	3.58516100
H	-2.30399700	3.42719500	4.35282900	C	2.50916300	-3.17037700	0.26005600
H	-3.63917300	2.26544700	4.53169500	C	1.89339900	-3.76715300	1.37840000
H	-3.79674700	3.65042200	3.41661800	C	0.89951500	-4.71868100	1.14965500
C	-2.27015100	-0.02457800	-0.05827100	H	0.39110600	-5.18716600	1.99268000
P	0.60577200	-0.88221800	0.02696200	C	0.53675900	-5.07389300	-0.14863300
N	4.67186900	-0.32524200	0.00699100	H	-0.25681700	-5.80525000	-0.30980900
N	3.47297700	-2.14444600	0.50409900	C	1.19818700	-4.51689100	-1.23609300
C	3.36746800	-0.83812500	0.01372700	H	0.92522800	-4.82286300	-2.24853900
C	5.58269200	-1.23406800	0.69556800	C	2.20944000	-3.56747300	-1.05508700
H	6.58263500	-1.22393100	0.23942400	C	2.27774100	-3.33976500	2.78857000
H	5.68518000	-0.94668400	1.75892000	H	3.36328000	-3.15333800	2.78339800
C	4.86807400	-2.56180200	0.54890200	C	1.59920000	-2.02403600	3.18828500
H	5.05052400	-3.25015800	1.38608000	H	0.50355000	-2.13059600	3.16170700
H	5.15417400	-3.07506800	-0.38879900	H	1.89762000	-1.73743700	4.20919800
C	4.96943000	1.06653900	0.13054300	H	1.86586600	-1.20753600	2.50362600
C	5.76704000	1.65365600	-0.87434300	C	2.00012800	-4.41790400	3.83579800
C	6.03102400	3.02117900	-0.78907400	H	2.42392700	-5.38967600	3.54363900
H	6.63742900	3.50721700	-1.55353500	H	2.43885300	-4.12502000	4.80036600
C	5.52058500	3.78250800	0.26234700	H	0.91977500	-4.55047400	3.99805300
H	5.72295700	4.85380900	0.30533600	C	2.92822200	-3.00136500	-2.27060700
C	4.77464600	3.17593500	1.26439800	H	3.65169400	-2.24847600	-1.92763800
H	4.40392300	3.77514800	2.09921500	C	1.96522800	-2.29874500	-3.23338100
C	4.50080400	1.80269200	1.23267400	H	1.38689400	-1.51764100	-2.72004000
C	6.27540500	0.81023400	-2.03761200	H	2.52534400	-1.83400900	-4.05901800
H	6.58850500	-0.15876700	-1.61893800	H	1.25483900	-3.01587700	-3.67341300
C	5.16772500	0.51708100	-3.05886800	C	3.71555500	-4.10114200	-2.99281400
H	4.77402400	1.45505800	-3.48047700	H	3.03967600	-4.87465600	-3.38827900
H	5.56794200	-0.08734700	-3.88715700	H	4.27650700	-3.67894400	-3.84015300
H	4.33152200	-0.03301400	-2.60586000	H	4.42809500	-4.59603500	-2.31638600
C	7.48810200	1.42270000	-2.73670900	C	2.22618300	-0.17181900	-0.38099000
H	8.28016400	1.68897400	-2.02204800	C	-2.36658900	-1.49409600	0.28079600

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H -3.38178800 -1.85469000 0.46003200  
C 2.27584900 1.16686900 -1.08042000  
H 1.60887600 1.14077600 -1.95820000  
H 1.90003500 1.98753600 -0.44261800  
H 3.27008100 1.44765700 -1.43312300

**<sup>3</sup>T-2a**

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C -4.91965300 2.22610600 -2.19128000  
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H -4.02219800 5.49174100 -2.60165100  
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H 3.44855100 1.92284500 4.50196900  
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C 4.15818000 0.19078700 -4.72568800  
H 3.66487700 -0.24586600 -5.60741500  
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H -0.89298000 0.47670300 -1.95805400  
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H 0.63387900 1.90345800 -0.23914000  
H 1.24378800 1.58680300 1.38945300  
H 2.24740800 2.45683700 0.21845200

### Z-2a

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C 4.15604100 -3.01413900 1.30636400  
C -3.66183400 2.06306100 0.88963800  
C -3.26689800 -1.98887200 -1.86655100  
C -1.75707000 -0.23541700 0.24323400  
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C 3.50570100 -1.86247100 1.79529300  
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C	3.44880100	2.30478700	-0.86794900	C	-4.37520300	-3.07732300	0.13793800
C	5.01991200	1.28789200	0.71839000	H	-3.86868100	-2.26002200	0.67683600
H	5.34054100	2.24711100	1.14836700	C	2.70804400	4.48602700	-1.55728100
H	5.73742900	1.00782400	-0.07685600	H	2.32474200	5.48102400	-1.33036200
C	-3.25350500	3.40512900	0.73749800	C	3.45859000	2.88273100	-3.19985700
C	2.65401200	-1.91316300	2.91511500	H	3.65525500	2.62453000	-4.24297300
C	-4.06024700	1.54254300	2.13234400	C	2.93114500	4.12927700	-2.88793200
C	5.09992100	-2.91856400	0.11712000	H	2.70836400	4.84113600	-3.68432200
H	5.63156700	-1.95701100	0.20298300	C	-2.72557700	-4.44628700	-3.03510900
C	-3.69930000	-3.16675100	-1.22117400	H	-2.51784300	-5.41273000	-3.49718800
C	3.74071200	1.94918300	-2.19477600	C	2.76073200	3.95395600	0.94207800
C	2.97326600	3.58742800	-0.52301400	H	3.63265500	3.56081200	1.48934000
C	-4.95741600	1.12708600	-0.97486600	C	-3.15660500	4.19318000	1.88501300
H	-5.25586000	2.08664200	-1.41983200	H	-2.83023300	5.23043200	1.80788100
H	-5.75996800	0.80099800	-0.28525800	C	-2.57288500	-0.44060900	-5.01529100
C	3.88023500	-4.23735000	1.91793100	H	-2.15699200	0.49076900	-5.42780300
H	4.35590000	-5.14738600	1.55153900	H	-3.66224900	-0.32388700	-4.92165700
C	2.40604000	-3.16128500	3.49453600	H	-2.38862500	-1.24448400	-5.74469800
H	1.73155700	-3.23103900	4.34959900	C	-3.47393000	3.67112200	3.13988100
C	-1.91582000	-0.77887200	-3.67267300	H	-3.37757900	4.29772300	4.02794800
H	-2.08709200	0.05520400	-2.97384800	C	-0.39809600	-0.92327900	-3.83675000
C	4.87051000	0.18521400	1.74556400	H	-0.15073500	-1.66127200	-4.61533700
H	5.78140700	-0.41397200	1.88411300	H	0.06903400	-1.25022900	-2.89618500
H	4.56596800	0.59322100	2.72666600	H	0.04793800	0.03846900	-4.13303400
C	2.99980800	-4.31343200	2.99456900	C	-4.19533800	-4.34012300	0.97728400
H	2.78634800	-5.27953200	3.45464200	H	-4.75601800	-5.19142500	0.56135300
C	-2.92689400	3.95332400	-0.64814400	H	-4.57252800	-4.16850700	1.99610700
H	-3.70959700	3.57447600	-1.32447200	H	-3.13353800	-4.61724800	1.04458500
C	-4.64522200	0.05960000	-2.00529100	C	5.73280500	0.80811000	-3.20368400
H	-5.51406700	-0.55412500	-2.27972600	H	5.64825600	1.33136000	-4.16847400
H	-4.23028100	0.50985600	-2.92586700	H	6.21531200	-0.16307700	-3.38942400
C	4.35403900	0.60501000	-2.56380000	H	6.39144100	1.40577200	-2.55643000
H	4.49913400	0.02460000	-1.64111900	C	-5.85758300	-2.71025300	0.01753800
C	-3.93847700	2.36761700	3.25771100	H	-5.99422800	-1.75669200	-0.51159000
H	-4.21600200	1.97943400	4.24045900	H	-6.31219300	-2.61206400	1.01562100
C	-4.63588100	0.14063300	2.28526500	H	-6.40711800	-3.48924100	-0.53327800
H	-4.69499100	-0.32093600	1.28926700	C	2.74446600	-0.23812100	4.78357200
C	-2.26633200	-3.27987000	-3.63211800	H	2.31417200	0.69352800	5.18094300
H	-1.68491900	-3.33788400	-4.55468500	H	3.81877000	-0.08069500	4.61360100
C	-3.42178100	-4.38996800	-1.82807800	H	2.64460600	-1.01586000	5.55647000
H	-3.73096900	-5.31765000	-1.34636700	C	6.15190700	-4.02684400	0.09144500
C	2.01152500	-0.66836600	3.50531600	H	6.67930400	-4.11140800	1.05270500
H	2.09854800	0.14059200	2.76273300	H	6.89390100	-3.82003700	-0.69311200



H 5.70123600 -5.00389200 -0.13896500  
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H 3.96731700 -1.14820500 -3.78496300  
H 3.18045000 0.32791600 -4.38902300  
C 1.52127200 3.28683100 1.55161800  
H 0.60317200 3.64701800 1.06271500  
H 1.44644300 3.53457300 2.62140100  
H 1.55256100 2.19356900 1.45411900  
C -3.76152900 -0.77259500 3.15081800  
H -3.62221000 -0.35228000 4.15929400  
H -2.77344500 -0.93037400 2.69621900  
H -4.24138700 -1.75730600 3.26103600  
C 2.71136300 5.46235100 1.17921600  
H 3.57634800 5.97633900 0.73593000  
H 2.70185300 5.67093600 2.25834400  
H 1.79608500 5.90298600 0.75472500  
C -2.96760700 5.47938500 -0.71026800  
H -2.13175200 5.92380000 -0.14817700  
H -3.90621800 5.88221700 -0.30332200  
H -2.87210700 5.81368200 -1.75299200  
C -6.06449400 0.21237500 2.83824500  
H -6.51204100 -0.79187200 2.87610000  
H -6.70321800 0.85372900 2.21310000  
H -6.07607200 0.62213000 3.85967500  
C 4.32128200 -2.88909800 -1.20283000  
H 3.73655200 -3.81357300 -1.32450400  
H 5.01556900 -2.79929900 -2.05353000  
H 3.61595100 -2.04748400 -1.23730200  
C -1.09644100 0.75933600 1.18305900  
H -1.10197000 1.78465400 0.79348600  
H -1.57303100 0.78977600 2.17534600  
H -0.04813300 0.47890400 1.33821400  
C 0.97777200 0.83701300 -1.04724300  
H -0.04186000 0.46968600 -1.20537500

H 0.89367700 1.83128000 -0.58923800  
H 1.42096300 0.98206900 -2.04234300

### TSR-2a

P -0.76248400 1.33576400 -1.11766200  
P 0.87303100 -0.09263100 -1.52228800  
N -3.65235500 2.00105000 -0.11345200  
N 4.47434700 -0.39175700 0.20716200  
N 3.07977800 -1.99392300 -0.53601600  
N -4.24288700 -0.09090300 0.43928700  
C -3.16082600 0.71128600 0.06392000  
C 1.28512100 -3.43952700 -1.37081100  
C -4.26810400 -1.50648900 0.23535200  
C -2.86431800 3.17395400 0.11540900  
C -1.85350800 0.29786000 -0.13629900  
C 3.15786700 -0.64490200 -0.18681200  
C -2.28646400 3.39849700 1.38116500  
C 1.91010800 -2.78987300 -0.28633300  
C 2.11683000 0.26379700 -0.28127000  
C 5.06262600 0.91176700 0.15308700  
C 5.33313700 -1.49940600 -0.20765600  
H 6.14262500 -1.67566200 0.51508600  
H 5.79305300 -1.27571600 -1.18719000  
C -4.51474900 -2.31936000 1.36202100  
C 1.45225800 -2.96735700 1.03505000  
C -4.07073400 -2.05492000 -1.04471000  
C 1.83178500 -3.32234700 -2.78280800  
H 2.51626700 -2.46143300 -2.78892100  
C -2.71280800 4.09712200 -0.93659700  
C 5.08835900 1.64522700 -1.04788000  
C 5.65701400 1.40395100 1.33452400  
C -5.49350500 0.62384100 0.19590400  
H -6.25864100 0.36156200 0.94025300  
H -5.88875300 0.37327300 -0.80586800  
C 0.16478400 -4.23381300 -1.11414000  
H -0.33999300 -4.73273800 -1.94366300  
C 0.32151200 -3.76658800 1.24128500  
H -0.06297700 -3.89731400 2.25557600  
C -2.47948500 2.45431100 2.55915200  
H -3.18142500 1.66290500 2.26080400  
C 4.35685500 -2.66180800 -0.30470100  
H 4.60383500 -3.35505500 -1.12102500  
H 4.31812100 -3.24052400 0.63612000

C -0.32356900 -4.39015900 0.18048200  
H -1.21356200 -4.99494400 0.36138000  
C -4.75197800 -1.68789400 2.72825500  
H -5.34881800 -0.77758500 2.56350300  
C -5.05593500 2.07726500 0.27234500  
H -5.62232300 2.73280100 -0.40435700  
H -5.15000000 2.47687700 1.29958500  
C 4.60368100 1.09011700 -2.38065100  
H 4.13288500 0.11183700 -2.21211300  
C -4.04182100 -3.45075300 -1.16009100  
H -3.87142100 -3.90072200 -2.14067200  
C -3.93011100 -1.20944800 -2.30310300  
H -3.92401600 -0.14792600 -2.02049200  
C -1.50299400 4.54363300 1.55202000  
H -1.02531500 4.72533600 2.51741900  
C -1.94640600 5.24193900 -0.70961700  
H -1.81197600 5.96570800 -1.51588800  
C 2.13870200 -2.34615700 2.24549900  
H 3.05776400 -1.84447800 1.91092000  
C -3.34921100 3.86336600 -2.29512400  
H -3.71603200 2.82624100 -2.30184500  
C 6.21196400 2.68436600 1.31304400  
H 6.67075300 3.09278900 2.21370700  
C 5.64445700 2.93054700 -1.01592400  
H 5.66154100 3.52618200 -1.93105800  
C 6.18818900 3.45227300 0.15035700  
H 6.61515900 4.45633200 0.15204700  
C -1.33107700 5.45873600 0.51901100  
H -0.71757000 6.34762700 0.67406900  
C 5.66194300 0.56020900 2.60284900  
H 5.81982000 -0.48485400 2.29441800  
C -4.49277700 -3.70466800 1.19503900  
H -4.67352100 -4.35806200 2.04891600  
C -3.10446500 3.18040500 3.75556200  
H -3.31305300 2.46707200 4.56711000  
H -4.04705700 3.67418000 3.47670100  
H -2.42814400 3.95121900 4.15463100  
C -4.24013500 -4.26831100 -0.05521100  
H -4.21602500 -5.35367800 -0.16794900  
C -1.16453400 1.77447900 2.95543900  
H -0.41026700 2.52034600 3.25168300  
H -0.76136100 1.19161100 2.11529600  
H -1.32053500 1.09503100 3.80762000

C -2.33966600 4.00320300 -3.43716200  
H -1.97642400 5.03826400 -3.52939900  
H -2.81145800 3.73319800 -4.39381600  
H -1.47782000 3.34196900 -3.27256400  
C 5.79362300 0.87883000 -3.32651700  
H 6.28010600 1.83686900 -3.56544700  
H 5.45616500 0.42632400 -4.27066800  
H 6.55562500 0.22292500 -2.87997200  
C -4.54180800 4.80463600 -2.50252200  
H -5.28653800 4.70165200 -1.69954200  
H -5.03760900 4.59989400 -3.46328400  
H -4.20860600 5.85427000 -2.51055900  
C 2.55564400 -3.42406000 3.25301500  
H 3.14300100 -2.97541100 4.06821500  
H 3.16454400 -4.20603300 2.77562500  
H 1.67872700 -3.91217100 3.70405000  
C 2.62549300 -4.58392300 -3.14774700  
H 3.42312700 -4.79047200 -2.41947100  
H 3.08321900 -4.48181800 -4.14316000  
H 1.96214400 -5.46282700 -3.16680600  
C -3.43666300 -1.24646400 3.38253800  
H -3.63132500 -0.80802000 4.37354700  
H -2.91475000 -0.49634400 2.77367300  
H -2.76413800 -2.10895300 3.51533400  
C 1.26402500 -1.28210100 2.91906800  
H 0.26963100 -1.68485200 3.16870900  
H 1.12471900 -0.41256300 2.26048400  
H 1.73404100 -0.93316900 3.85069200  
C 3.55040100 1.98783400 -3.03642200  
H 2.69090100 2.14882900 -2.37213400  
H 3.17330100 1.51661600 -3.95587100  
H 3.97497600 2.96687100 -3.30774300  
C 4.30665900 0.61513000 3.31533600  
H 4.06434100 1.64941300 3.60582900  
H 4.32614200 -0.00222700 4.22703300  
H 3.50187900 0.24275500 2.66877500  
C -2.61596700 -1.48463600 -3.03978100  
H -2.57276300 -2.52291700 -3.40510200  
H -1.74753600 -1.31004600 -2.38973300  
H -2.52045200 -0.81776700 -3.90977200  
C 6.78657100 0.93127700 3.56846700  
H 7.76365500 0.95928300 3.06505100  
H 6.83858200 0.19464900 4.38282100

H 6.61169700 1.91427300 4.03125000  
C -5.53838300 -2.59082000 3.67770200  
H -4.93701900 -3.45332100 4.00271900  
H -6.45761200 -2.97183600 3.21000200  
H -5.81710100 -2.03117800 4.58185400  
C -5.13108200 -1.43678200 -3.23016300  
H -5.05950800 -0.78699200 -4.11483800  
H -6.08188700 -1.22430200 -2.71904700  
H -5.16728200 -2.47984400 -3.57984700  
C 0.74329100 -3.05557300 -3.82295100  
H 0.05374900 -3.90867700 -3.91859500  
H 1.19971700 -2.89139000 -4.81033900  
H 0.16467700 -2.16089600 -3.55689300  
C -1.37229900 -1.03513900 0.39061600  
H -2.01625700 -1.45677000 1.16887800  
H -1.26864600 -1.80125400 -0.39629600  
H -0.37232800 -0.91218200 0.82548200  
C 2.13812100 1.58558100 0.45634600  
H 1.16164200 1.75805600 0.93497700  
H 2.90613700 1.62606000 1.23664900  
H 2.30738000 2.44263200 -0.21732600

**E-2b**

P -0.56707400 0.79468900 -0.38537800  
N -4.62854600 0.06942500 -0.08247100  
N -3.63792400 2.06235600 0.07189100  
C -3.39307600 0.70895200 -0.11304500  
C -5.70861400 1.04412700 -0.13359800  
H -6.57385400 0.71205200 0.45771600  
H -6.04435600 1.21398400 -1.17440900  
C -5.03036900 2.28226700 0.44271900  
H -5.41157800 3.22139400 0.01721800  
H -5.14406500 2.32795900 1.54197600  
C -4.81951600 -1.23136400 -0.63409600  
C -5.16470900 -2.27781400 0.24505100  
C -5.36723400 -3.55187700 -0.28978200  
H -5.63880500 -4.37936300 0.36614800  
C -5.22174100 -3.78184500 -1.65633200  
H -5.37781900 -4.78433600 -2.05804600  
C -4.87956600 -2.73874900 -2.50841100  
H -4.76849800 -2.92950100 -3.57815000  
C -4.67821700 -1.44337700 -2.01838000  
C -5.25408300 -2.01344600 1.73973400

H -5.68816100 -1.00904600 1.86478900  
C -3.85017900 -1.98241100 2.35859600  
H -3.36248900 -2.96326700 2.24530800  
H -3.90832900 -1.74944200 3.43328000  
H -3.21061100 -1.23081800 1.87398200  
C -6.14673000 -3.00670700 2.48115800  
H -7.13917900 -3.09050400 2.01496500  
H -6.28142100 -2.68365800 3.52331000  
H -5.69559900 -4.01017900 2.50893100  
C -4.31980300 -0.32526100 -2.98537100  
H -4.21194800 0.60746400 -2.41368200  
C -2.97669400 -0.58925700 -3.67435700  
H -2.16743300 -0.69618600 -2.93814400  
H -2.72233300 0.24649700 -4.34337300  
H -3.01908700 -1.50644300 -4.28218100  
C -5.43441100 -0.10986800 -4.01507900  
H -5.56139400 -0.99660600 -4.65463200  
H -5.19249900 0.74201500 -4.66790700  
H -6.39962800 0.09052500 -3.52682900  
C -2.62973600 2.95213800 0.55190300  
C -2.17828700 3.96614700 -0.31448700  
C -1.13715000 4.78753900 0.12021300  
H -0.75539100 5.57285700 -0.53252900  
C -0.56729600 4.60814100 1.37890800  
H 0.25806400 5.24781900 1.69664900  
C -1.05197800 3.62596700 2.23464100  
H -0.60553600 3.50404400 3.22420500  
C -2.09756200 2.78327500 1.84369600  
C -2.78355800 4.10570700 -1.70319400  
H -3.85924100 3.88858200 -1.60699100  
C -2.19506000 3.06763700 -2.66693300  
H -1.10851900 3.21158300 -2.76871800  
H -2.65518600 3.16676000 -3.66276600  
H -2.36038100 2.04220300 -2.30766300  
C -2.64171400 5.51243100 -2.28237000  
H -3.00045300 6.28041600 -1.58176300  
H -3.22193100 5.59518300 -3.21250300  
H -1.59430100 5.73917800 -2.53247700  
C -2.61728900 1.73359000 2.81535000  
H -3.35169500 1.10478200 2.29096600  
C -1.50488100 0.80527900 3.31307800  
H -0.98307900 0.32078700 2.47480800  
H -1.92651900 0.02150000 3.96024100

H -0.76094300 1.36051500 3.90557900  
C -3.33353200 2.40457700 3.99387100  
H -2.63262200 3.02315700 4.57526300  
H -3.75659500 1.64646000 4.67003700  
H -4.14864000 3.05941500 3.65183600  
C -2.20182300 0.06239300 -0.28226300  
P 0.56140800 -0.90018400 -0.18979200  
N 4.60535200 -0.03140000 -0.02477300  
N 3.66097800 -1.96899900 0.54137100  
C 3.38899600 -0.70590000 0.03801100  
C 5.63836800 -0.77662200 0.68019900  
H 6.61764800 -0.65692500 0.19514700  
H 5.72747400 -0.44010200 1.73076900  
C 5.09830200 -2.20000800 0.59643900  
H 5.36723400 -2.81712100 1.46539600  
H 5.45384600 -2.71295800 -0.31709200  
C 4.67894000 1.39079700 -0.09534700  
C 5.22838200 1.96569200 -1.25920300  
C 5.31126600 3.35761100 -1.33439600  
H 5.73532800 3.82959200 -2.22104800  
C 4.85236800 4.15536600 -0.28794300  
H 4.91722500 5.24192700 -0.36480200  
C 4.31554300 3.57163100 0.85321300  
H 3.96168900 4.20583500 1.66915800  
C 4.22514400 2.18055900 0.97777400  
C 5.66440600 1.07200100 -2.40956600  
H 6.11870000 0.17286400 -1.96452300  
C 4.44421300 0.61196900 -3.21799800  
H 3.95007100 1.47814000 -3.68485400  
H 4.75046400 -0.08027200 -4.01772600  
H 3.70565700 0.10417900 -2.58115200  
C 6.70278700 1.71912600 -3.32370700  
H 7.56018100 2.10894800 -2.75603700  
H 7.07573800 0.98120100 -4.04823200  
H 6.26848000 2.54920200 -3.90126300  
C 3.65553700 1.57868400 2.25333100  
H 3.66382000 0.48381700 2.15476400  
C 2.19945700 2.00127200 2.47576700  
H 1.55674000 1.70877300 1.63175800  
H 1.80262600 1.52653700 3.38640400  
H 2.12085900 3.09270000 2.60256200  
C 4.52336500 1.94095800 3.46382300  
H 4.51877500 3.02687100 3.64394500

H 4.13964500 1.44901300 4.37008700  
H 5.56880500 1.63153200 3.31726100  
C 2.77072600 -3.06893700 0.36412600  
C 2.14749400 -3.60510900 1.50803500  
C 1.22720100 -4.63916400 1.33074200  
H 0.71881800 -5.06847900 2.19449700  
C 0.94067400 -5.12712500 0.05741900  
H 0.20822400 -5.92659800 -0.06501900  
C 1.59028800 -4.60670700 -1.05519300  
H 1.36658900 -5.00630600 -2.04674000  
C 2.52318300 -3.57297100 -0.92515800  
C 2.44101200 -3.02325800 2.88279600  
H 3.50650200 -2.74382800 2.89265300  
C 1.63301500 -1.74121200 3.12182100  
H 0.55346100 -1.95332600 3.07139500  
H 1.85939900 -1.32498600 4.11638900  
H 1.85554000 -0.97480100 2.36580400  
C 2.20854900 -4.01883900 4.01849100  
H 2.72437700 -4.97292700 3.83702000  
H 2.57849500 -3.60036000 4.96542900  
H 1.13690600 -4.22914400 4.15422900  
C 3.22683600 -3.03651700 -2.16304700  
H 3.86197300 -2.18952000 -1.86466000  
C 2.23458500 -2.50829700 -3.20340200  
H 1.59735800 -1.71984000 -2.77872000  
H 2.77575100 -2.08971400 -4.06513100  
H 1.58273300 -3.31353800 -3.57573400  
C 4.13784900 -4.10927000 -2.77161700  
H 3.54921100 -4.97109700 -3.12170400  
H 4.68783400 -3.70370000 -3.63406600  
H 4.86778300 -4.48133100 -2.03746900  
C 2.19114500 -0.15878000 -0.32666000  
H -2.28791300 -1.02421500 -0.37580500  
H 2.25502500 0.88406200 -0.65170900

### Z-2b

P -0.81311900 -2.07938600 0.32137500  
P 1.22571900 -1.96674500 0.19565000  
N -3.78784300 -1.09123600 -0.39494700  
N 3.22988700 1.56011600 -0.54557100  
N 4.06474100 -0.22533200 0.49566000  
N -3.56106800 0.92622800 0.52946900  
C -2.86717300 -0.22352800 0.17196000

C 4.66929500 -2.48840500 1.14460600  
C -3.05278900 1.86705400 1.47209100  
C -3.44987900 -2.08765400 -1.36424900  
C -1.52461000 -0.43502100 0.35621000  
H -0.94764500 0.41311500 0.74049100  
C 2.91268100 0.29024400 -0.07744900  
C -2.90433900 -1.70289200 -2.60558600  
C 4.04334300 -1.26958500 1.46943600  
C 1.66538300 -0.27047200 -0.17856700  
H 0.90986600 0.38157900 -0.62858400  
C 2.48679300 2.18405900 -1.59085000  
C 4.66568100 1.79609600 -0.47187500  
H 4.88621200 2.84067200 -0.20973300  
H 5.15224000 1.57256800 -1.43964700  
C -2.86184000 3.19308100 1.03301700  
C 3.42532700 -1.05435100 2.71400600  
C -2.81006800 1.48328000 2.80375300  
C 5.35391600 -2.65866400 -0.20382700  
H 5.85532700 -1.70379900 -0.43006400  
C -3.72290900 -3.43542300 -1.06448900  
C 2.50487600 1.63654300 -2.88774600  
C 1.79617100 3.37562300 -1.29181700  
C -4.99828400 0.69327400 0.47014000  
H -5.53893500 1.59553900 0.15045300  
H -5.38770900 0.39180600 1.46048100  
C 4.61000300 -3.52399700 2.07766700  
H 5.07464100 -4.48453000 1.85430500  
C 3.37993100 -2.12503500 3.61316500  
H 2.88638900 -1.99407700 4.57870000  
C -2.60851700 -0.25443500 -2.96344800  
H -2.94292400 0.38704800 -2.13634200  
C 5.08833400 0.80754100 0.60794000  
H 6.09223100 0.39126700 0.44346000  
H 5.06730000 1.26985900 1.61233200  
C 3.95447600 -3.34945500 3.29528700  
H 3.90358900 -4.17511800 4.00680900  
C -3.15411200 3.54732400 -0.41640100  
H -4.06717100 3.00322300 -0.70318500  
C -5.08737900 -0.44472200 -0.53727100  
H -5.90600100 -1.14627500 -0.32357200  
H -5.21555000 -0.06561100 -1.56857800  
C 3.28634800 0.37817800 -3.23632400  
H 3.79310100 0.01846900 -2.32972600

C -2.28524400 2.44602300 3.67500900  
H -2.07179500 2.17046600 4.71034400  
C -3.18026800 0.10672700 3.33709700  
H -3.55515000 -0.50100600 2.50150500  
C -2.60460300 -2.70768200 -3.53005800  
H -2.16035600 -2.43467900 -4.48980400  
C -3.42847700 -4.40161500 -2.02864800  
H -3.62783000 -5.45321800 -1.81259300  
C 2.81816700 0.28422100 3.10851600  
H 2.94234300 0.98546600 2.27080800  
C -4.30723300 -3.84935500 0.27431100  
H -4.29447700 -2.95827200 0.91929100  
C 1.13281400 4.02617200 -2.33554900  
H 0.60751100 4.96233300 -2.14699400  
C 1.79474700 2.30457900 -3.89161400  
H 1.78333800 1.89423900 -4.90396300  
C 1.12128900 3.48979500 -3.62176100  
H 0.58600800 4.00687600 -4.41997500  
C -2.86543600 -4.04462500 -3.24966800  
H -2.62616800 -4.81307600 -3.98640400  
C 1.78338000 3.90666600 0.13639200  
H 2.82406100 3.86468100 0.49903500  
C -2.37276300 4.12925600 1.94586500  
H -2.21810000 5.16342900 1.63622500  
C -3.37682500 0.18365500 -4.21467600  
H -3.18826400 1.24763100 -4.42336500  
H -4.46093200 0.04074100 -4.09319600  
H -3.06084900 -0.39066400 -5.09864600  
C -2.06533700 3.75211500 3.25237700  
H -1.66633600 4.48982100 3.95064100  
C -1.10233500 -0.03249000 -3.13729200  
H -0.72514900 -0.59190100 -4.00788600  
H -0.55293400 -0.37500400 -2.24786600  
H -0.87556100 1.03382800 -3.29603200  
C -3.45984700 -4.92684500 0.95622100  
H -3.48023200 -5.87059800 0.38990800  
H -3.85131600 -5.13684500 1.96290000  
H -2.41553500 -4.59753200 1.04643300  
C 4.36839400 0.67784300 -4.28014300  
H 3.92204600 0.98718600 -5.23746000  
H 4.97565500 -0.21999800 -4.46837900  
H 5.03711200 1.48575700 -3.94774600  
C -5.76015600 -4.31191100 0.11611400

H -6.38461900 -3.53750100 -0.35337900  
H -6.19747800 -4.56350200 1.09396000  
H -5.81398500 -5.20981300 -0.51912000  
C 3.54855700 0.87803700 4.31827700  
H 3.14185800 1.87119300 4.56107600  
H 4.62721200 0.98074300 4.12767100  
H 3.42641700 0.23847700 5.20564700  
C 6.42052800 -3.75265300 -0.20181100  
H 7.13309000 -3.62713500 0.62632000  
H 6.98166900 -3.73033600 -1.14691000  
H 5.96835200 -4.75228100 -0.11648300  
C -2.02208900 3.05239400 -1.32245200  
H -2.29135300 3.15748600 -2.38569500  
H -1.77205100 1.99849300 -1.12927500  
H -1.11405500 3.64509700 -1.14777800  
C 1.31618100 0.16662200 3.37577000  
H 1.11622500 -0.50421500 4.22600500  
H 0.79582300 -0.23593300 2.49520400  
H 0.88239600 1.15116100 3.61201800  
C 2.36450100 -0.74894300 -3.70953300  
H 1.63871500 -1.01825600 -2.92935500  
H 2.95417000 -1.64517400 -3.95341800  
H 1.81022500 -0.45236200 -4.61395300  
C 0.94502200 3.01747800 1.06678700  
H -0.10928800 3.00416500 0.75293900  
H 0.97627700 3.40962500 2.09559000  
H 1.30429000 1.98127600 1.08193200  
C -1.98332100 -0.64044600 3.92571500  
H -1.52744200 -0.07806600 4.75569700  
H -1.21721000 -0.81562600 3.15973600  
H -2.30278800 -1.61798600 4.31629300  
C 1.30893200 5.35468200 0.23711600  
H 1.87377300 6.02436400 -0.42735700  
H 1.42483200 5.71447900 1.26920300  
H 0.24008900 5.43837700 -0.01773300  
C -3.40822500 5.03561900 -0.64278500  
H -2.49344400 5.62727100 -0.48334700  
H -4.18779300 5.42503300 0.02790300  
H -3.72812500 5.20749600 -1.68040100  
C -4.31070600 0.23191600 4.36676300  
H -4.63857200 -0.76423000 4.69873200  
H -5.17933400 0.76337500 3.95032300  
H -3.97424100 0.78901900 5.25445200

C 4.33365900 -2.90962700 -1.32037300  
H 3.76730100 -3.83258300 -1.12474500  
H 4.84745200 -3.01216000 -2.28933800  
H 3.60678500 -2.08942200 -1.39655700

### **<sup>3</sup>T-2b**

P 0.81721100 1.22040400 -1.09966600  
N 3.91842700 -0.69265000 0.87024300  
N 4.09479400 1.23873400 -0.23240400  
C 3.20501500 0.24309300 0.12863800  
C 5.24536900 -0.18455000 1.19190900  
H 5.99279300 -0.99065000 1.18416800  
H 5.25678000 0.28799300 2.19231900  
C 5.46141400 0.84255600 0.08580800  
H 6.05972300 1.70666400 0.40762700  
H 5.95317200 0.38947800 -0.79473600  
C 3.29247400 -1.59820500 1.77807900  
C 3.35381500 -2.97713200 1.48950700  
C 2.80962300 -3.87077300 2.41611700  
H 2.85024500 -4.94329800 2.22421600  
C 2.22284500 -3.40909700 3.59299100  
H 1.80531900 -4.12066700 4.30741400  
C 2.16207700 -2.04585400 3.85504200  
H 1.69047200 -1.69339600 4.77534300  
C 2.69269700 -1.11372100 2.95615300  
C 3.96981800 -3.45427200 0.18342200  
H 4.84305900 -2.81187100 -0.01243000  
C 2.98835700 -3.25566100 -0.97967500  
H 2.06490100 -3.83070600 -0.80712000  
H 3.43636400 -3.60282900 -1.92350000  
H 2.70422200 -2.20104100 -1.10044700  
C 4.45195200 -4.90273500 0.23421500  
H 5.10819300 -5.08650600 1.09729900  
H 5.01110000 -5.14278700 -0.68118200  
H 3.60645900 -5.60529900 0.29057800  
C 2.60518900 0.37082900 3.27793100  
H 3.12027900 0.93156200 2.48487300  
C 1.14945300 0.84800000 3.28908400  
H 0.67424300 0.69265500 2.30918500  
H 1.10125300 1.92208800 3.52466600  
H 0.56243300 0.30808100 4.04930300  
C 3.30274400 0.69698200 4.60266200  
H 2.79232900 0.21694900 5.45136400

H	3.29496800	1.78265000	4.77990200	C	-4.10079500	2.20428600	2.26951000
H	4.34769300	0.35300500	4.60323900	C	-4.14507800	3.57656600	2.52379700
C	3.86615500	2.11405500	-1.33776800	H	-4.02194400	3.94451000	3.54268700
C	3.67530800	3.48194100	-1.06486700	C	-4.34127200	4.48650100	1.48688600
C	3.41649500	4.33554800	-2.13842600	H	-4.36646500	5.55625700	1.70048400
H	3.25459400	5.39896300	-1.96103400	C	-4.50886400	4.03562800	0.18315200
C	3.35827100	3.84347100	-3.44070800	H	-4.66708000	4.75697200	-0.62157300
H	3.14528500	4.52254400	-4.26786700	C	-4.48433500	2.66882200	-0.11689100
C	3.57910500	2.49480500	-3.69166800	C	-3.82797800	1.19365000	3.37210300
H	3.54076000	2.12362500	-4.71804500	H	-4.43221800	0.30029700	3.14950800
C	3.84290100	1.60258800	-2.64766200	C	-2.35511600	0.76692600	3.34365800
C	3.71211000	3.98484800	0.37048500	H	-1.70513500	1.63231500	3.54684900
H	4.50463300	3.41986000	0.88732500	H	-2.15784400	0.00132900	4.11087000
C	2.39393200	3.68280600	1.09401400	H	-2.07187400	0.35469200	2.36441100
H	1.55500800	4.18733800	0.59077500	C	-4.21747500	1.68937900	4.76323700
H	2.43995500	4.03721000	2.13603800	H	-5.25193000	2.06148700	4.78947100
H	2.17208800	2.60656500	1.10081900	H	-4.12682500	0.87076000	5.49139500
C	4.05241500	5.47027700	0.47958000	H	-3.55344500	2.49902800	5.10190700
H	4.96275800	5.72326000	-0.08307300	C	-4.70257100	2.21451200	-1.55217900
H	4.21058000	5.74213600	1.53303400	H	-4.65425700	1.11671000	-1.58095600
H	3.23092900	6.09800900	0.10251900	C	-3.60480600	2.73855400	-2.48370100
C	4.09960800	0.13550400	-2.96089400	H	-2.61191900	2.39848300	-2.15744100
H	4.19569300	-0.41332000	-2.01227900	H	-3.77052800	2.37263900	-3.50807400
C	2.94067100	-0.50365000	-3.73228000	H	-3.60530600	3.83917600	-2.51450100
H	1.99471300	-0.40861400	-3.18116600	C	-6.09166400	2.62784900	-2.05152900
H	3.14007700	-1.57312500	-3.89641800	H	-6.18881400	3.72342000	-2.09269300
H	2.81227200	-0.03247700	-4.71884100	H	-6.26468600	2.23773600	-3.06553500
C	5.41676300	-0.02503300	-3.73030200	H	-6.88624300	2.24693500	-1.39286900
H	5.36000800	0.47588300	-4.70885900	C	-2.88572000	-2.51323100	-0.93078200
H	5.63266300	-1.08923500	-3.90803400	C	-2.97293000	-2.95133100	-2.26644500
H	6.26294900	0.41499000	-3.18192200	C	-2.07711800	-3.93199500	-2.69412000
C	1.86932000	0.11570600	-0.17594700	H	-2.10852700	-4.28412500	-3.72538100
P	-0.79056600	-0.24150600	-1.51144100	C	-1.13055100	-4.46322300	-1.81944300
N	-4.23239500	0.36106600	0.69203700	H	-0.42522800	-5.21619200	-2.17547800
N	-3.74708000	-1.45170400	-0.51594800	C	-1.09141200	-4.04957200	-0.49355700
C	-3.25318300	-0.22626100	-0.09974700	H	-0.35814600	-4.48532500	0.18978000
C	-5.48173100	-0.38100900	0.58854300	C	-1.97625800	-3.07593100	-0.01811600
H	-6.02739900	-0.37955000	1.54288100	C	-3.99467800	-2.33054100	-3.20815600
H	-6.13833700	0.05732100	-0.18667600	H	-4.90691500	-2.15316200	-2.61626600
C	-4.98735900	-1.76573000	0.18322300	C	-3.52200900	-0.96836300	-3.73047600
H	-5.68981500	-2.30040400	-0.47152800	H	-2.58250400	-1.07686500	-4.29324900
H	-4.78865400	-2.39967800	1.06763400	H	-4.28213500	-0.53268000	-4.39808100
C	-4.26686800	1.76548800	0.94044400	H	-3.32998500	-0.26309200	-2.91031200

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H -2.69106000 -1.90495400 1.62902800  
C -0.57568500 -2.05050700 1.82327500  
H -0.40667500 -1.12346100 1.25953600  
H -0.55261900 -1.80851700 2.89669300  
H 0.26156300 -2.73827300 1.61997600  
C -2.24207300 -3.86934400 2.34939400  
H -1.46777200 -4.64660800 2.25945200  
H -2.27929900 -3.55515800 3.40325900  
H -3.20805800 -4.32610800 2.08730500  
C -2.03440200 0.35090800 -0.38208600  
H 1.43610600 -0.81620000 0.19704900  
H -1.87276100 1.31244700 0.11428900

**TS<sub>R</sub>-2b**

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P 0.89557500 -1.45842000 -0.64491800  
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C 4.06540100 -2.37210400 -2.26447500  
C -3.07077800 2.30105000 -1.06153700  
C -4.04921100 -2.05657000 0.89180400  
C -1.86455200 -0.28860700 -0.28776900  
H -1.33632500 0.39051300 -0.96248500  
C 3.20102500 0.00845700 0.15993300  
C -3.91671400 -3.04501600 -0.09978300  
C 4.04919500 -2.05659900 -0.89179900  
C 1.86455000 -0.28862500 0.28778200  
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C 3.07079800 2.30102700 1.06154100  
C 5.17417300 1.25656000 0.26724800  
H 5.83938800 1.62995000 1.05880200  
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C -3.01662000 2.70549700 -2.41108600  
C 3.91671100 -3.04505800 0.09977600  
C -2.47754200 3.06299900 -0.03589300

C 4.21833300 -1.26825400 -3.30045200  
H 4.92339200 -0.53127200 -2.88388000  
C -4.06543500 -2.37209500 2.26447400  
C 2.47757500 3.06296000 0.03587700  
C 3.01664700 2.70551100 2.41107900  
C -5.17416000 1.25661200 -0.26720600  
H -5.83937400 1.63001400 -1.05875500  
H -5.21984600 1.96030200 0.58524100  
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C 3.74149600 -4.36846600 -0.31794500  
H 3.61868200 -5.15444400 0.43037700  
C -3.97239200 -2.73190800 -1.58776700  
H -4.05378700 -1.64261700 -1.71393800  
C 5.50111200 -0.16715200 -0.16794900  
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H 3.57913300 -5.73407200 -1.97364300  
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H -6.19050100 -0.21169500 1.02275200  
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H 3.11302500 1.73021400 -1.51536100  
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H -3.89682700 -3.98370100 3.68825300  
C 3.97240200 -2.73197300 1.58776400  
H 4.05388200 -1.64269000 1.71394900  
C -4.21837200 -1.26826800 3.30047200  
H -4.92338300 -0.53124500 2.88389400  
C 2.36722100 3.90391100 2.71757900  
H 2.31893700 4.24642000 3.75134800  
C 1.82485000 4.24902200 0.39187900  
H 1.35078400 4.85029500 -0.38755500  
C 1.77883300 4.67240300 1.71485300



H 1.27503600 5.60634200 1.97182600  
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C 3.62309900 1.82255700 3.49078900  
H 4.56450700 1.41875100 3.08599400  
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H -5.71830400 -2.33936000 4.48162500  
H -5.02007900 -0.90568100 5.27881600  
H -4.07400200 -2.39691400 5.16475800  
C 5.21607000 -3.36656300 2.22233100  
H 5.28588200 -3.09575900 3.28650400  
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H 5.17362600 -4.46446200 2.15584800  
C 4.79380400 -1.76167300 -4.62705100  
H 5.71818200 -2.33935900 -4.48170200  
H 5.01995900 -0.90564000 -5.27882300  
H 4.07384300 -2.39684900 -5.16475400  
C -2.70394400 0.62863700 -3.78267200  
H -3.14563300 -0.01703600 -4.55715700  
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H -1.72588300 0.98092900 -4.14623300  
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H 2.58124500 -4.26915600 2.27681300

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H 2.75214200 -2.88469100 3.37800300  
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H 1.72586300 0.98104400 4.14631800  
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C 3.94930500 2.57494900 4.77918000  
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H -3.29911500 3.37148300 3.32588500  
H -4.22270600 3.94772700 1.91207600  
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C 2.88768800 -0.54228800 -3.52951200  
H 2.13078800 -1.23930100 -3.92045200  
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### Z-SB

C -3.70033200 -0.26373200 0.53767800  
C -2.80449800 0.80161800 0.60445400  
C -1.59008900 0.76603500 -0.09500100  
C -1.31157800 -0.35206000 -0.89677500  
C -2.20913500 -1.41289700 -0.96918800  
C -3.40346600 -1.37659100 -0.24721100  
H -4.63637900 -0.22158600 1.09678800  
H -3.04248900 1.67609900 1.21416500  
H -0.38368700 -0.38015000 -1.47038600  
H -1.97847100 -2.27288000 -1.59993700  
H -4.10527000 -2.20984800 -0.30589300

C	1.59010800	0.76609700	0.09500900
C	1.31170400	-0.35188300	0.89697800
C	2.80439200	0.80156400	-0.60466400
C	2.20924900	-1.41273100	0.96938400
H	0.38389200	-0.37987400	1.47072600
C	3.70021500	-0.26379700	-0.53788900
H	3.04229100	1.67595300	-1.21454100
C	3.40346000	-1.37654200	0.24720400
H	1.97867100	-2.27262900	1.60028200
H	4.63616700	-0.22175100	-1.09716700
H	4.10525800	-2.20980500	0.30587800
C	-0.67166600	1.92224900	-0.01459000
H	-1.16477300	2.89935500	0.01118900
C	0.67165000	1.92228700	0.01461100
H	1.16470700	2.89942000	-0.01110500

#### **TSR-SB**

C	4.00982500	0.11232100	0.68055200
C	2.91042100	-0.69413700	0.92932600
C	1.74056200	-0.60101700	0.13172100
C	1.73372700	0.34714500	-0.92398800
C	2.83986000	1.14904100	-1.16433800
C	3.98421600	1.03895700	-0.36788500
H	4.89948300	0.02282000	1.30608300
H	2.93387600	-1.41708500	1.74764600
H	0.83950900	0.44261700	-1.54307800
H	2.81384200	1.87269500	-1.98070600
H	4.85063600	1.67255400	-0.56130000
C	-1.74056300	-0.60101800	-0.13170300
C	-1.73371500	0.34719600	0.92395900
C	-2.91043300	-0.69417900	-0.92928800
C	-2.83984600	1.14910200	1.16428500
H	-0.83948900	0.44270000	1.54303100
C	-4.00983500	0.11228900	-0.68053800
H	-2.93389800	-1.41716800	-1.74757200
C	-3.98421400	1.03897500	0.36785300
H	-2.81381900	1.87279600	1.98061700
H	-4.89950200	0.02275600	-1.30605200
H	-4.85063200	1.67258000	0.56125000
C	0.61353700	-1.43162700	0.39992400
H	0.68682200	-2.11782400	1.25248300
C	-0.61354100	-1.43164200	-0.39987700
H	-0.68683200	-2.11787900	-1.25240300

#### **E-SB**

C	-4.20028600	1.07403100	0.17102900
C	-2.82136400	1.27018000	0.15527600
C	-1.93600200	0.19419800	-0.00987200
C	-2.48052900	-1.09120300	-0.17138900
C	-3.85653700	-1.28855200	-0.15568300
C	-4.72418900	-0.20775700	0.01715300
H	-4.86787600	1.92676100	0.30353300
H	-2.41508100	2.27673800	0.27690800
H	-1.82136200	-1.94720700	-0.32192700
H	-4.25836000	-2.29476800	-0.28471000
H	-5.80341900	-0.36629500	0.02708700
C	1.93600200	-0.19419900	-0.00986600
C	2.48052900	1.09120200	-0.17138700
C	2.82136400	-1.27017900	0.15528900
C	3.85653800	1.28855200	-0.15567700
H	1.82136300	1.94720500	-0.32193100
C	4.20028600	-1.07403000	0.17104700
H	2.41508000	-2.27673700	0.27692400
C	4.72418900	0.20775800	0.01716600
H	4.25836000	2.29476700	-0.28470700
H	4.86787500	-1.92675900	0.30355600
H	5.80341900	0.36629600	0.02710400
C	0.48973300	-0.45957800	-0.00850300
H	0.22145300	-1.52011500	0.01084600
C	-0.48973300	0.45957700	-0.00850500
H	-0.22145300	1.52011500	0.01084300

#### **Z-AB**

C	3.33885600	-0.41634100	-0.67455700
C	2.49562200	0.68845600	-0.75927400
C	1.39810400	0.79151700	0.09896800
C	1.18339000	-0.17405000	1.08881000
C	2.05085100	-1.25808700	1.18711200
C	3.11931800	-1.39124600	0.29891600
H	4.18290600	-0.50721100	-1.35969300
H	2.66734300	1.48280200	-1.48696800
H	0.34356700	-0.06918800	1.77674100
H	1.88863500	-2.00771900	1.96292900
H	3.78992600	-2.24793400	0.37631100
N	0.61672000	1.98717300	0.00740900
N	-0.61682200	1.98715500	-0.00755600

C -1.39816200 0.79146300 -0.09900200  
C -1.18315900 -0.17434000 -1.08854600  
C -2.49588800 0.68857400 0.75899600  
C -2.05055300 -1.25843700 -1.18679300  
H -0.34315300 -0.06962200 -1.77627700  
C -3.33905900 -0.41627600 0.67434100  
H -2.66781900 1.48309200 1.48645300  
C -3.11924000 -1.39141500 -0.29883600  
H -1.88810700 -2.00826000 -1.96237800  
H -4.18327600 -0.50700900 1.35928900  
H -3.78979400 -2.24814800 -0.37618400

### **TS<sub>I</sub>-AB**

C -1.96906100 -3.98505800 -0.98026300  
C -1.08302400 -2.95780600 -1.27358300  
C -1.07015200 -1.79214200 -0.46435600  
C -1.96590200 -1.70728200 0.63273500  
C -2.83492800 -2.75876800 0.88965900  
C -2.85340300 -3.90720300 0.09671700  
H -1.96399700 -4.87132100 -1.61786300  
H -0.39849900 -3.02719000 -2.11812200  
H -1.96169300 -0.81386700 1.25597800  
H -3.51764600 -2.67104000 1.73713900  
H -3.54261600 -4.72260200 0.31239400  
N -0.22921300 -0.79677100 -0.73017000  
N 0.53667000 0.10860000 -0.98013400  
C 1.83962200 0.04914200 -0.34956100  
C 2.22878600 -0.97549900 0.51775800  
C 2.70393900 1.09523200 -0.66383100  
C 3.50340600 -0.94185100 1.07174600  
H 1.53076000 -1.78317300 0.74707600  
C 3.98052600 1.12220100 -0.10554400  
H 2.35008100 1.86963800 -1.34580600  
C 4.37806200 0.10454400 0.76079900  
H 3.82187200 -1.73398400 1.75076700  
H 4.66542900 1.93633400 -0.34548100  
H 5.37679500 0.12340200 1.19949300

### **E-AB**

C 4.00659300 1.09159100 0.00006200  
C 2.62706900 1.28696700 -0.00001100  
C 1.76543700 0.18753100 -0.00013400  
C 2.28210800 -1.11570000 -0.00001300

C 3.65870000 -1.30316100 0.00012900  
C 4.52287800 -0.20319600 0.00011500  
H 4.67940000 1.95019200 0.00008600  
H 2.18716600 2.28497100 -0.00006100  
H 1.58696500 -1.95447100 -0.00004800  
H 4.06760000 -2.31487500 0.00018900  
H 5.60265000 -0.35997200 0.00021000  
N 0.37756600 0.49039000 -0.00021700  
N -0.37757300 -0.49041300 -0.00017700  
C -1.76544000 -0.18754300 -0.00005900  
C -2.28209400 1.11569500 0.00004200  
C -2.62708300 -1.28696800 -0.00006300  
C -3.65868300 1.30317000 0.00007100  
H -1.58694000 1.95445600 0.00000700  
C -4.00660500 -1.09158000 0.00008500  
H -2.18719100 -2.28497700 -0.00012800  
C -4.52287400 0.20321500 0.00013100  
H -4.06757200 2.31488900 0.00009700  
H -4.67942200 -1.95017300 0.00009200  
H -5.60264400 0.36000300 0.00018700

### **Z-VP**

P 1.01600300 -0.95736500 -0.04560300  
P -1.01602400 -0.95734300 0.04567900  
C 2.91593400 1.00252400 0.06537700  
C 1.61252600 0.75734400 -0.12164700  
H 0.94281000 1.58909500 -0.35511400  
C -2.91574200 1.00251400 -0.06648000  
C -1.61264300 0.75729600 0.12269100  
H -0.94356600 1.58892300 0.35843800  
H 3.32031400 2.01657700 0.00865700  
H 3.62245400 0.19566600 0.28288500  
H -3.32037000 2.01645300 -0.00941600  
H -3.62177100 0.19583600 -0.28623600

### **TS<sub>I</sub>-VP**

P 1.07893600 -0.82177300 0.01071500  
P -0.81690000 -0.23160300 -0.09720900  
C 3.40527500 0.59622700 -0.05833400  
C 2.07670400 0.70986400 0.05724700  
H 1.58876700 1.67860700 0.20237800  
C -3.52799700 0.46954600 -0.29157900  
C -2.45177800 0.17385600 0.44905900

H -2.50246000 0.15034100 1.54319200  
H 4.06764500 1.46371900 0.00142300  
H 3.87887600 -0.37927500 -0.21429700  
H -4.47118800 0.69311000 0.20770300  
H -3.50539700 0.49718300 -1.38134800

#### **TS<sub>R</sub>-VP**

P -0.96700900 -0.75320400 -0.53427000  
P 0.96700800 -0.75320300 0.53427200  
C -3.09175100 0.86659600 0.09816200  
C -1.82925100 0.51032200 0.41093700  
H -1.33198400 1.00414600 1.25309700  
C 3.09175000 0.86659800 -0.09816100  
C 1.82925400 0.51031500 -0.41094300  
H 1.33199200 1.00412600 -1.25311400  
H -3.62284100 1.63553400 0.66395300  
H -3.62649700 0.39688200 -0.73240700  
H 3.62284100 1.63553100 -0.66395800  
H 3.62649000 0.39689700 0.73241800

#### **E-VP**

P 0.75986300 -0.67313900 -0.00022900  
C 3.42780200 -0.01486400 0.00015100  
C 2.17653200 0.46168200 0.00006800  
P -0.75990000 0.67320500 -0.00014400  
C -3.42778100 0.01477200 0.00003800  
C -2.17648100 -0.46171400 0.00002100  
H 2.00809600 1.54468600 0.00048800  
H -2.00800000 -1.54471100 0.00105400  
H 3.62767500 -1.09052700 0.00032000  
H 4.29287400 0.65276100 0.00077900  
H -3.62768600 1.09043000 0.00033500  
H -4.29282600 -0.65288400 0.00096000

#### **E-HP=PH**

P 0.00000000 1.00984800 -0.00001900  
H 1.42521500 1.11377100 0.00027900  
P 0.00000000 -1.00984800 -0.00001900  
H -1.42521500 -1.11377100 0.00027900

#### **TS<sub>R</sub>-HP=PH**

P 1.09811500 -0.06286900 -0.07152600  
P -1.09811500 -0.06286900 0.07152500

H 1.26373300 0.94304100 0.93227700  
H -1.26373300 0.94304200 -0.93227600

#### **TS<sub>I</sub>-HP=PH**

P 1.01727600 -0.09957600 0.00000800  
P -0.95498700 0.00777000 -0.00002100  
H -2.34646200 0.08350600 0.00018100  
H 1.41212200 1.29358400 0.00000000

#### **Z-HP=PH**

P 0.00000000 1.01446100 -0.08803000  
H 0.00001900 1.24239900 1.32044700  
P 0.00000000 -1.01446100 -0.08803000  
H -0.00001900 -1.24239900 1.32044700

#### **[AuCl( $\eta^2$ -E-2b)]**

P -0.70701400 0.78978300 0.57002700  
N -4.72679400 -0.12053100 0.95085000  
N -3.85596100 1.90828200 0.60425100  
C -3.53470600 0.57240500 0.75825300  
C -5.87702400 0.76251900 0.72716700  
H -6.70380600 0.52947200 1.42854100  
H -6.26521400 0.66049300 -0.31481300  
C -5.25640400 2.14716900 0.96644500  
H -5.69984100 2.94300300 0.33617300  
H -5.35453200 2.45662700 2.03451100  
C -4.81594300 -1.53682700 0.76620100  
C -5.02103700 -2.34753600 1.91356000  
C -5.09361500 -3.74174300 1.73424500  
H -5.24951300 -4.39663900 2.60430700  
C -4.95845500 -4.30918300 0.45730900  
H -5.01120100 -5.40271600 0.33589900  
C -4.75294900 -3.49209000 -0.66214000  
H -4.64317100 -3.94942100 -1.65818400  
C -4.68126800 -2.09010800 -0.53401400  
C -5.09064200 -1.70588100 3.29626800  
H -5.56030900 -0.70747800 3.16310200  
C -3.66801200 -1.46123100 3.84560400  
H -3.12971700 -2.42392200 3.97557800  
H -3.71023200 -0.95520100 4.83326100  
H -3.06976400 -0.83073400 3.15775800  
C -5.94473800 -2.49783500 4.29789900  
H -6.95658800 -2.71353700 3.89682200

H	-6.06279300	-1.92354400	5.23984700	N	4.41194500	0.30095300	-0.05533400
H	-5.47269400	-3.46611400	4.56814000	N	3.58551700	-1.75688300	-0.34985300
C	-4.45446400	-1.22104200	-1.76702100	C	3.31969200	-0.50994900	0.18572400
H	-4.40966800	-0.16422800	-1.43533600	C	5.54310300	-0.46826500	-0.58480900
C	-3.10608600	-1.53257800	-2.44028900	H	6.06519500	0.10222700	-1.37828600
H	-2.26302700	-1.37963100	-1.73568500	H	6.28531700	-0.70730100	0.21376100
H	-2.92678000	-0.86445700	-3.30714500	C	4.84084300	-1.73196900	-1.11877900
H	-3.05971000	-2.57885200	-2.80790500	H	5.42162800	-2.65800400	-0.94087700
C	-5.62761500	-1.33946500	-2.75933200	H	4.63302500	-1.64846900	-2.20909700
H	-5.71329600	-2.36912900	-3.16611600	C	4.44912600	1.70111600	0.22154200
H	-5.47935700	-0.65209400	-3.61811400	C	3.76268600	2.59854000	-0.64535300
H	-6.59581300	-1.08886800	-2.27780800	C	3.85666800	3.97435500	-0.36168200
C	-2.88861400	2.94661400	0.43374600	H	3.33609900	4.69339000	-1.01029000
C	-2.45681400	3.25303500	-0.88765600	C	4.60283400	4.44498100	0.73076200
C	-1.49175500	4.26499900	-1.03829600	H	4.67162200	5.52784200	0.92122000
H	-1.12509200	4.51880000	-2.04236500	C	5.23864700	3.54202800	1.59144900
C	-0.96997900	4.94049000	0.07651100	H	5.79351500	3.91745500	2.46606000
H	-0.21000200	5.72455200	-0.06731400	C	5.15330500	2.15311600	1.36539400
C	-1.38880800	4.60310600	1.36896900	C	2.95158100	2.08001400	-1.82754600
H	-0.94550500	5.11501700	2.23766600	H	2.44746000	1.14675500	-1.49070700
C	-2.34509800	3.58911600	1.57315100	C	1.83225300	3.03231800	-2.26802300
C	-2.97755700	2.45552800	-2.08148900	H	2.22774700	3.98149100	-2.68923900
H	-2.96498700	1.38951500	-1.76266000	H	1.23405400	2.53974600	-3.06006600
C	-2.08583000	2.56553600	-3.32370600	H	1.15369200	3.27435200	-1.42498100
H	-2.12321700	3.58215100	-3.77025500	C	3.84210700	1.69942500	-3.02627000
H	-2.42001200	1.84814000	-4.09927000	H	4.64383600	0.99058600	-2.73804000
H	-1.03194400	2.31718500	-3.09641900	H	3.22018900	1.21476700	-3.80672300
C	-4.43123100	2.82279000	-2.44049000	H	4.32860000	2.59819200	-3.46187500
H	-5.12443200	2.67895800	-1.59056100	C	5.76625000	1.17037500	2.35677600
H	-4.79237900	2.19120900	-3.27871800	H	5.47001500	0.15194700	2.03135000
H	-4.50030100	3.88435800	-2.75931600	C	5.18573900	1.36666700	3.76997600
C	-2.71270900	3.14905600	2.98588700	H	4.08075700	1.27811100	3.75926900
H	-3.38322600	2.26975800	2.89630600	H	5.58677700	0.60040000	4.46614400
C	-1.46983100	2.67567600	3.76405700	H	5.44488000	2.36318100	4.18552000
H	-0.93098300	1.88754400	3.19928700	C	7.30473400	1.24443700	2.35692800
H	-1.76236400	2.26117800	4.75133300	H	7.65742100	2.24166700	2.69595800
H	-0.75806300	3.50847400	3.94482200	H	7.73905800	0.48385400	3.03929900
C	-3.47478300	4.25357500	3.74260500	H	7.71938600	1.07474000	1.34188100
H	-2.84285900	5.15748200	3.87395300	C	2.97719200	-2.96276500	0.11955900
H	-3.77803900	3.90585800	4.75249700	C	3.23684000	-3.39759900	1.44813800
H	-4.38832100	4.56528900	3.19484300	C	2.62532600	-4.58773200	1.88688800
C	-2.28668300	-0.02874300	0.74469800	H	2.80450200	-4.93892400	2.91565600
P	0.59555200	-0.94945600	0.62492900	C	1.80300400	-5.33529800	1.03311200

H	1.33870400	-6.26696400	1.39351600
C	1.56277200	-4.89360500	-0.27504500
H	0.90019800	-5.47549000	-0.93302000
C	2.12864500	-3.69652700	-0.75285900
C	4.14077600	-2.62168000	2.39971300
H	4.53313700	-1.74268000	1.85065600
C	3.35059000	-2.08025200	3.60538400
H	2.93123800	-2.90621700	4.21796000
H	4.00600200	-1.47087100	4.26175300
H	2.51346700	-1.44044400	3.26147300
C	5.35641800	-3.45996400	2.83846100
H	5.93182100	-3.82682400	1.96331300
H	6.03921200	-2.85584400	3.47252300
H	5.04866600	-4.34727900	3.43085000
C	1.81597000	-3.18839900	-2.15240900
H	1.99907900	-2.09095700	-2.14092900
C	0.34450800	-3.40196500	-2.54310300
H	-0.33351400	-3.02977800	-1.74854200
H	0.11816400	-2.83689700	-3.46896500
H	0.11444800	-4.47390400	-2.72230100
C	2.75327700	-3.80920000	-3.20770000
H	2.57846600	-4.90312000	-3.29508700
H	2.56986000	-3.34860100	-4.20050100
H	3.82294000	-3.66552500	-2.95328600
C	2.15507300	-0.08881400	0.81267700
H	-2.31043100	-1.12894700	0.81641800
H	2.16712600	0.94891300	1.18452100
Au	0.06033400	-0.03436800	-1.63584000
Cl	0.42730400	-0.05483000	-3.96809300

### TS1-2b

P	0.61621600	-0.42665000	0.80404500
N	4.61590400	0.78719200	0.70691300
N	3.96521700	-1.35207300	0.56928300
C	3.49671100	-0.05025900	0.66662000
C	5.82646500	0.03483000	0.36772400
H	6.70354600	0.40840200	0.93472400
H	6.05981300	0.10765900	-0.72236200
C	5.41836900	-1.39234200	0.76032300
H	5.88637600	-2.16976100	0.12334500
H	5.67778700	-1.61163500	1.82372000
C	4.51064800	2.19977800	0.51313900
C	4.73603800	3.04028100	1.63620400

C	4.61165400	4.43148500	1.46163600
H	4.78114300	5.10563000	2.31455000
C	4.26132000	4.96980700	0.21333700
H	4.16220300	6.06066500	0.09558300
C	4.03358500	4.12521000	-0.88104500
H	3.75300500	4.55738400	-1.85474500
C	4.15676700	2.72643700	-0.75718100
C	5.02910400	2.42296700	3.00023900
H	5.57778100	1.47562800	2.81208600
C	3.70809200	2.04079600	3.70315500
H	3.10251700	2.94775800	3.91409300
H	3.90875300	1.52922000	4.66814000
H	3.09584200	1.36547900	3.07259300
C	5.90508700	3.30642800	3.90109100
H	6.83938300	3.61724500	3.38948500
H	6.18417400	2.75672400	4.82365200
H	5.37216400	4.22619000	4.22312600
C	3.90348100	1.82654700	-1.96079000
H	4.03888600	0.77835000	-1.63162600
C	2.45596000	1.94535500	-2.47258900
H	1.72263500	1.71471900	-1.67495000
H	2.27865800	1.23355400	-3.30476900
H	2.23744800	2.96771100	-2.84593500
C	4.92519800	2.09110700	-3.08346100
H	4.82256400	3.11797500	-3.49433900
H	4.77383500	1.37833400	-3.92088100
H	5.96768900	1.98031300	-2.71901400
C	3.11529900	-2.48732100	0.74841100
C	2.84370600	-3.30235100	-0.38436900
C	1.90186800	-4.33929500	-0.23114500
H	1.62804800	-4.95655300	-1.09649000
C	1.27065500	-4.56407300	1.00293800
H	0.51730800	-5.36233000	1.08846000
C	1.58754900	-3.77814100	2.11639900
H	1.09684900	-3.97574200	3.08181500
C	2.51820600	-2.72440700	2.01446200
C	3.56261700	-3.04696300	-1.71161500
H	4.62887600	-2.86522600	-1.44731700
C	3.06181000	-1.78736700	-2.45412200
H	2.08506900	-1.99124700	-2.93711100
H	3.78705000	-1.49635600	-3.24369700
H	2.92694400	-0.92833100	-1.77138200
C	3.51591000	-4.25458500	-2.66023700

H	3.88183000	-5.18319800	-2.17523000	C	-4.36337800	0.97088600	2.94876800
H	4.14689000	-4.06109600	-3.55224700	H	-4.24908100	1.68053300	2.10384800
H	2.47986900	-4.42604900	-3.01969300	C	-3.02093400	0.95936600	3.70587000
C	2.92507100	-1.92625300	3.25066600	H	-2.19280100	0.62853900	3.04787100
H	3.44098500	-1.00745000	2.90554700	H	-2.77612600	1.97615100	4.07687600
C	1.72981600	-1.47130700	4.10415900	H	-3.05664500	0.27991700	4.58339100
H	0.99728400	-0.91184500	3.48687300	C	-5.51250100	1.48907700	3.83524700
H	2.07318800	-0.81135200	4.92765700	H	-5.66302100	0.84114600	4.72441500
H	1.20169800	-2.33144300	4.56755400	H	-5.29314600	2.51398800	4.20120100
C	3.93204900	-2.73987200	4.09136700	H	-6.47231500	1.51848700	3.27886300
H	3.46358300	-3.66931600	4.47913900	C	-2.59433100	2.97989000	-1.54036800
H	4.29030000	-2.14902300	4.96096400	C	-2.23925400	4.21302400	-0.93441100
H	4.81446100	-3.04202200	3.49015500	C	-1.18501400	4.94959000	-1.50507300
C	2.20100100	0.42068000	0.71439100	H	-0.87538600	5.90161400	-1.04865500
P	-0.58201200	1.14442300	-0.05170200	C	-0.51568500	4.47759000	-2.64332300
N	-4.62951600	0.47323300	0.06413300	H	0.31259200	5.06288100	-3.07286600
N	-3.62888000	2.20817000	-0.91942600	C	-0.89094100	3.26416900	-3.23425700
C	-3.40715700	1.06471200	-0.18400300	H	-0.35024000	2.90027700	-4.12038300
C	-5.72885500	1.35786200	-0.33342100	C	-1.93422200	2.48486200	-2.69754400
H	-6.56590000	0.78159700	-0.77655200	C	-2.93275100	4.67617700	0.34307900
H	-6.12231300	1.91776100	0.54863400	H	-3.94743500	4.22360500	0.34330100
C	-5.03457500	2.28745400	-1.34206900	C	-2.19854700	4.12940300	1.58538800
H	-5.40301900	3.33226500	-1.30006400	H	-1.16164300	4.52313600	1.63270500
H	-5.14915300	1.92015200	-2.38770600	H	-2.72579900	4.42670700	2.51651100
C	-4.80255800	-0.61931400	0.97076900	H	-2.13074900	3.02416200	1.56022900
C	-5.06652500	-1.90113800	0.42039100	C	-3.10246600	6.20188700	0.42179400
C	-5.23367100	-2.97668700	1.31272700	H	-3.59579700	6.60727200	-0.48558300
H	-5.43385400	-3.98374100	0.91802800	H	-3.71970500	6.47549200	1.30240100
C	-5.13161100	-2.78342600	2.69917800	H	-2.12739100	6.72024200	0.53780800
H	-5.26022100	-3.63847900	3.38150800	C	-2.30763000	1.15293300	-3.34079400
C	-4.85573300	-1.51188300	3.21955300	H	-2.86427200	0.55868600	-2.58651600
H	-4.76565100	-1.37667900	4.30903300	C	-1.07283100	0.32713100	-3.74132800
C	-4.68535500	-0.40220100	2.36734600	H	-0.35279700	0.25079400	-2.90182400
C	-5.07197900	-2.10025300	-1.09105200	H	-1.35509400	-0.71114900	-4.00608600
H	-5.41624800	-1.14517800	-1.54364400	H	-0.54607400	0.77063500	-4.61277400
C	-3.63426400	-2.35103600	-1.59311100	C	-3.23778300	1.37138600	-4.55283100
H	-3.21867600	-3.28786300	-1.16993700	H	-2.71795800	1.94817600	-5.34699900
H	-3.59998200	-2.44522700	-2.69724400	H	-3.54666400	0.39738300	-4.98608600
H	-2.94104300	-1.53521900	-1.30647200	H	-4.15354600	1.93696500	-4.28174100
C	-6.02579100	-3.20996800	-1.55957600	C	-2.19620200	0.52327500	0.25681800
H	-7.05469600	-3.06523600	-1.16922700	H	2.13146300	1.52009800	0.76469100
H	-6.07462200	-3.22740700	-2.66758500	H	-2.31190600	-0.43665600	0.78867200
H	-5.67613400	-4.21399700	-1.23952200	Au	0.10229800	-1.80366700	-0.99923800

Cl -0.41032500 -3.24128100 -2.81779700

[AuCl( $\eta^1$ -E-2b)]

P 0.63280300 -0.10739100 0.07550700

N 4.73174600 0.47154200 0.11306500

N 3.71594500 -1.35068700 0.92346400

C 3.49335800 -0.13674300 0.29691300

C 5.81656600 -0.46858300 0.40902700

H 6.67603100 0.04772900 0.88291200

H 6.18144000 -0.96841300 -0.52046400

C 5.11702900 -1.46059300 1.34911000

H 5.48844600 -2.49957200 1.24042400

H 5.23073400 -1.16124100 2.41762800

C 4.90990400 1.59668500 -0.75075200

C 5.15892900 2.86032100 -0.15187600

C 5.32537300 3.97307800 -0.99781700

H 5.51875900 4.96488700 -0.56237300

C 5.23710800 3.83467500 -2.39182000

H 5.36606000 4.71668800 -3.03898200

C 4.98008200 2.58124600 -2.96329000

H 4.90538500 2.48652800 -4.05824700

C 4.81288200 1.43659000 -2.15781700

C 5.16680900 2.99797700 1.36742100

H 5.50329900 2.02146100 1.77638300

C 3.73119500 3.22990200 1.88779900

H 3.32211300 4.18485400 1.49538700

H 3.71862000 3.28014700 2.99694700

H 3.04751100 2.41712600 1.57191200

C 6.12761300 4.08194800 1.87958400

H 7.15297300 3.94548400 1.47814000

H 6.18439500 4.05274000 2.98731100

H 5.78705200 5.10178000 1.60137600

C 4.52116100 0.08385300 -2.79807700

H 4.43164200 -0.66401300 -1.98544500

C 3.17254600 0.08650000 -3.54349700

H 2.34200800 0.35071300 -2.85962200

H 2.95828800 -0.92008500 -3.95793500

H 3.17598300 0.80800900 -4.38784700

C 5.67668800 -0.36678800 -3.71237200

H 5.80023300 0.31532600 -4.58001300

H 5.48149400 -1.38374500 -4.11196000

H 6.64235700 -0.38928000 -3.16565200

C 2.66708100 -2.10476100 1.54046500

C 2.31698700 -3.35418400 0.96299500

C 1.21188400 -4.03795900 1.50748200

H 0.87852500 -4.98095800 1.05525200

C 0.49614600 -3.50384100 2.59081800

H -0.38374700 -4.04122100 2.97649200

C 0.88848200 -2.29349400 3.17331200

H 0.33075200 -1.89489700 4.03375200

C 1.98146800 -1.56636900 2.66211400

C 3.11077500 -3.90901800 -0.22186700

H 4.18459400 -3.74718600 0.02480800

C 2.83372800 -3.15868700 -1.54379500

H 1.82514800 -3.41385200 -1.92767700

H 3.58046400 -3.45180400 -2.31200400

H 2.87842800 -2.06088400 -1.41900600

C 2.90024200 -5.41644100 -0.43077300

H 3.09561200 -5.99849400 0.49351500

H 3.58209500 -5.78958600 -1.22239700

H 1.86249100 -5.62443200 -0.76546100

C 2.44353500 -0.28574600 3.35269600

H 3.13388700 0.24266600 2.66438000

C 1.29274400 0.68662000 3.66263300

H 0.71872200 0.93016500 2.74672500

H 1.69152400 1.63195200 4.08502500

H 0.58594800 0.26440300 4.40745100

C 3.23371000 -0.63490500 4.63205700

H 2.58239600 -1.14798200 5.37099200

H 3.63543300 0.28311800 5.11078900

H 4.08424900 -1.31421900 4.41609600

C 2.30329800 0.44661300 -0.10636800

P -0.59030300 1.58653000 0.02213400

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N -3.90247100 2.44196400 0.05512900

C -3.42281600 1.14737800 -0.04770000

C -5.74843300 1.01176500 0.20497300

H -6.58993600 0.62832200 -0.40715600

H -6.03056200 0.91341500 1.28086200

C -5.35792600 2.45857600 -0.14881900

H -5.84535100 3.21280500 0.50191900

H -5.60738100 2.70304400 -1.20848700

C -4.34671500 -1.11933200 0.15601000

C -4.45703000 -2.00406100 -0.94736300

C -4.25558900 -3.37693200 -0.71810800

H -4.29536900 -4.08086100 -1.56108400



C -3.94093300 -3.85417900 0.56103100  
H -3.75508500 -4.92825500 0.71113700  
C -3.80964700 -2.96280400 1.63255800  
H -3.52980800 -3.34486200 2.62719800  
C -4.00162300 -1.57881300 1.45345300  
C -4.65696100 -1.46361800 -2.35812100  
H -5.12357400 -0.45964700 -2.26070300  
C -3.28103700 -1.27208400 -3.03454000  
H -2.73303000 -2.23582100 -3.08846100  
H -3.40101900 -0.87098500 -4.06351100  
H -2.64519200 -0.56886000 -2.46011600  
C -5.58559500 -2.33827500 -3.21563100  
H -6.55981400 -2.51597700 -2.71459900  
H -5.78294500 -1.84979400 -4.19255500  
H -5.13082300 -3.32710400 -3.43399500  
C -3.77612200 -0.62438800 2.62137200  
H -3.91800600 0.41200800 2.25315700  
C -2.32576100 -0.72371600 3.13059800  
H -1.59883200 -0.55622900 2.31135300  
H -2.13346400 0.02884800 3.92312300  
H -2.12185900 -1.72711800 3.55847600  
C -4.79481000 -0.85658700 3.75342400  
H -4.69099200 -1.87331000 4.18785600  
H -4.64496100 -0.12388900 4.57434800  
H -5.83789900 -0.75743600 3.38725900  
C -3.06934600 3.57100200 -0.22642100  
C -2.70172200 4.41047600 0.85760300  
C -1.82614400 5.48062100 0.59774200  
H -1.51546200 6.14280600 1.41958200  
C -1.33080900 5.70439400 -0.69588100  
H -0.63754900 6.54035900 -0.87976300  
C -1.71224300 4.86947700 -1.75411100  
H -1.31572400 5.05570700 -2.76446100  
C -2.58981500 3.78714800 -1.54519400  
C -3.19102100 4.09757800 2.26834500  
H -4.17932600 3.60111700 2.16314400  
C -2.25169800 3.08107600 2.95079800  
H -1.23101600 3.50245800 3.06405900  
H -2.63033800 2.81079600 3.95915600  
H -2.15938400 2.15281000 2.35446600  
C -3.38397600 5.34894700 3.13884600  
H -4.02622900 6.10309500 2.63887900  
H -3.85930100 5.07604500 4.10359200

H -2.41593900 5.83538400 3.38295300  
C -2.99725000 2.89574800 -2.71480600  
H -3.55483300 2.02858100 -2.30714300  
C -1.77954100 2.32357300 -3.46312500  
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H -2.10885000 1.61172700 -4.24735100  
H -1.19037300 3.12262000 -3.96067900  
C -3.94269100 3.65181700 -3.67071900  
H -3.43242100 4.52328400 -4.13301100  
H -4.28614900 2.98644100 -4.49035500  
H -4.83792000 4.03647000 -3.13907700  
C -2.11542500 0.70059400 -0.12126900  
H 2.41817200 1.44226200 -0.56135300  
H -2.04210100 -0.39932700 -0.22969500  
Au -0.21043800 -2.11801200 -0.57195600  
Cl -1.00072100 -4.14181200 -1.46220200

#### TS2-2b

P 0.65857300 -2.11754400 0.32438500  
P -1.00163700 -0.76333000 -0.19423500  
N -3.14902400 0.48028000 3.13519700  
N -3.72325400 1.03318900 1.03584100  
N 4.19352200 0.02582200 0.17751100  
N 3.99621700 -2.17222000 0.57551300  
C 1.90095000 -0.83999200 0.35225000  
H 1.59402900 0.20369600 0.18275900  
C 3.28231200 -1.00541300 0.38214900  
C -1.70046000 -0.40626800 1.38837200  
H -1.10550500 -0.79314200 2.23071400  
C -2.80718800 0.33427200 1.79228400  
C 5.42829700 -1.88604500 0.70500500  
H 6.04071300 -2.67901300 0.22988400  
H 5.72333000 -1.81679000 1.77951400  
C 5.54248900 -0.52755500 -0.00454200  
H 6.31485800 0.13304600 0.43978200  
H 5.77416600 -0.64985300 -1.08946800  
C -4.50893300 1.03036000 3.23301600  
H -4.61971600 1.67304100 4.12689500  
H -5.26486800 0.21169200 3.29100200  
C -4.61883300 1.80212700 1.91258700  
H -5.65017000 1.83270600 1.50899600  
H -4.25374700 2.85109000 2.01680700  
C 3.39749000 -3.37843100 1.05704200

C	3.27346100	-4.46479500	0.15169800	C	1.65194000	-0.09849000	-3.06187800
C	2.62843100	-5.63048000	0.60380100	H	0.95073000	-0.08720500	-2.20417500
H	2.50084600	-6.48138900	-0.08304500	H	1.50962500	-1.06237500	-3.59153600
C	2.12061600	-5.71057100	1.90863600	H	1.35034700	0.71289000	-3.75702900
H	1.60501600	-6.62543400	2.24061100	C	-3.18606700	-3.44471000	2.26594900
C	2.25853400	-4.62908600	2.78923800	H	-2.26995100	-3.03926500	1.79321600
H	1.84957500	-4.70241600	3.80912400	H	-3.84863800	-3.80751200	1.45367200
C	2.90079000	-3.44242300	2.38660900	H	-2.89857400	-4.31929900	2.88687300
C	4.06614900	-2.62533600	4.47004300	C	-3.90523300	-2.36923600	3.10388600
H	3.71555700	-3.48099000	5.08511600	H	-4.20105200	-1.56803700	2.39956100
H	4.21804500	-1.76014200	5.14938200	C	-5.19745700	-2.91410300	3.74226800
H	5.05083200	-2.90661300	4.04209000	H	-4.98674300	-3.75663200	4.43438100
C	3.04723700	-2.28058800	3.36475200	H	-5.88737400	-3.28936000	2.95814700
H	3.44484300	-1.41143600	2.80224800	H	-5.72722200	-2.13043300	4.32322200
C	1.69515000	-1.84600200	3.95958200	C	-2.97581400	-1.76415100	4.15057600
H	0.97659100	-1.59248600	3.15446100	C	-2.42866600	-2.59309100	5.15021100
H	1.82328300	-0.95508800	4.60860900	H	-2.69817300	-3.66076200	5.16956900
H	1.23671000	-2.64213600	4.58209900	C	-1.54575700	-2.08220700	6.10928500
C	4.58707700	-5.54271700	-1.74659400	H	-1.12902000	-2.74353300	6.88516100
H	5.44709400	-5.71990200	-1.06774600	C	-1.18129400	-0.72928800	6.07102000
H	4.98255400	-5.37586700	-2.77017100	H	-0.46752100	-0.33172400	6.81055900
H	3.98566200	-6.47564700	-1.77810300	C	-2.61052600	-0.38919200	4.14251600
C	3.74520500	-4.33785100	-1.29244200	C	-1.69317100	0.14257300	5.08859500
H	4.38788500	-3.43411300	-1.34321800	C	-0.16593200	1.75282600	3.87352000
C	2.54838800	-4.08891800	-2.23318400	H	0.63706400	0.99107600	3.89714500
H	1.86245500	-4.96187800	-2.24587600	H	0.30689900	2.75612800	3.91436800
H	2.89548800	-3.90968900	-3.27252000	H	-0.68025500	1.65638000	2.89731900
H	1.95305200	-3.21399700	-1.89953400	C	-1.14900300	1.57049900	5.04630800
C	3.81407700	1.26947100	-0.42405300	H	-0.55742000	1.67551400	5.98279700
C	3.30256600	1.30976400	-1.74845500	C	-2.20144300	2.69399300	5.06845000
C	2.95983500	2.57101300	-2.27874300	H	-2.69468500	2.80446900	4.08338700
H	2.55669700	2.63084100	-3.30180600	H	-1.71372900	3.66338000	5.30185700
C	3.12432500	3.74301000	-1.53020700	H	-2.97973400	2.51455500	5.83866900
H	2.85455600	4.71691400	-1.96826500	C	-3.51903100	1.36080000	-0.34474400
C	3.62084000	3.68043000	-0.21876300	C	-2.41238400	2.16984700	-0.71832300
H	3.73011300	4.60653400	0.36444700	C	-2.18532600	2.37535800	-2.09362100
C	3.96557700	2.44512300	0.35892700	H	-1.32139800	2.97759700	-2.41332000
C	3.20693100	1.91538700	2.68805400	C	-3.03825400	1.81952100	-3.05361500
H	2.42801700	2.70530600	2.66889700	H	-2.83194300	1.96533400	-4.12497800
H	3.51395600	1.76204800	3.74414100	C	-4.15353000	1.06411100	-2.66116400
H	2.74092300	0.97857400	2.32285200	H	-4.79606900	0.61703400	-3.43015100
C	3.11467500	0.05862400	-2.60238200	C	-4.41781400	0.81435400	-1.30100500
H	3.35188000	-0.82557200	-1.97784700	C	-5.20582200	-1.43561500	-0.35372700

H	-4.91083600	-2.07629500	-1.20888700
H	-6.05978200	-1.91735900	0.16826900
H	-4.34885300	-1.39510400	0.34363500
C	-5.61240700	-0.03242500	-0.85584300
H	-6.07130300	0.50384100	0.00542300
C	-6.69082900	-0.16870000	-1.94152400
H	-7.02074300	0.81636500	-2.33140300
H	-7.57914700	-0.69120000	-1.53071100
H	-6.31442700	-0.77677100	-2.79020900
C	-1.98024000	4.33397400	0.49189900
H	-1.84234900	4.90674100	-0.44950300
H	-1.38744900	4.83350400	1.28722000
H	-3.05361100	4.40251500	0.76525200
C	-1.53179400	2.86812700	0.31383400
H	-1.67794300	2.35824000	1.28674200
C	-0.03315400	2.78451100	-0.01441500
H	0.26864700	1.73409600	-0.20203600
H	0.57837100	3.17510400	0.82420200
H	0.23394200	3.37489900	-0.91421800
C	4.40966300	2.32884300	1.81407300
C	5.08457700	3.59455700	2.36160200
H	4.36903100	4.43975000	2.44588300
H	5.92586200	3.92458300	1.71794800
H	5.48341900	3.40713800	3.37975500
C	4.08827600	0.05324200	-3.79792800
H	3.89027100	0.90210800	-4.48595800
H	3.98068200	-0.88465200	-4.38168700
H	5.14410500	0.13440700	-3.46460900
Au	-2.22910700	-1.50953800	-1.93741200
Cl	-3.52060600	-2.35441300	-3.70199100
H	5.14884000	1.50110300	1.86646200

[AuCl( $\eta^1$ -Z-2b)]

P	0.62682300	-1.87333500	-0.36714800
P	-1.12615100	-0.76725700	-0.32082900
N	-1.55033400	3.34692100	-0.07430300
N	-3.09093500	1.94861300	-0.89458200
N	4.30921200	-0.09523900	0.20543200
N	3.77939800	-2.24843500	0.47557700
C	1.96928400	-0.69474000	-0.27911400
H	1.79611300	0.37308600	-0.48952900
C	3.27229700	-1.01273300	0.09404300
C	-0.95496100	0.96959400	-0.01818200

H	0.01133000	1.29104500	0.40314200
C	-1.83581200	2.00313100	-0.31221400
C	5.12122100	-2.10749500	1.05181800
H	5.76813900	-2.96225800	0.76773800
H	5.07273200	-2.06619000	2.16548800
C	5.58571400	-0.77359000	0.45620100
H	6.22161100	-0.18327600	1.14689600
H	6.15196400	-0.91792200	-0.49532300
C	-2.76758100	4.15580000	-0.24165300
H	-2.52400500	5.16110500	-0.63547000
H	-3.29827200	4.27952200	0.73222200
C	-3.57364300	3.29683800	-1.21539800
H	-4.66911500	3.37481500	-1.06618600
H	-3.34817500	3.55396300	-2.27746700
C	2.94774600	-3.36553500	0.81168100
C	2.89746800	-4.45006300	-0.10162200
C	2.00805600	-5.50327100	0.17713300
H	1.92700500	-6.34921100	-0.52129200
C	1.20402000	-5.47902900	1.32712000
H	0.49552100	-6.30008900	1.51718800
C	1.29489600	-4.41569300	2.23426000
H	0.65616800	-4.41095300	3.13063000
C	2.16974300	-3.33730100	1.99996800
C	2.97960400	-2.61677900	4.27712500
H	2.41707200	-3.41612800	4.80403100
H	3.08861900	-1.76168600	4.97707500
H	3.99168200	-3.01590300	4.05669700
C	2.24572100	-2.18090200	2.99202100
H	2.84035100	-1.37022100	2.52334400
C	0.86135400	-1.58859300	3.31282200
H	0.32888900	-1.28961000	2.38806800
H	0.96603300	-0.69489000	3.96149300
H	0.21552800	-2.31543100	3.84790800
C	4.15526600	-5.81342600	-1.86225400
H	4.64505300	-6.39790600	-1.05631500
H	4.86754800	-5.72792500	-2.70877600
H	3.28755700	-6.40126800	-2.22877200
C	3.73400600	-4.41710800	-1.37791100
H	4.65919700	-3.84852200	-1.14046600
C	3.00516500	-3.63903300	-2.49395100
H	2.04476800	-4.13106500	-2.75280700
H	3.63089900	-3.59196600	-3.41050300
H	2.76940100	-2.60314600	-2.18097300

C 4.30396600 1.21995300 -0.35121500  
C 4.43986300 1.40081200 -1.75107000  
C 4.55164700 2.71997900 -2.23631400  
H 4.65684800 2.89109700 -3.31923400  
C 4.53685400 3.81254000 -1.36006600  
H 4.64219200 4.83485800 -1.75639900  
C 4.37822300 3.61271000 0.02069200  
H 4.35929200 4.47903900 0.69582900  
C 4.25045400 2.31597200 0.55181500  
C 2.54338000 1.72185100 2.31040600  
H 1.88694500 2.55567100 1.99529300  
H 2.37399600 1.54760000 3.39311400  
H 2.22541400 0.81262500 1.76577500  
C 4.44298700 0.22056100 -2.71612600  
H 4.42001800 -0.71030200 -2.11387300  
C 3.16711300 0.21956900 -3.57981800  
H 2.26133900 0.18709000 -2.94414700  
H 3.14623400 -0.66798400 -4.24537800  
H 3.11152600 1.12615200 -4.21917000  
C -1.33223500 1.61831300 3.48335200  
H -0.74919100 1.01380400 2.76215000  
H -2.16454200 0.98562800 3.85445200  
H -0.67551000 1.86479700 4.34457800  
C -1.88055000 2.89421900 2.81427700  
H -2.52673100 2.55680700 1.98098300  
C -2.76318400 3.70886500 3.77695100  
H -2.20349100 4.02625100 4.68198100  
H -3.62489500 3.09844100 4.11757800  
H -3.15979600 4.62444100 3.29064200  
C -0.74363800 3.72152800 2.22568700  
C 0.15759600 4.38722200 3.08074600  
H 0.01534500 4.32196100 4.17076300  
C 1.22090000 5.13737200 2.56260100  
H 1.89785000 5.67664100 3.24354300  
C 1.43769600 5.17885600 1.17755200  
H 2.29363100 5.73906300 0.77034000  
C -0.54170100 3.82851300 0.82205300  
C 0.57824300 4.51440400 0.27934500  
C 1.18674000 3.11966600 -1.76105100  
H 1.92589500 2.58087600 -1.13775400  
H 1.59823800 3.17799300 -2.78911800  
H 0.26329400 2.51141200 -1.79486400  
C 0.91869400 4.53202000 -1.21014100

H 1.87998400 5.08754200 -1.27314400  
C -0.09080900 5.29055900 -2.09293200  
H -1.02598400 4.71067700 -2.21955700  
H 0.33557600 5.45164900 -3.10506400  
H -0.34435500 6.28432800 -1.66935700  
C -3.61245000 0.79876600 -1.56906600  
C -2.98650200 0.34155200 -2.75831200  
C -3.47324600 -0.84535300 -3.34047800  
H -2.99577500 -1.23679400 -4.25192300  
C -4.54871600 -1.53454200 -2.76859400  
H -4.89905700 -2.47739600 -3.21573500  
C -5.18434100 -1.03719200 -1.61992400  
H -6.01505200 -1.60292900 -1.17903900  
C -4.73422600 0.14274500 -0.99632400  
C -4.57500600 0.51510900 1.54322500  
H -4.60471700 -0.54541800 1.86497700  
H -4.99070900 1.13981900 2.36229100  
H -3.51408500 0.79243900 1.39907900  
C -5.40935000 0.70611200 0.25678800  
H -5.50153100 1.80331200 0.08892600  
C -6.82350000 0.14759500 0.47700000  
H -7.46748100 0.27192400 -0.41798700  
H -7.31048100 0.66966800 1.32624600  
H -6.78032400 -0.93132100 0.73414800  
C -2.43779400 1.88810300 -4.66441100  
H -2.79788200 1.17595800 -5.43673700  
H -1.65608600 2.52716700 -5.12690300  
H -3.29590800 2.53524000 -4.38802000  
C -1.87600800 1.13540800 -3.43983300  
H -1.51284500 1.89687600 -2.72051700  
C -0.66162500 0.27583900 -3.82674800  
H -0.26480700 -0.27185700 -2.94868900  
H 0.14709400 0.91528700 -4.23616400  
H -0.91840600 -0.47314000 -4.60518200  
C 4.02602700 2.06167500 2.03969300  
C 4.50040400 3.21294800 2.93733100  
H 3.87628100 4.11912300 2.79752800  
H 5.55739700 3.48616700 2.73845800  
H 4.41515000 2.92365400 4.00468900  
C 5.71805800 0.18440100 -3.57873500  
H 5.78376800 1.06632800 -4.25026300  
H 5.72803500 -0.72186200 -4.21933100  
H 6.63327300 0.17364700 -2.95108300

Au -2.85278500 -2.07952700 0.32468000  
Cl -4.60939900 -3.37670800 1.15605700  
H 4.61857400 1.15819700 2.30383500

### TS3-2b

P 0.73880500 -1.75103900 -0.71329100  
P -1.06502800 -0.71879100 -0.54775100  
N -1.59229500 3.34474400 -0.03018400  
N -3.13479700 1.88559900 -0.72038700  
N 4.35909600 -0.00107000 0.16388100  
N 3.80180100 -2.16039700 0.35490600  
C 2.04822000 -0.57356900 -0.45169800  
H 1.86898400 0.50665300 -0.57582600  
C 3.33096800 -0.91129900 -0.02581100  
C -0.91346400 0.97769200 -0.02349500  
H 0.06133300 1.30580800 0.37242900  
C -1.83977800 1.98909000 -0.23834100  
C 5.10817700 -2.03928100 1.01334500  
H 5.76943800 -2.88963400 0.75009800  
H 4.99153400 -2.02187800 2.12248600  
C 5.61506600 -0.69307700 0.47687800  
H 6.21304300 -0.12505600 1.21834200  
H 6.23469400 -0.81901600 -0.44321500  
C -2.84482900 4.10992900 -0.12328500  
H -2.66165600 5.11288200 -0.55485300  
H -3.30941900 4.24157600 0.88286200  
C -3.69378800 3.20588600 -1.02063600  
H -4.77584300 3.24181600 -0.78190700  
H -3.56726200 3.46175800 -2.09924400  
C 2.91779600 -3.26274400 0.60935800  
C 2.89681800 -4.32328600 -0.33240900  
C 1.91561500 -5.31960100 -0.17948600  
H 1.85542000 -6.14171200 -0.90820000  
C 0.98415200 -5.25657300 0.86829400  
H 0.18932300 -6.01389900 0.94706200  
C 1.04884900 -4.22610100 1.81460500  
H 0.29992300 -4.18879900 2.61977500  
C 2.02450700 -3.21479800 1.71566600  
C 2.72386900 -2.64768200 4.06242100  
H 2.08849100 -3.43994700 4.51113700  
H 2.83608400 -1.83621500 4.81219200  
H 3.72446100 -3.09159800 3.87775500  
C 2.08996200 -2.10810500 2.76264400

H 2.75189800 -1.30735600 2.37245500  
C 0.72212500 -1.46115600 3.03772600  
H 0.27752200 -1.04978600 2.11064200  
H 0.83100800 -0.63723000 3.77191100  
H -0.00783700 -2.18610000 3.45274000  
C 4.27648500 -5.71974600 -1.97068000  
H 4.67314200 -6.31760200 -1.12441400  
H 5.06531800 -5.65522100 -2.74856700  
H 3.42923500 -6.28270000 -2.41552800  
C 3.85254900 -4.31212100 -1.52228300  
H 4.76789800 -3.77255200 -1.19653600  
C 3.25416500 -3.51005000 -2.69680700  
H 2.31518400 -3.98037200 -3.05535400  
H 3.96862000 -3.46474000 -3.54621200  
H 3.00578900 -2.47397500 -2.39449400  
C 4.36321500 1.31852600 -0.38443200  
C 4.48768700 1.51255300 -1.78414900  
C 4.55716800 2.83810600 -2.26028200  
H 4.65011700 3.01900200 -3.34273500  
C 4.51469300 3.92460200 -1.37743800  
H 4.58508600 4.95211900 -1.76812100  
C 4.37390300 3.71061800 0.00291600  
H 4.33311100 4.57043100 0.68507700  
C 4.28411200 2.40731400 0.52495400  
C 2.56913500 1.79301500 2.26161200  
H 1.91393800 2.63021100 1.95216500  
H 2.38941700 1.60135700 3.33964100  
H 2.25867400 0.89129100 1.70054200  
C 4.53037900 0.34389800 -2.76258400  
H 4.49516600 -0.59488500 -2.17367100  
C 3.28979400 0.34202100 -3.67713800  
H 2.35827000 0.29439300 -3.07955300  
H 3.30607300 -0.53854200 -4.35201200  
H 3.25276500 1.25398600 -4.30995300  
C -1.06255400 1.81102600 3.58647100  
H -0.52685400 1.17509000 2.85617600  
H -1.83787000 1.18473800 4.07278100  
H -0.33958400 2.13110900 4.36641300  
C -1.70305100 3.02359500 2.88438400  
H -2.38664000 2.61399200 2.11475800  
C -2.54962100 3.86600500 3.85540900  
H -1.94272300 4.25508400 4.70001400  
H -3.36475900 3.25066100 4.28931900

H	-3.00970100	4.73789600	3.34526600
C	-0.63223600	3.84806100	2.17833300
C	0.30885300	4.57263800	2.93687700
H	0.24062200	4.56217300	4.03593700
C	1.32296400	5.30826600	2.31077600
H	2.03210200	5.89512700	2.91543100
C	1.44625100	5.27995600	0.91412000
H	2.26104200	5.83282600	0.42183300
C	-0.52838200	3.88557600	0.76082600
C	0.53894400	4.56138000	0.10938100
C	1.08731100	3.10285000	-1.90552200
H	1.89602700	2.63723500	-1.30920100
H	1.42894100	3.13514200	-2.96052000
H	0.19970200	2.44300700	-1.85031200
C	0.77602800	4.52403600	-1.39999500
H	1.69838200	5.12629300	-1.55463800
C	-0.33218700	5.18510100	-2.24185600
H	-1.24193500	4.55384400	-2.27115400
H	0.01278300	5.31599400	-3.28877000
H	-0.60747100	6.18529600	-1.84796500
C	-3.69903400	0.67273500	-1.22575800
C	-3.29403400	0.18708100	-2.49828400
C	-3.78125000	-1.07057700	-2.90483500
H	-3.47491200	-1.48220800	-3.87848000
C	-4.61278200	-1.82145000	-2.06501300
H	-4.94511900	-2.82417700	-2.37437100
C	-5.02173100	-1.31091600	-0.82201700
H	-5.67071900	-1.91830400	-0.17550200
C	-4.59341800	-0.04089700	-0.38850700
C	-4.05102400	0.17124000	2.09258900
H	-4.09381600	-0.91508500	2.31514400
H	-4.31395200	0.72698200	3.01800000
H	-3.00354200	0.41131800	1.82492700
C	-5.02592200	0.54012200	0.95543700
H	-4.98800400	1.64564000	0.84474000
C	-6.46697400	0.15748300	1.33036200
H	-7.18242600	0.39360500	0.51561200
H	-6.78491200	0.70671400	2.24072000
H	-6.55212100	-0.92503000	1.55955000
C	-3.25609200	1.73132800	-4.48367400
H	-3.74451100	0.99196800	-5.15313900
H	-2.62927900	2.39897700	-5.11182400
H	-4.06158700	2.34139000	-4.02528600

C	-2.40036700	1.01749900	-3.41550300
H	-1.91809800	1.79765800	-2.78993500
C	-1.26843700	0.20537400	-4.06734200
H	-0.67740000	-0.33504400	-3.30072600
H	-0.58665900	0.87831200	-4.62766200
H	-1.66021700	-0.54278100	-4.78825500
C	4.05279200	2.14063200	2.00928700
C	4.51147200	3.28873100	2.91917300
H	3.87866000	4.18963400	2.78385100
H	5.56658200	3.57420600	2.72767900
H	4.42386900	2.98953700	3.98361900
C	5.83856000	0.33029800	-3.57592400
H	5.92386100	1.22469200	-4.22854600
H	5.88010800	-0.56518300	-4.23039600
H	6.72842400	0.31500600	-2.91293200
Au	-2.28501700	-2.29232200	0.57863100
Cl	-3.33773800	-3.86485400	1.94744500
H	4.64760800	1.23927500	2.27400900

[AuCl( $\eta^2$ -Z-**2b**)]

Au	0.07071200	-2.50975500	0.76728300
Cl	0.04762700	-3.72399500	2.79236500
P	0.95058200	-1.31108700	-1.19123400
P	-1.19642800	-1.26497700	-0.97434100
N	-3.22993200	1.95084200	0.58945000
N	-4.09490000	0.29354100	-0.62220900
N	3.57433800	1.74972100	-0.69674200
N	3.99153800	-0.44862700	-0.73642300
C	1.61601400	0.25871000	-0.66940700
H	0.97510800	1.12743500	-0.44937600
C	2.98352100	0.49876100	-0.69527000
C	-1.62698400	0.28386700	-0.21180200
H	-0.85336800	0.91276000	0.25803000
C	-2.91768600	0.79019700	-0.09509600
C	5.30412200	0.17828000	-0.93343000
H	5.66444600	0.03488200	-1.97801300
H	6.05068800	-0.27370400	-0.25033500
C	5.03681200	1.66851800	-0.62148900
H	5.41240600	1.95519200	0.38776100
H	5.50134400	2.35104100	-1.36221200
C	-4.64184300	2.31036900	0.42408200
H	-4.76127100	3.13422500	-0.31782300
H	-5.07396800	2.64958500	1.38649300

C	-5.26330300	1.00108200	-0.09144100	H	2.71833400	2.80698700	3.80058600
H	-5.74930600	0.41816700	0.72546200	H	1.40032000	2.65300000	2.59100700
H	-6.01586000	1.16464500	-0.88930100	C	2.34757400	2.54294000	-3.23381900
C	3.82586900	-1.77580600	-0.21926600	H	2.95380500	1.64763100	-2.98830500
C	3.85469200	-2.87168500	-1.11993600	C	0.95733400	2.04597300	-3.67251000
C	3.61548200	-4.15904200	-0.60657200	H	0.47466800	1.46331300	-2.86420300
H	3.61417400	-5.02309100	-1.28842900	H	1.03879000	1.38645700	-4.56121700
C	3.32283500	-4.34695000	0.75123300	H	0.28804700	2.89130200	-3.93827400
H	3.07967800	-5.35040200	1.13208000	C	-1.61715800	-0.40016500	3.31619500
C	3.30987600	-3.25419100	1.62843100	H	-1.01189200	-0.48800300	2.39260800
H	3.04490500	-3.41552900	2.68331500	H	-2.01295200	-1.41178800	3.53490600
C	3.58284400	-1.95121400	1.16954600	H	-0.93471700	-0.12069600	4.14606900
C	4.64834100	-1.00907400	3.25767200	C	-2.75048100	0.62785500	3.14403900
H	4.39411800	-1.88542200	3.88949900	H	-3.36570400	0.29373400	2.28443500
H	4.70737500	-0.12282400	3.92429300	C	-3.67678300	0.67100700	4.37372200
H	5.65527300	-1.18727500	2.82604700	H	-3.12306700	0.94558100	5.29614700
C	3.59157700	-0.78913200	2.15750300	H	-4.13080800	-0.32672200	4.54704400
H	3.88799900	0.12384600	1.60029600	H	-4.49713400	1.40731900	4.24260300
C	2.19910800	-0.52486500	2.76037900	C	-2.18874500	2.00338600	2.80385000
H	1.47381700	-0.26707100	1.96324600	C	-1.45505800	2.71344100	3.77325200
H	2.23964100	0.31916700	3.47937400	H	-1.30228100	2.26600900	4.76774000
H	1.80456700	-1.41698700	3.28849700	C	-0.93152900	3.98242500	3.49434700
C	5.57372600	-2.95483300	-2.96413800	H	-0.37720200	4.53191500	4.27093300
H	6.27969800	-2.36366300	-2.34487300	C	-1.08379400	4.53454500	2.21692100
H	5.77951900	-2.73141700	-4.03254800	H	-0.63254300	5.51227800	1.98315000
H	5.80368700	-4.02773100	-2.79082800	C	-2.37640800	2.60530500	1.52605200
C	4.10502400	-2.64791600	-2.60550600	C	-1.79112100	3.85830200	1.20073100
H	3.92155800	-1.56717400	-2.79154000	C	-1.85358300	3.64639200	-1.40103300
C	3.13155400	-3.43767000	-3.49646300	H	-1.07581500	2.86250200	-1.32103800
H	3.29764600	-4.53296400	-3.42080500	H	-1.62054300	4.25849400	-2.29674600
H	3.26837200	-3.15793100	-4.56210600	H	-2.82029000	3.14022800	-1.59177600
H	2.08242200	-3.22365400	-3.20872100	C	-1.88417700	4.55217700	-0.15907500
C	2.85026800	2.97569100	-0.74638300	H	-0.95487600	5.15906900	-0.20899000
C	2.25902300	3.39076200	-1.97017800	C	-3.05902500	5.55239200	-0.20456000
C	1.58972700	4.63001000	-1.99203100	H	-4.03907900	5.03557000	-0.14730900
H	1.12743300	4.97667200	-2.92965700	H	-3.04147100	6.13329900	-1.15079900
C	1.52055000	5.43659900	-0.84645800	H	-3.01175000	6.26869700	0.64093700
H	1.01958300	6.41640500	-0.89454700	C	-4.20635100	-0.91034100	-1.38292700
C	2.08856500	4.99840200	0.35852100	C	-4.10637100	-0.82566400	-2.79585900
H	2.01399200	5.62781600	1.25906500	C	-4.14820700	-2.02464200	-3.53178900
C	2.74712700	3.75624600	0.43548600	H	-4.04894500	-1.99284400	-4.62803200
C	2.28889100	3.24807400	2.87709200	C	-4.30718500	-3.25895700	-2.88617700
H	1.94027600	4.27087900	3.12776900	H	-4.32998800	-4.18781100	-3.47764100

C -4.43602000 -3.31762400 -1.49143000  
H -4.55482300 -4.29330800 -0.99598700  
C -4.38182700 -2.14861100 -0.71085300  
C -3.55516600 -3.27884700 1.41595100  
H -3.84431100 -4.30952400 1.12263000  
H -3.57727600 -3.23220600 2.52357400  
H -2.50473300 -3.11835200 1.10051200  
C -4.49061400 -2.22240700 0.80745700  
H -4.16583200 -1.23807900 1.20535600  
C -5.95361900 -2.45348000 1.23905700  
H -6.63629700 -1.68463900 0.82089500  
H -6.04502000 -2.43502900 2.34535600  
H -6.31546300 -3.44245200 0.88601700  
C -4.86234100 0.71351100 -4.67586600  
H -4.66026000 -0.00578700 -5.49737900  
H -4.75024200 1.73340700 -5.09955800  
H -5.91977200 0.58157200 -4.36658400  
C -3.89854900 0.51337600 -3.49297100  
H -4.11398000 1.30319600 -2.74240100  
C -2.42887200 0.68823000 -3.92360700  
H -1.74791800 0.59677700 -3.05509500  
H -2.26824100 1.68578100 -4.38349200  
H -2.13608400 -0.08484700 -4.66495300  
C 3.33646200 3.26787100 1.75358300  
C 4.57449900 4.09468600 2.15336100  
H 4.29732000 5.15128700 2.35535500  
H 5.34080300 4.10268200 1.35104000  
H 5.04181200 3.68674700 3.07400600  
C 3.06809400 3.29721700 -4.36797600  
H 2.49703200 4.19355300 -4.69032400  
H 3.18830300 2.64264500 -5.25641400  
H 4.07559900 3.63846800 -4.05191800  
H 3.65471400 2.21703300 1.59605100

[AuCl( $\eta^2$ -E-2b<sup>H</sup>)]

P 0.91154900 -1.06791200 -0.58523600  
P -0.91001400 -1.06902100 0.58752800  
N 4.05497500 -1.09136700 -0.96247100  
N -4.58282600 -1.56518100 -1.15261900  
N -4.05398100 -1.08963000 0.96181800  
N 4.58565200 -1.55899700 1.15334200  
C 3.52103000 -1.31000300 0.29494600  
C 2.17918600 -1.30408100 0.65058700

H 1.93915400 -1.44328200 1.71764900  
C -3.51891300 -1.31312000 -0.29422600  
C -2.17675100 -1.30876200 -0.64862700  
H -1.93563500 -1.45177300 -1.71493700  
C -5.84879600 -1.24498700 -0.49044300  
H -6.66915500 -1.91582100 -0.81807900  
H -6.16403700 -0.18875500 -0.67049200  
C 5.85112300 -1.24186000 0.48871500  
H 6.67153000 -1.91174800 0.81816400  
H 6.16695000 -0.18507300 0.66439700  
C -5.46748000 -1.45444500 0.98961900  
H -6.05002300 -0.80578700 1.67516200  
H -5.62777700 -2.51823700 1.29270900  
C 5.46833000 -1.45688600 -0.99015400  
H 6.05050000 -0.81111700 -1.67873600  
H 5.62790300 -2.52189800 -1.28929000  
H 4.46254300 -1.33496600 2.14238100  
H 3.45116600 -1.21185000 -1.77958200  
H -3.45100300 -1.20630300 1.78007200  
H -4.45870200 -1.34529200 -2.14245500  
Au -0.00087800 1.17022500 -0.00003800  
Cl -0.00236200 3.49407100 -0.00184400

TS1-2b<sup>H</sup>

P 0.57042200 -0.42918500 1.83353700  
N 4.61244800 0.51876900 1.24673900  
N 3.43487100 -0.87413300 -0.04107900  
C 3.32663600 0.00503600 1.02192900  
C 5.47901500 0.18815100 0.11492300  
H 6.53523700 0.05332700 0.42763100  
H 5.44787800 0.96089000 -0.69294300  
C 4.83237200 -1.12381700 -0.37113200  
H 4.97680800 -1.29762600 -1.45703100  
H 5.25375800 -1.99941800 0.18177200  
C 2.20747600 0.34441800 1.75281600  
P -0.57912800 0.76899300 0.39670400  
N -4.65054100 0.66062600 0.19460200  
N -3.20547000 1.75731800 -1.08446600  
C -3.31115600 0.91508800 -0.00148800  
C -5.47571700 1.53027500 -0.64442700  
H -6.38540700 1.01211300 -1.00968200  
H -5.79140700 2.45309700 -0.10112900  
C -4.48611900 1.86763300 -1.78200600



H	-4.64654100	2.88305600	-2.19744900
H	-4.56943200	1.13024000	-2.61569500
C	-2.26525300	0.40164600	0.77435900
H	2.36329800	1.09506900	2.54795200
H	-2.54902900	-0.27120000	1.60262200
Au	0.22503200	-1.59054000	-0.26672600
Cl	0.12856000	-3.15162100	-1.98870200
H	2.70343700	-1.58029400	-0.18684900
H	4.66877800	1.45572200	1.65020600
H	-2.31100800	1.80657000	-1.57942700
H	-4.97357400	0.32707600	1.10352900

[AuCl( $\eta^1$ -E-2b<sup>H</sup>)]

P	-0.19636900	-1.01167400	-0.05325900
N	-3.77559900	-3.00943300	0.21037400
N	-3.46251300	-0.83415900	-0.16834300
C	-2.80701800	-2.02601200	0.03748000
C	-5.09063300	-2.48367800	-0.16416000
H	-5.90124900	-2.92176100	0.45307100
H	-5.32772300	-2.66942900	-1.23993900
C	-4.89136900	-0.97673400	0.09918900
H	-5.50232600	-0.33969100	-0.57163200
H	-5.14740100	-0.71901200	1.15505600
C	-1.43483200	-2.25458900	0.08350700
P	1.69893800	-1.84574200	0.14564800
N	4.99797800	0.58078100	0.04599200
N	4.87631100	-1.65024000	-0.04870500
C	4.11569400	-0.49202000	0.05022800
C	6.37129500	0.10469600	0.20684000
H	7.09784500	0.73982800	-0.34003100
H	6.68180300	0.06005300	1.27932200
C	6.25957000	-1.31423800	-0.38662000
H	6.98200200	-2.02340900	0.06691100
H	6.43367900	-1.29406600	-1.49002600
C	2.73461200	-0.39948400	0.14379700
H	-1.09993100	-3.29450300	0.22473200
H	2.30404900	0.61374800	0.21862200
H	4.70156400	1.45186800	0.48967700
H	4.43376800	-2.47386700	-0.46429500
H	-2.96039500	0.05253900	-0.01490000
H	-3.52920300	-3.97235700	-0.02482000
Au	-0.74701400	1.19871700	-0.02776800
Cl	-1.33459400	3.43508200	0.02172200

TS2-2b<sup>H</sup>

P	-1.96380800	0.60147700	-1.65877800
P	0.23241600	0.53982600	-1.34660200
N	-4.93063400	0.63109300	-0.47476600
N	2.25057800	3.65923800	0.45103200
N	2.86379700	1.51812500	0.35211500
N	-4.37880400	0.13553400	1.63594600
C	-3.86323900	0.36946800	0.36700100
C	-2.51312500	0.34641700	0.01509300
H	-1.79854000	0.11124800	0.82153700
C	1.88307800	2.40369300	-0.00819900
C	0.69443600	2.11786900	-0.69387500
H	0.02848000	2.96843300	-0.91341100
C	3.64412100	3.63653600	0.90555600
H	3.80732600	4.30797700	1.77286000
H	4.34989700	3.93452700	0.09319100
C	-5.83299600	-0.02022200	1.55992900
H	-6.33995800	0.36419400	2.46842400
H	-6.13392400	-1.08586500	1.41403500
C	3.81714000	2.14461800	1.26614200
H	4.85063600	1.78015900	1.09924500
H	3.54889200	1.95489400	2.33257300
C	-6.15570500	0.81325800	0.30196800
H	-7.05037000	0.44068800	-0.23750100
H	-6.32980200	1.88372100	0.57066300
H	-3.83841900	-0.46002500	2.26690400
H	-4.75459800	1.18433100	-1.31765100
H	2.63125300	0.50988000	0.39064200
H	1.87951900	4.48127600	-0.02839100
Au	1.10297300	-1.26776900	-0.23435200
Cl	1.95934200	-3.04817700	0.98996400

[AuCl( $\eta^1$ -Z-2b<sup>H</sup>)]

P	1.99030200	-1.00347800	-0.06947900
P	0.18989000	0.00234900	0.25319400
N	5.12688000	-1.09535500	0.34090800
N	-0.83214000	3.97841200	0.05886300
N	-2.20267200	2.22607800	0.01714800
N	5.57806800	0.92988000	-0.48828200
C	4.54752700	0.04731400	-0.18310900
C	3.19081500	0.28067900	-0.37352600
H	2.90933100	1.26008800	-0.79533000

C	-0.88518200	2.59055600	0.09866600
C	0.23321300	1.76016900	0.19514200
H	1.21555300	2.24918900	0.28793300
C	-2.17653200	4.53445600	0.24077900
H	-2.31782600	5.46987100	-0.33786000
H	-2.39843400	4.74801100	1.31422700
C	6.86750800	0.23923300	-0.40902200
H	7.67865200	0.91275800	-0.06445500
H	7.17014900	-0.20172300	-1.38961400
C	-3.05249700	3.37469100	-0.28028600
H	-4.03064900	3.31007100	0.23731300
H	-3.24374900	3.47635000	-1.37545200
C	6.54571900	-0.87252400	0.61061800
H	7.14998500	-1.78810200	0.44652200
H	6.72640500	-0.51708400	1.65421600
H	5.41665900	1.60624200	-1.23679900
H	4.55854400	-1.68197200	0.95751800
H	-2.45715700	1.25426800	-0.21650900
H	-0.03005100	4.44010000	0.49086700
Au	-1.78842400	-1.09953900	0.02878600
Cl	-3.82818700	-2.15635800	-0.22931900

### TS3-2b<sup>H</sup>

P	1.89820200	-0.73550500	1.26260400
P	0.06811000	0.30302900	1.72624500
N	4.94669400	-1.07949400	0.46582900
N	-0.78514900	4.07591000	0.26139700
N	-1.99689400	2.20253000	0.07708000
N	5.14658100	0.85245500	-0.60823900
C	4.27561600	0.06411800	0.11382500
C	2.94863100	0.39479800	0.42770100
H	2.57266200	1.36584100	0.05782900
C	-0.80331700	2.71045900	0.54953400
C	0.21403200	2.00714000	1.17780700
H	1.10714900	2.57634400	1.48584500
C	-2.12123800	4.50666000	-0.16085100
H	-2.07615400	5.32321700	-0.91068700
H	-2.74294500	4.85525100	0.69945900
C	6.35592000	0.10026300	-0.95350900
H	7.26028700	0.74155300	-0.94175400
H	6.27332100	-0.37270300	-1.96081400
C	-2.68724200	3.19540400	-0.74241800
H	-3.78940900	3.12415700	-0.64159200

H	-2.43018000	3.09570600	-1.82454000
C	6.37159600	-0.97024300	0.16129300
H	6.79855100	-1.93439600	-0.18136000
H	6.95946300	-0.62188800	1.04414100
H	4.76430600	1.55404700	-1.24436900
H	4.57927300	-1.66115000	1.22336500
H	-2.02945800	1.20128400	-0.16516300
H	-0.25211100	4.67704000	0.89294200
Au	-0.89954800	-1.06793700	0.07394800
Cl	-2.07505100	-2.20926400	-1.58189300

### [AuCl( $\eta^2$ -Z-2b<sup>H</sup>)]

P	-0.90643000	-0.49105700	-1.39896500
P	1.22571400	-0.14857300	-1.20035100
N	-3.80833400	-1.29397100	-0.44432400
N	3.85738400	-2.14648100	1.21069500
N	4.23188400	-0.89632800	-0.59600700
N	-3.21501900	-3.02600400	0.83016600
C	-2.72366900	-2.01465300	0.01856700
C	-1.38184800	-1.77370100	-0.25927000
H	-0.64186900	-2.42084400	0.24004200
C	3.23739700	-1.38511000	0.22800500
C	1.86795800	-1.17429000	0.10961500
H	1.22597500	-1.61442400	0.89053400
C	5.30551700	-1.92736300	1.17735100
H	5.86946400	-2.84020000	1.45833700
H	5.62054800	-1.09678200	1.85403600
C	-4.66906100	-3.12695900	0.69071000
H	-5.15771100	-3.42379300	1.64118300
H	-4.96495200	-3.85886900	-0.09941900
C	5.51118400	-1.53377000	-0.30044800
H	6.36456600	-0.83927600	-0.44052700
H	5.68988200	-2.43864800	-0.93137200
C	-5.02555200	-1.68772100	0.26403900
H	-5.91979000	-1.64766900	-0.39085200
H	-5.21602300	-1.04434000	1.15628900
H	-2.65191100	-3.87053700	0.94276500
H	-3.65664300	-0.32024000	-0.72028000
H	3.98219200	-0.58682800	-1.53839400
H	3.38096100	-2.24000700	2.10960400
Au	-0.20652200	1.51922800	-0.08534900
Cl	-0.74068800	3.35875100	1.23442300

**Z-3**

P -1.06258200 -2.31570900 0.10939100  
P 1.00084800 -1.99188700 0.92139900  
N -4.02049000 -1.09485200 -0.42848600  
N 3.10013400 1.21119500 -0.79741500  
N 3.96860900 -0.23930000 0.64637700  
N -3.58825200 0.86853100 0.55194800  
C -2.99456700 -0.30036500 0.07195300  
C 4.77360200 -2.28857500 1.68654700  
C -2.96104600 1.68452700 1.53926300  
C -3.86100400 -1.98694600 -1.53261500  
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C 2.29679000 1.77329300 -1.82924300  
C 4.52678900 1.48535000 -0.76795300  
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H 5.05689300 0.98767700 -1.60229800  
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C 3.31096600 -0.76106300 2.94977800  
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H 6.20205200 -1.53908500 0.32500800  
C -4.19833200 -3.34242400 -1.35056500  
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H -1.76334900 1.62830300 4.71713300  
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H -3.48401300 -0.76604200 2.37074100  
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H -3.13036600 -2.01242400 -4.85521200  
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H 0.32040600 3.52286600 -4.66290600  
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H -3.71866700 -4.39981500 -4.56143800  
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C -3.99944200 0.59318100 -4.14315800  
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H -5.07238400 0.47788500 -3.92882000  
H -3.79995500 0.12408900 -5.11833000  
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H -1.32520400 3.99994200 4.16616900  
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H -1.38900400 1.20294700 -3.48355000  
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H 0.85587400 1.61216600 3.70503600  
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H 1.04716200 -1.25079800 -3.53416700  
H 2.47383400 -2.15821900 -4.09697400  
H 1.77804000 -0.87649600 -5.10954800  
C 0.95516100 2.90117000 0.84257500  
H -0.11560500 3.01404000 0.62660000  
H 1.13324900 3.30928000 1.85038000  
H 1.17815100 1.82695700 0.85720900  
C -1.85427400 -1.09464100 3.69374900  
H -1.35333100 -0.64038000 4.56274800  
H -1.11171300 -1.22122700 2.89442900  
H -2.19957600 -2.09621800 3.98973100  
C 1.45782600 5.13876400 -0.17399600  
H 2.03247300 5.70757900 -0.91928100  
H 1.67269200 5.55676400 0.81971500  
H 0.38596700 5.30264800 -0.36950000

C -3.34748200 5.06650200 -0.20998600  
H -2.39245300 5.59758800 -0.07516900  
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H -3.74455100 5.35757000 -1.19301400  
C -4.11050700 -0.17823500 4.33328900  
H -4.46235700 -1.18822000 4.59072400  
H -4.97701700 0.42323700 4.02042800  
H -3.70231100 0.27959000 5.24730200  
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H 5.75748900 -2.92616400 -1.62187100  
H 4.24207100 -2.16507600 -1.07114200  
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C -0.48961500 -2.91975500 -1.59782900  
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H 2.64077000 -3.77373300 0.60094000  
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C 1.47307900 -5.93049800 -0.08878800  
H 1.48756200 -5.97527600 1.01204400  
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#### TS4

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N 3.63992500 -1.12158500 0.79006100  
C 2.93981900 0.03658000 0.46092300  
C -5.25363000 1.24224800 0.24782500  
C 3.08641800 -2.29755900 1.37975400  
C 3.78512800 2.13748400 -0.61166900  
C 1.57932400 0.14958700 0.36431700  
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C -2.71202900 -0.97575700 0.03421500

C	3.78169500	1.88080400	-2.00004400	C	3.98128800	4.50494100	-1.02332100
C	-4.42280800	0.50472700	1.11417300	H	4.05662200	5.52866100	-0.65003700
C	-1.57235600	-0.21429300	0.00384200	C	-3.28367800	0.11421200	3.35315000
H	-0.78637700	-0.62065400	-0.63953200	H	-2.57688500	-0.46355700	2.73721400
C	-1.92260700	-2.71525700	-1.57907600	C	3.85435400	3.74031200	1.37925000
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H	-4.70785300	-2.38015700	-1.58009800	H	0.11388200	-5.40455100	-2.03519400
C	3.28927900	-3.50975000	0.68352800	C	-0.98377600	-2.71929000	-3.79654800
C	-4.10755100	0.97213700	2.40739000	H	-0.88108500	-2.26528400	-4.78468000
C	2.50966300	-2.27390500	2.66318900	C	-0.30966500	-3.89800700	-3.50855200
C	-5.65314600	0.73882400	-1.13118900	H	0.32051100	-4.36543100	-4.26716400
H	-5.15099100	-0.22373100	-1.29993900	C	4.00256800	4.26909800	-2.39402200
C	3.86641300	3.45128300	-0.11125600	H	4.09520300	5.10255500	-3.09226400
C	-1.81762000	-2.11486800	-2.84650800	C	-1.28842700	-4.45256900	0.15456700
C	-1.21417700	-3.89364100	-1.25721300	H	-2.35113100	-4.46516300	0.44801900
C	4.99672200	-0.78562000	1.20433200	C	2.92253200	-4.70508300	1.30392300
H	5.70641600	-1.57783500	0.92534700	H	3.08313500	-5.65524200	0.79384100
H	5.04431900	-0.65108800	2.30151200	C	4.69030300	0.16693200	-3.63606300
C	-5.74602500	2.47566500	0.69173500	H	4.60602400	-0.88345200	-3.95261500
H	-6.38869900	3.06574700	0.03431000	H	5.70696600	0.33039300	-3.24862200
C	-4.60601800	2.21413800	2.80112700	H	4.56728900	0.79057600	-4.53397700
H	-4.35613200	2.60830100	3.78624700	C	2.35472400	-4.69912800	2.57756600
C	3.62959400	0.48162600	-2.57759700	H	2.07169300	-5.64083600	3.05124100
H	3.75640000	-0.24887400	-1.76606900	C	2.21317100	0.30201600	-3.13900200
C	-4.79195400	-1.91997800	0.56808000	H	2.01451400	1.03858600	-3.93425400
H	-5.83501000	-1.60890600	0.41959600	H	1.46854500	0.44148900	-2.34200000
H	-4.74169800	-2.54503900	1.47659500	H	2.08154600	-0.70621300	-3.56090500
C	-5.41627900	2.96349900	1.94997900	C	2.76727000	4.75345300	1.74521500
H	-5.79643300	3.93333400	2.27540600	H	2.96512000	5.73899100	1.29491200
C	3.85253500	-3.47158100	-0.72744000	H	2.72728100	4.88804600	2.83651100
H	4.68636800	-2.75122000	-0.73006200	H	1.78493100	4.39884900	1.40306300
C	5.23506200	0.51985500	0.46762900	C	-3.56633200	-1.12255800	-4.36420800
H	5.87754400	1.21894000	1.02083300	H	-3.03879900	-1.43381000	-5.27868900
H	5.68924600	0.34575800	-0.52597400	H	-4.13503900	-0.21089500	-4.59968700
C	-2.58120200	-0.85535300	-3.22173600	H	-4.27880500	-1.91894300	-4.10215700
H	-3.16048000	-0.53012700	-2.34613600	C	5.23068100	4.21579300	1.85817100
C	2.14036400	-3.49729400	3.23860800	H	6.01985700	3.48879600	1.61675500
H	1.68556600	-3.50200700	4.23169100	H	5.22870000	4.37262300	2.94710800
C	2.28480500	-0.99029500	3.44552600	H	5.50205600	5.17013000	1.38028000
H	2.67815900	-0.14884000	2.85925500	C	-4.19854800	-0.87767800	4.08318200
C	3.88732500	2.96807000	-2.87326900	H	-3.60798200	-1.55297200	4.72030700
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H -1.02797700 0.04311700 -4.47239600  
C -0.54975800 -3.52357100 1.12716800  
H 0.51180000 -3.44703100 0.84315300  
H -0.59385200 -3.92427900 2.15106900  
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H 2.89679200 -0.05160600 5.30660000  
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H 1.51943700 3.38569600 -1.96019600  
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H 0.45455800 5.98122600 0.06562000  
H -0.07286400 6.44333400 -1.55765100  
H 1.48994200 5.61566600 -1.33537500  
C -2.19930300 5.29081000 0.11257400  
H -3.22766100 5.03781600 0.40265800  
H -2.22261400 6.23554200 -0.45219200  
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**TS6**

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C 5.17969800 -1.21765900 1.52411400  
H 5.68828500 -2.19120300 1.46338100  
H 5.22310200 -0.87328800 2.57185500  
C 4.62893200 1.70288500 -0.64761200  
C 4.32706600 2.86675500 0.08703300  
C 4.39692300 4.09789400 -0.57073600  
H 4.16201100 5.01315500 -0.02300900  
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H 4.00216300 1.75998000 1.87619300  
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H 2.27726900 4.24701400 1.38047200  
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H 5.86735700 3.38195600 2.32294300

H	4.52908000	3.55039600	3.48975500	N	-4.51085100	0.03786500	0.52585700
H	4.71962700	4.73164600	2.17914600	N	-3.34396300	1.83322000	1.12906700
C	5.20695900	0.49714000	-2.82121000	C	-3.26221000	0.64829800	0.39825700
H	5.03650700	-0.35970300	-2.15211700	C	-5.26472200	0.65286900	1.60614100
C	4.20050900	0.38245300	-3.97018800	H	-6.34588500	0.60516200	1.41368900
H	3.16832900	0.41027400	-3.59162400	H	-5.05961900	0.15983300	2.57634100
H	4.34118300	-0.56264500	-4.51524000	C	-4.70813700	2.06935400	1.57801300
H	4.32193200	1.20686400	-4.68947800	H	-4.72410300	2.56378900	2.55960400
C	6.64786500	0.42490000	-3.33457200	H	-5.26453300	2.70292900	0.85987400
H	6.85886000	1.25020700	-4.03217100	C	-4.84766500	-1.26520500	0.06389100
H	6.82068000	-0.52027500	-3.87096600	C	-5.79806000	-1.36040400	-0.97949300
H	7.37129000	0.49220100	-2.50887000	C	-6.17559100	-2.62906600	-1.42286100
C	3.12110300	-2.59138700	1.06698800	H	-6.90537400	-2.72784800	-2.22692600
C	3.35666200	-3.49764700	0.01492100	C	-5.64446900	-3.77707000	-0.83634400
C	2.65428200	-4.70780200	0.01895100	H	-5.95328600	-4.76176500	-1.19098100
H	2.80563000	-5.42104100	-0.79414600	C	-4.73306000	-3.66777700	0.20505800
C	1.76443000	-5.01269600	1.04356000	H	-4.33093000	-4.57212500	0.66667900
H	1.22034700	-5.95870700	1.02760500	C	-4.31589400	-2.41558600	0.67492800
C	1.57549300	-4.12148100	2.09817400	C	-6.38459100	-0.09755100	-1.59290800
H	0.88905300	-4.38237100	2.90532700	H	-6.48738200	0.63524800	-0.77813800
C	2.25128700	-2.90028300	2.13122100	C	-5.42320300	0.50776600	-2.62023600
C	4.37209400	-3.21254200	-1.08274100	H	-5.35085400	-0.14391000	-3.50502100
H	4.94567900	-2.32222500	-0.78642400	H	-5.78193700	1.49529300	-2.95123400
C	3.71116200	-2.88576600	-2.42528400	H	-4.41297900	0.62524300	-2.20166000
H	3.01827700	-3.68437800	-2.73286300	C	-7.76844800	-0.30341700	-2.20668200
H	4.47806700	-2.77427900	-3.20778400	H	-8.46223000	-0.77913300	-1.49845900
H	3.14573100	-1.94484200	-2.36576600	H	-8.19235100	0.66562200	-2.50682600
C	5.36903000	-4.36692600	-1.23004900	H	-7.71995600	-0.92893000	-3.11074300
H	5.82941200	-4.62560300	-0.26529900	C	-3.33640900	-2.34753000	1.83459000
H	6.16799900	-4.09220200	-1.93444600	H	-3.06733600	-1.29366400	1.99570100
H	4.88018400	-5.27101000	-1.62282200	C	-2.04412400	-3.10552500	1.51772900
C	2.12363300	-1.95145000	3.31010100	H	-1.52971200	-2.67542300	0.64559900
H	2.39367800	-0.94915600	2.94200200	H	-1.35130000	-3.05266900	2.36887100
C	0.71181600	-1.86392700	3.88376400	H	-2.24324300	-4.17050000	1.31720000
H	0.00126600	-1.54132200	3.10979500	C	-3.98318400	-2.87523600	3.12052100
H	0.68745400	-1.12797000	4.70090600	H	-4.23911600	-3.94183300	3.02412300
H	0.37598000	-2.82632200	4.30107000	H	-3.28976300	-2.76965800	3.96834100
C	3.12855400	-2.35288800	4.39862400	H	-4.90848500	-2.33040900	3.35939700
H	2.87763400	-3.34650200	4.80177200	C	-2.47161400	2.94032900	0.91799400
H	3.11322300	-1.63231000	5.23005300	C	-1.62311000	3.32606300	1.97713200
H	4.15345800	-2.40602000	4.00367900	C	-0.74327800	4.38669700	1.76118300
C	2.21728000	0.04700900	-0.26216000	H	-0.06973000	4.70486700	2.55707000
P	-0.56530400	0.87756100	-0.56765400	C	-0.70687500	5.04643600	0.53331900

H 0.00060200 5.86277900 0.37663400  
C -1.58099500 4.68230400 -0.48182900  
H -1.56248500 5.22233000 -1.43108000  
C -2.49162900 3.63494200 -0.30458300  
C -1.67659200 2.58641200 3.30632000  
H -2.73990100 2.38861500 3.51653000  
C -0.97435900 1.22715000 3.22808600  
H 0.09622700 1.35423100 2.99995000  
H -1.06493400 0.69866700 4.18969100  
H -1.40019200 0.59415800 2.43702200  
C -1.12086400 3.40369700 4.47148900  
H -1.57607700 4.40328900 4.52627500  
H -1.31525600 2.88320300 5.42013700  
H -0.03033900 3.52850200 4.38697200  
C -3.48156300 3.30799000 -1.41165400  
H -4.09767200 2.45989600 -1.08153800  
C -2.78656800 2.88668700 -2.70946500  
H -2.18664100 1.97790000 -2.55871100  
H -3.53374200 2.68422600 -3.49220600  
H -2.11946000 3.68128300 -3.07814900  
C -4.42310700 4.49361600 -1.65476400  
H -3.87000100 5.36648400 -2.03424400  
H -5.18745000 4.23032200 -2.40170300  
H -4.93232800 4.79811000 -0.72840400  
C -2.19623100 0.12988700 -0.27282200  
H 2.22677500 0.89654200 -0.95393600  
H -2.35295200 -0.87508500 -0.67908500  
C -1.10965600 -1.16567500 -3.07681200  
C -0.20426600 -0.14678000 -3.09769400  
H -0.39074800 0.74220600 -3.70427800  
H 0.80506800 -0.25609000 -2.69946700  
C -0.90868600 -2.35777700 -2.26468100  
C 0.24399700 -2.57026400 -1.56938000  
H 1.15300300 -2.01116800 -1.78035600  
H 0.35537000 -3.44669900 -0.92656900  
C -2.42602700 -1.01939800 -3.79487700  
H -3.27174200 -1.12957800 -3.10002800  
H -2.54565800 -1.79476500 -4.56884100  
H -2.50749600 -0.03655900 -4.27847900  
C -2.05714300 -3.33063900 -2.13931500  
H -1.79946000 -4.15648600 -1.46305600  
H -2.31518100 -3.76106500 -3.12005200  
H -2.97293100 -2.85235500 -1.75653900

*E-3*

P 2.47629800 4.70720700 12.59221100  
P 1.52998700 2.93385700 11.62143300  
N 1.62687900 7.63130400 11.05887800  
N -1.23948500 1.20151000 12.06728500  
N 3.01940200 7.24562800 9.35545100  
N -1.12139800 1.26713600 14.28790900  
C -0.43146700 1.59174400 13.12501700  
C 3.89032600 6.52392200 8.48901500  
C -0.88420300 1.05153500 10.69491300  
C 2.57388000 6.73346100 10.57409100  
C 0.79053300 2.18969700 13.09701800  
H 1.28239800 2.30046400 14.06962500  
C 3.02271600 5.56282200 11.09341600  
H 3.72069100 5.03180700 10.44170400  
C 1.40178100 7.86511200 12.44988600  
C 3.37689900 5.57301500 7.59148300  
C 4.87515800 3.39245700 11.84987500  
C 0.13216800 7.58629400 12.98746500  
C -1.41406200 1.94415800 9.74488000  
C -0.07199300 -0.03549300 10.29603700  
C 0.17179600 -0.21303100 8.93151200  
H 0.80616700 -1.03508700 8.60025300  
C -1.19706200 1.68936300 8.38787200  
H -1.62441000 2.36253100 7.64086200  
C 2.41854600 8.44255800 13.23830400  
C 5.27893900 6.76690600 8.58630600  
C 4.10285200 3.84135100 13.05934800  
H 4.69605400 4.53192800 13.67714800  
H 3.80324700 3.00317100 13.70994600  
C 4.35367900 2.44690700 11.03935600  
C 2.08258500 8.23846100 8.85770800  
H 1.29171300 7.78700900 8.22983500  
H 2.59483800 9.00781800 8.26339200  
C 1.50632900 8.77790800 10.16365900  
H 2.09878100 9.63401600 10.53939700  
H 0.45867500 9.09805200 10.07130500  
C 1.91935200 5.14739200 7.61465200  
H 1.42222700 5.67387000 8.44245800  
C 2.14272200 8.71378600 14.58109200  
H 2.92424000 9.14238600 15.21246200  
C 3.79482000 8.77516500 12.68312100



H	3.78844800	8.58142000	11.60128900	C	5.62406600	5.22169200	6.74665900
C	-2.15745300	3.19789800	10.16548000	H	6.30297600	4.72358000	6.05255100
H	-2.05991100	3.27538900	11.25788800	C	4.13697200	10.25565900	12.87938600
C	-0.95801000	6.93342300	12.15871200	H	3.37616800	10.90655300	12.42356600
H	-0.50619600	6.65628100	11.19572000	H	5.11010700	10.48847200	12.42203400
C	4.26390400	4.94690300	6.70619700	H	4.20235000	10.51396200	13.94697300
H	3.88024300	4.21573600	5.99120300	C	-3.64420000	3.12701700	9.80477200
C	-2.36901800	0.58100500	14.00530800	H	-3.77732500	3.08544800	8.71240200
H	-3.17500600	0.94621200	14.65780100	H	-4.17742400	4.01605900	10.17494100
H	-2.28240400	-0.51378000	14.14623000	H	-4.12259900	2.23335600	10.23171000
C	-1.50298900	4.44987800	9.57078200	C	6.12357500	4.18509000	11.57623500
H	-0.44888000	4.51911200	9.88376200	H	5.86831100	5.25897000	11.53651000
H	-2.03103700	5.35517200	9.90813600	H	6.61564100	3.92049300	10.63290500
H	-1.54174300	4.43853300	8.46992400	H	6.85275800	4.06183100	12.39349300
C	-0.40681500	0.62270800	7.97985800	C	-1.47092700	5.65151400	12.82166200
H	-0.22586400	0.44787500	6.91807500	H	-0.66170100	4.91307300	12.94832400
C	0.47797200	-1.01996800	11.31624300	H	-2.26581800	5.19956600	12.20937400
H	0.79193000	-0.43640700	12.19687700	H	-1.90380300	5.85891600	13.81344800
C	-0.50742400	1.20925900	15.57014400	C	1.81243300	3.65230800	7.92422100
C	-0.11398800	7.92159200	14.32113500	H	2.24513700	3.03931700	7.11734900
H	-1.10385600	7.73683000	14.74484400	H	0.76278600	3.35565100	8.05153300
C	0.88392500	8.46849300	15.11978700	H	2.33143900	3.41532200	8.86432500
H	0.68062500	8.70485400	16.16556800	C	7.29673900	7.48942600	9.96523900
C	5.81311300	7.69635900	9.66549600	H	7.52881300	6.43468700	10.17027900
H	5.24930300	7.44840100	10.58025100	H	7.58476100	8.08045600	10.84696700
C	-0.55503500	2.33460500	16.41322000	H	7.92841400	7.82468300	9.12811400
C	0.13556500	0.02173200	15.97773600	C	0.00025000	2.23128300	17.69328400
C	6.12993000	6.10735400	7.69781900	H	-0.03439300	3.09430500	18.36173500
H	7.20535700	6.27756200	7.74901500	C	0.60003800	1.05317300	18.12315700
C	-2.59503300	0.94707000	12.53543000	H	1.02472600	0.99037300	19.12633300
H	-3.05980200	0.13866800	11.95380100	C	0.67560400	-0.03943400	17.26441900
H	-3.23124400	1.84727300	12.44975000	H	1.17285200	-0.95416100	17.59519200
C	4.86842200	7.87403600	13.30085700	C	5.54906900	9.16960400	9.33587700
H	4.94031700	8.03448900	14.38782900	H	6.06385900	9.45368600	8.40500100
H	5.85494800	8.08837700	12.86006800	H	5.92444300	9.81609900	10.14381000
H	4.63120600	6.81583100	13.12117700	H	4.47695300	9.37019200	9.21237200
C	1.19709000	5.49958200	6.31150900	C	4.95512800	1.98362200	9.73913200
H	1.24789000	6.57753600	6.09766400	H	4.23527100	2.12768300	8.91688300
H	0.13789900	5.20643100	6.36745200	H	5.17536800	0.90422700	9.77991800
H	1.64754200	4.96893700	5.45847300	H	5.87792900	2.50915400	9.46956900
C	3.05410400	1.79454900	11.42368600	C	-1.15886800	3.64946200	15.95923100
H	3.14642300	1.28287100	12.39539900	H	-1.48813700	3.51782400	14.91813300
H	2.75999900	1.03673500	10.68110600	C	-2.10864700	7.90862700	11.89010700

H -2.60572600 8.19734400 12.82953800  
H -2.86594700 7.44623900 11.23831100  
H -1.75230300 8.82911700 11.40516700  
C 1.69777100 -1.79906100 10.82443000  
H 1.43032600 -2.51055100 10.02851700  
H 2.12470900 -2.38333400 11.65187900  
H 2.48397900 -1.13381400 10.44027400  
C -0.61841200 -2.00307600 11.74668000  
H -1.49220700 -1.48125600 12.16095000  
H -0.23935300 -2.69674400 12.51321300  
H -0.95540400 -2.59661600 10.88303800  
C 0.29280200 -1.16116500 15.03988900  
H -0.21837500 -0.91317500 14.10110000  
C -0.10712800 4.76170500 15.98022700  
H 0.32321400 4.88670300 16.98613400  
H -0.55576500 5.72071600 15.69067200  
H 0.71160900 4.55737800 15.27334100  
C -0.35018100 -2.42934500 15.60742400  
H 0.14840800 -2.74568300 16.53631600  
H -0.27164400 -3.25942300 14.88919500  
H -1.41418700 -2.27019300 15.83680400  
C 1.76756400 -1.38833700 14.69456400  
H 2.20655900 -0.48280300 14.24980400  
H 1.86913300 -2.21374200 13.97288000  
H 2.35110300 -1.64980800 15.59066600  
C -2.38092600 4.02330700 16.80344500  
H -3.13860400 3.22620100 16.78783500  
H -2.84321700 4.94620800 16.42157000  
H -2.09948300 4.19955100 17.85333500

### Z-3<sup>H</sup>

P -0.92138900 -1.01955600 -0.24934600  
P -1.24876300 1.22983500 -0.66080000  
N 1.97216900 -2.03052400 -0.89910700  
N 2.26974100 2.62661700 0.93038900  
N 1.86640100 1.50102100 -0.96682500  
N 2.88141600 -1.66643900 1.10224300  
C 1.70465600 -1.54615000 0.37968000  
C 0.52289300 -1.04705200 0.82325900  
H 0.49897200 -0.61269800 1.82575500  
C 1.25883000 2.05278000 0.15617700  
C -0.06319800 2.02155400 0.44909300  
H -0.39157500 2.45358400 1.39720800

C 3.47808500 2.72314400 0.12711700  
H 4.38674200 2.67032300 0.74200100  
H 3.51279700 3.64629800 -0.48020100  
C 3.96554500 -2.13169100 0.25832700  
H 4.63614300 -2.81911800 0.79174800  
H 4.57221400 -1.30534100 -0.15619400  
C 3.30556800 1.50483000 -0.77778400  
H 3.84842400 1.59876000 -1.72773900  
H 3.65020000 0.59380100 -0.25474700  
C 3.18405700 -2.83351300 -0.85701600  
H 3.71652200 -2.82073700 -1.81688000  
H 2.98215300 -3.88336000 -0.57783300  
H 3.04818500 -1.01430700 1.85731900  
H 1.16339200 -2.37919700 -1.40659800  
H 1.45689500 0.64205800 -1.32283900  
H 1.99774500 3.43327400 1.47899700  
C -3.62661400 -0.87459900 0.35275900  
C -2.31635100 -1.24810800 0.99428800  
H -2.30721800 -2.30258600 1.30598100  
H -2.09433200 -0.63520500 1.88282000  
C -3.85518200 0.41938800 0.04580000  
C -2.80413300 1.44301000 0.38768800  
H -2.51130100 1.37887800 1.44739200  
H -3.17347200 2.46330700 0.20765900  
C -4.53014600 -2.02956000 0.02207600  
H -3.98804500 -2.75299100 -0.60902000  
H -5.44314100 -1.73456600 -0.50636900  
H -4.82317400 -2.56525400 0.93913700  
C -5.05937600 0.95143600 -0.67987300  
H -4.73797100 1.47040600 -1.59780400  
H -5.58445800 1.69728400 -0.06176900  
H -5.77929900 0.17565500 -0.96227300

### TS4<sup>H</sup>

P -0.92990000 0.12780300 -1.17835500  
P 1.13590000 0.38576900 -1.02454600  
N -3.73222500 -0.90795500 -0.29936200  
N 4.08522700 -0.53879500 -0.61483000  
N -3.12408500 -2.95329800 0.33706800  
N 3.71427000 -2.09677300 0.92581600  
C 3.09073900 -1.15687900 0.11912200  
C -2.63712700 -1.74346700 -0.13814000  
C 1.75151600 -0.89876000 0.06252400

H 1.10622400 -1.45874000 0.74222800  
C -1.33561500 -1.43484700 -0.39670800  
H -0.58662000 -2.20569200 -0.20967000  
C -1.19830900 2.79726500 0.68114200  
C -1.57460900 1.51376600 0.97807300  
H -2.63143100 1.23778800 1.01202900  
H -0.88719300 0.79447200 1.42138500  
C 0.19249400 3.16588700 0.56867200  
C -4.50895100 -2.79910700 0.74636700  
H -4.60607700 -2.47555300 1.79917500  
H -5.08442900 -3.72363100 0.60571000  
C -4.95794200 -1.67971800 -0.19512900  
H -5.27459800 -2.10086400 -1.16650100  
H -5.78290700 -1.08548100 0.21903800  
C 5.15206100 -1.88778700 0.90561700  
H 5.70565500 -2.82866800 1.02369200  
H 5.48555000 -1.17803500 1.68466400  
C 5.33017500 -1.27192400 -0.48428000  
H 6.20491800 -0.61088000 -0.54238200  
H 5.43394300 -2.06609600 -1.24602900  
C 1.19117900 2.26238500 0.82223800  
H 1.02292200 1.37012100 1.42300500  
H 2.23676300 2.54486600 0.67975500  
C -2.24301300 3.78821800 0.23364700  
H -2.13737000 4.01941400 -0.83924500  
H -2.15790200 4.74198300 0.77588100  
H -3.25393400 3.39339400 0.39690600  
C 0.53416100 4.50529300 -0.03506500  
H 1.62086100 4.65245600 -0.07339500  
H 0.09960500 5.33297800 0.54610700  
H 0.14224200 4.59607800 -1.06118500  
H 3.25662300 -2.33393700 1.79636300  
H 3.81912900 -0.11553600 -1.49673400  
H -2.49683100 -3.51612900 0.89666800  
H -3.64801200 -0.17209700 -0.99328300

#### Z-2b<sup>H</sup>

P -1.01679900 1.60335800 -0.08183700  
P 1.01680100 1.60335700 0.08187600  
N -3.96012300 0.57419400 0.11593500  
N 3.53863500 -1.58436400 0.17246100  
N 3.96011900 0.57419300 -0.11600200  
N -3.53862800 -1.58435800 -0.17243300

C -2.94577700 -0.33597200 -0.08591400  
C -1.60608600 -0.07223600 -0.18109800  
H -0.95050300 -0.92381500 -0.36932500  
C 2.94578300 -0.33597400 0.08591000  
C 1.60609100 -0.07224600 0.18111700  
H 0.95051700 -0.92382300 0.36937600  
C 4.97866500 -1.43953000 0.30519400  
H 5.52023600 -2.27219300 -0.16259800  
H 5.29591100 -1.35610400 1.36055600  
C -4.97865700 -1.43955700 -0.30517900  
H -5.52022400 -2.27219600 0.16266300  
H -5.29591600 -1.35619700 -1.36054300  
C 5.20065900 -0.11089900 -0.42272000  
H 6.07600900 0.43370000 -0.04512800  
H 5.32965000 -0.28160400 -1.50713200  
C -5.20067700 -0.11088200 0.42264900  
H -6.07601700 0.43368100 0.04497700  
H -5.32972700 -0.28151700 1.50706400  
H -3.05416900 -2.28965800 -0.71244200  
H -3.72612000 1.46236400 0.54336200  
H 3.72610400 1.46235400 -0.54344300  
H 3.05420100 -2.28961600 0.71255600

#### TSS<sup>H</sup>

P -0.99633700 1.40407900 -0.40521600  
N -3.82769100 -1.26090300 0.81778700  
N -3.96241900 0.41159900 -0.64073200  
C -3.10422900 -0.24896100 0.21170700  
C -5.10283400 -1.42460000 0.14005800  
H -5.89491500 -1.74989200 0.82715600  
H -5.04191700 -2.14165200 -0.69885200  
C -5.32969700 -0.00549200 -0.38924100  
H -5.93984800 0.01046100 -1.30180100  
H -5.82302500 0.61718100 0.37905600  
C -1.77907800 0.05131700 0.42669200  
P 0.98666200 1.36126000 0.55932700  
N 3.86836200 -1.06059800 -1.00746100  
N 3.92917300 0.28543400 0.76057000  
C 3.12527300 -0.15716200 -0.26673700  
C 5.26479300 -0.98457600 -0.61049400  
H 5.77209700 -1.95372700 -0.70384800  
H 5.82493300 -0.23112100 -1.19357800  
C 5.12500700 -0.53158300 0.84582100

H 5.99348200 0.04379300 1.19223600  
H 4.98993000 -1.40504900 1.50956700  
C 1.82405300 0.22060500 -0.50487800  
H -1.24176800 -0.57672900 1.14146700  
H 1.33443900 -0.22281100 -1.37538800  
H 3.63043600 -1.16479300 -1.98562100  
H 3.47536400 0.64373700 1.59356800  
H -3.74348400 1.37576700 -0.86762500  
H -3.31687500 -2.07501000 1.13431400

### **E-2b<sup>H</sup>**

P -0.84609600 0.56305500 -0.06235300  
N -4.53289200 -1.15594900 0.15344900  
N -3.95892500 0.97235000 -0.12778800  
C -3.44775800 -0.30235500 0.02703300  
C -5.75508600 -0.45469200 -0.19956500  
H -6.61943700 -0.82521300 0.36719500  
H -5.98211100 -0.52042700 -1.27942200  
C -5.37731300 0.98019900 0.17625200  
H -5.92066000 1.72744400 -0.41701000  
H -5.57883100 1.16217800 1.24786300  
C -2.13188100 -0.66483900 0.05467800  
P 0.84608400 -0.56301300 0.06231200  
N 4.53288700 1.15584200 -0.15411500  
N 3.95892200 -0.97225200 0.12847000  
C 3.44775900 0.30232300 -0.02714900  
C 5.75509500 0.45483600 0.19931800  
H 6.61941500 0.82495600 -0.36775500  
H 5.98220100 0.52132800 1.27911100  
C 5.37732100 -0.98033500 -0.17546800  
H 5.92063200 -1.72710800 0.41842700  
H 5.57893600 -1.16318100 -1.24690800  
C 2.13188500 0.66479900 -0.05507700  
H -1.90987200 -1.72891100 0.16576200  
H 1.90991100 1.72879100 -0.16700600  
H 4.40305500 2.11542300 0.13929600  
H 3.36720100 -1.75259600 -0.13164400  
H -3.36723800 1.75246800 0.13307200  
H -4.40308800 -2.11534000 -0.14060800

### **TS6<sup>H</sup>**

P 0.41116500 -1.44754200 -0.27512700  
P -1.22398400 -0.67011000 0.71732400

N 3.51330000 -1.25243800 -0.67069200  
N -4.24598600 0.08874400 0.94006600  
N 4.02015000 -0.40891000 1.33111900  
N -4.91254800 -0.71181900 -1.02462100  
C -3.80575100 -0.54875500 -0.20732400  
C 2.97204400 -0.87673800 0.54351200  
C -2.52683100 -0.93497800 -0.48240400  
H -2.33821900 -1.40150400 -1.45253400  
C 1.65780800 -0.91835200 0.89355500  
H 1.38764800 -0.53746300 1.88168900  
C 1.27644700 1.55910700 -1.08102400  
C 0.65068300 0.72972700 -1.96878300  
H 1.18076000 0.37256300 -2.85580300  
H -0.42720500 0.56826100 -1.95955500  
C 0.61023900 2.03916500 0.11030200  
C 5.28376700 -0.82188800 0.73854400  
H 5.60044900 -1.82213100 1.08526200  
H 6.08792500 -0.10453300 0.94803000  
C 4.91076300 -0.86851200 -0.74646200  
H 5.04958900 0.12405600 -1.21115500  
H 5.50944600 -1.60269200 -1.30252000  
C -6.02227800 0.07509800 -0.51575000  
H -6.99136100 -0.39367700 -0.73170400  
H -6.02758100 1.10541600 -0.91637400  
C -5.69704200 0.08856100 0.97979000  
H -6.09399600 0.97683000 1.48862300  
H -6.10573800 -0.81422000 1.46918900  
C -0.73537800 1.85602300 0.30109200  
H -1.40467500 1.64128700 -0.53275800  
H -1.21088300 2.23223300 1.20918300  
C 2.73820800 1.88872600 -1.25795200  
H 3.33785700 1.56151300 -0.39371000  
H 2.88516300 2.97653400 -1.35334600  
H 3.14235800 1.41715400 -2.16517800  
C 1.45350800 2.65233700 1.20220500  
H 0.84043400 2.88797800 2.08191700  
H 1.92799700 3.58761600 0.86388000  
H 2.26583000 1.97558000 1.51415800  
H -4.75052900 -0.76682300 -2.02168800  
H -3.70857900 -0.05960500 1.78712700  
H 3.90224000 -0.50180100 2.33261500  
H 2.91180800 -1.18393900 -1.48522300

**E-3<sup>H</sup>**

P 0.75182900 0.05546300 -1.00118000  
P -0.98142100 0.61237900 0.30117300  
N 2.54043500 -2.51129500 -0.65163900  
N -3.58631300 -0.99717500 1.02716200  
N 3.74555400 -1.80415200 1.07628500  
N -4.50597800 -1.00683100 -0.99655900  
C -3.41203200 -0.55107200 -0.27162000  
C 2.71566100 -1.44640700 0.21339400  
C -2.37820200 0.18678400 -0.75507600  
H -2.40982400 0.46620300 -1.81213100  
C 2.02826700 -0.27393700 0.22816600  
H 2.25253300 0.43676100 1.02821200  
C 1.46610400 2.74369100 -0.41889200  
C 1.23438000 1.79298500 -1.56378400  
H 2.14033000 1.68026700 -2.17736500  
H 0.42865000 2.13542900 -2.23381500  
C 0.42848200 3.07224900 0.37836900  
C 4.04166500 -3.21854000 0.92887700  
H 3.42370400 -3.85286200 1.59079700  
H 5.10116700 -3.43823200 1.11691300  
C 3.64635300 -3.43939900 -0.53335700  
H 4.49063600 -3.18537600 -1.20109400  
H 3.33852900 -4.47433200 -0.73386600  
C -5.52127500 -1.51339200 -0.09012700  
H -6.10093200 -2.33138500 -0.53843800  
H -6.21984300 -0.72589100 0.24796300  
C -4.64854000 -1.98213800 1.07643000  
H -5.18317800 -1.96298800 2.03554300  
H -4.28493400 -3.01027200 0.89353000  
C -0.92438200 2.49240100 0.07005800  
H -1.23000700 2.70013100 -0.96781100

H -1.70126400 2.90917500 0.72746600  
C 2.89251900 3.18145900 -0.23238200  
H 3.54044700 2.29427300 -0.14086200  
H 3.04558200 3.81351700 0.64971100  
H 3.24222000 3.73939400 -1.11624300  
C 0.50277600 3.92884500 1.61217000  
H 0.14331200 3.35813100 2.48434300  
H -0.15755300 4.80566400 1.51532300  
H 1.51340200 4.28866500 1.83509800  
H -4.78332500 -0.46179200 -1.80243000  
H -2.75492100 -1.08954200 1.59947800  
H 3.73011200 -1.39316700 2.00069100  
H 2.09250100 -2.32440300 -1.54100000

**DMBD**

C 0.74508700 0.12718500 -0.02454300  
C -0.74509200 0.12711400 0.02465900  
C -1.42595600 1.19407300 0.46023500  
H -0.90808400 2.08321500 0.82476500  
H -2.51825500 1.19839400 0.47446500  
C 1.44050200 -1.13430300 0.41911500  
H 1.20054900 -1.97447600 -0.25085400  
H 1.11739600 -1.42581400 1.43066000  
H 2.52994000 -1.00273800 0.42355100  
C -1.44043200 -1.13435600 -0.41914100  
H -2.52988900 -1.00295500 -0.42343200  
H -1.20030500 -1.97462900 0.25064400  
H -1.11736000 -1.42572700 -1.43074800  
C 1.42587700 1.19413900 -0.46025800  
H 2.51817000 1.19844000 -0.47453800  
H 0.90792600 2.08317600 -0.82491800

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