# Supplementary Information for

# Ion Mobility Mass Spectrometry Uncovers Regioselectivity in the Carboxylate-Assisted C-H activation of Palladium N-Heterocyclic Carbene Complexes

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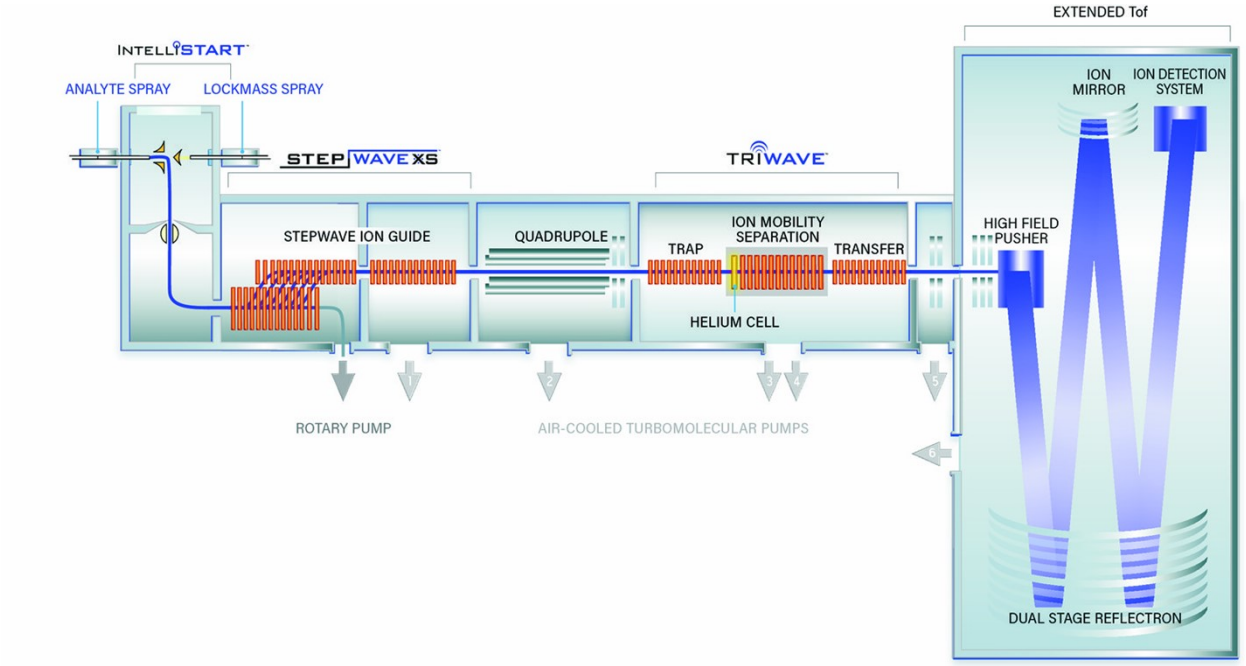
## 1.- Electrospray Ionization Ion Mobility Spectrometry Mass Spectrometry (ESI IM-MS)

**1.1 Schematic representation of the IM-MS instrument**: experiments were performed using a SYNAPT XS High Definition Mass Spectrometer (Waters Corporation, Manchester, UK) equipped with an electrospray ionization (ESI) source. After electrospray ionization, the ions generated are transmitted through the StepWave XS ion guide to the first quadrupole (Q), then to the traveling wave ion mobility (TWIM) cell, and finally analyzed with a time-of flight (TOF) mass analyzer. The ion mobility separation occurs through the so-called *triwave* device that operates with three regions: trap, ion mobility separation, and transfer with a helium cell located between the trap and ion mobility separation regions. A schematic view is given in scheme S1.




**Scheme S1**. Schematic view of the Synapt XS High Definition Mass Spectrometer. Reprinted from the waters.com webpage with permission from the Waters Corporation.

A capillary voltage was set to 2.5 kV operated in the positive ionization mode and in the resolution mode (FWHM ca. 20000 at m/z 556). Source settings were adjusted to keep intact the complexes of interest. Typical values were cone voltage 20 to 40 V and source offset 4 V; source and desolvation temperatures were set to 110 and 350 ºC, respectively. Cone and desolvation gas flows were 150 and 500 (L/h), respectively. Calibration of the *m/z* axis up to *m/z* 1000 was performed using the routine implemented in intellistart from a mixture of sodium hydroxide and formic acid in 1:9 *v/v* $H_2O$:isopropanol. The instrument was switched from TOF acquisition to

mobility TOF acquisition mode and left for 30 minutes before recording Travelling Wave Ion Mobility (TWIM) mass spectra. The ion mobility separation occurs through the so-called *triwave* device that operates with three regions: trap, ion mobility separation, and transfer with a helium cell located between the trap and ion mobility separation regions. The *m/z* 50-900 range was investigated and ion mobility separation settings were used as follows: the traveling wave height was set to 40 V and wave velocity was set to 650 m/s. The drift gas was nitrogen ($N_2$) at a flow rate set to 90 mL/min. The helium cell gas flow was 180.00 mL/min. IMS DC values were as follow: Entrance 20; Helium cell DC 50; Helium exit -20; Bias 3; Exit 0. Trap DC bias was 45 V; entrance, 3; Exit 0. Different traveling wave height, wave velocity and drift gas nitrogen flow rate were used aimed at providing improved resolution of the three mobility peaks associated to the isomers of formula $[(NHC^1 - H)Pd]^+$. As shown in figure S1, three mobility peaks were invariably observed regardless the set of values used in the CID IM mass spectra.

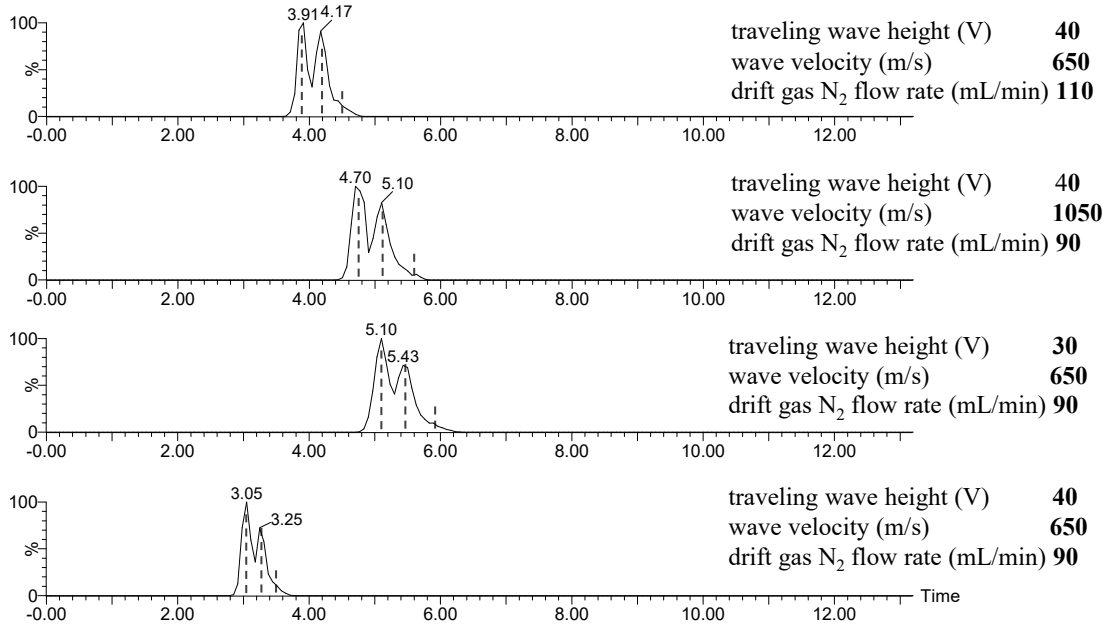
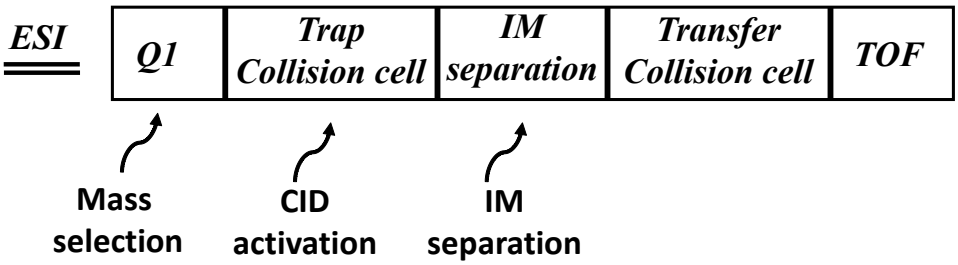



Figure S1. ATDs of the product ion formulated as $[(NHC^1 - H)Pd]^+$ obtained upon CID of the precursor $[(NHC^1)PdCl]^+$ using different experimental setups.

The TWIM-MS data were processed using Masslynx 4.2 (SCN 982). Ion mobility spectra of the species of interest were extracted using a 0.15 Da mass window and were converted from waters.raw to .txt files. Gaussian fitting of the IM data was applied to improve the precision of the drift time measurements. The reported drift times values were obtained by Gaussian peak

fitting using origin 6.0 (Microcal) rendering good correlation in all cases. In those cases where partial overlapping of the ATD profiles was observed, deconvolution to several gaussian functions was performed. Each sample was recorded by triplicate on the same day and the deviation in the drift time values was less than 0.5 %.

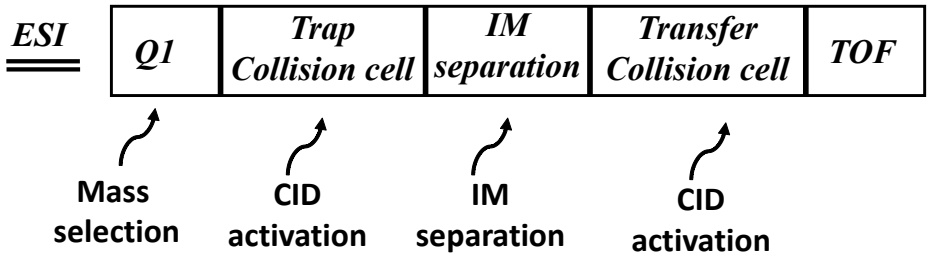
***1.2 CID prior to IM separation***: CID experiments were performed by mass selecting the $[(NHC^n)LMX]^+$ (X = $Cl^-$, carboxylates and bicarbonate) of interest in the first quadrupole and increasing the collision voltage (V) in the trap collision cell (see scheme S2) starting from 5 V and stepped by 5 V up to a maximum of 30 V. An isolation width of approximately 1 Da was selected (LM resolution set to 9). The resulting product ions were then separated according to their mobilities in the IM separation region (see conditions in the experimental section).




**Scheme S2**. Schematic representation of the CID followed by IM-MS experiment.

***1.3 CID prior to IM separation and subsequent CID of the IM-resolved isomers***:

CID experiments were performed by mass selecting the $[(NHC^n)LMX]^+$ (X = $Cl^-$, carboxylates and bicarbonate) of interest in the first quadrupole and subjected to CID fragmentation in the trap collision cell; the voltage (Utrap) was adjusted for each sample to promote the competitive C-H activation. The resulting product ions were then separated according to their mobilities in the IM separation region (see conditions in the experimental section) and CID of the IM-resolved isomers was performed in the second transfer collision cell; typical Utransfer values were 30-45 V. The resulting second generation product ions were drift-time aligned with the IM-resolved isomers. Some of these second generation product ions proved to be diagnostic of specific isomers, thus providing crucial insights on the identification of the IM-resolved isomers.




**Scheme S3**. Schematic representation of the CID followed by IM-MS experiment and subsequent CID of the IM-resolved isomers.

## 2.- Additional CID IM mass spectra.

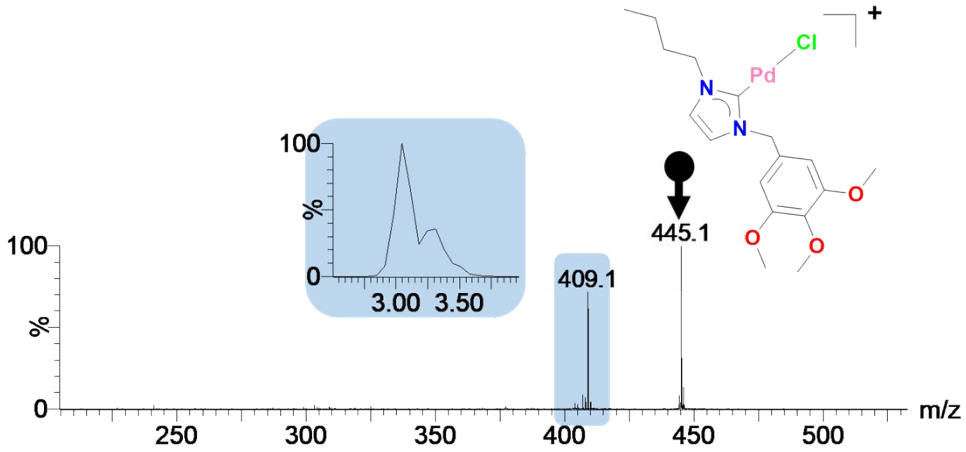



**Figure S2**. CID mass spectrum of the precursor ion $[(NHC^1)PdCl)]^+$ (m/z 445.1; the isotopomer with $^{35}Cl$ was mass-selected to observe exclusively the $H^{35}Cl$ loss (Δm 36)) registered at a collision energy of 8 V. The inset shows the arrival time distribution (ATD) of the product ion of formula $[(NHC^1 – H)Pd]^+$ (m/z 409.1).

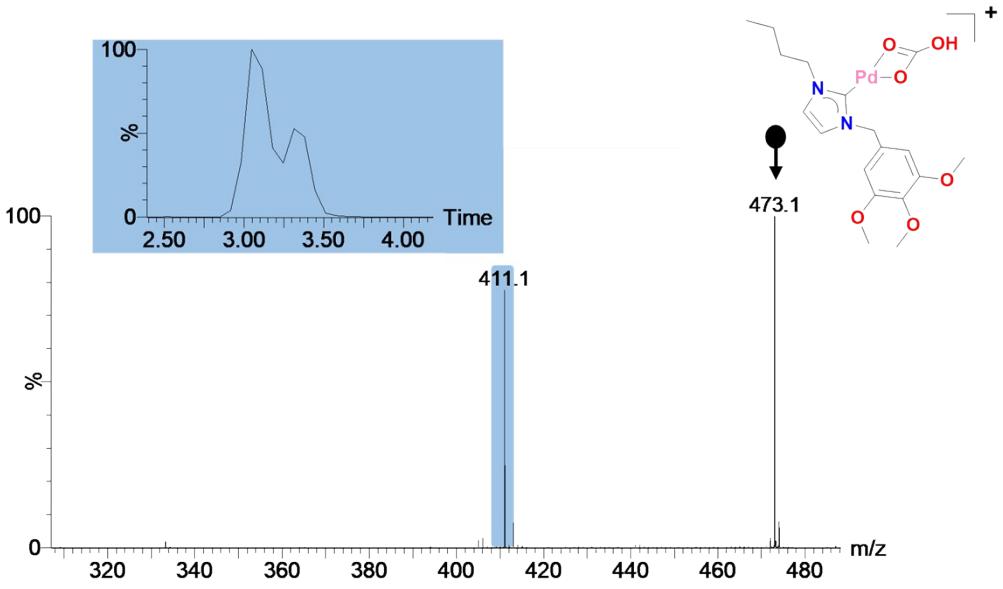



**Figure S3**. CID mass spectrum of the precursor ion $[(NHC^1)Pd(HCO_3)]^+$ (m/z 473.1) registered at a collision energy of 12 V along with the arrival time distribution (ATD) of the product ion of formula $[(NHC^1 – H)Pd]^+$ (m/z 411.1).

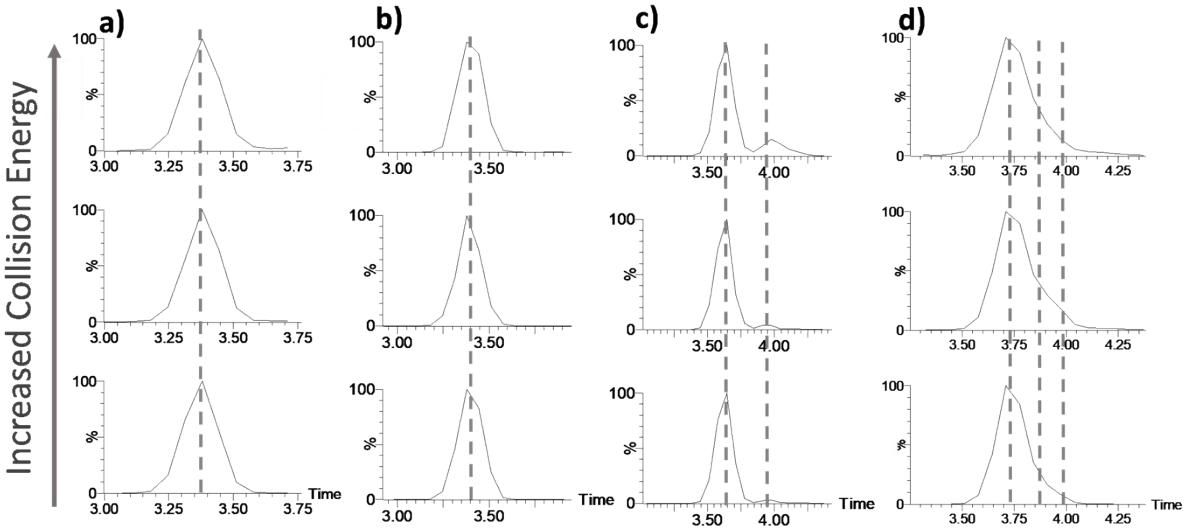



**Figure S4**. Arrival time distributions (ATDs) of the precursor ions of formula $[(NHC^{1})PdX]^{+}$ a) X = $Cl^{-}$; b) X = $HCO_2^{-}$; c) X = $CH_3CO_2^{-}$ and d) X = $HCO_3^{-}$. For the precursors $[(NHC^{1})PdX]^{+}$ (X = $Cl^{-}$ and $HCO_2^{-}$) a single gaussian-type mobility peak was observed (Fig. S4 a) and b)), thus pointing to a single isomer or a mixture of isomers not distinguishable by size and shape. However, for the precursors $[(NHC^{1})PdX]^{+}$ (X = $HCO_3^{-}$ and $CH_3CO_2^{-}$) deviations from a gaussian-shaped ATDs are observed upon increasing the collision energy where three and two mobility peaks can be identified for X = $HCO_3^{-}$ and $CH_3CO_2^{-}$, respectively.

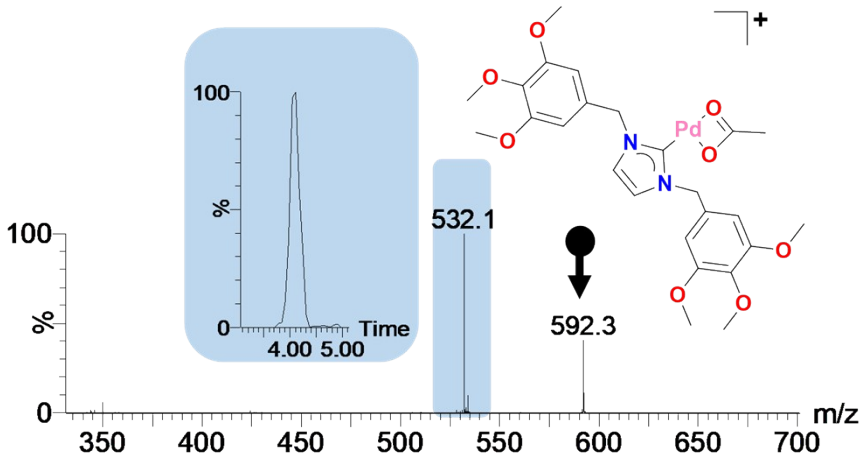



**Figure S5**. CID mass spectra of the precursor ion $[(NHC^{2})Pd(CH_3CO_2)]^{+}$ (m/z 592.3) registered at a collision energy of 12 V along with the arrival time distributions (ATDs) of the product ions of formula $[(NHC^{2} - H)Pd]^{+}$ (m/z 532.2).

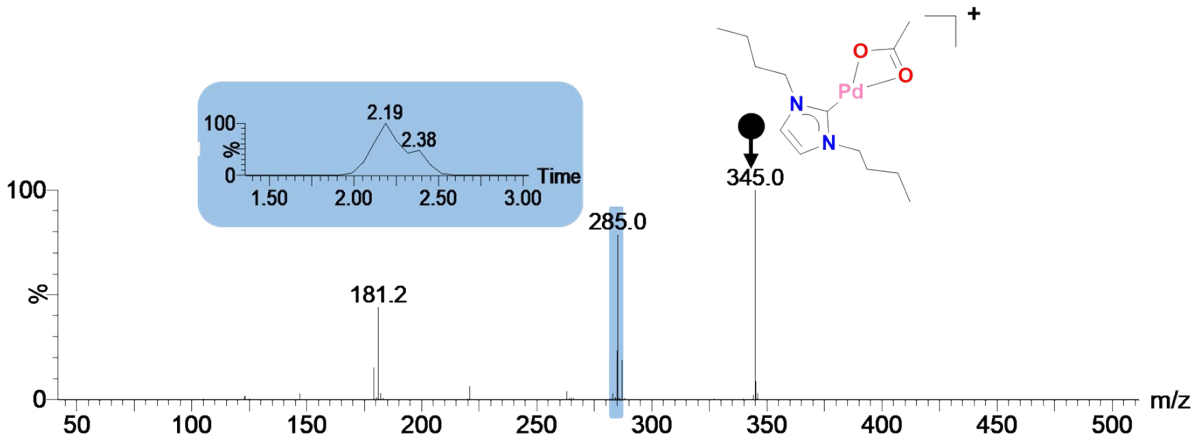



**Figure S6**. CID mass spectra of the precursor ion $[(NHC^3)Pd(CH_3CO_2)]^+$ (m/z 345.0) registered at a collision energy of 12 V along with the arrival time distributions (ATDs) of the product ion of formula $[(NHC^3 - H)Pd]^+$ (m/z 285.1). A loss of the ketene (Δm 58, $CH_2CO_2$) is also observed to afford the product $[(NHC^3)PdH]^+$ ion at m/z 287.0 which presumably transforms into the $[NHC^3 + H]^+$ cation at m/z 181.2 via reductive elimination concomitant with the ¨Pd¨ release.

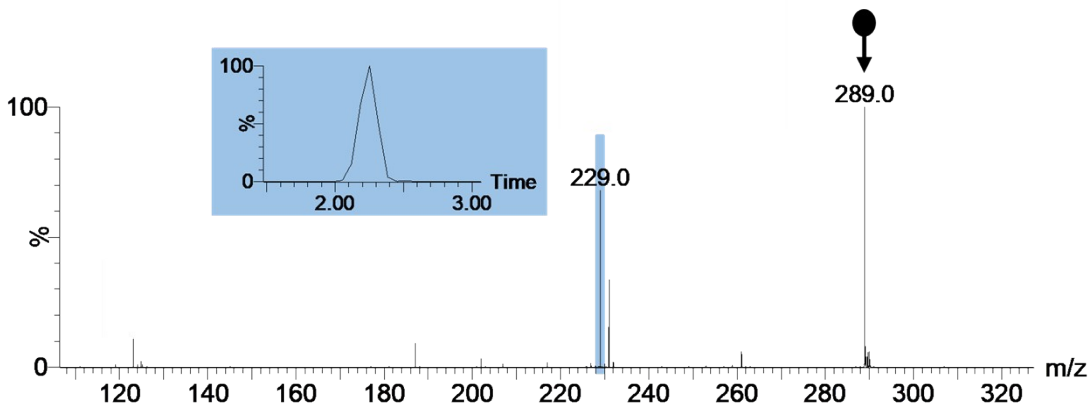



**Figure S7**. CID mass spectra of the precursor ion $[(NHC^4)Pd(CH_3CO_2)]^+$ (m/z 289.0) registered at a collision energy of 5 V along with the arrival time distributions (ATDs) of the product ions of formula $[(NHC^4 - H)Pd]^+$ (m/z 229.0).

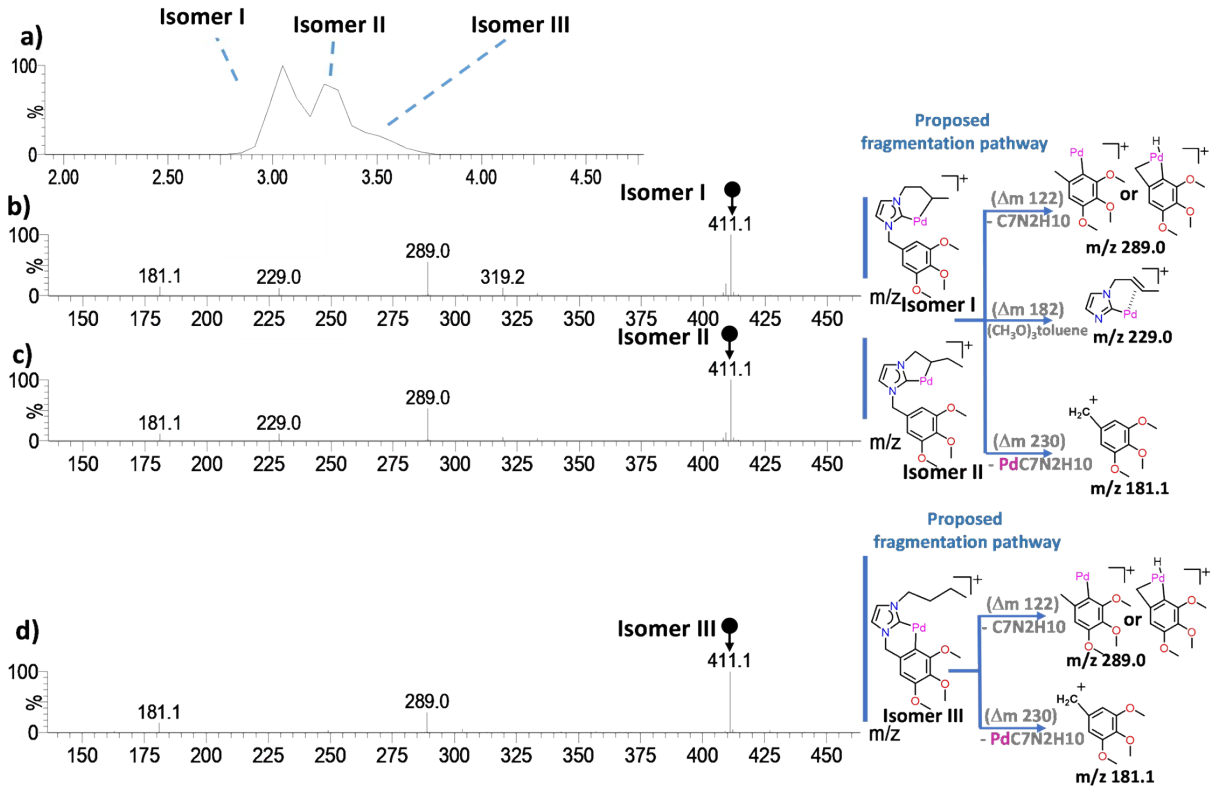



**Figure S8**. a) ATDs of the product ion at m/z 411.1 that is formed upon CID from the precursor $[(NHC^1)Pd(CH_3CO_2)]^+$ ion. Second-generation product ions from the ion mobility-resolved isomers using 15 V and 30 V in the trap and transfer regions, respectively; b) isomer **I** at 3.05 ms; c) isomer **II** at 3.25 ms. Proposed fragmentation pathways are shown in the right panel. Isomers **I** and **II** display a prominent product ion at m/z 289.0 (loss of Δm 122); plausible structures are shown whose formation is not intuitive and most likely involve partial isomer **I-II** to isomer **III** isomerization followed by a single hydrogen migration from the butyl N-donor group to the benzylic group. A second product ion that results from the $(OCH_3)_3$toluene loss (Δm 182) is observed and it is proposed as diagnostic of non-activated aryl N-donor groups. Formation of the product ion at m/z 181.1 is due to the heterolytic rupture of the $C_{benzyl}$-$N_{imidazol}$ bond. Figure S8 d) shows the second-generation product ions from the ion mobility-resolved isomer **III** at 3.50 ms. Proposed fragmentation pathways are shown in the right panel and are common to the ones observed from isomer **I** and **II**, thus pointing that partial isomerization is occurring upon CID conditions. This is particularly evident due to the formation of the product ion at m/z 181.1 from the isomer **III** which can be explained by isomer **III** to isomer **I-II** isomerization followed by an heterolytic rupture of the $C_{benzyl}$-$N_{imidazol}$ bond.

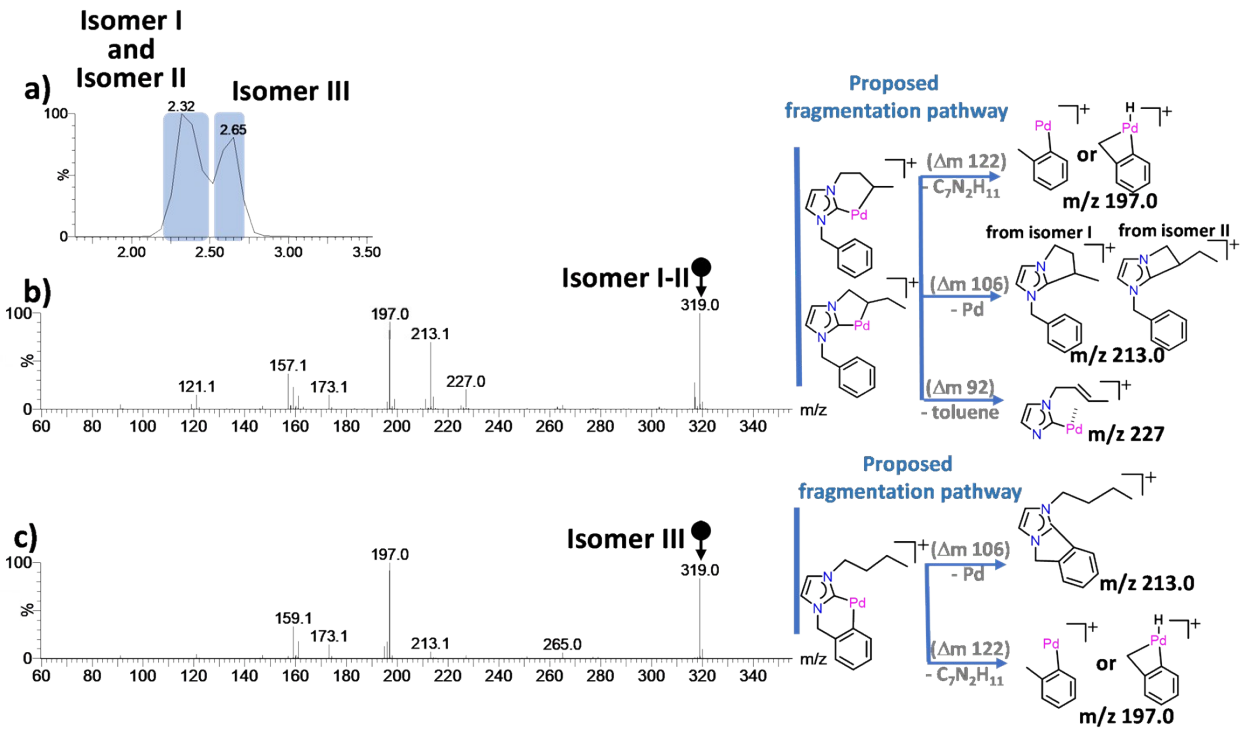



**Figure S9**. a) ATDs of the product ion at m/z 319.0 that is formed upon CID from the precursor $[(NHC^5)Pd(CH_3CO_2)]^+$ ion. Second-generation product ions from the ion mobility-resolved isomers using 15 V and 30 V in the trap and transfer regions, respectively; b) isomer **I** and **II** are associated to mobility peaks overlapped between 2.32 and 2.47 ms. Proposed fragmentation pathways are shown in the right panel. Isomers **I** and **II** display a prominent product ion at m/z 197.0 (loss of Δm 122); like the members with the structure-related $NHC^1$ ligand, plausible structures are shown whose formation most likely involve partial isomer **I-II** to isomer **III** isomerization followed by a single hydrogen migration from the butyl N-donor group to the benzylic group. A second major fragmentation channel involve a reductive elimination concomitant with loss of ¨Pd¨. A third product ion that results from the toluene loss (Δm 92) is observed and it is proposed as diagnostic of non-activated aryl N-donor groups. Figure S9 c) shows the second-generation product ions from the ion mobility-resolved isomer **III** at 2.65 ms. Proposed fragmentation pathways are shown in the right panel and comprise a reductive elimination concomitant with loss of ¨Pd¨ to afford a product ion at m/z 213.0 competitive with a prominent product ion at m/z 197.0 (loss of Δm 122) whose formation most likely involve a single hydrogen migration from the butyl N-donor group to the benzylic group.

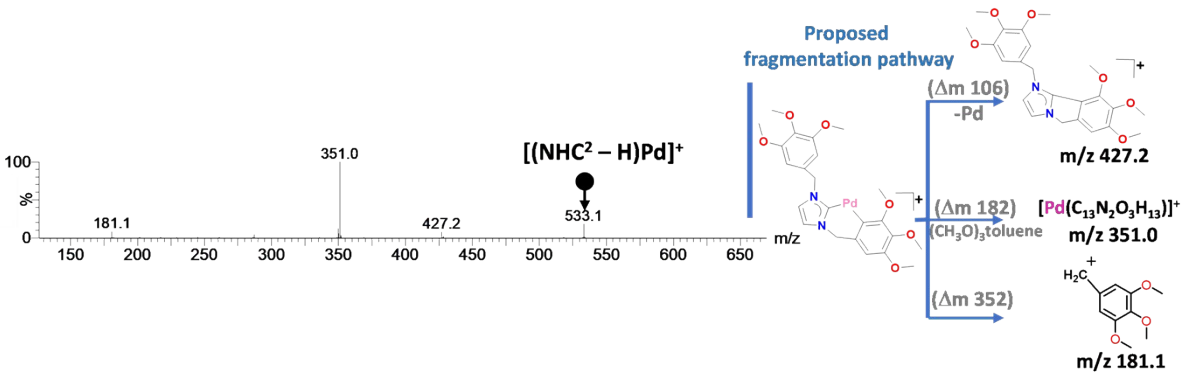



**Figure S10**. Second-generation product ions from the ion mobility-resolved isomer $[(NHC^2 - H)Pd]^+$ (m/z 533.1) using 20 V and 30 V in the trap and transfer regions, respectively. The right panel shows its fragmentation pathways that comprises a reductive elimination concomitant with the release of ¨Pd¨ (Δm 106) competitive with the loss of $(OCH_3)_3$toluene (Δm 182). Formation of the product ion at m/z 181.1 is due to the heterolytic rupture of the $C_{benzyl}$-$N_{imidazol}$ bond.

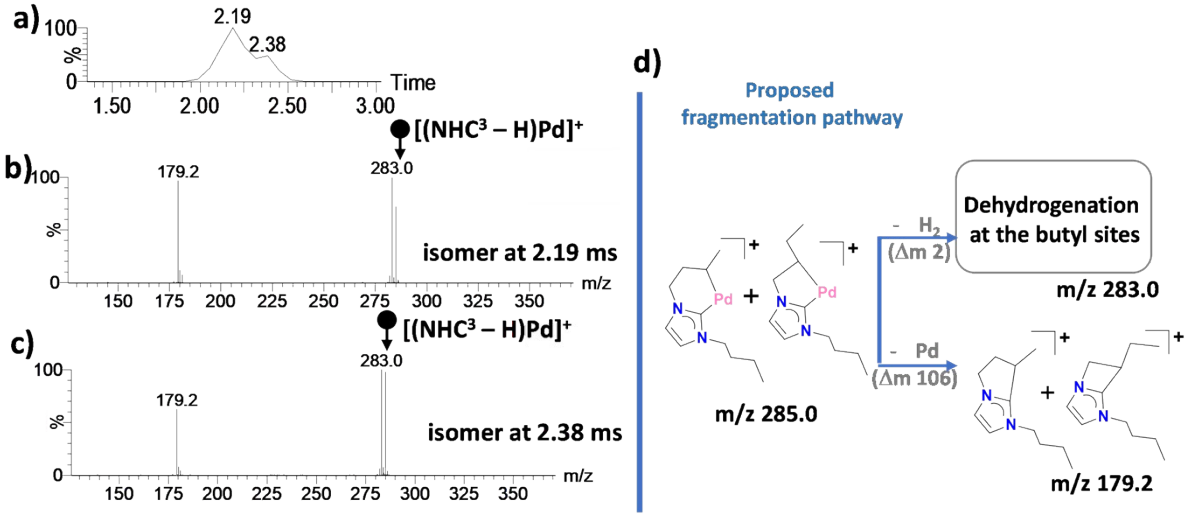



**Figure S11**. a) ATDs of the product ion at m/z 285.0 that is formed upon CID from the precursor $[(NHC^3)Pd(CH_3CO_2)]^+$ ion. Second-generation product ions from the ion mobility-resolved isomers at 2.19 b) and 2.38 c) ms using 12 V and 20 V in the trap and transfer regions; The right panel d) shows their fragmentation pathways that comprises a reductive elimination concomitant with the release of ¨Pd¨ (Δm 106) competitive with dehydrogenation (Δm 2) from the butyl chains.

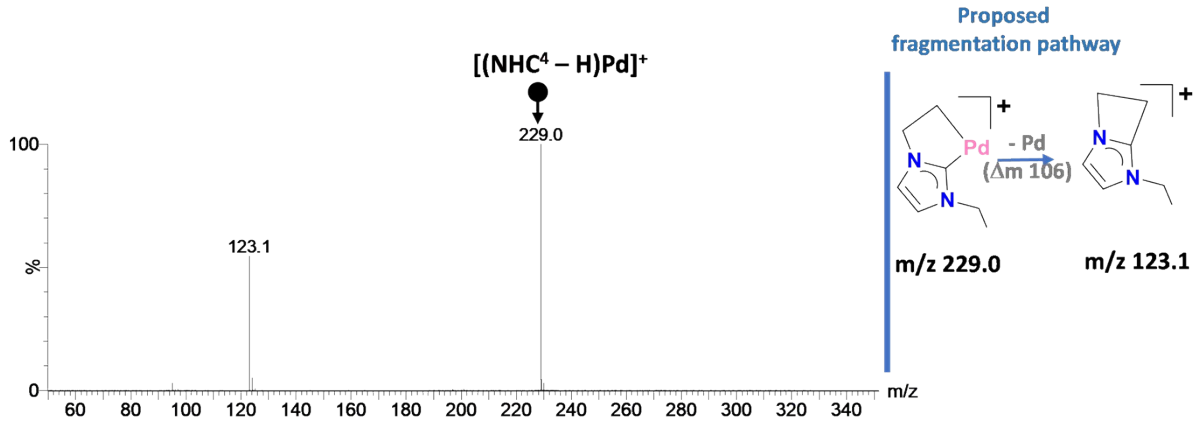



**Figure S12**. Second-generation product ions from the ion mobility-resolved $[(NHC^4 – H)Pd]^+$ cation (m/z 229.0) using 10 V and 15 V in the trap and transfer regions. The right panel shows its fragmentation pathway that comprises a reductive elimination concomitant with the release of ¨Pd¨ (Δm 106).

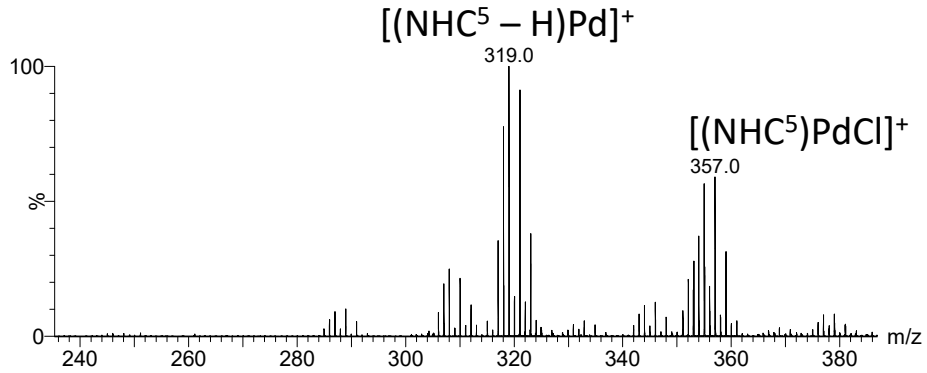



**Figure S13**. ESI mass spectrum of $CH_2Cl_2$/methanol solutions (1 x $10^{-6}$ M) of complex $(NHC^5)PdCl_2(py)$.

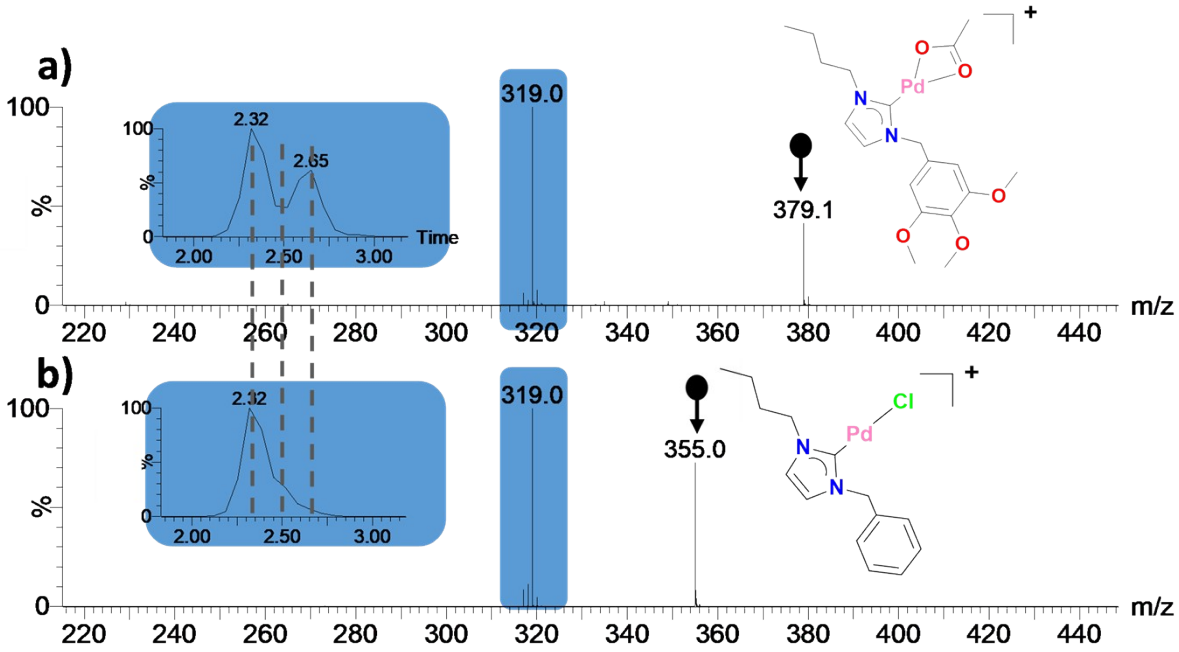
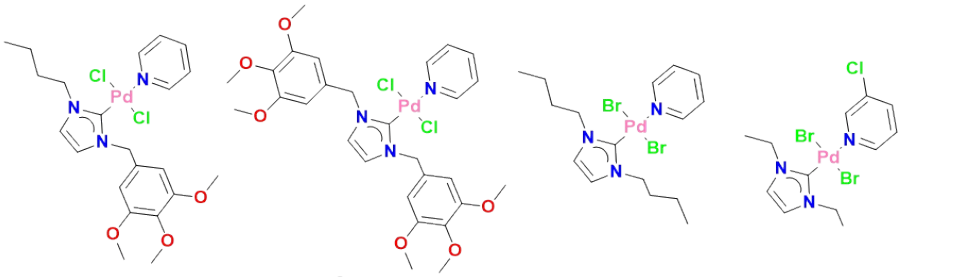


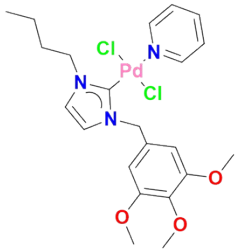

**Figure S14**. CID mass spectra of the precursor ion a) $[(NHC^5)PdCl]^+$ (m/z 355.0) and b) $[(NHC^5)Pd(CH_3CO_2)]^+$ (m/z 379.1) along with the arrival time distributions (ATDs) of the product ions of formula $[(NHC^5 - H)Pd]^+$ (m/z 319.0).

## 3 Synthesis and characterization of palladium NHC complexes



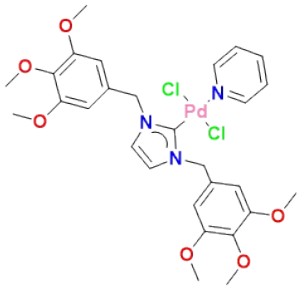
[(NHC[1])PdCl$_2$(py)] [(NHC[2])PdCl$_2$(py)] [(NHC[3])PdBr$_2$(py)] [(NHC[4])PdBr$_2$(py)]

### 3.1 Synthesis and characterization



[(NHC[1])PdCl$_2$(py)]

**Synthesis of (NHC[1])PdCl$_2$(py):** Complex [(NHC[1])PdCl$_2$(py)] was prepared by following a reported method in the literature.[1] A mixture of 1-butyl-3-(3,4,5-trimethoxy)benzyl imidazolium chloride[2] (262 mg, 0.77 mmol), $PdCl_2$ (137 mg, 0.77 mmol), and $K_2CO_3$ (213 mg, 1.54 mmol) was stirred in pyridine (5 mL) as solvent at 60ºC during 17h under inert atmosphere. Pyridine was removed under reduced pressure. The mixture was redissolved in $CH_2Cl_2$, filtered through celite and concentrated to dryness. Precipitation from dichloromethane/diethylether produced the pure product as a pale yellow solid. Yield: 261 mg (59%). $^1$H NMR ($CDCl_3$, 400 MHz): δ=9.02–9.00 (m, 2H, Py), 7.77(t, 1H, Py), 7.38–7.34 (m, 2H, Py), 6.92 (d, J=2.1 Hz, 1H, Ar), 6.77 (m, 3H, $ArH_{imid}$), 5.77 (s,2H, $NCH_2Ar$), 4.60 (t, 2H, $NCH_2$), 3.85 (s, 6H, $OCH_3$), 3.84 (s, 3H, $OCH_3$), 2.14–2.07 (m, 2H, $NCH_2CH_2$), 1.56–1.47 (m, 2H, $NCH_2CH_2CH_2$), 1.04 (t, 3H, $CH_3$); $^{13}$C NMR ($CDCl_3$, 100 MHz): δ =153.8 ($C_{carbene}$), 151.4, 138.2 (Py), 138.2, 131.3 (Ar), 124.6 (Py), 122.3, 121.3 ($CH_{imid}$), 106.2 (Ar), 61.0, 56.6 (OMe), 55.1 ($NCH_2Ar$), 51.0, 32.7, 20.1, 13.9 (n-Bu); ESI-MS (cone 20 V): m/z (fragment) = 447.1 [M – Cl - py]$^+$ and 411.1 [M - Cl - Py - HCl]$^+$.

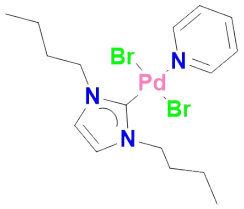


[(NHC[2])PdCl$_2$(py)]

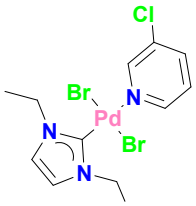
**Synthesis of (NHC[2])PdCl$_2$(py):** Palladium complex [(NHC[2])PdCl$_2$(py)] was prepared by adapting a reported method in the literature.[1] A mixture of 1,3-bis(3,4,5-trimethoxybenzyl)imidazolium chloride[3] (190 mg, 0.56 mmol), $PdCl_2$ (100 mg, 0.56 mmol), and $K_2CO_3$ (154 mg, 1.12 mmol) was stirred in pyridine (4 mL) as solvent at 60ºC during 17h under inert atmosphere. Pyridine was removed under reduced pressure. The mixture was redissolved in $CH_2Cl_2$, filtered through celite and concentrated to dryness. The crude solid was purified by column chromatography using an elution of dichloromethane/acetone (8:2). Precipitation from dichloromethane/pentane produced the pure product as a pale yellow solid. Yield: 272 mg (71%).

$^1$H NMR ($CDCl_3$, 400 MHz): δ =9.02–9.00 (m, 2H, Py), 7.78 (t, 1H, Py), 7.38–7.35 (m, 2H, Py), 6.81 (s, 4H, Ar), 6.79 (s, 2H, $H_{imid}$), 5.80 (s, 4H, $NCH_2$), 3.86 (s, 12H, $OCH_3$), 3.84 (s, 6H, $OCH_3$); $^{13}$C NMR ($CDCl_3$, 100 MHz): δ =153.8 ($C_{carbene}$), 151.4, 138.3 (Py), 131.2 (Ar), 124.7 (Py), 122.1 ($CH_{imid}$), 106.2 (Ar), 61.0, 56.6 (OMe), 55.1 ($NCH_2Ar$); ESI-MS (cone 20 V): m/z (fragment) = 571.1 $[M - Cl - py]^+$ and 533.1 $[M - Cl - Py - HCl]^+$.

**Synthesis of $(NHC^3)PdBr_2(py)$:** A mixture of 1,3-dibutylimidazolium chloride[4,5] (100 mg, 0.35 mmol), $PdCl_2$ (56 mg, 0.31 mmol), NaBr (319 mg, 3.1 mmol) and $K_2CO_3$ (221 mg, 1.6 mmol) was stirred in pyridine (4 mL) as solvent at 80ºC during 16h under inert atmosphere. Pyridine was removed under reduced pressure. The mixture was redissolved in $CH_2Cl_2$, filtered through celite and concentrated to dryness. The crude solid was purified by column chromatography using an elution of dichloromethane/acetone (9:1). Precipitation from dichloromethane/pentane produced the pure product as a pale yellow solid. Yield: 121 mg (74%). $^1$H NMR ($CDCl_3$, 400 MHz): δ =9.05-9.03 (m, 2H, Py), 7.75 (t, 1H, Py), 7.35-7.31 (m, 2H, Py), 6.92 (s, 2H, $H_{imid}$), 4.51 (t, 4H, $NCH_2$), 2.11-2.04 (m, 4H, $NCH_2CH_2$), 1.54-1.44 (m, 4H, $NCH_2CH_2CH_2$), 1.03 t, 6H, $CH_3$); $^{13}$C NMR ($CDCl_3$, 100 MHz): δ = 152.8 (Py), 146.8 ($C_{carbene}$), 137.9, 124.6 (Py), 121.7 ($CH_{imid}$), 51.3, 32.3, 20.1, 13.9 (n-Bu); ESI-MS (cone 20 V): m/z (fragment) = 367.9 $[M – Br - py]^+$ and 287.0 $[M - Br - Py - HBr]^+$.



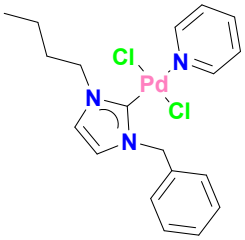
$[(NHC^3)PdBr_2(py)]$



$(NHC^4)PdBr_2(py^{Cl})$

**Synthesis of $(NHC^4)PdBr_2(py^{Cl})$:** A mixture of 1,3-diethylimidazolium bromide[6] (168 mg, 0.82 mmol), $PdCl_2$ (134 mg, 0.75 mmol), NaBr (780 mg, 7.5 mmol) and $K_2CO_3$ (521 mg, 3.8 mmol) was stirred in 3-chloropyridine (4 mL) as solvent at 80ºC during 16h under inert atmosphere. The mixture was filtered through celite and concentrated to dryness. The crude solid was purified by column chromatography using an elution of dichloromethane/acetone (9:1). Precipitation from dichloromethane/diethylether produced the pure product as a pale yellow solid. Yield: 160 mg (43%). $^1$H NMR ($CDCl_3$, 400 MHz): δ = 9.11 (d, J=1.98 Hz, 1H, Py), 9.01 (dd, J= 5.5, 1.3 Hz, 1H, Py), 7.77-7.74 (m, 1H, Py), 7.32-7.28 (m, 1H, Py), 6.96 (s, 2H, $CH_{imid}$), 4.59 (q, 4H, $NCH_2$), 1.61 (t, 6H, $CH_3$); $^{13}$C NMR ($CDCl_3$, 100 MHz): δ = 151.9 ($CH_{Py}$), 150.8 ($CH_{Py}$), 145.1 ($C_{carbene}$), 138.0 ($CH_{Py}$), 132.7 ($C_{Py}$), 125.0 ($CH_{Py}$), 121.4 ($CH_{imid}$), 46.4 ($NCH_2$), 15.7 ($CH_3$); ESI-MS (cone 20 V): m/z (fragment) = 310.9 $[M – Br - py^{Cl}]^+$ and 231.0 $[M - Br - Py^{Cl} - HBr]^+$.

**Synthesis of $[(NHC^5)PdCl_2(py)]$:** A mixture of 1-butyl-3-benzyl imidazolium chloride[7] (322 mg, 1.28 mmol), $PdCl_2$ (195 mg, 1.1 mmol), and $K_2CO_3$ (760 mg, 5.5 mmol) was stirred in pyridine (10 mL) as solvent at 80ºC during 17h under inert atmosphere. Pyridine was removed under reduced pressure. The mixture was redissolved in $CH_2Cl_2$, filtered through celite and concentrated to dryness. The crude solid was purified by column chromatography using an elution of dichloromethane/acetone (9:1).



$[(NHC^5)PdCl_2(py)]$

Precipitation from dichloromethane/pentane produced the pure product as a pale yellow solid. Yield: 281 mg (56%). $^{1}$H NMR ($CDCl_3$, 400 MHz): δ= 9.01-8.99 (m, 2H, Py), 7.76 (t, 1H, Py), 7.52-7.49 (m, 2H, Py), 7.40-7.33 (m, 5H, Ar), 6.90 (d, J= 2.1 Hz, 1H, $H_{imid}$), 6.71 (d, J=2.1Hz, 1H, $H_{imid}$), 5.85 (s, 2H, $NCH_2Ar$), 4.59 (t, 2H, $NCH_2$), 2.14-2.06 (m, 2H, $NCH_2CH_2$), 1.56-1.47 (m,2H, $NCH_2CH_2CH_2$), 1.04 (t,3H, $CH_3$); $^{13}$C NMR ($CDCl_3$, 100 MHz): δ = 151.4 (Py), 149.2 ($C_{carbene}$), 138.1 (Py), 135.6 (Ar), 129.1 (Py), 129.1 (Ar), 128.6 (Ar), 124.6 (Ar), 122.1 ($CH_{imid}$), 121.3 ($CH_{imid}$), 54.9 ($NCH_2Ar$), 51.0, 32.7, 20.1, 13.9 (n-Bu); ESI-MS (cone 20 V): m/z (fragment) = 355.0 $[M – Cl - py]^+$ and 319.1 $[M - Cl - Py - HCl]^+$.

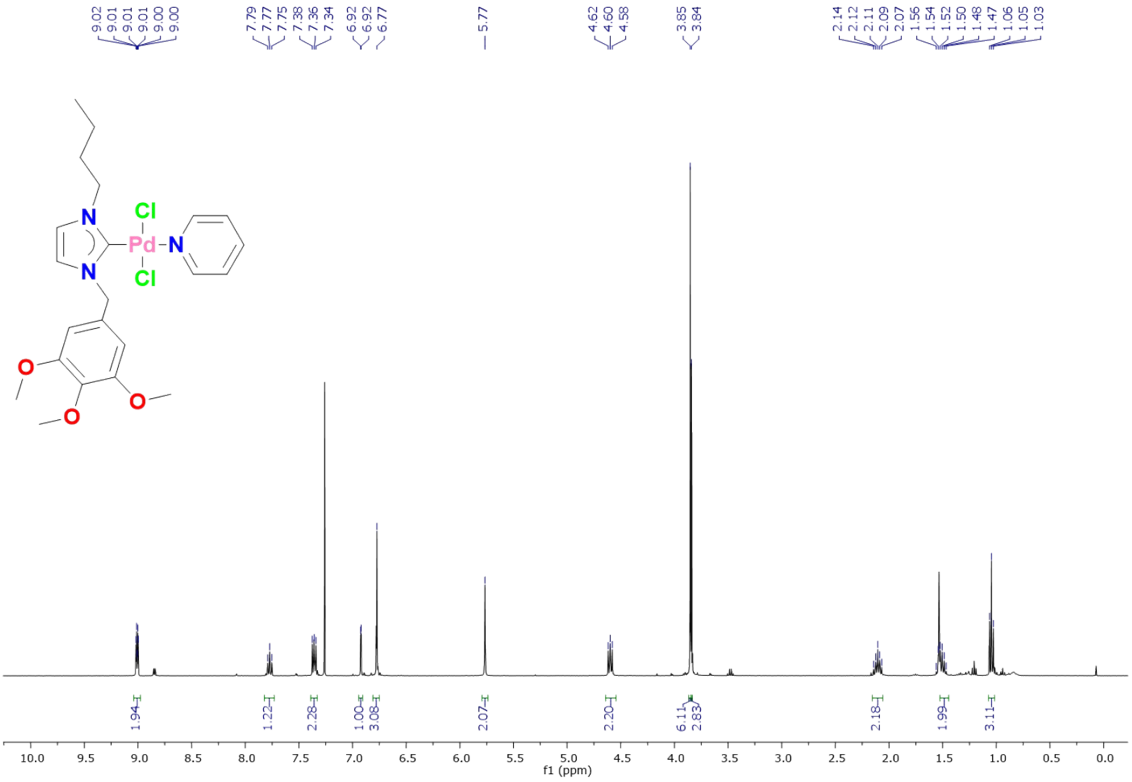



**Figure S15.** $^{1}$H NMR of $(NHC^1)PdCl_2(py)$ in $CDCl_3$

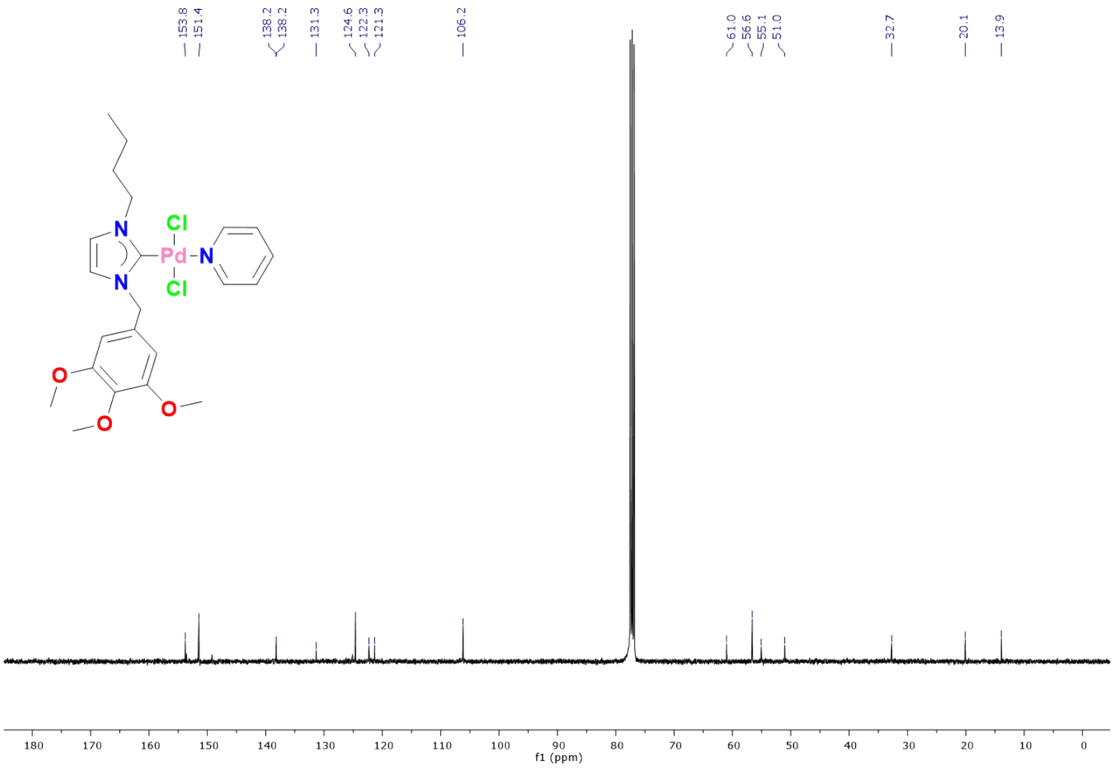



**Figure S16.** $^{13}C$ NMR of $(NHC^1)PdCl_2(py)$ in $CDCl_3$.

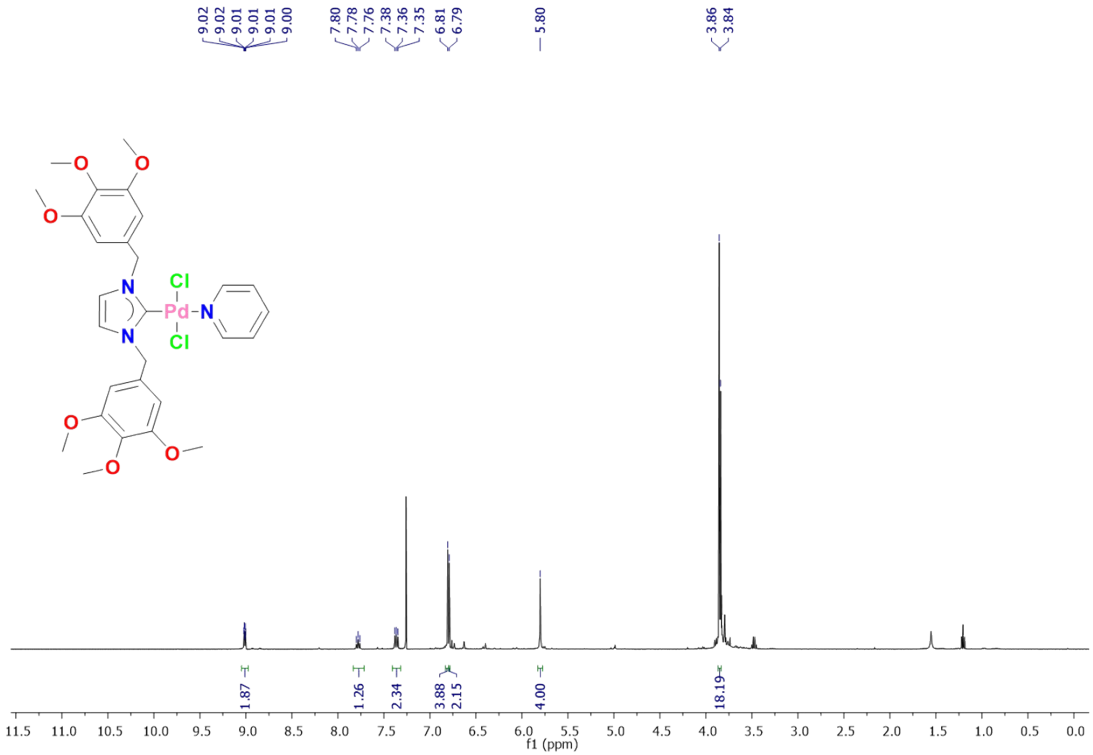



**Figure S17.** $^{1}H$ NMR of $(NHC^2)PdCl_2(py)$ in $CDCl_3$.

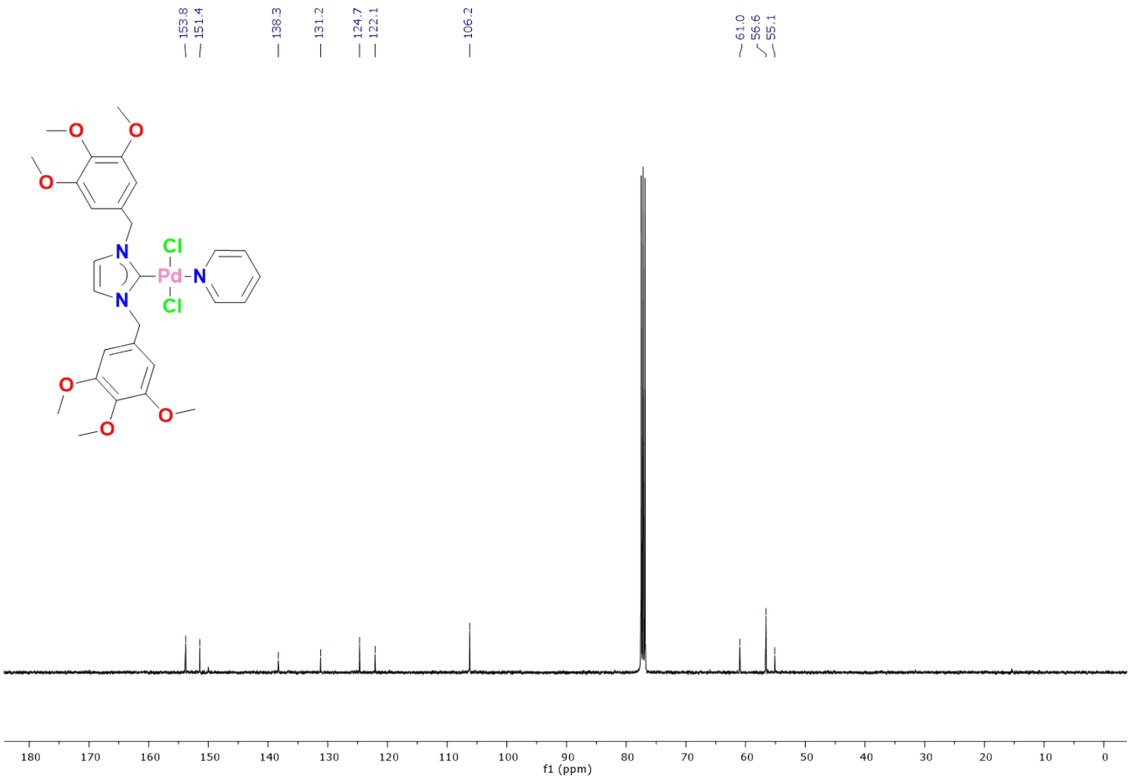



**Figure S18.** $^{13}C$ NMR of $(NHC^2)PdCl_2(py)$ in $CDCl_3$.

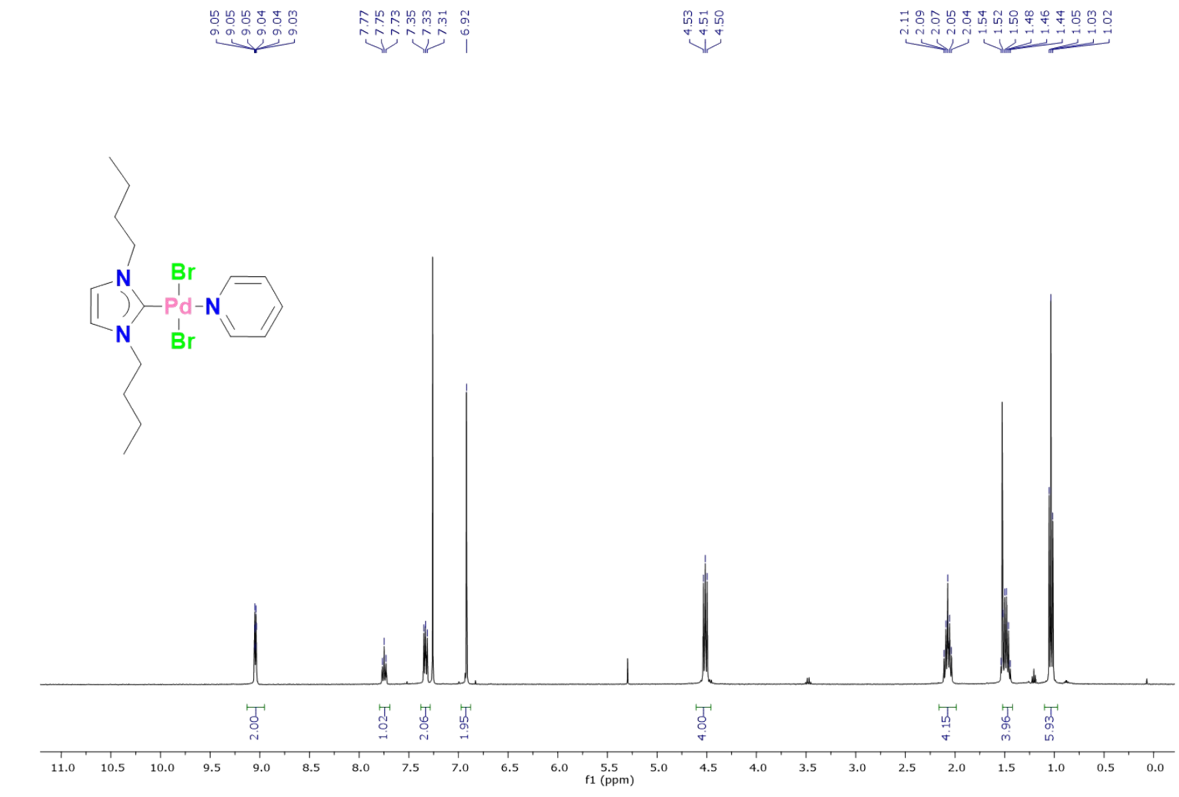



**Figure S19.** $^{1}H$ NMR of $(NHC^3)PdCl_2(py)$ in $CDCl_3$.

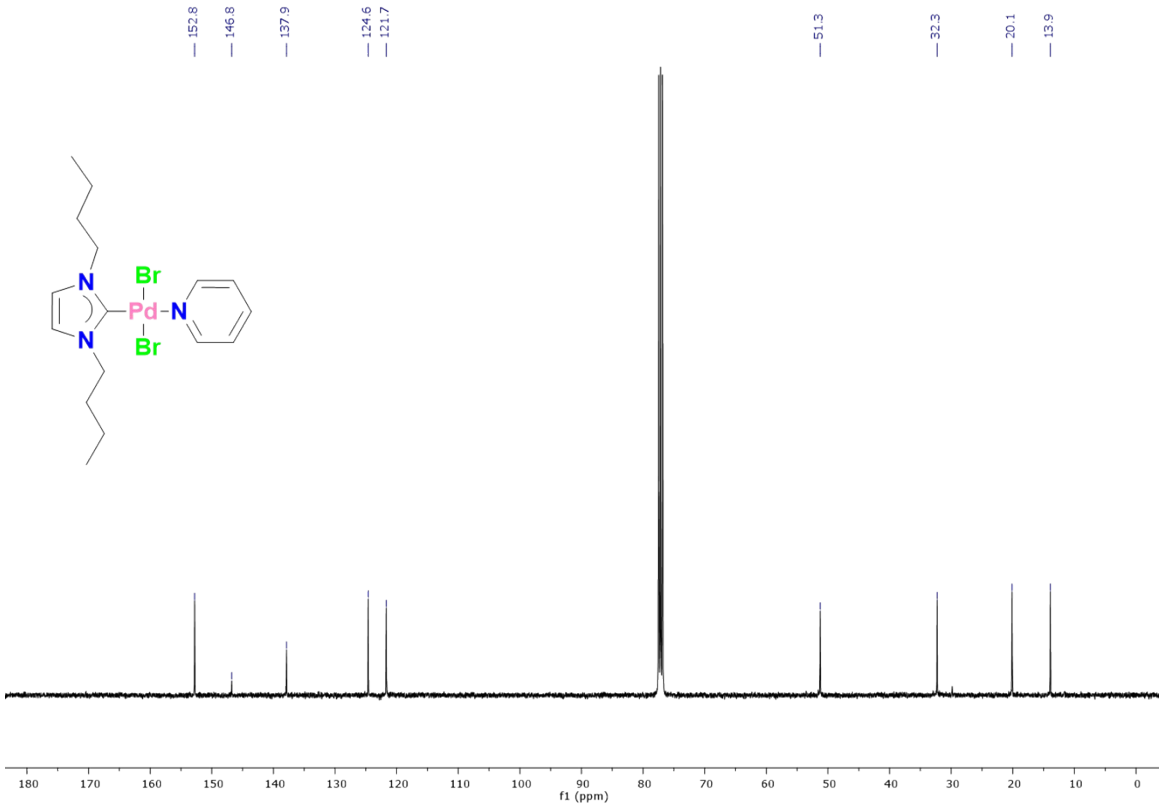



**Figure S20**. $^{13}C$ NMR of $(NHC^3)PdCl_2(py)$ in $CDCl_3$.

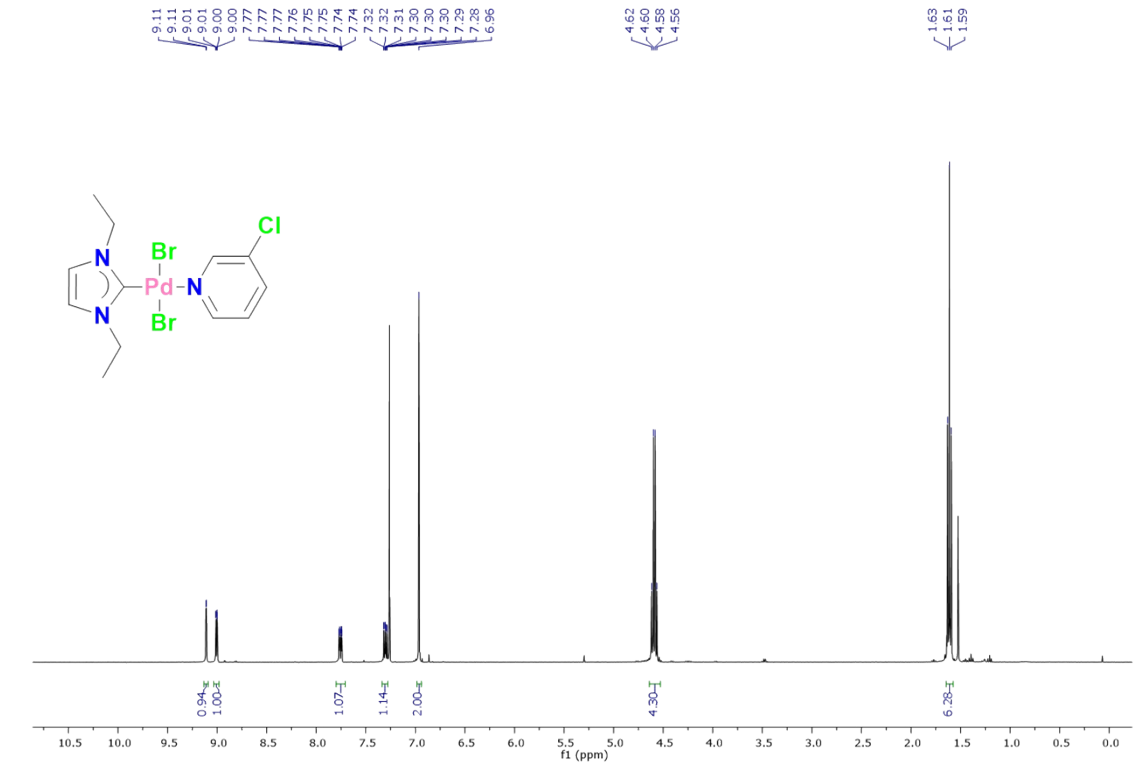



**Figure S21.** $^{1}H$ NMR of $(NHC^4)PdCl_2(py)$ in $CDCl_3$.

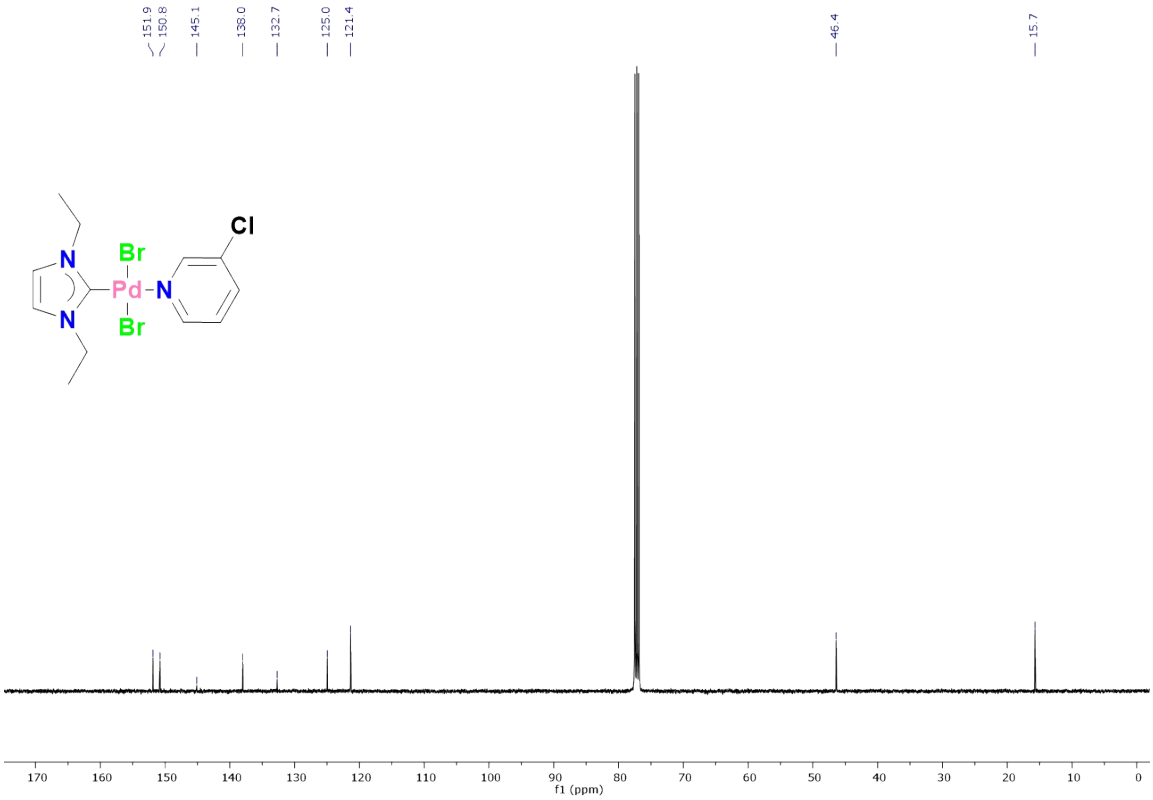



**Figure S22.** $^{13}C$ NMR of $(NHC^4)PdCl_2(py)$ in $CDCl_3$.

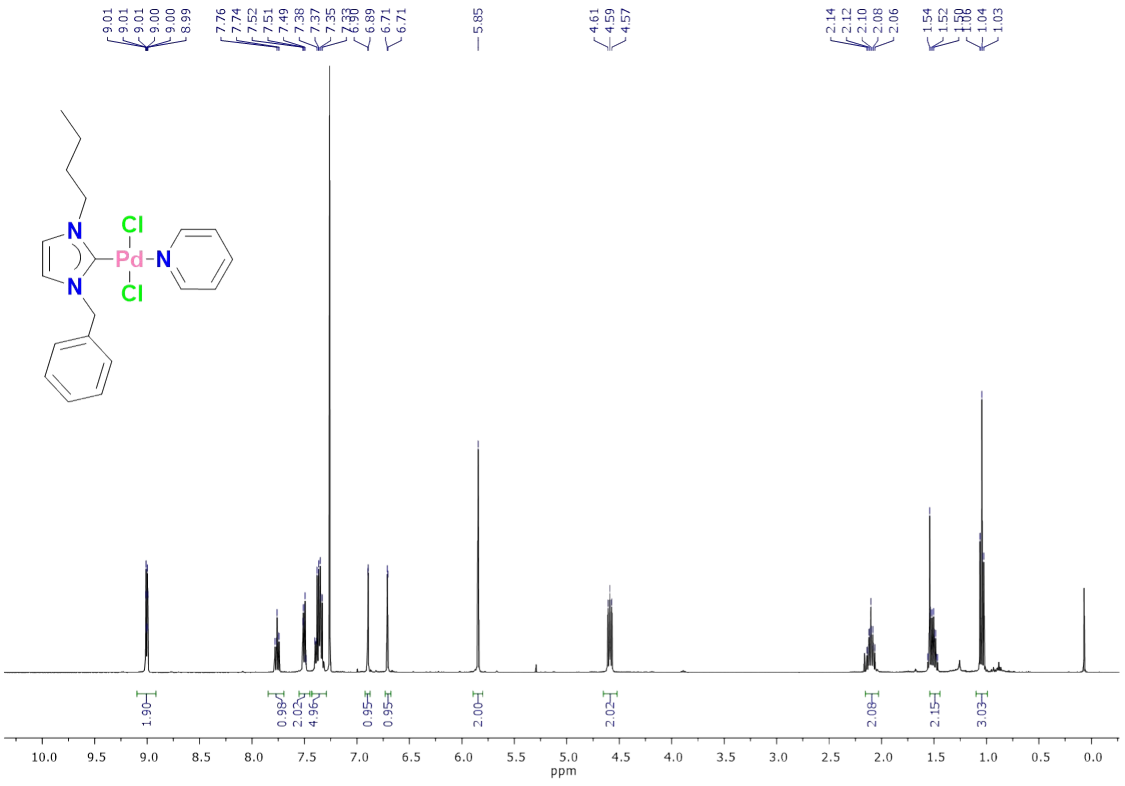



**Figure S23.** $^{1}H$ NMR of $(NHC^5)PdCl_2(py)$ in $CDCl_3$.

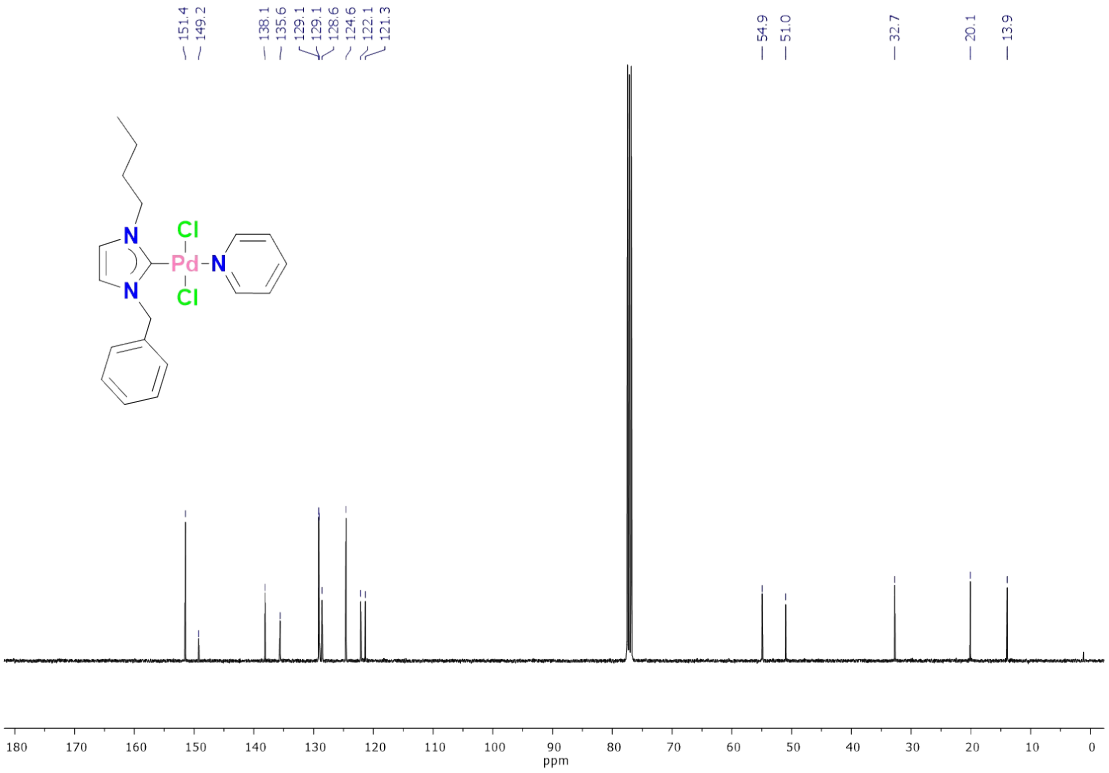



**Figure S24.** $^{13}C$ NMR of $(NHC^5)PdCl_2(py)$ in $CDCl_3$.

### 3.2 Single crystal X-ray diffraction data of $(NHC^3)PdBr_2(py)$

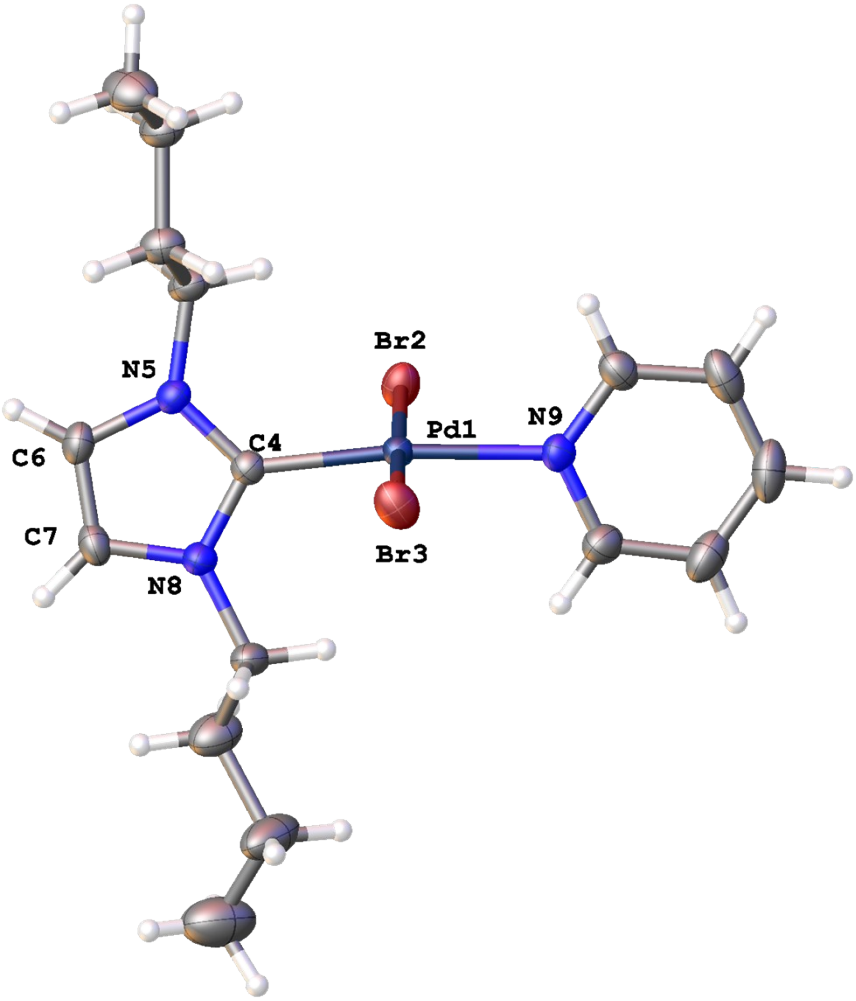



**Figure S25**. Ortep representation of complex **$(NHC^3)PdBr_2(py)$**. Ellipsoids are at 50% probability level.

**Table S1 Crystal data and structure refinement for complex (NHC$^3$)PdBr$_2$(py)**.

| | |
|---|---|
| Identification code | str2251_auto |
| Empirical formula | $C_{16}H_{25}Br_2N_3Pd$ |
| Formula weight | 525.619 |
| Temperature/K | 200.0(3) |
| Crystal system | monoclinic |
| Space group | $P2_1/n$ |
| a/Å | 13.8237(2) |
| b/Å | 8.7247(1) |
| c/Å | 16.4465(2) |
| α/° | 90 |
| β/° | 101.415(1) |
| γ/° | 90 |
| Volume/Å$^3$ | 1944.34(4) |
| Z | 4 |
| $\rho_{calc}$g/cm$^3$ | 1.796 |
| μ/mm$^{-1}$ | 12.503 |
| F(000) | 1029.8 |
| Crystal size/mm$^3$ | 0.12 × 0.1 × 0.07 |
| Radiation | Cu Kα (λ = 1.54184) |
| 2Θ range for data collection/° | 7.64 to 143.3 |
| Index ranges | $-16 \le h \le 17$, $-10 \le k \le 10$, $-20 \le l \le 20$ |
| Reflections collected | 34828 |
| Independent reflections | 3785 [$R_{int}$ = 0.0261, $R_{sigma}$ = 0.0108] |
| Data/restraints/parameters | 3785/0/202 |
| Goodness-of-fit on F$^2$ | 1.039 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0234, $wR_2$ = 0.0584 |
| Final R indexes [all data] | $R_1$ = 0.0239, $wR_2$ = 0.0588 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.91/-0.57 |

## Experimental

A single crystal of $C_{16}H_{25}Br_2N_3Pd$ (complex **(NHC$^3$)PdBr$_2$(py)** was mounted on a MicroMount® polymer tip (MiteGen) in a random orientation. Data collection was performed on a SuperNova, Dual, Cu at home/near, Atlas diffractometer. The crystal was kept at 200.0(3) K during data collection. Using Olex2,[8] the structure was solved with the SHELXT[9] structure solution program using Intrinsic Phasing and refined with the olex2.refine[10] refinement package using Gauss-Newton minimisation.

Crystal structure determination of complex **(NHC$^3$)PdBr$_2$(py): Crystal Data** for $C_{16}H_{25}Br_2N_3Pd$ ($M$ =525.619 g/mol): monoclinic, space group $P2_1/n$ (no. 14), $a$ = 13.8237(2) Å, $b$ = 8.7247(1) Å, $c$ = 16.4465(2) Å, $\beta$ = 101.415(1)°, $V$ = 1944.34(4) Å$^3$, $Z$ =

4, $T$ = 200.0(3) K, μ(Cu Kα) = 12.503 $mm^{-1}$, *Dcalc* = 1.796 $g/cm^3$, 34828 reflections measured (7.64° ≤ 2Θ ≤ 143.3°), 3785 unique ($R_{int}$ = 0.0261, $R_{sigma}$ = 0.0108) which were used in all calculations. The final $R_1$ was 0.0234 (I>=2u(I)) and $wR_2$ was 0.0588 (all data).

**Refinement model description;** Number of restraints - 0, number of constraints - 40.

Details:

1. Fixed Uiso

At 1.2 times of:

All C(H) groups, All C(H,H) groups

At 1.5 times of:

All C(H,H,H) groups

2.a Secondary CH2 refined with riding coordinates:

C19(H19a,H19b), C16(H16a,H16b), C15(H15a,H15b), C17(H17a,H17b), C20(H20a, H20b), C21(H21a,H21b)

2.b Aromatic/amide H refined with riding coordinates:

C10(H10), C6(H6), C7(H7), C14(H14), C11(H11), C13(H13), C12(H12)

2.c Idealised Me refined as rotating group:

C18(H18a,H18b,H18c), C22(H22a,H22b,H22c)

# 4 Computational part

## 4.1 Free Energy profile for different probable processes

### 4.1.1. C-H activation

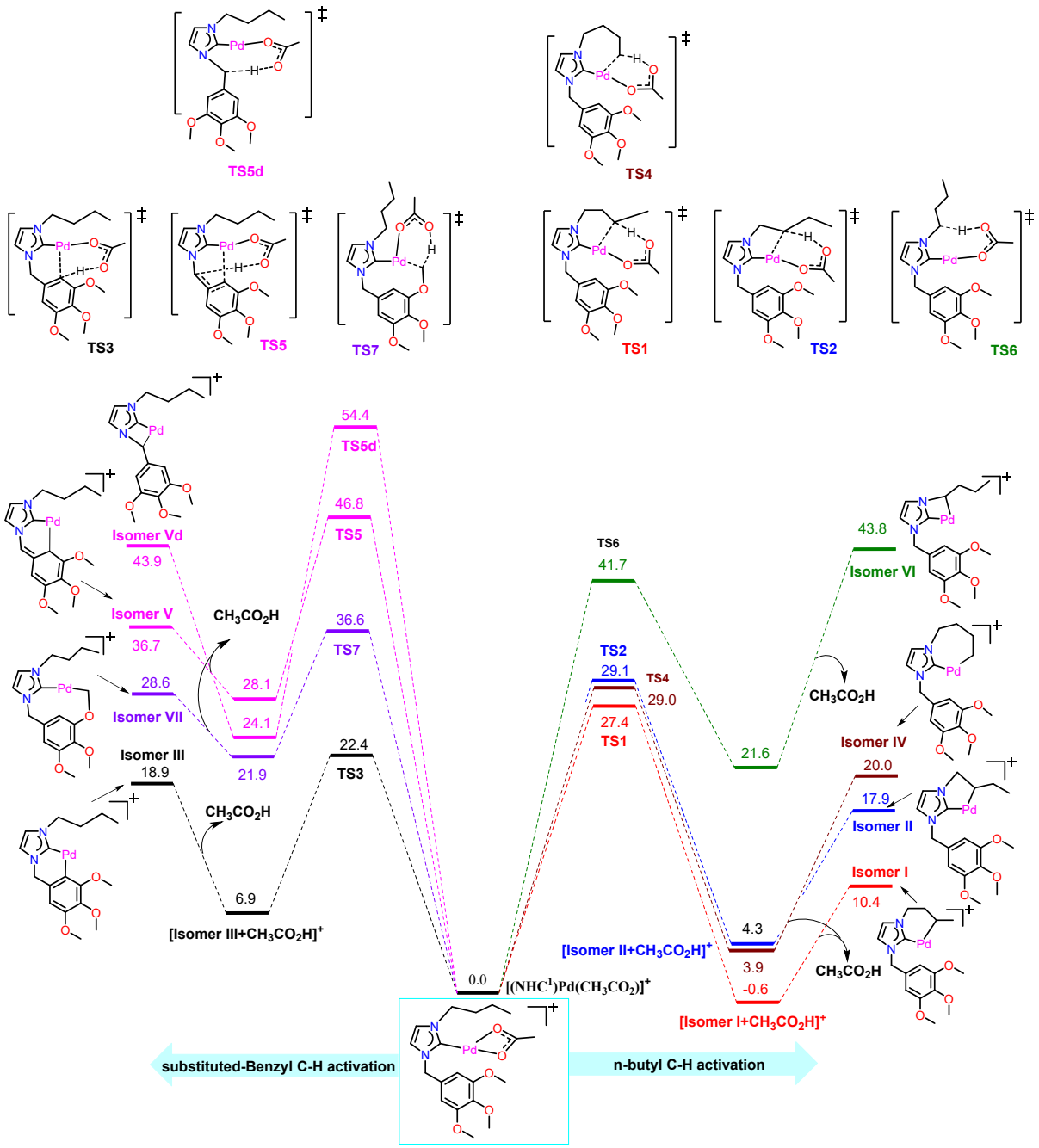



**Figure S26.** Computed free energy profile (kcal/mol) for all probable C-H activation in $[(NHC^1)Pd(CH_3CO_2)]^+$ assuming a temperature of 298 K. Note that the isomers **V**, **Vd**, **VI**, and **VII** complex with $CH_3CO_2H$, [Isomer+$CH_3CO_2H$] have relatively higher energy than isomer **I-IV** complex with $CH_3CO_2H$ by >15 kcal/mol. Besides, isomers **V-VII** are also of higher energy

than isomer **I-IV**. Hence, these isomers are less likely to be involved in the CID IM mass spectra. Strained 4-membered ring is responsible for higher energy of Isomer **Vd** and **VI**. Isomer **V** is higher in energy due to loss of aromaticity. Isomer **VII** is higher in energy due to ring strain.

### 4.1.2. Isomerization

Isomerization probably occurs through Pd-catalyzed C-H activation. Conversion of Isomer **I** to **II**, first involve C-H activation at C2-carbon leading to formation of Pd-hydride and alkene (**Int1**). It is followed by hydride transfer to C3-carbon forming isomer **II**. The barrier for this process is very high (51.6 kcal/mol, Figure S23). The mechanism of isomer **I** to isomer **IV** is similar, and have 33.6 kcal/mol barrier (Figure S24). The conversion of isomer **I** to **III** involves C-H activation of aromatic C-H bond and simultaneous H-transfer to C3 butyl carbon (Figure S25a). The isomerization between isomer **II** and **III** also follow similar mechanism (Figure S25b). The barrier for these two pathways is very high (>58 kcal/mol).

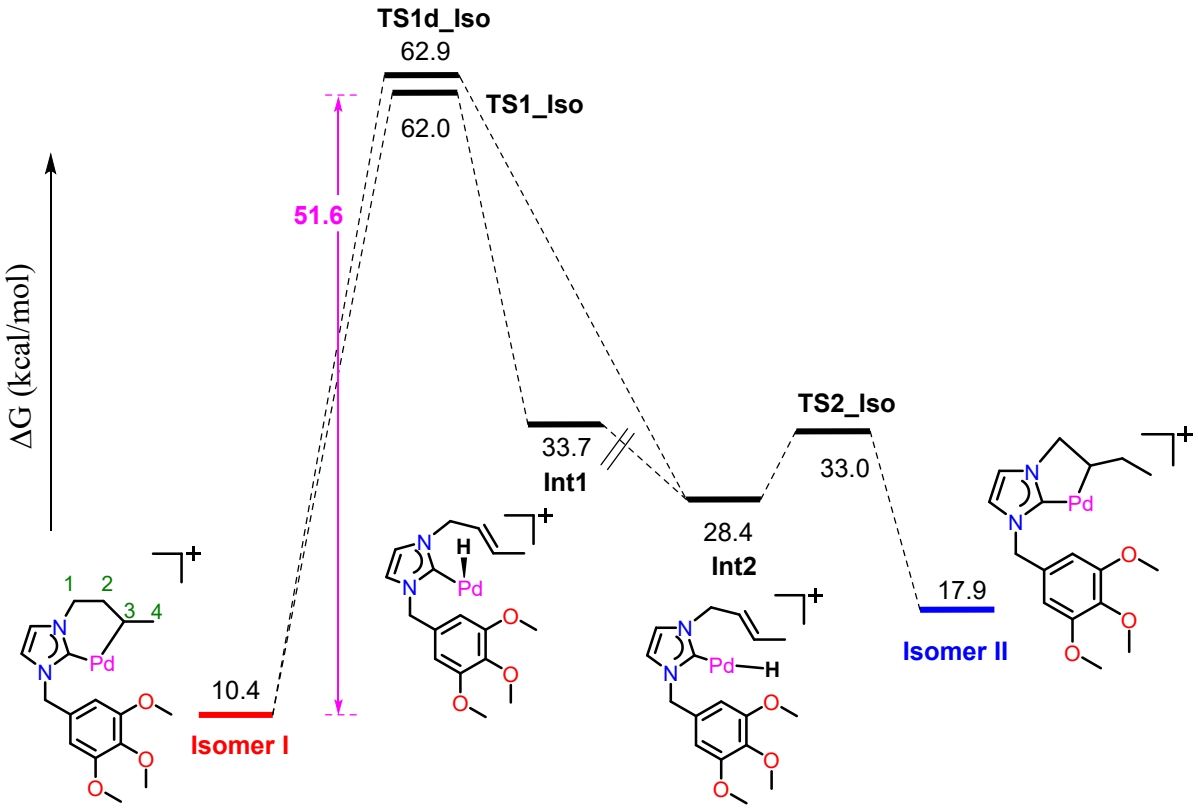



**Figure S27.** Computed free energy profile (kcal/mol) for isomerization of Isomer **I** to **II**.

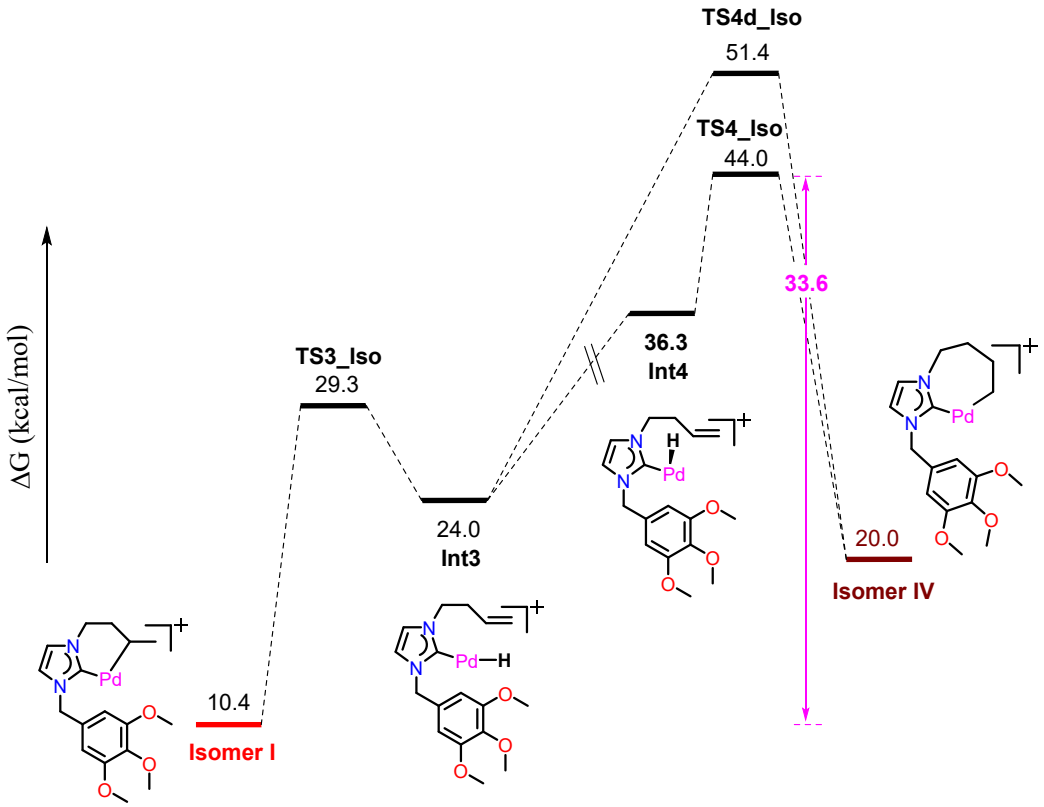



**Figure S28.** Computed free energy profile (kcal/mol) for isomerization of Isomer **I** to **IV**.

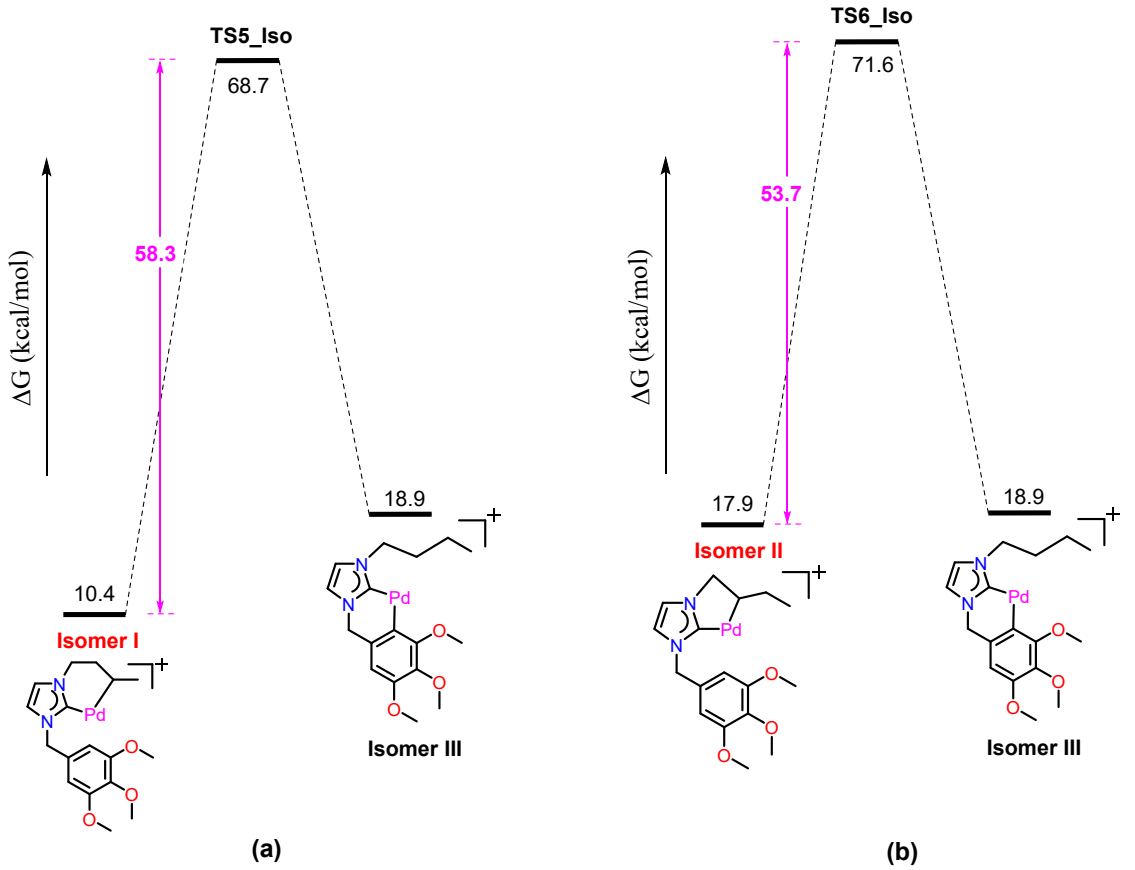
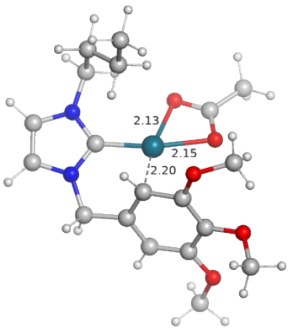
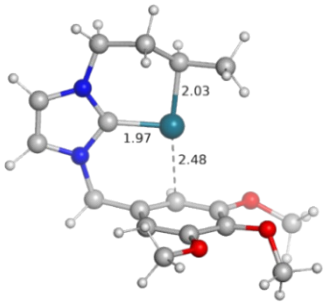



**Figure S29.** Computed free energy profile (kcal/mol) for isomerization of (a) Isomer **I** to **III** and (b) Isomer **II** to **III**.

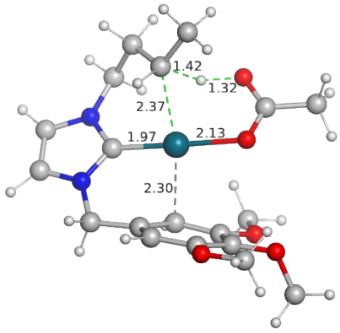
## 4.2 Molecular Images of Optimized Geometries of Stationary Points



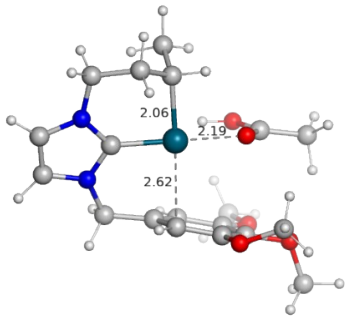

**[(NHC$^1$)Pd(CH$_3$CO$_2$)]$^+$** (0.0)



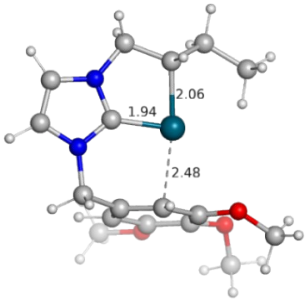

**Isomer I** (10.4)



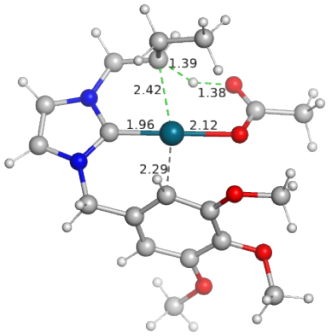

**TS1** (27.4)



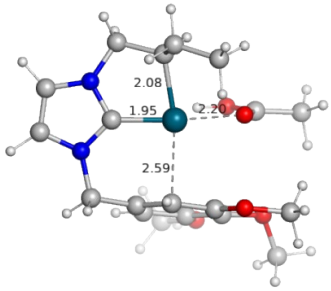

**[Isomer I+CH$_3$CO$_2$H]$^+$** (-0.6)



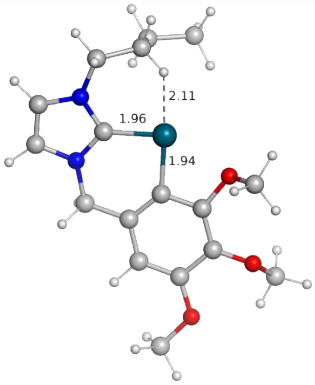

**Isomer II** (17.9)



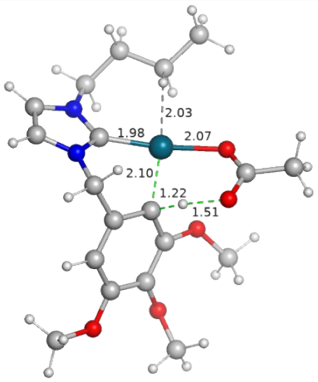

**TS2** (29.1)



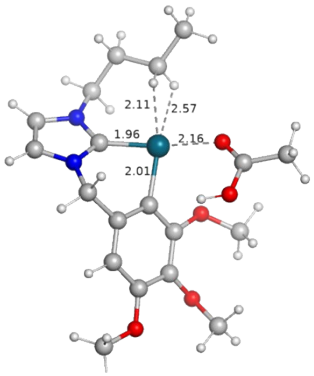

**[Isomer II+CH$_3$CO$_2$H]$^+$** (4.3)




**Isomer III** (18.9)

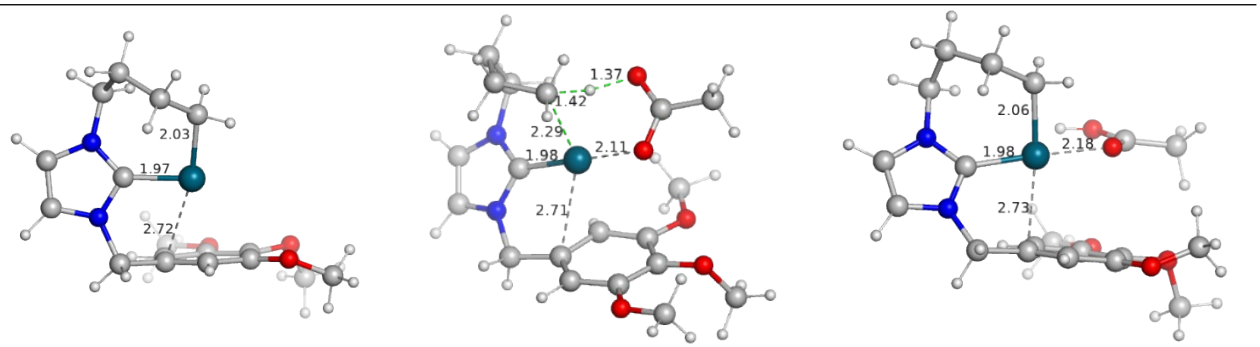



**TS3** (22.4)

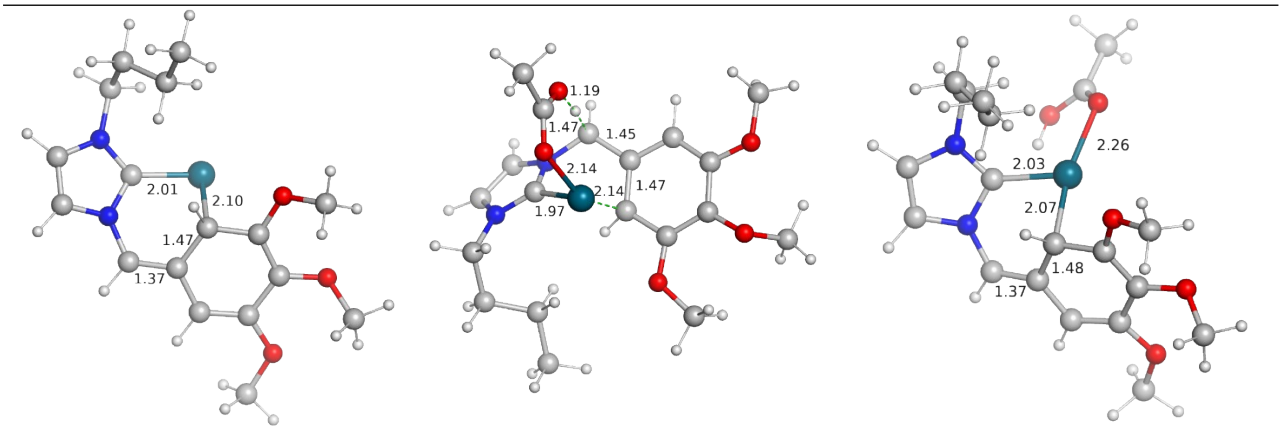



**[Isomer III+CH$_3$CO$_2$H]$^+$** (6.9)

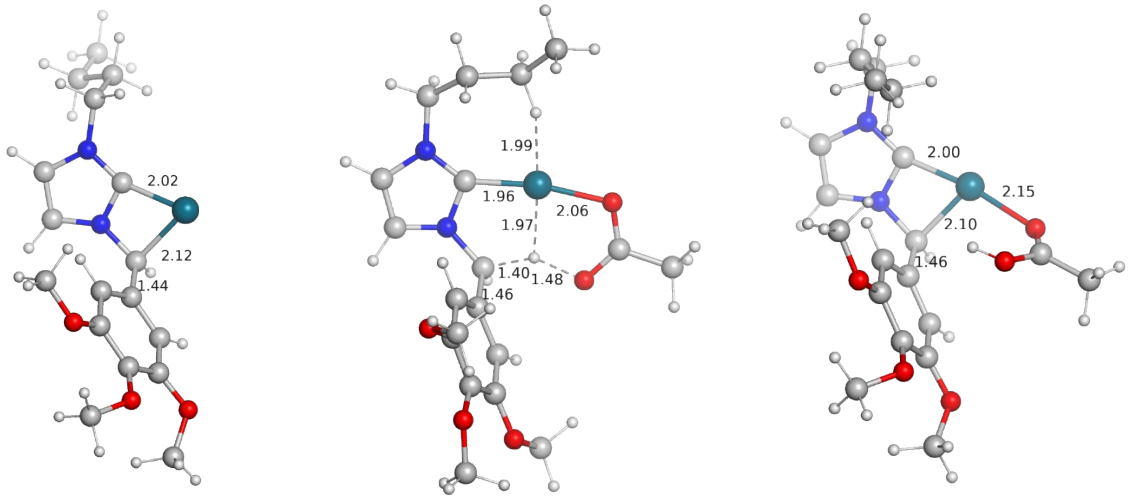
**Figure S30.** The optimized stationary points for C-H activation in **[(NHC$^1$)Pd(CH$_3$CO$_2$)]$^+$** with the respective free energy (kcal/mol) in the parentheses. (*continued on next page*).




**Isomer IV** (20.0) | **TS4** (29.0) | **[Isomer IV+$CH_3CO_2H$]$^+$** (3.9)




**Isomer V** (36.7) | **TS5 (46.8)** | **[Isomer V+$CH_3CO_2H$]$^+$** (28.1)




**Isomer Vd** (43.9) | **TS5d (54.4)** | **[Isomer Vd+$CH_3CO_2H$]$^+$** (24.1)

**Figure S30.** The optimized stationary points for C-H activation in **[(NHC$^1$)Pd($CH_3CO_2$)]$^+$** with the respective free energy (kcal/mol) in the parentheses.

### 4.3 Stationary Point Energies

**Table S2.** Computed total potential energies ($E_{SPC}$) at BS2, total potential energy at BS1 (E), zero-point energy correction (ZPE), enthalpy (H), temperature*entropy (T.S) term, T.S term with quasiharmonic correction by Grimme (T.qh-S), free energy (with quasiharmonic corrections for entropy(qh-G(T)_SPC). All energies are in Hartree.

| Structure | E_SPC | E | ZPE | H_SPC | T.S | T.qh-S | G(T)_SPC | qh-G(T)_SPC |
|---|---|---|---|---|---|---|---|---|
| **Acetic_acid** | -229.187969 | -229.084611 | 0.062036 | -229.120403 | 0.032907 | 0.032422 | -229.15331 | -229.152824 |
| **[(NHC$^1$)Pd($CH_3CO_2$)]$^+$** | -1353.818898 | -1352.563105 | 0.448997 | -1353.339107 | 0.094786 | 0.087648 | -1353.433893 | -1353.426755 |
| **[Isomer I+$CH_3CO_2H$]$^+$** | -1353.822598 | -1352.569866 | 0.449782 | -1353.342845 | 0.089659 | 0.084896 | -1353.432504 | -1353.427741 |
| **[Isomer II+$CH_3CO_2H$]$^+$** | -1353.81284 | -1352.558703 | 0.448842 | -1353.3336 | 0.092386 | 0.086358 | -1353.425986 | -1353.419958 |
| **[Isomer III+$CH_3CO_2H$]$^+$** | -1353.808465 | -1352.550776 | 0.448953 | -1353.328859 | 0.092738 | 0.086909 | -1353.421597 | -1353.415768 |
| **[Isomer IV+$CH_3CO_2H$]$^+$** | -1353.815774 | -1352.562074 | 0.450169 | -1353.335879 | 0.089727 | 0.084693 | -1353.425606 | -1353.420572 |
| **[Isomer V+$CH_3CO_2H$]$^+$** | -1353.772211 | -1352.51785 | 0.446943 | -1353.294754 | 0.094354 | 0.087185 | -1353.389108 | -1353.381939 |
| **[Isomer Vd+$CH_3CO_2H$]$^+$** | -1353.777609 | -1352.520239 | 0.447299 | -1353.298846 | 0.097941 | 0.089562 | -1353.396787 | -1353.388407 |
| **[Isomer VI+$CH_3CO_2H$]$^+$** | -1353.782504 | -1352.527679 | 0.447402 | -1353.303984 | 0.095206 | 0.088278 | -1353.39919 | -1353.392262 |
| **[Isomer VII+$CH_3CO_2H$]$^+$** | -1353.785732 | -1352.529359 | 0.448521 | -1353.307964 | 0.089439 | 0.083967 | -1353.397403 | -1353.391931 |
| **TS1** | -1353.774122 | -1352.517462 | 0.445552 | -1353.299269 | 0.088733 | 0.083748 | -1353.388002 | -1353.383017 |
| **TS2** | -1353.770158 | -1352.51294 | 0.444962 | -1353.295599 | 0.090304 | 0.08486 | -1353.385903 | -1353.380459 |
| **TS3** | -1353.781093 | -1352.524444 | 0.445365 | -1353.30614 | 0.090748 | 0.084983 | -1353.396888 | -1353.391123 |
| **TS4** | -1353.771051 | -1352.513247 | 0.444781 | -1353.297092 | 0.088668 | 0.08345 | -1353.38576 | -1353.380543 |
| **TS5** | -1353.737393 | -1352.483406 | 0.442169 | -1353.264691 | 0.094869 | 0.08742 | -1353.35956 | -1353.352111 |
| **TS5d** | -1353.720878 | -1352.460484 | 0.439729 | -1353.249947 | 0.099406 | 0.090073 | -1353.349353 | -1353.340021 |
| **TS6** | -1353.745683 | -1352.48741 | 0.44211 | -1353.273056 | 0.094359 | 0.08722 | -1353.367415 | -1353.360276 |
| **TS7** | -1353.758264 | -1352.499106 | 0.444832 | -1353.284213 | 0.090313 | 0.084257 | -1353.374526 | -1353.36847 |
| **Isomer_I** | -1124.590836 | -1123.434468 | 0.384086 | -1124.181855 | 0.079975 | 0.075443 | -1124.26183 | -1124.257298 |
| **Isomer_II** | -1124.578254 | -1123.42216 | 0.383726 | -1124.16938 | 0.081032 | 0.076075 | -1124.250411 | -1124.245455 |
| **Isomer_III** | -1124.576282 | -1123.417729 | 0.3843 | -1124.166724 | 0.08239 | 0.077154 | -1124.249114 | -1124.243878 |
| **Isomer_IV** | -1124.577146 | -1123.420761 | 0.385239 | -1124.167533 | 0.079148 | 0.074567 | -1124.246681 | -1124.242101 |
| **Isomer_V** | -1124.54711 | -1123.392456 | 0.383256 | -1124.138399 | 0.082154 | 0.076979 | -1124.220554 | -1124.215379 |
| **Isomer_Vd** | -1124.533886 | -1123.377149 | 0.383119 | -1124.124878 | 0.086044 | 0.079075 | -1124.210922 | -1124.203952 |
| **Isomer_VI** | -1124.534325 | -1123.377956 | 0.382342 | -1124.126159 | 0.084037 | 0.077896 | -1124.210196 | -1124.204055 |
| **Isomer_VII** | -1124.562428 | -1123.403697 | 0.383574 | -1124.154668 | 0.077807 | 0.073756 | -1124.232475 | -1124.228424 |
| **TS1d_Iso** | -1124.500683 | -1123.338658 | 0.377163 | -1124.098833 | 0.078849 | 0.074839 | -1124.177682 | -1124.173672 |
| **TS1_Iso** | -1124.501252 | -1123.342623 | 0.377091 | -1124.098938 | 0.081004 | 0.076223 | -1124.179942 | -1124.175161 |
| **Int1** | -1124.548814 | -1123.385304 | 0.379338 | -1124.144436 | 0.080505 | 0.075824 | -1124.224942 | -1124.22026 |
| **Int2** | -1124.558481 | -1123.394174 | 0.380567 | -1124.153037 | 0.080325 | 0.075657 | -1124.233362 | -1124.228694 |
| **TS2_Iso** | -1124.549947 | -1123.385012 | 0.378632 | -1124.146671 | 0.078754 | 0.074644 | -1124.225425 | -1124.221314 |
| **TS3_Iso** | -1124.557399 | -1123.391715 | 0.380083 | -1124.152962 | 0.078915 | 0.074349 | -1124.231877 | -1124.227311 |
| **Int3** | -1124.566819 | -1123.402202 | 0.381701 | -1124.160653 | 0.07989 | 0.075066 | -1124.240544 | -1124.235719 |
| **Int4** | -1124.545935 | -1123.384631 | 0.380184 | -1124.14075 | 0.079247 | 0.075272 | -1124.219996 | -1124.216022 |
| **TS4_Iso** | -1124.533719 | -1123.368616 | 0.379482 | -1124.130076 | 0.077802 | 0.073714 | -1124.207878 | -1124.20379 |
| **TS4d_Iso** | -1124.521689 | -1123.357778 | 0.379225 | -1124.118321 | 0.078015 | 0.073775 | -1124.196337 | -1124.192096 |
| **TS5_Iso** | -1124.493308 | -1123.324607 | 0.378792 | -1124.089968 | 0.07806 | 0.074453 | -1124.168028 | -1124.164421 |
| **TS6_Iso** | -1124.487313 | -1123.317929 | 0.378172 | -1124.08417 | 0.079911 | 0.075676 | -1124.164081 | -1124.159846 |

## 4.4 Conformational study of isomer III

The different conformations for the Isomer **III** were explored to find lower energy conformers. The CREST program in combination with XTB was used for conformation sampling. The obtained conformations were further refined with the DFT methods described in the main text. The conformers with one small imaginary frequency (< -20 $cm^{-1}$) were discarded. The energy of the four most stable conformers with respect to the lowest energy conformer is given in Table 1.

**Table S3.** Relative free energy in kcal/mol of the four lowest energy conformers of isomer **III**

| **Isomer** | energy with respect to the lowest energy conformer | Calculated CCS ($Å^2$) [a] |
|---|---|---|
| **Isomer III** | 0.0 | 170.9 |
| **Isomer III_c1** | 0.1 | 168.5 |
| **Isomer III_c2** | 0.1 | 171.2 |
| **Isomer III_c3** | 0.6 | 170.8 |

[a] CCS were calculated using Trajectory Methods (TM) as implemented in the IMoS software.

## 4.5 Cartesian Coordinates

(Besides coordinates, the Gibbs energies at B3LYP-D3BJ/BS1 at 298.15 K are given in hartree (Eh).)

Acetic_acid
Energy (FREE) = -229.049952 Eh

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | C | -0.9211 | 2.3566 | 1.1037 |
| 2 | H | -0.9952 | 1.2747 | 0.9527 |
| 3 | H | -0.2713 | 2.5216 | 1.9693 |
| 4 | H | -1.9094 | 2.7753 | 1.2938 |
| 5 | C | -0.3254 | 3.0076 | -0.1188 |
| 6 | O | -0.8455 | 3.8637 | -0.7977 |
| 7 | O | 0.9092 | 2.5115 | -0.3905 |
| 8 | H | 1.2164 | 2.9832 | -1.1876 |

$[(NHC^1)Pd(CH_3CO_2)]^+$
Energy (FREE) = -1352.178099 Eh

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | C | 0.9247 | -2.2534 | 0.0248 |
| 2 | C | 2.2729 | -3.9499 | -0.5605 |
| 3 | C | 1.0443 | -4.2189 | -1.0746 |
| 4 | N | 0.2256 | -3.1591 | -0.7067 |
| 5 | N | 2.1797 | -2.7406 | 0.1155 |
| 6 | C | -1.2126 | -3.0711 | -0.9678 |
| 7 | H | -1.3790 | -3.3451 | -2.0166 |
| 8 | H | -1.7331 | -3.8036 | -0.3434 |
| 9 | C | -1.7585 | -1.6852 | -0.7096 |
| 10 | C | -2.9926 | -1.5283 | -0.1049 |
| 11 | C | -1.0173 | -0.5417 | -1.1449 |
| 12 | C | -3.5449 | -0.2360 | 0.0196 |
| 13 | H | -3.5216 | -2.3903 | 0.2807 |
| 14 | C | -1.6206 | 0.7652 | -1.0689 |
| 15 | H | -0.2380 | -0.6547 | -1.8942 |
| 16 | C | -2.8720 | 0.9158 | -0.4717 |
| 17 | O | -3.4379 | 2.1449 | -0.3210 |
| 18 | O | -4.7194 | 0.0154 | 0.6017 |
| 19 | O | -0.8717 | 1.7371 | -1.5925 |
| 20 | C | -5.4859 | -1.0616 | 1.1539 |
| 21 | H | -4.9257 | -1.5675 | 1.9467 |
| 22 | H | -6.3766 | -0.5952 | 1.5724 |
| 23 | H | -5.7721 | -1.7758 | 0.3747 |
| 24 | C | -4.5351 | 2.4339 | -1.2050 |
| 25 | H | -5.3693 | 1.7494 | -1.0301 |
| 26 | H | -4.8419 | 3.4540 | -0.9715 |
| 27 | H | -4.2116 | 2.3732 | -2.2509 |
| 28 | C | -0.9473 | 3.0985 | -1.1088 |
| 29 | H | -0.0223 | 3.5591 | -1.4563 |
| 30 | H | -1.8086 | 3.6160 | -1.5317 |
| 31 | H | -0.9933 | 3.1026 | -0.0196 |
| 32 | C | 3.3147 | -2.0628 | 0.7694 |
| 33 | H | 2.9018 | -1.4441 | 1.5673 |
| 34 | H | 3.9242 | -2.8477 | 1.2253 |
| 35 | C | 4.1402 | -1.2234 | -0.2097 |
| 36 | H | 5.0253 | -0.8758 | 0.3381 |
| 37 | H | 4.5105 | -1.8632 | -1.0221 |

| | | | | |
|---|---|---|---|---|
| 38 | C | 3.3926 | -0.0177 | -0.7879 |
| 39 | H | 2.5136 | -0.3616 | -1.3491 |
| 40 | H | 3.0080 | 0.5933 | 0.0399 |
| 41 | C | 4.2750 | 0.8355 | -1.7021 |
| 42 | H | 4.6482 | 0.2504 | -2.5505 |
| 43 | H | 3.7183 | 1.6885 | -2.1035 |
| 44 | H | 5.1434 | 1.2269 | -1.1600 |
| 45 | Pd | 0.1923 | -0.5507 | 0.6967 |
| 46 | C | 0.6282 | 1.0117 | 2.5932 |
| 47 | O | 1.3151 | -0.0635 | 2.4345 |
| 48 | O | -0.3008 | 1.2541 | 1.7542 |
| 49 | C | 0.9113 | 1.9256 | 3.7437 |
| 50 | H | 1.9904 | 2.0587 | 3.8598 |
| 51 | H | 0.4198 | 2.8884 | 3.5930 |
| 52 | H | 0.5317 | 1.4699 | 4.6654 |
| 53 | H | 3.1964 | -4.5053 | -0.6079 |
| 54 | H | 0.6813 | -5.0587 | -1.6461 |

Isomer_I

Energy (FREE) = -1123.105462 Eh

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | C | 1.0167 | -0.6132 | 1.1843 |
| 2 | C | 2.7490 | 0.0138 | -0.1042 |
| 3 | C | 2.9846 | -1.2630 | 0.2998 |
| 4 | H | 3.3262 | 0.6752 | -0.7311 |
| 5 | H | 3.8052 | -1.9318 | 0.0921 |
| 6 | N | 1.5316 | 0.3922 | 0.4464 |
| 7 | N | 1.9049 | -1.6342 | 1.0886 |
| 8 | C | 1.7438 | -2.9300 | 1.7796 |
| 9 | H | 2.2718 | -3.6783 | 1.1836 |
| 10 | H | 2.2322 | -2.8631 | 2.7561 |
| 11 | C | 0.2837 | -3.2918 | 1.9317 |
| 12 | C | -0.3895 | -2.9935 | 3.1289 |
| 13 | C | -0.4068 | -3.8766 | 0.8653 |
| 14 | C | -1.7715 | -3.2842 | 3.2644 |
| 15 | H | 0.1488 | -2.6750 | 4.0166 |
| 16 | C | -1.7759 | -4.1345 | 0.9814 |
| 17 | H | 0.1159 | -4.0863 | -0.0594 |
| 18 | C | -2.4784 | -3.8296 | 2.1787 |
| 19 | O | -3.8321 | -3.9616 | 2.2535 |
| 20 | O | -2.3066 | -2.9308 | 4.4542 |
| 21 | O | -2.5386 | -4.6304 | -0.0153 |
| 22 | C | -3.4378 | -3.6285 | 5.0009 |
| 23 | H | -3.3100 | -4.7106 | 4.8944 |
| 24 | H | -3.4441 | -3.3657 | 6.0594 |
| 25 | H | -4.3661 | -3.3139 | 4.5243 |
| 26 | C | -4.3764 | -5.2905 | 2.1574 |
| 27 | H | -5.4468 | -5.1811 | 2.3346 |
| 28 | H | -4.2015 | -5.7160 | 1.1684 |
| 29 | H | -3.9396 | -5.9378 | 2.9271 |
| 30 | C | -1.9244 | -4.9345 | -1.2662 |
| 31 | H | -2.7249 | -5.3137 | -1.9009 |
| 32 | H | -1.4912 | -4.0350 | -1.7191 |
| 33 | H | -1.1511 | -5.7024 | -1.1499 |
| 34 | C | 0.9236 | 1.7262 | 0.3094 |
| 35 | H | 1.2668 | 2.1386 | -0.6423 |
| 36 | H | 1.3116 | 2.3622 | 1.1133 |
| 37 | Pd | -0.6909 | -0.7356 | 2.1570 |
| 38 | C | -0.6025 | 1.6775 | 0.3554 |
| 39 | H | -0.9823 | 1.0659 | -0.4711 |
| 40 | H | -0.9549 | 2.7052 | 0.1797 |
| 41 | C | -1.1481 | 1.1810 | 1.6800 |
| 42 | H | -0.7414 | 1.7637 | 2.5163 |
| 43 | C | -2.6531 | 1.0089 | 1.7781 |
| 44 | H | -3.0955 | 0.6827 | 0.8326 |
| 45 | H | -2.9328 | 0.2671 | 2.5553 |
| 46 | H | -3.1443 | 1.9381 | 2.0990 |

Isomer_II

Energy (FREE) = -1123.094317 Eh

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | C | -2.0768 | 0.6759 | -0.1889 |
| 2 | C | -3.9482 | 1.8354 | 0.2441 |
| 3 | C | -3.1408 | 2.6127 | -0.5342 |
| 4 | N | -1.9844 | 1.8807 | -0.7886 |
| 5 | N | -3.2698 | 0.6425 | 0.4401 |
| 6 | C | -0.8147 | 2.3001 | -1.5937 |
| 7 | H | -1.0155 | 2.0658 | -2.6435 |
| 8 | H | -0.7229 | 3.3838 | -1.4932 |
| 9 | C | 0.4254 | 1.5922 | -1.0960 |
| 10 | C | 1.1870 | 2.1514 | -0.0751 |
| 11 | C | 0.7225 | 0.2999 | -1.5694 |
| 12 | C | 2.2339 | 1.4173 | 0.5033 |
| 13 | H | 0.9363 | 3.1338 | 0.3053 |
| 14 | C | 1.7780 | -0.4452 | -0.9929 |
| 15 | H | 0.2508 | -0.0942 | -2.4650 |
| 16 | C | 2.5273 | 0.1018 | 0.0672 |
| 17 | O | 3.4418 | -0.6748 | 0.7109 |
| 18 | O | 2.9834 | 1.8597 | 1.5339 |
| 19 | O | 1.9247 | -1.6986 | -1.4885 |
| 20 | C | 2.7386 | 3.1640 | 2.0586 |
| 21 | H | 1.7236 | 3.2392 | 2.4654 |
| 22 | H | 3.4637 | 3.2968 | 2.8611 |
| 23 | H | 2.8920 | 3.9322 | 1.2923 |
| 24 | C | 4.8154 | -0.2447 | 0.6876 |
| 25 | H | 4.9473 | 0.6774 | 1.2549 |
| 26 | H | 5.3822 | -1.0539 | 1.1492 |
| 27 | H | 5.1524 | -0.1005 | -0.3456 |
| 28 | C | 3.2106 | -2.3427 | -1.5204 |
| 29 | H | 3.1038 | -3.1462 | -2.2501 |
| 30 | H | 3.9816 | -1.6429 | -1.8579 |
| 31 | H | 3.4747 | -2.7462 | -0.5431 |
| 32 | C | -3.5531 | -0.5469 | 1.2475 |
| 33 | H | -3.3870 | -0.2998 | 2.3012 |
| 34 | H | -4.6034 | -0.8308 | 1.1214 |
| 35 | C | -2.5907 | -1.6568 | 0.7830 |
| 36 | H | -3.0292 | -2.2080 | -0.0584 |
| 37 | C | -2.0912 | -2.6025 | 1.8638 |
| 38 | H | -1.7373 | -2.0285 | 2.7287 |
| 39 | H | -2.9181 | -3.2346 | 2.2228 |
| 40 | C | -0.9596 | -3.5005 | 1.3368 |
| 41 | H | -0.0790 | -2.9143 | 1.0129 |
| 42 | H | -0.5927 | -4.1759 | 2.1154 |
| 43 | H | -1.2910 | -4.1074 | 0.4875 |
| 44 | Pd | -0.9068 | -0.8651 | -0.1092 |
| 45 | H | -4.9223 | 2.0325 | 0.6630 |
| 46 | H | -3.2865 | 3.6078 | -0.9246 |

Isomer_III

Energy (FREE) = -1123.090561 Eh

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | C | -1.8481 | -1.0295 | 0.1576 |
| 2 | N | -1.3367 | -2.2654 | -0.0443 |
| 3 | C | -2.3574 | -3.2093 | -0.0199 |
| 4 | C | -3.5153 | -2.5385 | 0.2052 |
| 5 | N | -3.1854 | -1.1951 | 0.3108 |
| 6 | C | -4.1383 | -0.1292 | 0.6625 |
| 7 | H | -4.1933 | -0.0659 | 1.7539 |
| 8 | C | -3.7874 | 1.2314 | 0.0615 |
| 9 | C | -3.7747 | 1.2883 | -1.4697 |
| 10 | C | -3.1776 | 2.5942 | -1.9976 |

| | | | | |
|---|---|---|---|---|
| 11 | H | -3.2273 | 2.6361 | -3.0894 |
| 12 | H | -2.1201 | 2.6845 | -1.7122 |
| 13 | H | -3.7079 | 3.4676 | -1.6019 |
| 14 | H | -4.8067 | 1.1751 | -1.8249 |
| 15 | H | -3.2101 | 0.4392 | -1.8721 |
| 16 | H | -2.8249 | 1.6033 | 0.4915 |
| 17 | H | -4.5093 | 1.9556 | 0.4578 |
| 18 | H | -5.1166 | -0.4493 | 0.2936 |
| 19 | H | -4.5300 | -2.8905 | 0.3048 |
| 20 | H | -2.1667 | -4.2603 | -0.1698 |
| 21 | C | 0.0589 | -2.6493 | -0.3246 |
| 22 | C | 1.0830 | -1.5605 | -0.1281 |
| 23 | C | 0.7546 | -0.2408 | 0.0685 |
| 24 | C | 1.7074 | 0.7662 | 0.1750 |
| 25 | C | 3.0645 | 0.4892 | 0.1031 |
| 26 | C | 3.4301 | -0.8791 | -0.0664 |
| 27 | C | 2.4555 | -1.8747 | -0.1920 |
| 28 | H | 2.7564 | -2.9060 | -0.3372 |
| 29 | O | 4.7634 | -1.1064 | -0.0950 |
| 30 | C | 5.2263 | -2.4446 | -0.2520 |
| 31 | H | 6.3143 | -2.3836 | -0.2329 |
| 32 | H | 4.8800 | -3.0796 | 0.5719 |
| 33 | H | 4.8985 | -2.8671 | -1.2096 |
| 34 | O | 3.9836 | 1.4816 | 0.2526 |
| 35 | C | 4.7986 | 1.7674 | -0.9002 |
| 36 | H | 5.4296 | 0.9124 | -1.1505 |
| 37 | H | 5.4178 | 2.6191 | -0.6172 |
| 38 | H | 4.1663 | 2.0354 | -1.7543 |
| 39 | O | 1.1099 | 2.0248 | 0.2982 |
| 40 | C | 1.5409 | 2.8308 | 1.4239 |
| 41 | H | 0.9407 | 3.7398 | 1.3835 |
| 42 | H | 2.6011 | 3.0598 | 1.3199 |
| 43 | H | 1.3575 | 2.2913 | 2.3589 |
| 44 | Pd | -0.9345 | 0.6994 | 0.2154 |
| 45 | H | 0.0909 | -3.0076 | -1.3607 |
| 46 | H | 0.2856 | -3.5034 | 0.3219 |

Isomer_IV

Energy (FREE) = -1123.090296 Eh

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | C | -1.3071 | 1.2457 | -0.0510 |
| 2 | C | -2.3562 | 3.2346 | -0.1233 |
| 3 | C | -1.5266 | 3.1760 | -1.1985 |
| 4 | N | -0.8840 | 1.9490 | -1.1344 |
| 5 | N | -2.2034 | 2.0432 | 0.5729 |
| 6 | C | 0.1411 | 1.4584 | -2.0760 |
| 7 | H | -0.3485 | 0.8712 | -2.8580 |
| 8 | H | 0.5939 | 2.3382 | -2.5397 |
| 9 | C | 1.1745 | 0.6294 | -1.3467 |
| 10 | C | 2.1388 | 1.2550 | -0.5459 |
| 11 | C | 1.1376 | -0.7711 | -1.4387 |
| 12 | C | 3.0425 | 0.4808 | 0.1846 |
| 13 | H | 2.1498 | 2.3348 | -0.4671 |
| 14 | C | 2.0691 | -1.5624 | -0.7186 |
| 15 | H | 0.4993 | -1.2732 | -2.1598 |
| 16 | C | 3.0105 | -0.9402 | 0.1180 |
| 17 | O | 3.8038 | -1.7031 | 0.9177 |
| 18 | O | 3.9625 | 0.9887 | 1.0311 |
| 19 | O | 1.9056 | -2.8954 | -0.8705 |
| 20 | C | 4.0471 | 2.4037 | 1.1873 |
| 21 | H | 3.1079 | 2.8118 | 1.5788 |
| 22 | H | 4.8469 | 2.5717 | 1.9080 |
| 23 | H | 4.2980 | 2.8912 | 0.2381 |
| 24 | C | 5.2289 | -1.6095 | 0.7374 |
| 25 | H | 5.6039 | -0.6410 | 1.0699 |
| 26 | H | 5.6524 | -2.4069 | 1.3490 |
| 27 | H | 5.4919 | -1.7721 | -0.3144 |
| 28 | C | 3.0103 | -3.8050 | -0.7342 |
| 29 | H | 2.6748 | -4.7258 | -1.2129 |
| 30 | H | 3.8917 | -3.4210 | -1.2579 |
| 31 | H | 3.2479 | -3.9850 | 0.3141 |
| 32 | C | -2.8401 | 1.7322 | 1.8597 |
| 33 | H | -2.0505 | 1.3697 | 2.5209 |
| 34 | H | -3.2044 | 2.6769 | 2.2693 |
| 35 | C | -3.9776 | 0.7157 | 1.7607 |
| 36 | H | -4.3001 | 0.5225 | 2.7912 |
| 37 | H | -4.8329 | 1.1641 | 1.2432 |
| 38 | C | -3.6011 | -0.6110 | 1.0783 |
| 39 | H | -4.3466 | -1.3634 | 1.3732 |
| 40 | H | -3.6937 | -0.5197 | -0.0094 |
| 41 | C | -2.2177 | -1.1347 | 1.4291 |
| 42 | H | -2.1149 | -2.2044 | 1.1745 |
| 43 | H | -1.9452 | -0.9789 | 2.4791 |
| 44 | H | -3.0220 | 4.0126 | 0.2155 |
| 45 | H | -1.3339 | 3.8875 | -1.9858 |
| 46 | Pd | -0.6307 | -0.5754 | 0.2946 |

**Isomer_V**

Energy (FREE) = -1123.065900 Eh

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | C | -1.8122 | -0.1171 | 0.4694 |
| 2 | C | -3.5702 | -0.1787 | 1.8879 |
| 3 | C | -2.5090 | -0.6830 | 2.5642 |
| 4 | N | -1.4111 | -0.6064 | 1.7058 |
| 5 | N | -3.1215 | 0.1752 | 0.6207 |
| 6 | C | -0.1059 | -0.9803 | 2.0255 |
| 7 | H | -0.0140 | -1.8301 | 2.6920 |
| 8 | C | 0.9684 | -0.3911 | 1.4149 |
| 9 | C | 2.2582 | -1.0194 | 1.4200 |
| 10 | C | 0.7842 | 0.8538 | 0.6490 |
| 11 | C | 3.2693 | -0.5260 | 0.6407 |
| 12 | H | 2.3760 | -1.9534 | 1.9542 |
| 13 | C | 1.9110 | 1.3961 | -0.0685 |
| 14 | H | 0.1613 | 1.6130 | 1.1224 |
| 15 | C | 3.1057 | 0.6990 | -0.1385 |
| 16 | O | 4.0721 | 1.1641 | -0.9507 |
| 17 | O | 4.4699 | -1.1111 | 0.4709 |
| 18 | O | 1.6578 | 2.5964 | -0.6571 |
| 19 | C | 4.7442 | -2.3232 | 1.1746 |
| 20 | H | 4.0500 | -3.1136 | 0.8681 |
| 21 | H | 5.7618 | -2.5988 | 0.9000 |
| 22 | H | 4.6795 | -2.1676 | 2.2574 |
| 23 | C | 5.4439 | 1.2596 | -0.5098 |
| 24 | H | 5.9835 | 0.3425 | -0.7432 |
| 25 | H | 5.8645 | 2.1001 | -1.0641 |
| 26 | H | 5.4934 | 1.4605 | 0.5637 |
| 27 | C | 2.6958 | 3.5870 | -0.7473 |
| 28 | H | 2.1736 | 4.5339 | -0.8903 |
| 29 | H | 3.2742 | 3.6220 | 0.1825 |
| 30 | H | 3.3581 | 3.3887 | -1.5905 |
| 31 | C | -3.9507 | 0.8143 | -0.4089 |

| | | | | |
|---|---|---|---|---|
| 32 | H | -3.4355 | 0.6560 | -1.3605 |
| 33 | H | -4.9055 | 0.2821 | -0.4468 |
| 34 | C | -4.1553 | 2.3086 | -0.1420 |
| 35 | H | -4.7918 | 2.6951 | -0.9478 |
| 36 | H | -4.7234 | 2.4393 | 0.7885 |
| 37 | C | -2.8541 | 3.1143 | -0.0732 |
| 38 | H | -2.2496 | 2.7604 | 0.7724 |
| 39 | H | -2.2566 | 2.9195 | -0.9756 |
| 40 | C | -3.1043 | 4.6172 | 0.0714 |
| 41 | H | -3.6783 | 4.8365 | 0.9792 |
| 42 | H | -2.1612 | 5.1698 | 0.1302 |
| 43 | H | -3.6693 | 5.0079 | -0.7824 |
| 44 | Pd | -0.4886 | 0.3852 | -0.9528 |
| 45 | H | -4.6031 | -0.0696 | 2.1806 |
| 46 | H | -2.4219 | -1.0600 | 3.5708 |

**Isomer_Vd**

Energy (FREE) = -1123.054186 Eh

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | C | -1.4035 | 1.3834 | 1.0461 |
| 2 | C | -2.7835 | -0.2244 | 0.3249 |
| 3 | C | -1.7437 | -0.1856 | -0.5574 |
| 4 | H | -3.6760 | -0.8300 | 0.3287 |
| 5 | H | -1.5400 | -0.7557 | -1.4494 |
| 6 | N | -2.5513 | 0.7354 | 1.3144 |
| 7 | N | -0.9214 | 0.8263 | -0.0825 |
| 8 | C | 0.3862 | 1.4054 | -0.3352 |
| 9 | H | 0.3646 | 2.1989 | -1.0827 |
| 10 | C | 1.5679 | 0.5784 | -0.2929 |
| 11 | C | 2.7547 | 1.0962 | -0.8426 |
| 12 | C | 1.5748 | -0.6908 | 0.3278 |
| 13 | C | 3.9442 | 0.3760 | -0.7818 |
| 14 | H | 2.7667 | 2.0567 | -1.3470 |
| 15 | C | 2.7539 | -1.4173 | 0.3996 |
| 16 | H | 0.6658 | -1.0720 | 0.7730 |
| 17 | C | 3.9623 | -0.8952 | -0.1549 |
| 18 | O | 5.1567 | -1.4976 | -0.0459 |
| 19 | O | 5.0377 | 0.9806 | -1.2962 |
| 20 | O | 2.8727 | -2.6147 | 1.0207 |
| 21 | C | 6.0071 | 0.2279 | -2.0440 |
| 22 | H | 5.5189 | -0.5338 | -2.6612 |
| 23 | H | 6.4985 | 0.9585 | -2.6885 |
| 24 | H | 6.7367 | -0.2411 | -1.3831 |
| 25 | C | 5.3114 | -2.9258 | -0.1649 |
| 26 | H | 6.3423 | -3.0696 | -0.4912 |
| 27 | H | 5.1452 | -3.4131 | 0.7953 |
| 28 | H | 4.6232 | -3.3288 | -0.9125 |
| 29 | C | 1.7230 | -3.1721 | 1.6488 |
| 30 | H | 2.0517 | -4.1171 | 2.0808 |
| 31 | H | 1.3517 | -2.5137 | 2.4434 |
| 32 | H | 0.9257 | -3.3590 | 0.9193 |
| 33 | C | -3.4739 | 1.0694 | 2.4123 |
| 34 | H | -2.8631 | 1.2458 | 3.3008 |
| 35 | H | -4.0858 | 0.1813 | 2.5938 |
| 36 | Pd | 0.2466 | 2.4627 | 1.4913 |
| 37 | C | -4.3443 | 2.2857 | 2.0894 |
| 38 | H | -3.6918 | 3.1543 | 1.9314 |
| 39 | H | -4.9430 | 2.5020 | 2.9834 |
| 40 | C | -5.2671 | 2.0957 | 0.8813 |
| 41 | H | -5.8964 | 1.2087 | 1.0418 |
| 42 | C | -6.1545 | 3.3178 | 0.6310 |
| 43 | H | -5.5494 | 4.2119 | 0.4409 |
| 44 | H | -6.8039 | 3.1625 | -0.2361 |
| 45 | H | -6.7939 | 3.5250 | 1.4964 |
| 46 | H | -4.6653 | 1.8930 | -0.0147 |

**Isomer_VI**

Energy (FREE) = -1123.053827 Eh

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | C | 1.0558 | 1.4766 | -0.0867 |
| 2 | C | 2.8803 | 2.7512 | -0.2716 |
| 3 | C | 1.9870 | 3.3799 | 0.5570 |
| 4 | H | 3.8524 | 3.0623 | -0.6207 |
| 5 | H | 2.0359 | 4.3523 | 1.0228 |
| 6 | N | 2.2477 | 1.5814 | -0.6694 |
| 7 | N | 0.8614 | 2.5591 | 0.6809 |
| 8 | C | -0.3339 | 2.7297 | 1.5508 |
| 9 | H | 0.0074 | 2.7093 | 2.5901 |
| 10 | H | -0.7714 | 3.7096 | 1.3448 |
| 11 | C | -1.2957 | 1.6077 | 1.2400 |
| 12 | C | -0.9985 | 0.3064 | 1.6879 |
| 13 | C | -2.3294 | 1.8057 | 0.3291 |
| 14 | C | -1.6725 | -0.7997 | 1.1349 |
| 15 | C | -3.0571 | 0.7151 | -0.1756 |
| 16 | H | -2.5492 | 2.8083 | -0.0177 |
| 17 | C | -2.6952 | -0.6047 | 0.1809 |
| 18 | O | -3.3402 | -1.6925 | -0.3097 |
| 19 | O | -1.2621 | -2.0493 | 1.5101 |
| 20 | O | -4.0923 | 0.8225 | -1.0343 |
| 21 | C | -2.2351 | -2.8870 | 2.1714 |
| 22 | H | -3.0701 | -3.1094 | 1.5058 |
| 23 | H | -1.7020 | -3.8006 | 2.4346 |
| 24 | H | -2.5919 | -2.3916 | 3.0811 |
| 25 | C | -3.2523 | -1.9149 | -1.7275 |
| 26 | H | -3.7330 | -2.8773 | -1.9042 |
| 27 | H | -3.7674 | -1.1287 | -2.2820 |
| 28 | H | -2.1998 | -1.9661 | -2.0344 |
| 29 | C | -4.5282 | 2.1229 | -1.4294 |
| 30 | H | -5.3916 | 1.9585 | -2.0732 |
| 31 | H | -4.8266 | 2.7173 | -0.5586 |
| 32 | H | -3.7463 | 2.6481 | -1.9907 |
| 33 | C | 2.4816 | 0.1960 | -1.1521 |
| 34 | H | 2.3201 | 0.1315 | -2.2290 |
| 35 | Pd | 0.6655 | -0.4116 | -0.2172 |
| 36 | C | 3.7278 | -0.4788 | -0.6407 |
| 37 | H | 3.8452 | -0.2782 | 0.4312 |
| 38 | H | 4.6066 | -0.0433 | -1.1439 |
| 39 | C | 3.6995 | -1.9938 | -0.8915 |
| 40 | H | 3.5359 | -2.1828 | -1.9607 |
| 41 | C | 4.9820 | -2.6879 | -0.4293 |
| 42 | H | 5.1512 | -2.5326 | 0.6424 |
| 43 | H | 4.9308 | -3.7659 | -0.6088 |
| 44 | H | 5.8544 | -2.2994 | -0.9670 |
| 45 | H | 2.8362 | -2.4261 | -0.3623 |
| 46 | H | -0.2600 | 0.1277 | 2.4636 |

**Isomer_VII**

Energy (FREE) = -1123.073745 Eh

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | C | 2.1111 | -1.2311 | 0.0189 |
| 2 | C | 3.5534 | -2.9247 | 0.4236 |
| 3 | C | 2.5008 | -3.4437 | -0.2615 |
| 4 | H | 4.4435 | -3.3944 | 0.8123 |
| 5 | H | 2.3040 | -4.4485 | -0.6014 |
| 6 | N | 3.2952 | -1.5692 | 0.5832 |
| 7 | N | 1.6266 | -2.3893 | -0.4939 |
| 8 | C | 0.3906 | -2.4851 | -1.2890 |
| 9 | H | 0.6336 | -2.2518 | -2.3330 |
| 10 | H | 0.0550 | -3.5231 | -1.2471 |
| 11 | C | -0.7024 | -1.5647 | -0.7970 |
| 12 | C | -1.8458 | -2.0521 | -0.2424 |
| 13 | C | -0.5473 | -0.1328 | -0.9529 |
| 14 | C | -2.9228 | -1.1888 | 0.1607 |
| 15 | H | -2.0090 | -3.1155 | -0.1018 |

| | | | | |
|---|---|---|---|---|
| 16 | C | -1.5987 | 0.7235 | -0.4386 |
| 17 | H | -0.1675 | 0.2031 | -1.9298 |
| 18 | C | -2.7992 | 0.2144 | 0.0734 |
| 19 | O | -3.7422 | 1.0371 | 0.6117 |
| 20 | O | -3.9534 | -1.8597 | 0.6548 |
| 21 | O | -1.3822 | 2.0361 | -0.4636 |
| 22 | C | -5.2157 | -1.2578 | 1.0172 |
| 23 | H | -5.6459 | -0.7317 | 0.1621 |
| 24 | H | -5.8445 | -2.1042 | 1.2913 |
| 25 | H | -5.0916 | -0.5766 | 1.8574 |
| 26 | C | -4.3951 | 1.9389 | -0.3007 |
| 27 | H | -5.1101 | 2.4997 | 0.3016 |
| 28 | H | -3.6742 | 2.6226 | -0.7548 |
| 29 | H | -4.9250 | 1.3768 | -1.0793 |
| 30 | C | -0.0078 | 2.3354 | -0.0680 |
| 31 | H | -0.0494 | 2.5853 | 1.0008 |
| 32 | H | 0.3156 | 3.1897 | -0.6636 |
| 33 | C | 4.1332 | -0.6439 | 1.3619 |
| 34 | H | 5.1714 | -0.9688 | 1.2441 |
| 35 | H | 3.8668 | -0.7461 | 2.4189 |
| 36 | Pd | 1.1664 | 0.6212 | -0.0598 |
| 37 | C | 3.9965 | 0.8109 | 0.9125 |
| 38 | H | 4.5290 | 1.4356 | 1.6392 |
| 39 | H | 2.9341 | 1.1350 | 1.0330 |
| 40 | C | 4.5035 | 1.0990 | -0.5051 |
| 41 | H | 4.1903 | 0.2965 | -1.1827 |
| 42 | C | 4.0014 | 2.4397 | -1.0423 |
| 43 | H | 4.2696 | 3.2680 | -0.3767 |
| 44 | H | 4.4163 | 2.6525 | -2.0319 |
| 45 | H | 2.9048 | 2.4285 | -1.1381 |
| 46 | H | 5.6004 | 1.0863 | -0.4893 |

TS1

Energy (FREE) = -1352.131342 Eh

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | C | -2.0151 | -1.2716 | -0.2172 |
| 2 | C | -3.9229 | -2.4120 | -0.5431 |
| 3 | C | -2.9141 | -3.3203 | -0.4565 |
| 4 | N | -1.7433 | -2.5956 | -0.2583 |
| 5 | N | -3.3489 | -1.1570 | -0.3954 |
| 6 | C | -0.4048 | -3.1837 | -0.0973 |
| 7 | H | -0.3967 | -3.7836 | 0.8169 |
| 8 | H | -0.2443 | -3.8619 | -0.9443 |
| 9 | C | 0.6975 | -2.1506 | -0.0442 |
| 10 | C | 0.7668 | -1.1153 | -1.0434 |
| 11 | C | 1.6554 | -2.2239 | 0.9318 |
| 12 | C | 1.9211 | -0.2770 | -1.0646 |
| 13 | H | 0.2147 | -1.2518 | -1.9680 |
| 14 | C | 2.7665 | -1.3319 | 0.9458 |
| 15 | H | 1.6050 | -2.9576 | 1.7286 |
| 16 | C | 2.9096 | -0.3633 | -0.0627 |
| 17 | O | 3.9453 | 0.5258 | -0.0579 |
| 18 | O | 2.1365 | 0.6501 | -2.0020 |
| 19 | O | 3.5766 | -1.5271 | 1.9876 |
| 20 | C | 1.1363 | 0.9005 | -2.9890 |
| 21 | H | 0.1839 | 1.1571 | -2.5107 |
| 22 | H | 1.5045 | 1.7464 | -3.5682 |
| 23 | H | 1.0038 | 0.0347 | -3.6473 |
| 24 | C | 4.9651 | 0.2986 | -1.0444 |
| 25 | H | 4.5591 | 0.3853 | -2.0554 |
| 26 | H | 5.7146 | 1.0738 | -0.8806 |
| 27 | H | 5.4202 | -0.6904 | -0.9086 |
| 28 | C | 4.7131 | -0.6970 | 2.2923 |
| 29 | H | 5.0652 | -1.0691 | 3.2545 |
| 30 | H | 5.4956 | -0.8173 | 1.5401 |
| 31 | H | 4.4238 | 0.3510 | 2.3679 |
| 32 | C | -4.0216 | 0.1475 | -0.5223 |
| 33 | H | -3.5584 | 0.6664 | -1.3669 |
| 34 | H | -5.0645 | -0.0516 | -0.7778 |
| 35 | C | -3.9229 | 1.0063 | 0.7418 |
| 36 | H | -4.3207 | 1.9935 | 0.4770 |
| 37 | H | -4.5864 | 0.5942 | 1.5145 |
| 38 | C | -2.5130 | 1.1616 | 1.3232 |
| 39 | H | -2.2507 | 0.2388 | 1.8504 |
| 40 | H | -1.8396 | 1.9660 | 0.3655 |
| 41 | C | -2.4009 | 2.2725 | 2.3829 |
| 42 | H | -3.0544 | 2.0357 | 3.2324 |
| 43 | H | -1.3758 | 2.3451 | 2.7587 |
| 44 | H | -2.6890 | 3.2482 | 1.9838 |
| 45 | Pd | -0.7625 | 0.2328 | 0.0310 |
| 46 | C | -0.1040 | 3.0097 | -0.0775 |
| 47 | O | -1.3746 | 3.0800 | -0.1756 |
| 48 | O | 0.5147 | 1.9278 | 0.1728 |
| 49 | C | 0.6987 | 4.2738 | -0.2420 |
| 50 | H | 1.7419 | 4.0393 | -0.4570 |
| 51 | H | 0.2664 | 4.8944 | -1.0302 |
| 52 | H | 0.6473 | 4.8434 | 0.6932 |
| 53 | H | -4.9813 | -2.5452 | -0.7032 |
| 54 | H | -2.9234 | -4.3976 | -0.5113 |

TS2

Energy (FREE) = -1352.128685 Eh

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | C | -1.9183 | 1.3911 | -0.1062 |
| 2 | C | -3.6891 | 2.7236 | 0.2616 |
| 3 | C | -2.7223 | 3.4771 | -0.3322 |
| 4 | N | -1.6343 | 2.6367 | -0.5442 |
| 5 | N | -3.1716 | 1.4437 | 0.3894 |
| 6 | C | -0.3343 | 3.0155 | -1.1155 |
| 7 | H | -0.4367 | 3.0951 | -2.2038 |
| 8 | H | -0.0737 | 4.0021 | -0.7257 |
| 9 | C | 0.7345 | 2.0066 | -0.7562 |
| 10 | C | 1.7230 | 2.3184 | 0.1505 |
| 11 | C | 0.7033 | 0.7153 | -1.3705 |
| 12 | C | 2.7331 | 1.3678 | 0.4364 |
| 13 | H | 1.7201 | 3.2776 | 0.6523 |
| 14 | C | 1.8150 | -0.1779 | -1.1920 |
| 15 | H | 0.1410 | 0.5811 | -2.2926 |
| 16 | C | 2.7961 | 0.1255 | -0.2340 |
| 17 | O | 3.7870 | -0.7635 | 0.0613 |
| 18 | O | 3.6987 | 1.5677 | 1.3430 |
| 19 | O | 1.7890 | -1.2244 | -2.0084 |
| 20 | C | 3.7382 | 2.7928 | 2.0817 |
| 21 | H | 2.8208 | 2.9253 | 2.6648 |
| 22 | H | 4.5895 | 2.6963 | 2.7543 |
| 23 | H | 3.8899 | 3.6479 | 1.4144 |
| 24 | C | 5.1082 | -0.4110 | -0.3839 |
| 25 | H | 5.4565 | 0.5025 | 0.1032 |
| 26 | H | 5.7482 | -1.2472 | -0.1001 |
| 27 | H | 5.1252 | -0.2851 | -1.4733 |
| 28 | C | 2.5853 | -2.4104 | -1.8137 |
| 29 | H | 2.1544 | -3.1371 | -2.5024 |
| 30 | H | 3.6278 | -2.2213 | -2.0766 |
| 31 | H | 2.4996 | -2.7571 | -0.7872 |
| 32 | C | -3.7230 | 0.2877 | 1.1009 |
| 33 | H | -3.5686 | 0.4442 | 2.1732 |
| 34 | H | -4.8026 | 0.2555 | 0.9132 |
| 35 | C | -3.0689 | -1.0191 | 0.6453 |
| 36 | H | -3.4283 | -1.7646 | 1.3716 |
| 37 | H | -1.8985 | -1.5016 | 1.2149 |
| 38 | C | -3.5191 | -1.5144 | -0.7377 |

| | | | | |
|---|---|---|---|---|
| 39 | H | -4.6105 | -1.6518 | -0.6991 |
| 40 | H | -3.3345 | -0.7520 | -1.5035 |
| 41 | C | -2.8647 | -2.8355 | -1.1540 |
| 42 | H | -3.0144 | -3.6064 | -0.3895 |
| 43 | H | -3.2976 | -3.2012 | -2.0900 |
| 44 | H | -1.7862 | -2.7170 | -1.3031 |
| 45 | Pd | -0.8743 | -0.2638 | -0.0361 |
| 46 | C | -0.1300 | -2.7202 | 1.2443 |
| 47 | O | -1.1811 | -2.4636 | 1.9003 |
| 48 | O | 0.2577 | -2.0298 | 0.2427 |
| 49 | C | 0.7186 | -3.9041 | 1.6388 |
| 50 | H | 0.3286 | -4.3777 | 2.5396 |
| 51 | H | 0.7286 | -4.6279 | 0.8171 |
| 52 | H | 1.7493 | -3.5749 | 1.8027 |
| 53 | H | -4.6793 | 2.9859 | 0.5994 |
| 54 | H | -2.7128 | 4.5165 | -0.6207 |

TS3

Energy (FREE) = -1352.140239 Eh

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | C | -1.5707 | -1.5218 | 0.1287 |
| 2 | C | -2.5434 | -3.5450 | -0.0055 |
| 3 | C | -1.5925 | -3.6141 | 0.9655 |
| 4 | N | -1.0092 | -2.3579 | 1.0309 |
| 5 | N | -2.5134 | -2.2502 | -0.5110 |
| 6 | C | 0.0786 | -1.9106 | 1.9170 |
| 7 | H | -0.3422 | -1.2435 | 2.6768 |
| 8 | H | 0.4915 | -2.7911 | 2.4119 |
| 9 | C | 1.1143 | -1.2015 | 1.0796 |
| 10 | C | 2.3330 | -1.7913 | 0.8487 |
| 11 | C | 0.7689 | 0.0547 | 0.4803 |
| 12 | C | 3.2472 | -1.1939 | -0.0538 |
| 13 | H | 2.5832 | -2.7316 | 1.3243 |
| 14 | C | 1.6763 | 0.5937 | -0.5083 |
| 15 | H | 0.6304 | 0.9694 | 1.2684 |
| 16 | C | 2.9274 | 0.0019 | -0.7346 |
| 17 | O | 3.7557 | 0.4942 | -1.6996 |
| 18 | O | 4.4328 | -1.7278 | -0.3635 |
| 19 | O | 1.2332 | 1.6888 | -1.1236 |
| 20 | C | 4.8402 | -2.9642 | 0.2339 |
| 21 | H | 4.1532 | -3.7718 | -0.0388 |
| 22 | H | 5.8281 | -3.1695 | -0.1761 |
| 23 | H | 4.9031 | -2.8697 | 1.3229 |
| 24 | C | 5.0260 | 1.0117 | -1.2652 |
| 25 | H | 5.6577 | 0.2170 | -0.8645 |
| 26 | H | 5.4877 | 1.4397 | -2.1556 |
| 27 | H | 4.8850 | 1.7933 | -0.5094 |
| 28 | C | 2.1068 | 2.7255 | -1.6096 |
| 29 | H | 1.4513 | 3.5844 | -1.7551 |
| 30 | H | 2.8657 | 2.9629 | -0.8594 |
| 31 | H | 2.5748 | 2.4335 | -2.5485 |
| 32 | C | -3.3678 | -1.7334 | -1.5917 |
| 33 | H | -2.7104 | -1.3073 | -2.3561 |
| 34 | H | -3.8710 | -2.5975 | -2.0308 |
| 35 | C | -4.3974 | -0.6960 | -1.1288 |
| 36 | H | -5.0692 | -0.5197 | -1.9781 |
| 37 | H | -5.0110 | -1.1181 | -0.3238 |
| 38 | C | -3.8074 | 0.6506 | -0.6942 |
| 39 | H | -3.2792 | 0.5053 | 0.2818 |
| 40 | H | -3.1017 | 1.0055 | -1.4597 |
| 41 | C | -4.8442 | 1.7459 | -0.4309 |
| 42 | H | -5.5578 | 1.4362 | 0.3398 |
| 43 | H | -4.3501 | 2.6622 | -0.0962 |
| 44 | H | -5.4036 | 1.9711 | -1.3450 |
| 45 | Pd | -1.2585 | 0.4330 | 0.1120 |
| 46 | C | -0.3551 | 2.9882 | 1.2267 |
| 47 | O | -1.1639 | 2.4820 | 0.3686 |
| 48 | O | 0.5239 | 2.3500 | 1.8591 |
| 49 | C | -0.5138 | 4.4742 | 1.4795 |
| 50 | H | -1.4447 | 4.6444 | 2.0313 |
| 51 | H | 0.3245 | 4.8557 | 2.0631 |
| 52 | H | -0.5950 | 5.0071 | 0.5281 |
| 53 | H | -3.2206 | -4.2933 | -0.3862 |
| 54 | H | -1.2869 | -4.4297 | 1.6016 |

TS4

Energy (FREE) = -1352.127956 Eh

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | C | -2.5418 | -0.8024 | -0.1016 |
| 2 | C | -4.5560 | -1.5749 | -0.7353 |
| 3 | C | -3.8090 | -2.6485 | -0.3630 |
| 4 | N | -2.5677 | -2.1517 | 0.0189 |
| 5 | N | -3.7542 | -0.4522 | -0.5815 |
| 6 | C | -1.4387 | -2.9581 | 0.4964 |
| 7 | H | -1.6351 | -3.2773 | 1.5242 |
| 8 | H | -1.3958 | -3.8571 | -0.1300 |
| 9 | C | -0.1203 | -2.2191 | 0.4269 |
| 10 | C | 0.1686 | -1.3640 | -0.6953 |
| 11 | C | 0.8180 | -2.3989 | 1.4097 |
| 12 | C | 1.4910 | -0.8380 | -0.8181 |
| 13 | H | -0.4131 | -1.4893 | -1.6027 |
| 14 | C | 2.1122 | -1.8144 | 1.3083 |
| 15 | H | 0.6116 | -2.9870 | 2.2972 |
| 16 | C | 2.4579 | -1.0432 | 0.1821 |
| 17 | O | 3.6749 | -0.4333 | 0.0821 |
| 18 | O | 1.8848 | -0.0929 | -1.8562 |
| 19 | O | 2.8818 | -2.0676 | 2.3670 |
| 20 | C | 0.9352 | 0.2786 | -2.8567 |
| 21 | H | 0.0859 | 0.8027 | -2.4028 |
| 22 | H | 1.4702 | 0.9462 | -3.5310 |
| 23 | H | 0.5818 | -0.5972 | -3.4120 |
| 24 | C | 4.5815 | -1.0061 | -0.8742 |
| 25 | H | 4.1835 | -0.9253 | -1.8889 |
| 26 | H | 5.5032 | -0.4286 | -0.7928 |
| 27 | H | 4.7818 | -2.0578 | -0.6348 |
| 28 | C | 4.1944 | -1.5092 | 2.5661 |
| 29 | H | 4.4731 | -1.8350 | 3.5683 |
| 30 | H | 4.9022 | -1.9089 | 1.8368 |
| 31 | H | 4.1700 | -0.4213 | 2.5083 |
| 32 | C | -4.1414 | 0.9428 | -0.8354 |
| 33 | H | -3.2776 | 1.4300 | -1.2919 |
| 34 | H | -4.9475 | 0.9322 | -1.5725 |
| 35 | C | -4.5696 | 1.6650 | 0.4472 |
| 36 | H | -4.6408 | 2.7334 | 0.2091 |
| 37 | H | -5.5766 | 1.3368 | 0.7305 |
| 38 | C | -3.6292 | 1.4427 | 1.6390 |
| 39 | H | -4.0403 | 2.0015 | 2.4899 |
| 40 | H | -3.6666 | 0.3883 | 1.9331 |
| 41 | C | -2.1747 | 1.8765 | 1.4449 |
| 42 | H | -2.1236 | 2.9742 | 1.4980 |
| 43 | H | -1.5180 | 2.2576 | 0.2468 |
| 44 | H | -1.5478 | 1.5481 | 2.2809 |
| 45 | Pd | -0.9681 | 0.3500 | 0.2309 |
| 46 | C | 0.4771 | 2.7286 | -0.1588 |
| 47 | O | 0.7267 | 1.5937 | 0.3640 |
| 48 | O | -0.7032 | 3.1001 | -0.4614 |
| 49 | C | 1.6341 | 3.6618 | -0.4008 |

| | | | | |
|---|---|---|---|---|
| 50 | H | 1.8532 | 4.1977 | 0.5301 |
| 51 | H | 2.5213 | 3.0876 | -0.6762 |
| 52 | H | 1.3839 | 4.3937 | -1.1701 |
| 53 | H | -5.5677 | -1.5109 | -1.1040 |
| 54 | H | -4.0422 | -3.7014 | -0.3396 |

**TS5**

Energy (FREE) = -1352.105572 Eh

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | C | -1.5460 | 0.9689 | -0.5164 |
| 2 | C | -3.4853 | 1.9055 | -1.0935 |
| 3 | C | -2.5153 | 2.4547 | -1.8798 |
| 4 | N | -1.3211 | 1.8461 | -1.5213 |
| 5 | N | -2.8667 | 0.9743 | -0.2647 |
| 6 | C | 0.0275 | 2.0084 | -2.0129 |
| 7 | H | 0.1663 | 2.8787 | -2.6479 |
| 8 | H | 0.6316 | 2.3521 | -0.7141 |
| 9 | C | 0.6798 | 0.7645 | -2.3563 |
| 10 | C | 2.0222 | 0.7449 | -2.7566 |
| 11 | C | 0.0145 | -0.5131 | -2.0648 |
| 12 | C | 2.7086 | -0.4647 | -2.8306 |
| 13 | H | 2.5397 | 1.6811 | -2.9231 |
| 14 | C | 0.7374 | -1.7604 | -2.2475 |
| 15 | H | -1.0311 | -0.5849 | -2.3562 |
| 16 | C | 2.0826 | -1.7411 | -2.5656 |
| 17 | O | 2.8362 | -2.8781 | -2.5786 |
| 18 | O | 4.0089 | -0.5621 | -3.1157 |
| 19 | O | -0.0472 | -2.8314 | -2.0349 |
| 20 | C | 4.7687 | 0.6233 | -3.3821 |
| 21 | H | 4.7716 | 1.2825 | -2.5081 |
| 22 | H | 5.7804 | 0.2769 | -3.5882 |
| 23 | H | 4.3691 | 1.1518 | -4.2534 |
| 24 | C | 3.3297 | -3.3220 | -3.8547 |
| 25 | H | 4.0470 | -2.6112 | -4.2690 |
| 26 | H | 3.8216 | -4.2763 | -3.6635 |
| 27 | H | 2.5002 | -3.4678 | -4.5572 |
| 28 | C | 0.3760 | -4.1742 | -2.3244 |
| 29 | H | -0.5046 | -4.7856 | -2.1257 |
| 30 | H | 0.6608 | -4.2708 | -3.3757 |
| 31 | H | 1.2042 | -4.4749 | -1.6832 |
| 32 | C | -3.5385 | 0.0979 | 0.7065 |
| 33 | H | -2.7609 | -0.2425 | 1.3952 |
| 34 | H | -4.2470 | 0.7103 | 1.2708 |
| 35 | C | -4.2327 | -1.0923 | 0.0380 |
| 36 | H | -4.6648 | -1.7015 | 0.8419 |
| 37 | H | -5.0767 | -0.7358 | -0.5670 |
| 38 | C | -3.2971 | -1.9457 | -0.8244 |
| 39 | H | -2.9688 | -1.3563 | -1.6897 |
| 40 | H | -2.3861 | -2.1849 | -0.2586 |
| 41 | C | -3.9533 | -3.2362 | -1.3173 |
| 42 | H | -4.8528 | -3.0247 | -1.9068 |
| 43 | H | -3.2637 | -3.8038 | -1.9508 |
| 44 | H | -4.2471 | -3.8774 | -0.4787 |
| 45 | Pd | -0.0283 | -0.1514 | 0.0406 |
| 46 | C | 0.8748 | 2.2032 | 1.5000 |
| 47 | O | 0.4272 | 1.0521 | 1.7561 |
| 48 | O | 0.9662 | 2.7777 | 0.3498 |
| 49 | C | 1.3799 | 3.0386 | 2.6546 |
| 50 | H | 1.2321 | 2.5187 | 3.6008 |
| 51 | H | 2.4439 | 3.2489 | 2.5063 |
| 52 | H | 0.8573 | 3.9997 | 2.6628 |
| 53 | H | -4.5410 | 2.1161 | -1.0231 |
| 54 | H | -2.5681 | 3.2129 | -2.6446 |

**TS5d**

Energy (FREE) = -1352.088958 Eh

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | C | 2.0635 | 0.9328 | -0.9169 |
| 2 | C | 1.9343 | 2.9646 | -1.8373 |
| 3 | C | 0.7402 | 2.3510 | -2.0658 |
| 4 | N | 0.8527 | 1.0932 | -1.4819 |
| 5 | N | 2.7393 | 2.0755 | -1.1192 |
| 6 | C | -0.0883 | -0.0136 | -1.3588 |
| 7 | H | -0.1368 | -0.5899 | -2.2848 |
| 8 | H | 0.2357 | -1.1337 | -0.5773 |
| 9 | C | -1.3848 | 0.3231 | -0.7865 |
| 10 | C | -2.4876 | -0.5069 | -1.0729 |
| 11 | C | -1.5355 | 1.3892 | 0.1190 |
| 12 | C | -3.7323 | -0.2562 | -0.5164 |
| 13 | H | -2.3408 | -1.3686 | -1.7102 |
| 14 | C | -2.7739 | 1.6739 | 0.6656 |
| 15 | H | -0.6993 | 2.0203 | 0.3964 |
| 16 | C | -3.9100 | 0.8784 | 0.3330 |
| 17 | O | -5.0564 | 1.2752 | 0.8889 |
| 18 | O | -4.8251 | -1.0302 | -0.7221 |
| 19 | O | -2.8958 | 2.7730 | 1.4538 |
| 20 | C | -4.6807 | -2.2085 | -1.5131 |
| 21 | H | -3.9355 | -2.8833 | -1.0763 |
| 22 | H | -5.6602 | -2.6860 | -1.5093 |
| 23 | H | -4.3975 | -1.9585 | -2.5424 |
| 24 | C | -6.3622 | 0.8670 | 0.4366 |
| 25 | H | -6.5724 | -0.1601 | 0.7346 |
| 26 | H | -7.0454 | 1.5577 | 0.9307 |
| 27 | H | -6.4419 | 0.9662 | -0.6474 |
| 28 | C | -3.2741 | 2.5608 | 2.8250 |
| 29 | H | -3.2251 | 3.5430 | 3.2960 |
| 30 | H | -4.2868 | 2.1606 | 2.9019 |
| 31 | H | -2.5639 | 1.8824 | 3.3127 |
| 32 | C | 4.1334 | 2.3241 | -0.7127 |
| 33 | H | 4.7946 | 1.8331 | -1.4353 |
| 34 | H | 4.2845 | 3.4019 | -0.8053 |
| 35 | C | 4.4642 | 1.8771 | 0.7183 |
| 36 | H | 5.3662 | 2.4300 | 1.0100 |
| 37 | H | 3.6681 | 2.2071 | 1.3966 |
| 38 | C | 4.7634 | 0.3885 | 0.9299 |
| 39 | H | 3.8435 | -0.2294 | 0.7387 |
| 40 | H | 5.4924 | 0.0391 | 0.1888 |
| 41 | C | 5.2290 | 0.0670 | 2.3481 |
| 42 | H | 4.4842 | 0.3784 | 3.0885 |
| 43 | H | 5.4036 | -1.0057 | 2.4706 |
| 44 | H | 6.1661 | 0.5901 | 2.5712 |
| 45 | Pd | 2.0869 | -0.7981 | -0.0029 |
| 46 | C | 0.6078 | -3.0990 | 0.5541 |
| 47 | O | 1.7714 | -2.6537 | 0.8450 |
| 48 | O | -0.2385 | -2.4644 | -0.1408 |
| 49 | C | 0.2593 | -4.4788 | 1.0589 |
| 50 | H | -0.8199 | -4.6347 | 1.0361 |
| 51 | H | 0.7397 | -5.2199 | 0.4097 |
| 52 | H | 0.6496 | -4.6209 | 2.0691 |
| 53 | H | 2.2868 | 3.9432 | -2.1234 |
| 54 | H | -0.1520 | 2.6935 | -2.5642 |

**TS6**

Energy (FREE) = -1352.109143 Eh

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | C | -0.2936 | 2.1687 | 0.7680 |
| 2 | C | -1.3682 | 3.7743 | 1.8673 |
| 3 | C | -0.3215 | 4.3455 | 1.1938 |
| 4 | N | 0.3417 | 3.3177 | 0.5159 |
| 5 | N | -1.3145 | 2.4129 | 1.5814 |
| 6 | C | 1.5398 | 3.3262 | -0.3428 |
| 7 | H | 1.2554 | 3.6643 | -1.3454 |
| 8 | H | 2.2571 | 4.0385 | 0.0701 |

| | | | | |
|---|---|---|---|---|
| 9 | C | 2.1385 | 1.9287 | -0.3838 |
| 10 | C | 3.3091 | 1.6647 | 0.2849 |
| 11 | C | 1.4463 | 0.8638 | -1.0648 |
| 12 | C | 3.8548 | 0.3541 | 0.2740 |
| 13 | H | 3.8071 | 2.4505 | 0.8388 |
| 14 | C | 2.0754 | -0.4260 | -1.1780 |
| 15 | H | 0.7550 | 1.1161 | -1.8680 |
| 16 | C | 3.2510 | -0.6929 | -0.4527 |
| 17 | O | 3.8013 | -1.9388 | -0.4496 |
| 18 | O | 4.9679 | 0.0146 | 0.9339 |
| 19 | O | 1.4634 | -1.2496 | -2.0207 |
| 20 | C | 5.6753 | 0.9967 | 1.6991 |
| 21 | H | 5.0425 | 1.3980 | 2.4975 |
| 22 | H | 6.5214 | 0.4665 | 2.1342 |
| 23 | H | 6.0374 | 1.8068 | 1.0573 |
| 24 | C | 5.0231 | -2.0904 | -1.1947 |
| 25 | H | 5.8231 | -1.4845 | -0.7628 |
| 26 | H | 5.2817 | -3.1474 | -1.1243 |
| 27 | H | 4.8679 | -1.8154 | -2.2448 |
| 28 | C | 1.6200 | -2.6859 | -1.9858 |
| 29 | H | 0.7791 | -3.0586 | -2.5699 |
| 30 | H | 2.5617 | -2.9801 | -2.4517 |
| 31 | H | 1.5604 | -3.0458 | -0.9614 |
| 32 | C | -2.0822 | 1.1907 | 1.9315 |
| 33 | H | -1.6934 | -0.1966 | 1.7408 |
| 34 | H | -2.0984 | 1.0966 | 3.0214 |
| 35 | C | -3.4700 | 1.1726 | 1.3087 |
| 36 | H | -3.9815 | 0.2772 | 1.6796 |
| 37 | H | -4.0471 | 2.0367 | 1.6741 |
| 38 | C | -3.4639 | 1.1679 | -0.2224 |
| 39 | H | -2.9784 | 2.0808 | -0.5924 |
| 40 | H | -2.8425 | 0.3254 | -0.5643 |
| 41 | C | -4.8679 | 1.0519 | -0.8199 |
| 42 | H | -5.4992 | 1.8935 | -0.5124 |
| 43 | H | -4.8319 | 1.0433 | -1.9138 |
| 44 | H | -5.3588 | 0.1289 | -0.4918 |
| 45 | Pd | -0.1767 | 0.3063 | 0.3962 |
| 46 | C | -1.2201 | -2.2244 | 1.0999 |
| 47 | O | -1.9087 | -1.4798 | 1.8757 |
| 48 | O | -0.3447 | -1.7920 | 0.2855 |
| 49 | C | -1.4564 | -3.7108 | 1.1792 |
| 50 | H | -2.5301 | -3.9152 | 1.1924 |
| 51 | H | -0.9795 | -4.2256 | 0.3446 |
| 52 | H | -1.0399 | -4.0851 | 2.1210 |
| 53 | H | -2.1128 | 4.2172 | 2.5100 |
| 54 | H | 0.0006 | 5.3736 | 1.1396 |

**TS7**

Energy (FREE) = -1352.115368 Eh

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | C | -1.2988 | -1.4434 | -0.6424 |
| 2 | C | -2.8262 | -2.9389 | 0.0732 |
| 3 | C | -1.6788 | -3.6245 | -0.1629 |
| 4 | N | -0.7515 | -2.6921 | -0.5972 |
| 5 | N | -2.5775 | -1.6087 | -0.2245 |
| 6 | C | 0.6512 | -2.9994 | -0.9076 |
| 7 | H | 0.8587 | -4.0002 | -0.5248 |
| 8 | H | 0.7819 | -3.0118 | -1.9949 |
| 9 | C | 1.5440 | -1.9667 | -0.2705 |
| 10 | C | 2.1813 | -2.1777 | 0.9203 |
| 11 | C | 1.6226 | -0.6915 | -0.9282 |
| 12 | C | 2.9521 | -1.1301 | 1.5063 |
| 13 | H | 2.0887 | -3.1260 | 1.4352 |
| 14 | C | 2.3789 | 0.3688 | -0.2957 |
| 15 | H | 1.7618 | -0.7574 | -2.0134 |
| 16 | C | 3.0368 | 0.1619 | 0.9179 |
| 17 | O | 3.7903 | 1.0669 | 1.5712 |
| 18 | O | 3.6054 | -1.2602 | 2.6519 |
| 19 | O | 2.4357 | 1.5629 | -0.8851 |
| 20 | C | 3.6043 | -2.5113 | 3.3533 |
| 21 | H | 4.0348 | -3.3033 | 2.7328 |
| 22 | H | 4.2301 | -2.3462 | 4.2289 |
| 23 | H | 2.5902 | -2.7788 | 3.6672 |
| 24 | C | 3.3314 | 2.4275 | 1.6692 |
| 25 | H | 2.2618 | 2.4569 | 1.9042 |
| 26 | H | 3.9015 | 2.8590 | 2.4924 |
| 27 | H | 3.5236 | 2.9758 | 0.7463 |
| 28 | C | 1.3267 | 1.8658 | -1.7893 |
| 29 | H | 1.4613 | 2.9316 | -1.9998 |
| 30 | H | 1.4823 | 1.3708 | -2.7549 |
| 31 | H | 0.1054 | 2.3312 | -1.2090 |
| 32 | C | -3.5685 | -0.5408 | -0.0030 |
| 33 | H | -3.6295 | 0.0527 | -0.9131 |
| 34 | H | -4.5280 | -1.0400 | 0.1548 |
| 35 | C | -3.2059 | 0.3405 | 1.1917 |
| 36 | H | -3.1121 | -0.2789 | 2.0932 |
| 37 | H | -2.2215 | 0.7892 | 1.0121 |
| 38 | C | -4.2456 | 1.4441 | 1.4130 |
| 39 | H | -4.4373 | 1.9539 | 0.4598 |
| 40 | H | -5.1997 | 0.9925 | 1.7147 |
| 41 | C | -3.7971 | 2.4667 | 2.4594 |
| 42 | H | -2.8725 | 2.9673 | 2.1463 |
| 43 | H | -4.5604 | 3.2356 | 2.6147 |
| 44 | H | -3.6050 | 1.9872 | 3.4261 |
| 45 | Pd | -0.2916 | 0.2272 | -1.1925 |
| 46 | C | -1.9320 | 2.5928 | -1.3916 |
| 47 | O | -2.0435 | 1.3537 | -1.6579 |
| 48 | O | -0.8525 | 3.1233 | -0.9726 |
| 49 | C | -3.1283 | 3.4865 | -1.5887 |
| 50 | H | -2.8787 | 4.2586 | -2.3233 |
| 51 | H | -3.9932 | 2.9174 | -1.9295 |
| 52 | H | -3.3573 | 3.9955 | -0.6474 |
| 53 | H | -3.7917 | -3.2726 | 0.4188 |
| 54 | H | -1.4442 | -4.6731 | -0.0715 |

[Isomer I+$CH_3CO_2H$]$^+$

Energy (FREE) = -1352.179772 Eh

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | C | 2.2384 | -1.5025 | -0.5002 |
| 2 | C | 3.8006 | -3.1134 | -0.6963 |
| 3 | C | 2.5965 | -3.7307 | -0.5839 |
| 4 | N | 1.6457 | -2.7254 | -0.4655 |
| 5 | N | 3.5583 | -1.7470 | -0.6453 |
| 6 | C | 0.2182 | -2.9755 | -0.2049 |
| 7 | H | -0.0969 | -3.7753 | -0.8835 |
| 8 | H | 0.1221 | -3.3505 | 0.8185 |
| 9 | C | -0.6648 | -1.7598 | -0.3899 |
| 10 | C | -1.5054 | -1.3553 | 0.6585 |
| 11 | C | -0.7174 | -1.0971 | -1.6263 |
| 12 | C | -2.4110 | -0.3090 | 0.4521 |
| 13 | H | -1.4495 | -1.8584 | 1.6156 |
| 14 | C | -1.6390 | -0.0483 | -1.8429 |
| 15 | H | -0.1270 | -1.4305 | -2.4732 |
| 16 | C | -2.4969 | 0.3376 | -0.8030 |
| 17 | O | -3.3646 | 1.3855 | -0.9595 |
| 18 | O | -3.2393 | 0.1874 | 1.3996 |
| 19 | O | -1.6208 | 0.4911 | -3.0779 |
| 20 | C | -3.1836 | -0.3678 | 2.7123 |
| 21 | H | -2.1898 | -0.2264 | 3.1516 |
| 22 | H | -3.9226 | 0.1821 | 3.2948 |
| 23 | H | -3.4435 | -1.4324 | 2.7029 |
| 24 | C | -4.7434 | 1.0081 | -1.1274 |
| 25 | H | -5.1093 | 0.4779 | -0.2441 |

| | | | | |
|---|---|---|---|---|
| 26 | H | -5.2950 | 1.9404 | -1.2552 |
| 27 | H | -4.8598 | 0.3821 | -2.0191 |
| 28 | C | -1.8710 | 1.8953 | -3.2684 |
| 29 | H | -1.4225 | 2.1305 | -4.2347 |
| 30 | H | -2.9401 | 2.1109 | -3.2905 |
| 31 | H | -1.3897 | 2.4782 | -2.4794 |
| 32 | C | 4.6170 | -0.7245 | -0.6407 |
| 33 | H | 5.0853 | -0.7359 | 0.3490 |
| 34 | H | 5.3712 | -1.0325 | -1.3696 |
| 35 | C | 4.0963 | 0.6690 | -0.9791 |
| 36 | H | 4.9634 | 1.3437 | -0.9043 |
| 37 | H | 3.7689 | 0.6963 | -2.0240 |
| 38 | C | 2.9911 | 1.1973 | -0.0709 |
| 39 | H | 2.6912 | 2.1918 | -0.4190 |
| 40 | C | 3.3429 | 1.2336 | 1.4101 |
| 41 | H | 4.2626 | 1.8184 | 1.5664 |
| 42 | H | 2.5559 | 1.7140 | 1.9997 |
| 43 | H | 3.5117 | 0.2357 | 1.8277 |
| 44 | Pd | 1.2331 | 0.1926 | -0.4368 |
| 45 | C | -0.4988 | 2.2658 | 0.8635 |
| 46 | O | -0.2710 | 1.5350 | 1.9521 |
| 47 | O | 0.0649 | 2.0345 | -0.2130 |
| 48 | C | -1.5230 | 3.3366 | 1.0368 |
| 49 | H | -1.5872 | 3.6593 | 2.0768 |
| 50 | H | -1.2969 | 4.1757 | 0.3772 |
| 51 | H | -2.4862 | 2.9070 | 0.7324 |
| 52 | H | 4.7942 | -3.5158 | -0.8174 |
| 53 | H | 2.3330 | -4.7769 | -0.5854 |
| 54 | H | 0.3547 | 0.8126 | 1.7035 |

[Isomer II+$CH_3CO_2H$]$^+$
Energy (FREE) = -1352.171850 Eh

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | C | -2.1836 | 1.1103 | -0.1721 |
| 2 | C | -4.0414 | 2.2486 | 0.3842 |
| 3 | C | -3.1920 | 3.1120 | -0.2426 |
| 4 | N | -2.0468 | 2.3923 | -0.5725 |
| 5 | N | -3.3974 | 1.0216 | 0.4122 |
| 6 | C | -0.8349 | 2.9133 | -1.2367 |
| 7 | H | -1.0162 | 2.9478 | -2.3154 |
| 8 | H | -0.6828 | 3.9355 | -0.8823 |
| 9 | C | 0.3640 | 2.0458 | -0.9168 |
| 10 | C | 1.1733 | 2.3330 | 0.1827 |
| 11 | C | 0.6056 | 0.8992 | -1.6885 |
| 12 | C | 2.2207 | 1.4617 | 0.5130 |
| 13 | H | 0.9690 | 3.2060 | 0.7897 |
| 14 | C | 1.6972 | 0.0440 | -1.3982 |
| 15 | H | 0.0543 | 0.7115 | -2.6045 |
| 16 | C | 2.4913 | 0.3111 | -0.2673 |
| 17 | O | 3.4629 | -0.5704 | 0.1298 |
| 18 | O | 3.0219 | 1.6162 | 1.5898 |
| 19 | O | 1.8248 | -0.9739 | -2.2674 |
| 20 | C | 2.8138 | 2.7379 | 2.4454 |
| 21 | H | 1.8127 | 2.7114 | 2.8917 |
| 22 | H | 3.5649 | 2.6511 | 3.2301 |
| 23 | H | 2.9543 | 3.6805 | 1.9039 |
| 24 | C | 4.8217 | -0.1164 | -0.0017 |
| 25 | H | 5.0111 | 0.7379 | 0.6510 |
| 26 | H | 5.4473 | -0.9590 | 0.2962 |
| 27 | H | 5.0349 | 0.1515 | -1.0432 |
| 28 | C | 2.8331 | -1.9865 | -2.1689 |
| 29 | H | 2.6524 | -2.6320 | -3.0290 |
| 30 | H | 3.8358 | -1.5577 | -2.2382 |
| 31 | H | 2.7297 | -2.5567 | -1.2459 |
| 32 | C | -3.7089 | -0.2405 | 1.0860 |
| 33 | H | -3.5745 | -0.0981 | 2.1629 |
| 34 | H | -4.7572 | -0.5011 | 0.9017 |
| 35 | C | -2.7527 | -1.3214 | 0.5346 |
| 36 | H | -2.4340 | -1.9920 | 1.3384 |
| 37 | H | 0.0131 | -0.6349 | 1.9120 |
| 38 | C | -3.3630 | -2.1090 | -0.6242 |
| 39 | H | -4.2421 | -2.6409 | -0.2249 |
| 40 | H | -3.7466 | -1.4117 | -1.3799 |
| 41 | C | -2.4250 | -3.1250 | -1.2817 |
| 42 | H | -1.9824 | -3.7961 | -0.5374 |
| 43 | H | -2.9701 | -3.7352 | -2.0083 |
| 44 | H | -1.6019 | -2.6297 | -1.8092 |
| 45 | Pd | -1.0103 | -0.4425 | -0.1790 |
| 46 | C | 0.9037 | -2.1779 | 1.3072 |
| 47 | O | 0.6794 | -1.2787 | 2.2578 |
| 48 | O | 0.3154 | -2.1547 | 0.2193 |
| 49 | C | 1.9527 | -3.1844 | 1.6516 |
| 50 | H | 2.9244 | -2.7075 | 1.4789 |
| 51 | H | 1.8916 | -3.4660 | 2.7050 |
| 52 | H | 1.8572 | -4.0588 | 1.0074 |
| 53 | H | -5.0242 | 2.4056 | 0.8001 |
| 54 | H | -3.3030 | 4.1573 | -0.4855 |

[Isomer III+$CH_3CO_2H$]$^+$
Energy (FREE) = -1352.163909 Eh

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | C | 1.5663 | -1.6764 | 0.1049 |
| 2 | C | 2.5679 | -3.6565 | 0.4496 |
| 3 | C | 1.5812 | -3.8490 | -0.4675 |
| 4 | N | 0.9784 | -2.6164 | -0.6621 |
| 5 | N | 2.5425 | -2.3102 | 0.7943 |
| 6 | C | -0.1401 | -2.2996 | -1.5629 |
| 7 | H | 0.2708 | -1.8119 | -2.4540 |
| 8 | H | -0.5932 | -3.2432 | -1.8714 |
| 9 | C | -1.1464 | -1.4209 | -0.8543 |
| 10 | C | -2.5029 | -1.7527 | -0.9025 |
| 11 | C | -0.7221 | -0.3084 | -0.1246 |
| 12 | C | -3.4355 | -1.0029 | -0.1793 |
| 13 | H | -2.8225 | -2.6145 | -1.4755 |
| 14 | C | -1.6475 | 0.4224 | 0.6510 |
| 15 | H | -0.8241 | 1.4110 | -1.3545 |
| 16 | C | -3.0137 | 0.0901 | 0.6131 |
| 17 | O | -3.8860 | 0.7497 | 1.4291 |
| 18 | O | -4.7596 | -1.2789 | -0.1296 |
| 19 | O | -1.1174 | 1.4041 | 1.4292 |
| 20 | C | -5.2504 | -2.4067 | -0.8480 |
| 21 | H | -4.7919 | -3.3346 | -0.4861 |
| 22 | H | -6.3232 | -2.4327 | -0.6572 |
| 23 | H | -5.0714 | -2.3001 | -1.9247 |
| 24 | C | -4.9459 | 1.4824 | 0.7944 |
| 25 | H | -5.6365 | 0.8113 | 0.2817 |
| 26 | H | -5.4628 | 2.0079 | 1.5985 |
| 27 | H | -4.5367 | 2.2102 | 0.0822 |
| 28 | C | -1.8448 | 2.6094 | 1.6997 |
| 29 | H | -1.0869 | 3.3315 | 2.0108 |
| 30 | H | -2.3485 | 2.9704 | 0.7958 |
| 31 | H | -2.5754 | 2.4632 | 2.4944 |
| 32 | C | 3.4217 | -1.6675 | 1.7831 |
| 33 | H | 2.7834 | -1.1365 | 2.4961 |
| 34 | H | 3.9212 | -2.4747 | 2.3230 |
| 35 | C | 4.4581 | -0.7175 | 1.1719 |
| 36 | H | 5.1623 | -0.4618 | 1.9734 |
| 37 | H | 5.0348 | -1.2475 | 0.4042 |
| 38 | C | 3.8878 | 0.5851 | 0.5985 |
| 39 | H | 3.2895 | 0.3476 | -0.3112 |
| 40 | H | 3.2379 | 1.0608 | 1.3472 |
| 41 | C | 4.9587 | 1.5865 | 0.1560 |
| 42 | H | 5.6117 | 1.1531 | -0.6090 |

| | | | | |
|---|---|---|---|---|
| 43 | H | 4.4975 | 2.4878 | -0.2585 |
| 44 | H | 5.5818 | 1.8836 | 1.0061 |
| 45 | Pd | 1.2055 | 0.2482 | 0.0037 |
| 46 | C | 0.2238 | 2.9643 | -1.0540 |
| 47 | O | 1.0486 | 2.3760 | -0.3454 |
| 48 | O | -0.8030 | 2.3623 | -1.6287 |
| 49 | C | 0.2985 | 4.4351 | -1.3257 |
| 50 | H | 0.2484 | 4.6176 | -2.4033 |
| 51 | H | -0.5668 | 4.9300 | -0.8713 |
| 52 | H | 1.2184 | 4.8463 | -0.9111 |
| 53 | H | 3.2647 | -4.3483 | 0.8958 |
| 54 | H | 1.2574 | -4.7387 | -0.9839 |

Isomer_IV+AcOH
Energy (FREE) = -1352.171906 Eh

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | C | 2.2312 | -0.9996 | 0.2130 |
| 2 | C | 4.1272 | -2.0250 | 0.8755 |
| 3 | C | 3.1291 | -2.9454 | 0.9287 |
| 4 | N | 1.9698 | -2.2972 | 0.5222 |
| 5 | N | 3.5544 | -0.8379 | 0.4431 |
| 6 | C | 0.6609 | -2.9570 | 0.3862 |
| 7 | H | 0.6715 | -3.5660 | -0.5222 |
| 8 | H | 0.5566 | -3.6333 | 1.2418 |
| 9 | C | -0.4980 | -1.9863 | 0.3361 |
| 10 | C | -0.6424 | -0.9869 | 1.3330 |
| 11 | C | -1.4447 | -2.1045 | -0.6698 |
| 12 | C | -1.7757 | -0.1573 | 1.3059 |
| 13 | H | 0.0470 | -0.9523 | 2.1669 |
| 14 | C | -2.5718 | -1.2575 | -0.7095 |
| 15 | H | -1.3403 | -2.8388 | -1.4609 |
| 16 | C | -2.7475 | -0.2903 | 0.2912 |
| 17 | O | -3.8125 | 0.5731 | 0.2732 |
| 18 | O | -2.0155 | 0.8347 | 2.1955 |
| 19 | O | -3.4108 | -1.4699 | -1.7414 |
| 20 | C | -1.1082 | 1.0104 | 3.2803 |
| 21 | H | -0.1003 | 1.2429 | 2.9161 |
| 22 | H | -1.4917 | 1.8549 | 3.8518 |
| 23 | H | -1.0747 | 0.1179 | 3.9152 |
| 24 | C | -4.8736 | 0.2271 | 1.1808 |
| 25 | H | -4.5198 | 0.2489 | 2.2156 |
| 26 | H | -5.6487 | 0.9817 | 1.0394 |
| 27 | H | -5.2730 | -0.7648 | 0.9411 |
| 28 | C | -4.1656 | -0.3909 | -2.3165 |
| 29 | H | -4.4282 | -0.7357 | -3.3176 |
| 30 | H | -5.0716 | -0.1858 | -1.7437 |
| 31 | H | -3.5565 | 0.5148 | -2.3790 |
| 32 | C | 4.2580 | 0.4314 | 0.2365 |
| 33 | H | 3.6164 | 1.2143 | 0.6456 |
| 34 | H | 5.1726 | 0.4013 | 0.8334 |
| 35 | C | 4.5686 | 0.7019 | -1.2369 |
| 36 | H | 4.9595 | 1.7258 | -1.2918 |
| 37 | H | 5.3750 | 0.0395 | -1.5724 |
| 38 | C | 3.3643 | 0.5521 | -2.1797 |
| 39 | H | 3.6531 | 0.9828 | -3.1497 |
| 40 | H | 3.1705 | -0.5078 | -2.3783 |
| 41 | C | 2.0840 | 1.2383 | -1.7241 |
| 42 | H | 2.2739 | 2.2363 | -1.3098 |
| 43 | H | 0.6330 | 2.4027 | 0.7490 |
| 44 | H | 1.3672 | 1.3276 | -2.5471 |
| 45 | Pd | 0.8472 | 0.2824 | -0.3822 |
| 46 | C | -0.9639 | 2.6580 | -0.2074 |
| 47 | O | -0.7426 | 1.6735 | -0.9233 |
| 48 | O | -0.1224 | 3.0388 | 0.7476 |
| 49 | C | -2.2085 | 3.4736 | -0.3228 |
| 50 | H | -2.4165 | 3.6722 | -1.3770 |
| 51 | H | -3.0265 | 2.8594 | 0.0717 |
| 52 | H | -2.1326 | 4.4045 | 0.2390 |
| 53 | H | 5.1753 | -2.1019 | 1.1185 |
| 54 | H | 3.1368 | -3.9842 | 1.2192 |

**[Isomer_V+CH3CO2H]+**
Energy (FREE) = -1352.134747 Eh

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | C | -1.5703 | -0.4049 | 1.0989 |
| 2 | C | -3.2914 | -0.0667 | 2.5203 |
| 3 | C | -2.2036 | -0.3614 | 3.2790 |
| 4 | N | -1.1335 | -0.5313 | 2.4055 |
| 5 | N | -2.8818 | -0.0815 | 1.1949 |
| 6 | C | 0.2015 | -0.7653 | 2.7664 |
| 7 | H | 0.3580 | -1.4380 | 3.6008 |
| 8 | H | -1.5671 | -2.3636 | -0.2576 |
| 9 | C | 1.2046 | -0.2715 | 1.9796 |
| 10 | C | 2.5472 | -0.7665 | 2.0613 |
| 11 | C | 0.8682 | 0.7237 | 0.9373 |
| 12 | C | 3.4705 | -0.3979 | 1.1206 |
| 13 | H | 2.7766 | -1.5208 | 2.8029 |
| 14 | C | 1.9285 | 1.1798 | 0.0490 |
| 15 | H | 0.2289 | 1.5408 | 1.2755 |
| 16 | C | 3.1731 | 0.5888 | 0.0800 |
| 17 | O | 4.1022 | 0.8910 | -0.8617 |
| 18 | O | 4.7112 | -0.9108 | 1.0198 |
| 19 | O | 1.5138 | 2.1855 | -0.7663 |
| 20 | C | 5.1206 | -1.8966 | 1.9673 |
| 21 | H | 4.4785 | -2.7824 | 1.9063 |
| 22 | H | 6.1416 | -2.1611 | 1.6940 |
| 23 | H | 5.1002 | -1.4914 | 2.9853 |
| 24 | C | 5.3412 | 1.4942 | -0.4412 |
| 25 | H | 5.9391 | 0.7979 | 0.1463 |
| 26 | H | 5.8626 | 1.7546 | -1.3627 |
| 27 | H | 5.1410 | 2.4027 | 0.1389 |
| 28 | C | 2.4506 | 3.0929 | -1.3641 |
| 29 | H | 1.8411 | 3.9117 | -1.7481 |
| 30 | H | 3.1466 | 3.4764 | -0.6102 |
| 31 | H | 3.0041 | 2.6179 | -2.1743 |
| 32 | C | -3.7353 | 0.2655 | 0.0510 |
| 33 | H | -3.2255 | -0.1062 | -0.8403 |
| 34 | H | -4.6801 | -0.2750 | 0.1614 |
| 35 | C | -3.9649 | 1.7760 | -0.0579 |
| 36 | H | -4.6178 | 1.9404 | -0.9244 |
| 37 | H | -4.5234 | 2.1268 | 0.8201 |
| 38 | C | -2.6752 | 2.5884 | -0.2148 |
| 39 | H | -2.0563 | 2.4673 | 0.6837 |
| 40 | H | -2.0855 | 2.1795 | -1.0474 |
| 41 | C | -2.9465 | 4.0759 | -0.4501 |
| 42 | H | -3.5129 | 4.5111 | 0.3814 |
| 43 | H | -2.0107 | 4.6355 | -0.5468 |
| 44 | H | -3.5271 | 4.2316 | -1.3664 |
| 45 | Pd | -0.3050 | -0.2281 | -0.4739 |
| 46 | C | -1.7917 | -2.3633 | -2.1298 |
| 47 | O | -1.2380 | -1.2672 | -2.2554 |
| 48 | O | -1.9583 | -2.9500 | -0.9487 |
| 49 | C | -2.3371 | -3.1512 | -3.2811 |
| 50 | H | -2.2401 | -2.5782 | -4.2026 |
| 51 | H | -1.7842 | -4.0928 | -3.3681 |
| 52 | H | -3.3850 | -3.4063 | -3.0961 |
| 53 | H | -4.3157 | 0.1230 | 2.8017 |

| | | | | |
|---|---|---|---|---|
| 54 | H | -2.0845 | -0.4373 | 4.3481 |

**[Isomer_Vd+CH3CO2H]+**

Energy (FREE) = -1352.139417 Eh

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | C | -2.4208 | -0.2242 | -0.6666 |
| 2 | C | -2.5574 | -2.4448 | -0.4055 |
| 3 | C | -1.5018 | -2.2181 | -1.2388 |
| 4 | H | -2.9905 | -3.3710 | -0.0611 |
| 5 | H | -0.8298 | -2.8953 | -1.7411 |
| 6 | N | -3.1077 | -1.2067 | -0.0564 |
| 7 | N | -1.4652 | -0.8394 | -1.3914 |
| 8 | C | -0.5576 | 0.2026 | -1.8518 |
| 9 | H | -0.6867 | 0.4493 | -2.9049 |
| 10 | C | 0.8181 | 0.1897 | -1.3571 |
| 11 | C | 1.8136 | 0.7949 | -2.1245 |
| 12 | C | 1.1225 | -0.3109 | -0.0714 |
| 13 | C | 3.1242 | 0.9158 | -1.6390 |
| 14 | H | 1.6010 | 1.1861 | -3.1138 |
| 15 | C | 2.4185 | -0.1906 | 0.4221 |
| 16 | H | 0.3435 | -0.7688 | 0.5234 |
| 17 | C | 3.4390 | 0.4290 | -0.3540 |
| 18 | O | 4.6712 | 0.6612 | 0.1643 |
| 19 | O | 3.9765 | 1.5677 | -2.4579 |
| 20 | O | 2.7976 | -0.5884 | 1.6590 |
| 21 | C | 5.3857 | 1.2957 | -2.4467 |
| 22 | H | 5.5738 | 0.2174 | -2.4084 |
| 23 | H | 5.7556 | 1.6941 | -3.3926 |
| 24 | H | 5.8793 | 1.7887 | -1.6090 |
| 25 | C | 5.4775 | -0.4729 | 0.5325 |
| 26 | H | 6.4459 | -0.0599 | 0.8161 |
| 27 | H | 5.0388 | -1.0133 | 1.3721 |
| 28 | H | 5.6001 | -1.1447 | -0.3252 |
| 29 | C | 1.8121 | -1.1418 | 2.5249 |
| 30 | H | 2.3312 | -1.3701 | 3.4554 |
| 31 | H | 1.0091 | -0.4202 | 2.7204 |
| 32 | H | 1.3859 | -2.0613 | 2.1059 |
| 33 | C | -4.1423 | -1.0075 | 0.9660 |
| 34 | H | -4.9496 | -1.7196 | 0.7734 |
| 35 | H | -4.5366 | 0.0002 | 0.8160 |
| 36 | Pd | -1.6904 | 1.6350 | -0.8067 |
| 37 | C | -3.5773 | -1.1780 | 2.3805 |
| 38 | H | -3.2103 | -2.2062 | 2.5009 |
| 39 | H | -4.4108 | -1.0638 | 3.0845 |
| 40 | C | -2.4627 | -0.1854 | 2.7293 |
| 41 | H | -2.8443 | 0.8396 | 2.6226 |
| 42 | C | -1.9136 | -0.3914 | 4.1432 |
| 43 | H | -1.4975 | -1.3990 | 4.2625 |
| 44 | H | -1.1212 | 0.3302 | 4.3694 |
| 45 | H | -2.6996 | -0.2672 | 4.8961 |
| 46 | H | -1.6449 | -0.2812 | 2.0023 |
| 47 | C | 0.4585 | 3.8065 | -0.5448 |
| 48 | O | -0.6224 | 3.4853 | -1.0550 |
| 49 | O | 1.1833 | 2.9969 | 0.2104 |
| 50 | H | 0.7956 | 2.0941 | 0.2291 |
| 51 | C | 1.0763 | 5.1538 | -0.7465 |
| 52 | H | 1.9529 | 5.0436 | -1.3956 |
| 53 | H | 0.3585 | 5.8288 | -1.2115 |
| 54 | H | 1.4251 | 5.5553 | 0.2089 |

**[Isomer_VI+CH3CO2H]+**

Energy (FREE) = -1352.144364 Eh

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | C | 1.1500 | 1.8654 | 0.1060 |
| 2 | C | 3.1089 | 2.9688 | 0.0383 |
| 3 | C | 2.1815 | 3.7647 | 0.6532 |
| 4 | H | 4.1476 | 3.1456 | -0.1918 |
| 5 | H | 2.2684 | 4.7692 | 1.0374 |
| 6 | N | 2.4199 | 1.8116 | -0.2983 |
| 7 | N | 0.9721 | 3.0620 | 0.6958 |
| 8 | C | -0.3133 | 3.5041 | 1.2947 |
| 9 | H | -0.1657 | 3.6177 | 2.3728 |
| 10 | H | -0.5702 | 4.4791 | 0.8720 |
| 11 | C | -1.3394 | 2.4514 | 0.9662 |
| 12 | C | -1.3221 | 1.2555 | 1.6858 |
| 13 | C | -2.0624 | 2.5349 | -0.2278 |
| 14 | C | -1.9414 | 0.1236 | 1.1487 |
| 15 | C | -2.7333 | 1.4211 | -0.7448 |
| 16 | H | -2.0639 | 3.4674 | -0.7796 |
| 17 | C | -2.6279 | 0.1728 | -0.0801 |
| 18 | O | -3.2082 | -0.9771 | -0.4965 |
| 19 | O | -1.8585 | -1.0772 | 1.8330 |
| 20 | O | -3.4890 | 1.4301 | -1.8661 |
| 21 | C | -3.0748 | -1.4651 | 2.5209 |
| 22 | H | -3.8868 | -1.6040 | 1.8038 |
| 23 | H | -2.8445 | -2.4042 | 3.0245 |
| 24 | H | -3.3336 | -0.6981 | 3.2563 |
| 25 | C | -3.0972 | -1.3596 | -1.8804 |
| 26 | H | -3.2732 | -2.4362 | -1.8922 |
| 27 | H | -3.8399 | -0.8451 | -2.4893 |
| 28 | H | -2.0911 | -1.1411 | -2.2542 |
| 29 | C | -3.5978 | 2.6450 | -2.6057 |
| 30 | H | -4.2570 | 2.4203 | -3.4438 |
| 31 | H | -4.0399 | 3.4390 | -1.9932 |
| 32 | H | -2.6192 | 2.9656 | -2.9825 |
| 33 | C | 2.5779 | 0.4188 | -0.7693 |
| 34 | H | 2.6275 | 0.3750 | -1.8589 |
| 35 | Pd | 0.5764 | 0.0206 | -0.2452 |
| 36 | C | 3.6413 | -0.3763 | -0.0530 |
| 37 | H | 3.4763 | -0.3267 | 1.0301 |
| 38 | H | 4.6119 | 0.1151 | -0.2413 |
| 39 | C | 3.7259 | -1.8352 | -0.5161 |
| 40 | H | 3.8651 | -1.8595 | -1.6053 |
| 41 | C | 4.8640 | -2.5935 | 0.1706 |
| 42 | H | 4.7305 | -2.6068 | 1.2588 |
| 43 | H | 4.9088 | -3.6317 | -0.1732 |
| 44 | H | 5.8348 | -2.1305 | -0.0405 |
| 45 | H | 2.7693 | -2.3300 | -0.3172 |
| 46 | H | -0.7660 | 1.1542 | 2.6117 |
| 47 | C | -0.2275 | -3.0849 | -0.5665 |
| 48 | O | 0.3314 | -2.0260 | -0.8845 |
| 49 | O | -1.1304 | -3.2011 | 0.3786 |
| 50 | H | -1.3407 | -2.3370 | 0.8360 |
| 51 | C | 0.1066 | -4.3793 | -1.2491 |
| 52 | H | -0.7989 | -4.9642 | -1.4276 |
| 53 | H | 0.6354 | -4.1853 | -2.1822 |
| 54 | H | 0.7533 | -4.9680 | -0.5875 |

**[Isomer_VII+CH3CO2H]+**

Energy (FREE) = -1352.141031 Eh

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | C | -1.2193 | 1.4989 | -0.6151 |
| 2 | C | -2.5013 | 3.3368 | -0.2447 |
| 3 | C | -1.2411 | 3.7718 | -0.4902 |
| 4 | H | -3.4055 | 3.8797 | -0.0190 |
| 5 | H | -0.8301 | 4.7683 | -0.5347 |
| 6 | N | -2.4677 | 1.9533 | -0.3278 |
| 7 | N | -0.4717 | 2.6387 | -0.7085 |
| 8 | C | 0.9290 | 2.7286 | -1.1457 |
| 9 | H | 0.9414 | 2.8333 | -2.2382 |
| 10 | H | 1.3421 | 3.6452 | -0.7197 |
| 11 | C | 1.7686 | 1.5470 | -0.7430 |
| 12 | C | 2.7923 | 1.6695 | 0.1498 |
| 13 | C | 1.5027 | 0.2716 | -1.3570 |

| | | | | |
|---|---|---|---|---|
| 14 | C | 3.6585 | 0.5691 | 0.4532 |
| 15 | H | 3.0155 | 2.6093 | 0.6435 |
| 16 | C | 2.3372 | -0.8439 | -0.9741 |
| 17 | H | 1.2601 | 0.2873 | -2.4286 |
| 18 | C | 3.4255 | -0.7082 | -0.1049 |
| 19 | O | 4.1400 | -1.7947 | 0.3060 |
| 20 | O | 4.6084 | 0.8861 | 1.3241 |
| 21 | O | 2.0155 | -2.0449 | -1.4655 |
| 22 | C | 5.6992 | 0.0129 | 1.6861 |
| 23 | H | 6.2543 | -0.2941 | 0.7968 |
| 24 | H | 6.3310 | 0.6273 | 2.3268 |
| 25 | H | 5.3345 | -0.8611 | 2.2236 |
| 26 | C | 4.9065 | -2.4696 | -0.7076 |
| 27 | H | 5.4053 | -3.2953 | -0.1992 |
| 28 | H | 4.2554 | -2.8563 | -1.4950 |
| 29 | H | 5.6549 | -1.7918 | -1.1363 |
| 30 | C | 0.5743 | -2.2435 | -1.3601 |
| 31 | H | 0.4249 | -2.8903 | -0.4893 |
| 32 | H | 0.2384 | -2.7352 | -2.2748 |
| 33 | C | -3.6503 | 1.1208 | -0.0803 |
| 34 | H | -3.3792 | 0.1027 | -0.3513 |
| 35 | H | -4.4382 | 1.4507 | -0.7651 |
| 36 | Pd | -0.4295 | -0.4641 | -0.9636 |
| 37 | C | -4.1283 | 1.2084 | 1.3731 |
| 38 | H | -5.0055 | 0.5553 | 1.4688 |
| 39 | H | -4.4864 | 2.2252 | 1.5821 |
| 40 | C | -3.0700 | 0.8214 | 2.4106 |
| 41 | H | -2.1951 | 1.4747 | 2.2982 |
| 42 | C | -3.5988 | 0.9128 | 3.8442 |
| 43 | H | -4.4575 | 0.2479 | 3.9933 |
| 44 | H | -2.8284 | 0.6325 | 4.5696 |
| 45 | H | -3.9249 | 1.9324 | 4.0796 |
| 46 | H | -2.7164 | -0.1989 | 2.2154 |
| 47 | C | -2.3103 | -2.3778 | 0.4717 |
| 48 | C | -3.4241 | -3.3267 | 0.7839 |
| 49 | H | -4.0324 | -3.4929 | -0.1046 |
| 50 | H | -3.0187 | -4.2720 | 1.1558 |
| 51 | H | -4.0426 | -2.8999 | 1.5818 |
| 52 | O | -2.2399 | -1.7349 | -0.5808 |
| 53 | O | -1.4094 | -2.2629 | 1.4416 |
| 54 | H | -0.7399 | -1.5951 | 1.1607 |

## Stationary points for Isomerization

**TS1_Iso**

Energy (FREE) = -1123.021313 Eh

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | C | -2.1936 | -1.0552 | -0.2607 |
| 2 | C | -4.1154 | -1.0180 | 0.9548 |
| 3 | C | -3.2490 | -1.8554 | 1.5831 |
| 4 | N | -2.0791 | -1.8552 | 0.8274 |
| 5 | N | -3.4482 | -0.5362 | -0.1679 |
| 6 | C | -0.8082 | -2.4868 | 1.2216 |
| 7 | H | -0.8688 | -2.6736 | 2.2989 |
| 8 | H | -0.7106 | -3.4541 | 0.7206 |
| 9 | C | 0.3840 | -1.6079 | 0.8884 |
| 10 | C | 1.4569 | -2.1323 | 0.1841 |
| 11 | C | 0.3790 | -0.2382 | 1.2353 |
| 12 | C | 2.5246 | -1.3000 | -0.2064 |
| 13 | H | 1.4399 | -3.1700 | -0.1239 |
| 14 | C | 1.4713 | 0.5956 | 0.8918 |
| 15 | H | -0.3604 | 0.1627 | 1.9209 |
| 16 | C | 2.5399 | 0.0737 | 0.1307 |
| 17 | O | 3.5000 | 0.9185 | -0.3398 |
| 18 | O | 3.5581 | -1.7171 | -0.9638 |
| 19 | O | 1.3678 | 1.8792 | 1.3168 |
| 20 | C | 3.6039 | -3.0790 | -1.3921 |
| 21 | H | 2.7377 | -3.3215 | -2.0177 |
| 22 | H | 4.5164 | -3.1678 | -1.9808 |
| 23 | H | 3.6504 | -3.7600 | -0.5350 |
| 24 | C | 4.8592 | 0.6739 | 0.0647 |
| 25 | H | 5.2401 | -0.2476 | -0.3768 |
| 26 | H | 5.4304 | 1.5286 | -0.2992 |
| 27 | H | 4.9292 | 0.6216 | 1.1578 |
| 28 | C | 2.5403 | 2.6547 | 1.6204 |
| 29 | H | 2.1800 | 3.4752 | 2.2426 |
| 30 | H | 3.2607 | 2.0572 | 2.1875 |
| 31 | H | 3.0063 | 3.0387 | 0.7132 |
| 32 | C | -3.9045 | 0.5330 | -1.0626 |
| 33 | H | -4.1316 | 0.1133 | -2.0470 |
| 34 | H | -4.8289 | 0.9455 | -0.6497 |
| 35 | C | -2.8551 | 1.6467 | -1.2135 |
| 36 | C | -2.1770 | 2.1879 | -0.1039 |
| 37 | H | -2.3341 | 1.7231 | 0.8680 |
| 38 | H | -1.8504 | 0.8674 | -1.8959 |
| 39 | C | -1.4480 | 3.4926 | -0.1177 |
| 40 | H | -2.0409 | 4.2556 | 0.4086 |
| 41 | H | -0.4944 | 3.4060 | 0.4151 |
| 42 | H | -1.2611 | 3.8477 | -1.1354 |
| 43 | Pd | -0.7039 | 0.3648 | -0.8461 |
| 44 | H | -5.1303 | -0.7411 | 1.1953 |
| 45 | H | -3.3638 | -2.4451 | 2.4795 |
| 46 | H | -3.0241 | 2.3132 | -2.0616 |

**TS1d_Iso**

Energy (FREE) = -1123.015658 Eh

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | C | -2.0181 | -0.8534 | 0.0219 |
| 2 | C | -3.9877 | -1.2315 | -1.0257 |
| 3 | C | -3.1524 | -2.2599 | -1.3285 |
| 4 | N | -1.9440 | -1.9970 | -0.6840 |
| 5 | N | -3.2715 | -0.3648 | -0.1994 |
| 6 | C | -0.6646 | -2.7042 | -0.8951 |
| 7 | H | -0.6118 | -3.5747 | -0.2362 |
| 8 | H | -0.6733 | -3.0643 | -1.9297 |
| 9 | C | 0.5200 | -1.7906 | -0.6445 |
| 10 | C | 0.6218 | -0.5275 | -1.3169 |
| 11 | C | 1.4670 | -2.1453 | 0.2797 |
| 12 | C | 1.7475 | 0.2893 | -1.0664 |
| 13 | H | -0.0084 | -0.3304 | -2.1772 |
| 14 | C | 2.5703 | -1.2967 | 0.5834 |
| 15 | H | 1.3937 | -3.0703 | 0.8412 |
| 16 | C | 2.7125 | -0.0732 | -0.0816 |
| 17 | O | 3.7217 | 0.7994 | 0.2155 |
| 18 | O | 2.0217 | 1.4278 | -1.7286 |
| 19 | O | 3.3625 | -1.7950 | 1.5439 |
| 20 | C | 1.0916 | 1.9154 | -2.6906 |
| 21 | H | 0.1248 | 2.1208 | -2.2115 |
| 22 | H | 1.5215 | 2.8411 | -3.0714 |
| 23 | H | 0.9595 | 1.2040 | -3.5137 |
| 24 | C | 4.7869 | 0.8761 | -0.7471 |
| 25 | H | 4.4193 | 1.2369 | -1.7105 |
| 26 | H | 5.5070 | 1.5851 | -0.3367 |
| 27 | H | 5.2631 | -0.1040 | -0.8727 |
| 28 | C | 4.5037 | -1.1023 | 2.0735 |
| 29 | H | 4.8589 | -1.7443 | 2.8801 |
| 30 | H | 5.2855 | -0.9980 | 1.3172 |
| 31 | H | 4.2279 | -0.1209 | 2.4604 |
| 32 | C | -3.6165 | 1.0589 | 0.0084 |
| 33 | H | -3.7949 | 1.5003 | -0.9762 |
| 34 | H | -4.5501 | 1.1255 | 0.5803 |
| 35 | C | -2.5451 | 1.8651 | 0.7433 |
| 36 | C | -1.9498 | 1.2887 | 1.9140 |

| | | | | |
|---|---|---|---|---|
| 37 | H | -2.3890 | 0.3731 | 2.2996 |
| 38 | H | -2.7416 | 2.9359 | 0.7271 |
| 39 | C | -1.1624 | 2.1113 | 2.8913 |
| 40 | H | -0.3987 | 1.5063 | 3.3904 |
| 41 | H | -0.6786 | 2.9662 | 2.4088 |
| 42 | H | -1.8328 | 2.4933 | 3.6748 |
| 43 | Pd | -0.6830 | 0.7098 | 0.3143 |
| 44 | H | -5.0084 | -1.0449 | -1.3223 |
| 45 | H | -3.3126 | -3.1449 | -1.9252 |
| 46 | H | -1.1645 | 2.3046 | -0.0918 |

**Int1**

Energy (FREE) = -1123.061432 Eh

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | C | -1.8345 | -0.7543 | -0.1726 |
| 2 | C | -3.8904 | -1.2837 | 0.5536 |
| 3 | C | -3.0028 | -1.9135 | 1.3658 |
| 4 | N | -1.7361 | -1.5746 | 0.9079 |
| 5 | N | -3.1552 | -0.5833 | -0.3931 |
| 6 | C | -0.4794 | -2.0961 | 1.4746 |
| 7 | H | -0.5752 | -2.0476 | 2.5641 |
| 8 | H | -0.3845 | -3.1478 | 1.1902 |
| 9 | C | 0.7365 | -1.3216 | 1.0075 |
| 10 | C | 1.7690 | -1.9868 | 0.3339 |
| 11 | C | 0.8396 | 0.0587 | 1.2685 |
| 12 | C | 2.8829 | -1.2653 | -0.1134 |
| 13 | H | 1.6753 | -3.0432 | 0.1191 |
| 14 | C | 1.9890 | 0.7870 | 0.8654 |
| 15 | H | 0.1152 | 0.5733 | 1.8907 |
| 16 | C | 3.0003 | 0.1336 | 0.1331 |
| 17 | O | 4.0249 | 0.8545 | -0.3934 |
| 18 | O | 3.8847 | -1.7987 | -0.8353 |
| 19 | O | 1.9616 | 2.0912 | 1.1952 |
| 20 | C | 3.8320 | -3.1853 | -1.1779 |
| 21 | H | 2.9491 | -3.4012 | -1.7900 |
| 22 | H | 4.7350 | -3.3765 | -1.7564 |
| 23 | H | 3.8292 | -3.8114 | -0.2788 |
| 24 | C | 5.3617 | 0.5471 | 0.0478 |
| 25 | H | 5.6806 | -0.4291 | -0.3185 |
| 26 | H | 5.9928 | 1.3308 | -0.3721 |
| 27 | H | 5.4165 | 0.5746 | 1.1423 |
| 28 | C | 3.1594 | 2.8804 | 1.2993 |
| 29 | H | 2.8477 | 3.7842 | 1.8236 |
| 30 | H | 3.9164 | 2.3568 | 1.8912 |
| 31 | H | 3.5575 | 3.1281 | 0.3158 |
| 32 | C | -3.7433 | 0.3347 | -1.3733 |
| 33 | H | -3.1537 | 0.2515 | -2.2915 |
| 34 | H | -4.7459 | -0.0437 | -1.6012 |
| 35 | C | -3.7951 | 1.7607 | -0.8949 |
| 36 | C | -3.3630 | 2.2133 | 0.2833 |
| 37 | H | -2.9371 | 1.5121 | 1.0010 |
| 38 | H | -1.0557 | 0.1770 | -2.2560 |
| 39 | C | -3.4210 | 3.6467 | 0.7204 |
| 40 | H | -4.0138 | 3.7534 | 1.6377 |
| 41 | H | -2.4164 | 4.0261 | 0.9467 |
| 42 | H | -3.8625 | 4.2868 | -0.0491 |
| 43 | Pd | -0.2402 | 0.0500 | -0.9429 |
| 44 | H | -4.9686 | -1.2618 | 0.5637 |
| 45 | H | -3.1530 | -2.5690 | 2.2092 |
| 46 | H | -4.2302 | 2.4504 | -1.6168 |

**Int2**

Energy (FREE) = -1123.069056 Eh

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | C | 2.1564 | -0.8262 | 0.0985 |
| 2 | C | 4.1285 | -1.8098 | -0.3644 |
| 3 | C | 3.2030 | -2.7944 | -0.1779 |
| 4 | N | 1.9961 | -2.1595 | 0.1020 |
| 5 | N | 3.4543 | -0.6064 | -0.1934 |
| 6 | C | 0.6988 | -2.7835 | 0.4209 |
| 7 | H | 0.5398 | -3.6111 | -0.2740 |
| 8 | H | 0.7599 | -3.1995 | 1.4334 |
| 9 | C | -0.4467 | -1.7953 | 0.3168 |
| 10 | C | -0.5740 | -0.7157 | 1.2709 |
| 11 | C | -1.3693 | -1.9310 | -0.6814 |
| 12 | C | -1.7667 | 0.0682 | 1.2360 |
| 13 | H | -0.0587 | -0.8203 | 2.2231 |
| 14 | C | -2.4977 | -1.0611 | -0.7816 |
| 15 | H | -1.2821 | -2.7034 | -1.4380 |
| 16 | C | -2.7084 | -0.0706 | 0.1832 |
| 17 | O | -3.7704 | 0.7864 | 0.1184 |
| 18 | O | -2.1107 | 0.9424 | 2.1841 |
| 19 | O | -3.2571 | -1.3204 | -1.8511 |
| 20 | C | -1.2135 | 1.2128 | 3.2606 |
| 21 | H | -0.2667 | 1.6020 | 2.8657 |
| 22 | H | -1.7081 | 1.9696 | 3.8680 |
| 23 | H | -1.0341 | 0.3144 | 3.8616 |
| 24 | C | -4.8471 | 0.5164 | 1.0317 |
| 25 | H | -4.5140 | 0.6086 | 2.0682 |
| 26 | H | -5.6101 | 1.2667 | 0.8210 |
| 27 | H | -5.2566 | -0.4868 | 0.8594 |
| 28 | C | -4.3848 | -0.5181 | -2.2445 |
| 29 | H | -4.6749 | -0.9201 | -3.2155 |
| 30 | H | -5.2097 | -0.6308 | -1.5375 |
| 31 | H | -4.1089 | 0.5329 | -2.3313 |
| 32 | C | 3.9662 | 0.7669 | -0.1757 |
| 33 | H | 4.5640 | 0.9076 | 0.7291 |
| 34 | H | 4.6257 | 0.9118 | -1.0385 |
| 35 | C | 2.8307 | 1.7991 | -0.2032 |
| 36 | C | 1.9582 | 1.9526 | -1.2689 |
| 37 | H | 1.9910 | 1.2016 | -2.0596 |
| 38 | H | 2.9564 | 2.6346 | 0.4820 |
| 39 | C | 1.2377 | 3.2250 | -1.6105 |
| 40 | H | 0.2165 | 3.0296 | -1.9463 |
| 41 | H | 1.2021 | 3.9119 | -0.7621 |
| 42 | H | 1.7705 | 3.7115 | -2.4400 |
| 43 | Pd | 0.9066 | 0.7724 | 0.3897 |
| 44 | H | 5.1784 | -1.8686 | -0.6058 |
| 45 | H | 3.2989 | -3.8679 | -0.2299 |
| 46 | H | -0.0065 | 2.0665 | 0.6255 |

**TS2_Iso**

Energy (FREE) = -1123.060490 Eh

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | C | -1.8667 | -1.0721 | -0.5435 |
| 2 | C | -3.8443 | -1.9820 | -1.1223 |
| 3 | C | -2.8513 | -2.7309 | -1.6846 |
| 4 | N | -1.6412 | -2.1483 | -1.3117 |
| 5 | N | -3.2124 | -0.9592 | -0.4271 |
| 6 | C | -0.2733 | -2.6454 | -1.5796 |
| 7 | H | -0.1592 | -3.6044 | -1.0628 |
| 8 | H | -0.1774 | -2.8229 | -2.6535 |
| 9 | C | 0.7631 | -1.6441 | -1.1109 |
| 10 | C | 1.4519 | -0.8810 | -2.0351 |
| 11 | C | 0.9672 | -1.4256 | 0.2800 |
| 12 | C | 2.3759 | 0.0966 | -1.6035 |
| 13 | H | 1.2649 | -1.0186 | -3.0928 |
| 14 | C | 1.9501 | -0.4971 | 0.7162 |
| 15 | C | 2.6327 | 0.2940 | -0.2341 |
| 16 | O | 3.5317 | 1.2322 | 0.1777 |
| 17 | O | 3.0719 | 0.8922 | -2.4383 |
| 18 | O | 2.2351 | -0.5246 | 2.0309 |
| 19 | C | 2.9060 | 0.7392 | -3.8480 |
| 20 | H | 1.8721 | 0.9455 | -4.1474 |

| | | | | |
|---|---|---|---|---|
| 21 | H | 3.5695 | 1.4756 | -4.3004 |
| 22 | H | 3.1961 | -0.2663 | -4.1731 |
| 23 | C | 4.9149 | 0.9101 | -0.0564 |
| 24 | H | 5.1210 | 0.8356 | -1.1268 |
| 25 | H | 5.4872 | 1.7331 | 0.3733 |
| 26 | H | 5.1786 | -0.0279 | 0.4457 |
| 27 | C | 2.4987 | 0.6850 | 2.7590 |
| 28 | H | 2.4094 | 0.4057 | 3.8095 |
| 29 | H | 3.4932 | 1.0767 | 2.5501 |
| 30 | H | 1.7440 | 1.4392 | 2.5068 |
| 31 | C | -3.7109 | 0.0706 | 0.4998 |
| 32 | H | -4.6458 | 0.4872 | 0.1116 |
| 33 | H | -3.9128 | -0.3891 | 1.4727 |
| 34 | C | -2.6370 | 1.1573 | 0.6072 |
| 35 | C | -2.0718 | 1.6680 | 1.8197 |
| 36 | H | -2.3477 | 1.1570 | 2.7416 |
| 37 | H | -0.4317 | 1.2197 | 1.8813 |
| 38 | C | -1.7692 | 3.1453 | 1.9613 |
| 39 | H | -2.7049 | 3.6717 | 2.1879 |
| 40 | H | -1.0648 | 3.3379 | 2.7734 |
| 41 | H | -1.3588 | 3.5591 | 1.0366 |
| 42 | Pd | -0.8004 | 0.1567 | 0.6480 |
| 43 | H | -4.9166 | -2.0895 | -1.1727 |
| 44 | H | -2.9038 | -3.6069 | -2.3124 |
| 45 | H | -2.6167 | 1.8330 | -0.2488 |
| 46 | H | 0.5981 | -2.1388 | 1.0128 |

**TS3_Iso**

Energy (FREE) = -1123.066194 Eh

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | C | -1.9896 | 0.7492 | -0.2828 |
| 2 | C | -3.4397 | 2.4102 | 0.1871 |
| 3 | C | -2.6173 | 2.8525 | -0.8040 |
| 4 | N | -1.7328 | 1.8149 | -1.0701 |
| 5 | N | -3.0370 | 1.1142 | 0.4880 |
| 6 | C | -0.5599 | 1.8290 | -1.9619 |
| 7 | H | -0.8073 | 1.3032 | -2.8884 |
| 8 | H | -0.3414 | 2.8713 | -2.2040 |
| 9 | C | 0.6086 | 1.1748 | -1.2535 |
| 10 | C | 1.3704 | 1.9098 | -0.3590 |
| 11 | C | 0.8425 | -0.2137 | -1.4199 |
| 12 | C | 2.4049 | 1.2818 | 0.3598 |
| 13 | H | 1.1547 | 2.9595 | -0.2018 |
| 14 | C | 1.9490 | -0.8270 | -0.7582 |
| 15 | H | 0.4383 | -0.7380 | -2.2841 |
| 16 | C | 2.7024 | -0.0865 | 0.1654 |
| 17 | O | 3.7231 | -0.6694 | 0.8582 |
| 18 | O | 3.1886 | 1.9090 | 1.2542 |
| 19 | O | 2.2297 | -2.0790 | -1.1523 |
| 20 | C | 2.9944 | 3.3030 | 1.4945 |
| 21 | H | 1.9930 | 3.4960 | 1.8956 |
| 22 | H | 3.7436 | 3.5775 | 2.2364 |
| 23 | H | 3.1500 | 3.8860 | 0.5798 |
| 24 | C | 5.0442 | -0.3323 | 0.4000 |
| 25 | H | 5.2341 | 0.7383 | 0.5125 |
| 26 | H | 5.7312 | -0.8961 | 1.0323 |
| 27 | H | 5.1740 | -0.6296 | -0.6473 |
| 28 | C | 2.7446 | -3.0545 | -0.2305 |
| 29 | H | 2.5286 | -4.0182 | -0.6937 |
| 30 | H | 3.8185 | -2.9404 | -0.0825 |
| 31 | H | 2.2302 | -2.9748 | 0.7317 |
| 32 | C | -3.4392 | 0.3133 | 1.6491 |
| 33 | H | -2.6163 | 0.3485 | 2.3697 |
| 34 | H | -4.3059 | 0.7957 | 2.1064 |
| 35 | C | -3.7800 | -1.1499 | 1.3091 |
| 36 | H | -3.8122 | -1.6876 | 2.2632 |
| 37 | H | -4.7935 | -1.1820 | 0.8951 |
| 38 | C | -2.8847 | -1.8992 | 0.3289 |
| 39 | H | -3.3080 | -1.9929 | -0.6697 |
| 40 | C | -1.9396 | -2.8883 | 0.6846 |
| 41 | H | -1.7992 | -3.7468 | 0.0368 |
| 42 | H | -1.6796 | -3.0437 | 1.7285 |
| 43 | Pd | -0.9673 | -1.0322 | -0.1356 |
| 44 | H | -4.2553 | 2.8981 | 0.6976 |
| 45 | H | -2.5913 | 3.7904 | -1.3365 |
| 46 | H | -0.2465 | -2.4614 | 0.1196 |

**Int3**

Energy (FREE) = -1123.075927 Eh

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | C | -2.2040 | 0.6342 | -0.2685 |
| 2 | C | -4.1331 | 1.7439 | -0.6735 |
| 3 | C | -3.1131 | 2.5368 | -1.0924 |
| 4 | N | -1.9415 | 1.8366 | -0.8329 |
| 5 | N | -3.5539 | 0.5832 | -0.1758 |
| 6 | C | -0.5967 | 2.3575 | -1.1252 |
| 7 | H | -0.5302 | 2.5203 | -2.2078 |
| 8 | H | -0.5028 | 3.3316 | -0.6377 |
| 9 | C | 0.5294 | 1.4527 | -0.6790 |
| 10 | C | 1.5013 | 1.9402 | 0.1762 |
| 11 | C | 0.6423 | 0.1316 | -1.2030 |
| 12 | C | 2.6373 | 1.1555 | 0.4763 |
| 13 | H | 1.3954 | 2.9285 | 0.6052 |
| 14 | C | 1.8351 | -0.6247 | -0.9640 |
| 15 | H | 0.0554 | -0.1626 | -2.0710 |
| 16 | C | 2.8215 | -0.1167 | -0.1025 |
| 17 | O | 3.9279 | -0.8557 | 0.1956 |
| 18 | O | 3.6179 | 1.5497 | 1.3048 |
| 19 | O | 1.9293 | -1.7589 | -1.6658 |
| 20 | C | 3.5354 | 2.8308 | 1.9325 |
| 21 | H | 2.6407 | 2.9020 | 2.5607 |
| 22 | H | 4.4262 | 2.9062 | 2.5550 |
| 23 | H | 3.5371 | 3.6347 | 1.1880 |
| 24 | C | 5.1518 | -0.4082 | -0.4126 |
| 25 | H | 5.4115 | 0.5976 | -0.0726 |
| 26 | H | 5.9182 | -1.1144 | -0.0914 |
| 27 | H | 5.0655 | -0.4257 | -1.5056 |
| 28 | C | 2.5855 | -2.9229 | -1.1286 |
| 29 | H | 2.2165 | -3.7521 | -1.7331 |
| 30 | H | 3.6692 | -2.8452 | -1.2123 |
| 31 | H | 2.3004 | -3.0601 | -0.0820 |
| 32 | C | -4.3080 | -0.5125 | 0.4480 |
| 33 | H | -4.4590 | -0.2789 | 1.5078 |
| 34 | H | -5.2932 | -0.5293 | -0.0237 |
| 35 | C | -3.6580 | -1.8845 | 0.2767 |
| 36 | H | -4.3946 | -2.6301 | 0.6103 |
| 37 | H | -3.4935 | -2.0838 | -0.7884 |
| 38 | C | -2.3835 | -2.1626 | 1.0399 |
| 39 | H | -1.9636 | -3.1494 | 0.8572 |
| 40 | C | -1.8997 | -1.4507 | 2.1230 |
| 41 | H | -1.1560 | -1.8893 | 2.7783 |
| 42 | H | -2.4005 | -0.5599 | 2.4903 |
| 43 | Pd | -0.7701 | -0.7959 | 0.3180 |
| 44 | H | -5.2009 | 1.8987 | -0.6884 |
| 45 | H | -3.1182 | 3.5141 | -1.5495 |
| 46 | H | 0.3289 | -1.8557 | 0.7691 |

**Int4**

Energy (FREE) = -1123.058692 Eh

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | C | 2.1598 | 1.0899 | -0.1878 |
| 2 | C | 3.9629 | 1.4321 | 1.1080 |
| 3 | C | 2.9848 | 2.2721 | 1.5391 |
| 4 | N | 1.8765 | 2.0409 | 0.7313 |

| | | | | |
|---|---|---|---|---|
| 5 | N | 3.4354 | 0.7059 | 0.0427 |
| 6 | C | 0.5322 | 2.6103 | 0.8850 |
| 7 | H | 0.4625 | 2.9923 | 1.9086 |
| 8 | H | 0.4182 | 3.4566 | 0.2017 |
| 9 | C | -0.5511 | 1.5766 | 0.6219 |
| 10 | C | -1.6965 | 1.9514 | -0.0797 |
| 11 | C | -0.4295 | 0.2609 | 1.1132 |
| 12 | C | -2.7186 | 1.0148 | -0.2976 |
| 13 | H | -1.7734 | 2.9509 | -0.4882 |
| 14 | C | -1.4847 | -0.6707 | 0.9435 |
| 15 | H | 0.3769 | -0.0192 | 1.7832 |
| 16 | C | -2.6247 | -0.3084 | 0.2077 |
| 17 | O | -3.5616 | -1.2477 | -0.1084 |
| 18 | O | -3.8215 | 1.2665 | -1.0283 |
| 19 | O | -1.2448 | -1.8815 | 1.4924 |
| 20 | C | -3.9897 | 2.5591 | -1.6119 |
| 21 | H | -3.1794 | 2.7785 | -2.3162 |
| 22 | H | -4.9377 | 2.5157 | -2.1470 |
| 23 | H | -4.0367 | 3.3359 | -0.8405 |
| 24 | C | -4.8915 | -1.0497 | 0.4029 |
| 25 | H | -5.3540 | -0.1656 | -0.0382 |
| 26 | H | -5.4498 | -1.9433 | 0.1214 |
| 27 | H | -4.8712 | -0.9559 | 1.4953 |
| 28 | C | -2.3077 | -2.7863 | 1.8356 |
| 29 | H | -1.8382 | -3.5336 | 2.4765 |
| 30 | H | -3.0908 | -2.2664 | 2.3954 |
| 31 | H | -2.7322 | -3.2553 | 0.9484 |
| 32 | C | 4.0669 | -0.4590 | -0.5960 |
| 33 | H | 4.1022 | -0.2820 | -1.6744 |
| 34 | H | 5.0936 | -0.4896 | -0.2268 |
| 35 | C | 3.3518 | -1.7996 | -0.2814 |
| 36 | H | 4.1130 | -2.5864 | -0.3760 |
| 37 | H | 3.0246 | -1.8034 | 0.7644 |
| 38 | C | 2.2110 | -2.1761 | -1.2017 |
| 39 | H | 2.4663 | -2.2129 | -2.2605 |
| 40 | C | 0.9894 | -2.6257 | -0.8166 |
| 41 | H | 0.2925 | -3.0295 | -1.5464 |
| 42 | H | 0.6987 | -2.6949 | 0.2281 |
| 43 | Pd | 0.8412 | -0.0656 | -1.0665 |
| 44 | H | 4.9757 | 1.2931 | 1.4519 |
| 45 | H | 2.9829 | 3.0120 | 2.3238 |
| 46 | H | 1.7198 | 0.2674 | -2.2988 |

**TS4_Iso**

Energy (FREE) = -1123.042774 Eh

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | C | -2.0802 | 0.9976 | 0.1128 |
| 2 | C | -3.9556 | 1.6164 | -0.9883 |
| 3 | C | -2.9544 | 2.4435 | -1.3892 |
| 4 | N | -1.8111 | 2.0369 | -0.7090 |
| 5 | N | -3.4023 | 0.7283 | -0.0698 |
| 6 | C | -0.4551 | 2.5724 | -0.8974 |
| 7 | H | -0.3914 | 2.9223 | -1.9337 |
| 8 | H | -0.3143 | 3.4384 | -0.2441 |
| 9 | C | 0.6242 | 1.5396 | -0.6268 |
| 10 | C | 1.7036 | 1.8775 | 0.1709 |
| 11 | C | 0.5431 | 0.2401 | -1.1946 |
| 12 | C | 2.7387 | 0.9438 | 0.3851 |
| 13 | H | 1.7398 | 2.8494 | 0.6464 |
| 14 | C | 1.6186 | -0.6791 | -1.0324 |
| 15 | H | -0.1662 | 0.0278 | -1.9907 |
| 16 | C | 2.7110 | -0.3336 | -0.2157 |
| 17 | O | 3.7164 | -1.2259 | 0.0236 |
| 18 | O | 3.8083 | 1.1793 | 1.1641 |
| 19 | O | 1.4967 | -1.8083 | -1.7514 |
| 20 | C | 3.9415 | 2.4490 | 1.8058 |
| 21 | H | 3.1118 | 2.6267 | 2.4988 |
| 22 | H | 4.8768 | 2.3959 | 2.3620 |
| 23 | H | 3.9957 | 3.2583 | 1.0692 |
| 24 | C | 4.9670 | -0.9384 | -0.6251 |
| 25 | H | 5.3805 | 0.0099 | -0.2734 |
| 26 | H | 5.6368 | -1.7554 | -0.3539 |
| 27 | H | 4.8371 | -0.9106 | -1.7138 |
| 28 | C | 2.1722 | -3.0253 | -1.3898 |
| 29 | H | 1.6518 | -3.8049 | -1.9480 |
| 30 | H | 3.2226 | -2.9993 | -1.6819 |
| 31 | H | 2.0940 | -3.2090 | -0.3162 |
| 32 | C | -4.0985 | -0.4391 | 0.5033 |
| 33 | H | -4.1190 | -0.3280 | 1.5923 |
| 34 | H | -5.1299 | -0.3836 | 0.1504 |
| 35 | C | -3.4968 | -1.8159 | 0.1090 |
| 36 | H | -4.2882 | -2.5648 | 0.2369 |
| 37 | H | -3.2351 | -1.8012 | -0.9538 |
| 38 | C | -2.2842 | -2.2658 | 0.9354 |
| 39 | H | -2.5316 | -2.6272 | 1.9374 |
| 40 | C | -1.0908 | -2.7932 | 0.3625 |
| 41 | H | -0.4396 | -3.4105 | 0.9736 |
| 42 | H | -1.0144 | -2.9240 | -0.7131 |
| 43 | Pd | -0.8447 | -0.5789 | 0.5174 |
| 44 | H | -4.9980 | 1.5887 | -1.2654 |
| 45 | H | -2.9582 | 3.2757 | -2.0757 |
| 46 | H | -1.9034 | -0.9921 | 1.6423 |

**TS4d_Iso**

Energy (FREE) = -1123.032426 Eh

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | C | -2.1336 | 0.9861 | 0.1222 |
| 2 | C | -3.9166 | 1.3856 | -1.2137 |
| 3 | C | -2.9644 | 2.3052 | -1.5188 |
| 4 | N | -1.8789 | 2.0344 | -0.6942 |
| 5 | N | -3.3883 | 0.5741 | -0.2122 |
| 6 | C | -0.5585 | 2.6745 | -0.7599 |
| 7 | H | -0.4711 | 3.1247 | -1.7545 |
| 8 | H | -0.5081 | 3.4818 | -0.0233 |
| 9 | C | 0.5694 | 1.6849 | -0.5272 |
| 10 | C | 1.6413 | 2.0492 | 0.2721 |
| 11 | C | 0.5324 | 0.3950 | -1.1160 |
| 12 | C | 2.7150 | 1.1543 | 0.4614 |
| 13 | H | 1.6430 | 3.0138 | 0.7639 |
| 14 | C | 1.6389 | -0.4862 | -0.9697 |
| 15 | H | -0.1917 | 0.1535 | -1.8892 |
| 16 | C | 2.7252 | -0.1137 | -0.1590 |
| 17 | O | 3.7647 | -0.9736 | 0.0473 |
| 18 | O | 3.7865 | 1.4202 | 1.2288 |
| 19 | O | 1.5693 | -1.6183 | -1.6923 |
| 20 | C | 3.8783 | 2.6856 | 1.8850 |
| 21 | H | 3.0520 | 2.8216 | 2.5916 |
| 22 | H | 4.8228 | 2.6635 | 2.4276 |
| 23 | H | 3.8891 | 3.5061 | 1.1587 |
| 24 | C | 4.9792 | -0.6431 | -0.6485 |
| 25 | H | 5.3725 | 0.3187 | -0.3094 |
| 26 | H | 5.6870 | -1.4365 | -0.4051 |
| 27 | H | 4.8062 | -0.6186 | -1.7310 |
| 28 | C | 2.0898 | -2.8554 | -1.1770 |
| 29 | H | 1.5925 | -3.6328 | -1.7589 |
| 30 | H | 3.1702 | -2.9219 | -1.3043 |
| 31 | H | 1.8377 | -2.9594 | -0.1171 |
| 32 | C | -4.0686 | -0.6229 | 0.3198 |
| 33 | H | -4.4200 | -0.4092 | 1.3326 |
| 34 | H | -4.9600 | -0.7558 | -0.2965 |
| 35 | C | -3.2850 | -1.9599 | 0.2815 |
| 36 | H | -4.0267 | -2.7415 | 0.4949 |
| 37 | H | -2.9308 | -2.1471 | -0.7373 |
| 38 | C | -2.1329 | -2.1383 | 1.2806 |

| | | | | |
|---|---|---|---|---|
| 39 | H | -1.9084 | -3.1765 | 1.5239 |
| 40 | C | -1.9509 | -1.1443 | 2.2974 |
| 41 | H | -1.2819 | -1.3606 | 3.1280 |
| 42 | H | -2.7248 | -0.4187 | 2.5092 |
| 43 | Pd | -0.7820 | -0.4666 | 0.6943 |
| 44 | H | -4.9096 | 1.2423 | -1.6105 |
| 45 | H | -2.9674 | 3.1158 | -2.2307 |
| 46 | H | -0.6802 | -2.1685 | 0.6639 |

**TS5_Iso**

Energy (FREE) = -1122.999327 Eh

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | C | -1.9730 | 1.0811 | 0.1111 |
| 2 | C | -3.3840 | 2.7107 | 0.6871 |
| 3 | C | -2.2108 | 3.2903 | 0.3149 |
| 4 | H | -4.3035 | 3.1425 | 1.0498 |
| 5 | H | -1.9191 | 4.3279 | 0.2723 |
| 6 | N | -3.2229 | 1.3442 | 0.5462 |
| 7 | N | -1.3411 | 2.2733 | -0.0424 |
| 8 | C | 0.0031 | 2.5626 | -0.6068 |
| 9 | H | -0.1389 | 2.7161 | -1.6836 |
| 10 | H | 0.3060 | 3.5198 | -0.1762 |
| 11 | C | 1.0505 | 1.5001 | -0.3668 |
| 12 | C | 0.6717 | 0.1719 | -0.3259 |
| 13 | C | 2.4052 | 1.8344 | -0.2616 |
| 14 | C | 1.6185 | -0.8417 | -0.1822 |
| 15 | C | 3.3605 | 0.8123 | -0.1362 |
| 16 | H | 2.7227 | 2.8707 | -0.2873 |
| 17 | C | 2.9787 | -0.5611 | -0.0800 |
| 18 | O | 3.9037 | -1.5620 | -0.0272 |
| 19 | O | 1.0184 | -2.0961 | -0.2032 |
| 20 | O | 4.6925 | 1.0296 | -0.0727 |
| 21 | C | 1.5850 | -3.1729 | 0.5669 |
| 22 | H | 1.7876 | -2.8437 | 1.5923 |
| 23 | H | 0.8289 | -3.9591 | 0.5709 |
| 24 | H | 2.5028 | -3.5284 | 0.1002 |
| 25 | C | 4.7162 | -1.6334 | 1.1563 |
| 26 | H | 5.3340 | -2.5241 | 1.0356 |
| 27 | H | 5.3493 | -0.7500 | 1.2531 |
| 28 | H | 4.0848 | -1.7405 | 2.0473 |
| 29 | C | 5.1837 | 2.3609 | -0.2070 |
| 30 | H | 6.2697 | 2.2777 | -0.1703 |
| 31 | H | 4.8799 | 2.7958 | -1.1660 |
| 32 | H | 4.8362 | 2.9961 | 0.6165 |
| 33 | C | -4.2569 | 0.3476 | 0.8996 |
| 34 | H | -5.2095 | 0.8807 | 0.8737 |
| 35 | H | -4.0738 | 0.0286 | 1.9317 |
| 36 | Pd | -1.1818 | -0.6684 | -0.1785 |
| 37 | C | -4.2692 | -0.8540 | -0.0418 |
| 38 | H | -4.4159 | -0.5079 | -1.0730 |
| 39 | H | -5.1644 | -1.4397 | 0.2191 |
| 40 | C | -3.0172 | -1.7041 | 0.0658 |
| 41 | H | -2.9085 | -2.0661 | 1.1034 |
| 42 | C | -2.9666 | -2.8747 | -0.9088 |
| 43 | H | -3.1414 | -2.5493 | -1.9404 |
| 44 | H | -1.9980 | -3.3938 | -0.8826 |
| 45 | H | -3.7294 | -3.6307 | -0.6672 |
| 46 | H | -1.4729 | -0.3375 | -1.6283 |

**TS6_Iso**

Energy (FREE) = -1122.994698 Eh

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | C | 2.0252 | 0.9669 | 0.2204 |
| 2 | C | 3.7953 | 2.2907 | 0.4132 |
| 3 | C | 2.6997 | 3.0720 | 0.1770 |
| 4 | N | 1.5975 | 2.2318 | 0.0503 |
| 5 | N | 3.3522 | 0.9806 | 0.4276 |
| 6 | C | 0.2383 | 2.7050 | -0.3131 |
| 7 | H | 0.0564 | 3.6023 | 0.2850 |
| 8 | H | 0.2945 | 3.0172 | -1.3630 |
| 9 | C | -0.8885 | 1.7059 | -0.1226 |
| 10 | C | -2.2113 | 2.1732 | -0.0835 |
| 11 | C | -0.6655 | 0.3417 | -0.0302 |
| 12 | C | -3.2749 | 1.2658 | 0.0368 |
| 13 | H | -2.4169 | 3.2359 | -0.1483 |
| 14 | C | -1.7165 | -0.5561 | 0.1251 |
| 15 | C | -3.0384 | -0.1345 | 0.1729 |
| 16 | O | -4.0579 | -1.0299 | 0.2916 |
| 17 | O | -4.5775 | 1.6206 | 0.0567 |
| 18 | O | -1.2740 | -1.8646 | 0.3156 |
| 19 | C | -4.9216 | 2.9952 | -0.0985 |
| 20 | H | -4.5543 | 3.3860 | -1.0544 |
| 21 | H | -6.0108 | 3.0284 | -0.0839 |
| 22 | H | -4.5245 | 3.5977 | 0.7272 |
| 23 | C | -4.8090 | -0.9736 | 1.5179 |
| 24 | H | -5.3334 | -0.0201 | 1.6100 |
| 25 | H | -5.5292 | -1.7903 | 1.4595 |
| 26 | H | -4.1456 | -1.1256 | 2.3771 |
| 27 | C | -1.8255 | -2.8754 | -0.5567 |
| 28 | H | -1.3171 | -3.8037 | -0.2945 |
| 29 | H | -2.8992 | -2.9625 | -0.3906 |
| 30 | H | -1.6255 | -2.6170 | -1.6027 |
| 31 | C | 4.0654 | -0.3140 | 0.5495 |
| 32 | H | 4.6416 | -0.4495 | -0.3717 |
| 33 | H | 4.7711 | -0.2252 | 1.3822 |
| 34 | C | 3.0365 | -1.4422 | 0.7312 |
| 35 | H | 2.8918 | -1.6279 | 1.8078 |
| 36 | C | 3.4124 | -2.7424 | 0.0291 |
| 37 | H | 3.6273 | -2.5402 | -1.0287 |
| 38 | H | 4.3387 | -3.1587 | 0.4558 |
| 39 | C | 2.3017 | -3.7926 | 0.1295 |
| 40 | H | 1.3853 | -3.4478 | -0.3726 |
| 41 | H | 2.5959 | -4.7335 | -0.3457 |
| 42 | H | 2.0510 | -4.0084 | 1.1748 |
| 43 | Pd | 1.0763 | -0.6813 | 0.2297 |
| 44 | H | 4.8271 | 2.5575 | 0.5796 |
| 45 | H | 2.6046 | 4.1439 | 0.0990 |
| 46 | H | 1.2609 | -0.5585 | -1.2716 |

## Conformers of Isomer III

Isomer_III_c1

Energy (FREE) = -1123.089259 Eh

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | C | 1.8249 | -0.9509 | 0.1273 |
| 2 | N | 1.3194 | -2.1937 | -0.0667 |
| 3 | C | 2.3030 | -3.1500 | 0.1478 |
| 4 | C | 3.4332 | -2.4844 | 0.4943 |
| 5 | N | 3.1211 | -1.1332 | 0.4875 |
| 6 | C | 4.0680 | -0.0713 | 0.8603 |
| 7 | H | 4.7758 | -0.5163 | 1.5636 |
| 8 | C | 4.8157 | 0.5320 | -0.3340 |
| 9 | C | 3.9262 | 1.2252 | -1.3741 |
| 10 | C | 3.1074 | 2.3928 | -0.8147 |
| 11 | H | 3.7489 | 3.2077 | -0.4604 |
| 12 | H | 2.5247 | 2.1208 | 0.0970 |
| 13 | H | 2.4218 | 2.8057 | -1.5601 |
| 14 | H | 3.2596 | 0.4900 | -1.8401 |
| 15 | H | 4.5659 | 1.6049 | -2.1783 |
| 16 | H | 5.3992 | -0.2570 | -0.8228 |
| 17 | H | 5.5387 | 1.2492 | 0.0749 |
| 18 | H | 3.5046 | 0.6833 | 1.4133 |
| 19 | H | 4.4141 | -2.8438 | 0.7630 |

| | | | | |
|---|---|---|---|---|
| 20 | H | 2.1064 | -4.2053 | 0.0441 |
| 21 | C | -0.0394 | -2.5623 | -0.4988 |
| 22 | C | -1.0898 | -1.5263 | -0.1970 |
| 23 | C | -0.7772 | -0.1974 | -0.0332 |
| 24 | C | -1.7472 | 0.7888 | 0.1027 |
| 25 | C | -3.0999 | 0.4767 | 0.1221 |
| 26 | C | -3.4431 | -0.9012 | 0.0037 |
| 27 | C | -2.4530 | -1.8754 | -0.1720 |
| 28 | H | -2.7356 | -2.9152 | -0.2896 |
| 29 | O | -4.7691 | -1.1621 | 0.0685 |
| 30 | C | -5.2067 | -2.5131 | -0.0461 |
| 31 | H | -4.7883 | -3.1316 | 0.7567 |
| 32 | H | -6.2920 | -2.4798 | 0.0473 |
| 33 | H | -4.9343 | -2.9359 | -1.0208 |
| 34 | O | -4.0272 | 1.4550 | 0.3073 |
| 35 | C | -4.9327 | 1.6891 | -0.7881 |
| 36 | H | -4.3723 | 1.9373 | -1.6966 |
| 37 | H | -5.5427 | 2.5410 | -0.4863 |
| 38 | H | -5.5661 | 0.8170 | -0.9609 |
| 39 | O | -1.1883 | 2.0695 | 0.1318 |
| 40 | C | -1.5300 | 2.8867 | 1.2793 |
| 41 | H | -1.2130 | 2.3857 | 2.1999 |
| 42 | H | -2.6058 | 3.0608 | 1.2912 |
| 43 | H | -0.9870 | 3.8229 | 1.1488 |
| 44 | Pd | 0.8953 | 0.7856 | -0.0468 |
| 45 | H | -0.2793 | -3.5091 | -0.0072 |
| 46 | H | -0.0014 | -2.7537 | -1.5785 |

Isomer_III_c2

Energy (FREE) = -1123.088881 Eh

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | C | 1.7601 | -1.1413 | 0.0151 |
| 2 | N | 1.1851 | -2.3491 | -0.1879 |
| 3 | C | 2.1028 | -3.3614 | 0.0585 |
| 4 | C | 3.2603 | -2.7620 | 0.4358 |
| 5 | N | 3.0338 | -1.3923 | 0.4091 |
| 6 | C | 3.9903 | -0.3952 | 0.9234 |
| 7 | H | 4.8374 | -0.9684 | 1.3051 |
| 8 | C | 4.4832 | 0.6372 | -0.0936 |
| 9 | C | 3.4720 | 1.7265 | -0.4714 |
| 10 | C | 4.0970 | 2.9036 | -1.2287 |
| 11 | H | 3.3391 | 3.6437 | -1.5021 |
| 12 | H | 4.5831 | 2.5608 | -2.1479 |
| 13 | H | 4.8510 | 3.4010 | -0.6099 |
| 14 | H | 2.9856 | 2.1056 | 0.4427 |
| 15 | H | 2.7065 | 1.2895 | -1.1500 |
| 16 | H | 4.8461 | 0.1286 | -0.9946 |
| 17 | H | 5.3541 | 1.1234 | 0.3634 |
| 18 | H | 3.5210 | 0.1019 | 1.7791 |
| 19 | H | 4.2094 | -3.1793 | 0.7328 |
| 20 | H | 1.8492 | -4.4036 | -0.0544 |
| 21 | C | -0.1929 | -2.6179 | -0.6340 |
| 22 | C | -1.1768 | -1.5330 | -0.2747 |
| 23 | C | -0.7822 | -0.2267 | -0.0956 |
| 24 | C | -1.6891 | 0.8120 | 0.0747 |
| 25 | C | -3.0572 | 0.5769 | 0.1239 |
| 26 | C | -3.4826 | -0.7769 | -0.0013 |
| 27 | C | -2.5560 | -1.8045 | -0.2182 |
| 28 | H | -2.9022 | -2.8239 | -0.3444 |
| 29 | O | -4.8195 | -0.9618 | 0.0968 |
| 30 | C | -5.3378 | -2.2834 | -0.0219 |
| 31 | H | -6.4165 | -2.1886 | 0.1012 |
| 32 | H | -5.1163 | -2.7088 | -1.0082 |
| 33 | H | -4.9354 | -2.9357 | 0.7622 |
| 34 | O | -3.9226 | 1.6049 | 0.3393 |
| 35 | C | -4.8379 | 1.8999 | -0.7327 |
| 36 | H | -5.5269 | 1.0688 | -0.8944 |
| 37 | H | -4.2854 | 2.1192 | -1.6534 |
| 38 | H | -5.3879 | 2.7853 | -0.4126 |
| 39 | O | -1.0603 | 2.0592 | 0.0919 |
| 40 | C | -1.3209 | 2.8866 | 1.2522 |
| 41 | H | -2.3875 | 3.1037 | 1.3098 |
| 42 | H | -0.7477 | 3.8013 | 1.0997 |
| 43 | H | -0.9856 | 2.3720 | 2.1589 |
| 44 | Pd | 0.9537 | 0.6408 | -0.1781 |
| 45 | H | -0.4866 | -3.5714 | -0.1873 |
| 46 | H | -0.1690 | -2.7577 | -1.7219 |

Isomer_III_c3

Energy (FREE) = -1123.089011 Eh

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | C | -1.7607 | 1.1282 | -0.1323 |
| 2 | N | -1.1945 | 2.3428 | 0.0526 |
| 3 | C | -2.1095 | 3.3451 | -0.2432 |
| 4 | C | -3.2558 | 2.7318 | -0.6326 |
| 5 | N | -3.0253 | 1.3646 | -0.5636 |
| 6 | C | -3.9620 | 0.3430 | -1.0641 |
| 7 | H | -3.4446 | -0.2178 | -1.8498 |
| 8 | C | -4.5219 | -0.6123 | -0.0077 |
| 9 | C | -3.5022 | -1.5806 | 0.6071 |
| 10 | C | -4.1406 | -2.7936 | 1.2926 |
| 11 | H | -4.8217 | -2.4702 | 2.0868 |
| 12 | H | -3.3796 | -3.4373 | 1.7438 |
| 13 | H | -4.7135 | -3.3909 | 0.5760 |
| 14 | H | -2.8986 | -1.0461 | 1.3583 |
| 15 | H | -2.8382 | -1.9577 | -0.2023 |
| 16 | H | -5.3017 | -1.1963 | -0.5120 |
| 17 | H | -5.0199 | -0.0422 | 0.7851 |
| 18 | H | -4.7788 | 0.8904 | -1.5390 |
| 19 | H | -4.1985 | 3.1375 | -0.9643 |
| 20 | H | -1.8614 | 4.3908 | -0.1531 |
| 21 | C | 0.1681 | 2.6345 | 0.5308 |
| 22 | C | 1.1617 | 1.5267 | 0.2879 |
| 23 | C | 0.7743 | 0.2142 | 0.1564 |
| 24 | C | 1.6847 | -0.8351 | 0.0802 |
| 25 | C | 3.0560 | -0.6063 | 0.0991 |
| 26 | C | 3.4762 | 0.7517 | 0.2141 |
| 27 | C | 2.5439 | 1.7909 | 0.3076 |
| 28 | H | 2.8878 | 2.8122 | 0.4235 |
| 29 | O | 4.8179 | 0.9283 | 0.2610 |
| 30 | C | 5.3300 | 2.2424 | 0.4603 |
| 31 | H | 5.0511 | 2.9063 | -0.3669 |
| 32 | H | 4.9758 | 2.6624 | 1.4091 |
| 33 | H | 6.4140 | 2.1340 | 0.4916 |
| 34 | O | 3.9225 | -1.6551 | 0.0998 |
| 35 | C | 4.8690 | -1.7214 | -0.9832 |
| 36 | H | 5.4055 | -2.6606 | -0.8442 |
| 37 | H | 5.5646 | -0.8823 | -0.9480 |
| 38 | H | 4.3439 | -1.7338 | -1.9462 |
| 39 | O | 1.0318 | -2.0669 | 0.0919 |
| 40 | C | 1.4660 | -3.0716 | -0.8508 |
| 41 | H | 2.4461 | -3.4460 | -0.5576 |
| 42 | H | 1.5016 | -2.6492 | -1.8606 |
| 43 | H | 0.7221 | -3.8669 | -0.8011 |
| 44 | Pd | -0.9648 | -0.6491 | 0.1411 |
| 45 | H | 0.1027 | 2.8490 | 1.6048 |
| 46 | H | 0.4845 | 3.5545 | 0.0318 |

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