Electronic Supplementary Information

for

Reactivity of NHC/diphosphene-coordinated Au(I)-hydride

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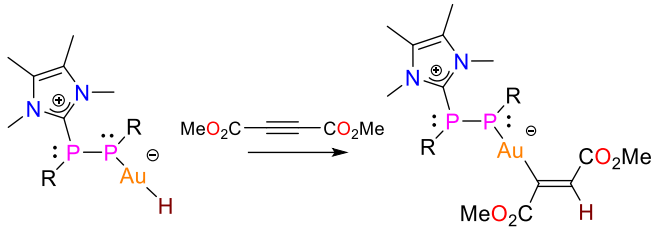
General Considerations

All experiments were carried out under argon atmosphere using standard Schlenk techniques, in a PL-HE-2GB Innovative Technology and MBraun Unilab GloveBox. Hexane, diethyl ether, THF, and toluene were dried by PS-MD-5 Innovative Technology solvent purification system. Benzene was refluxed over sodium/benzophenone, then distilled and stored under argon. Compounds **1a**[S1] and **3**[S2] were prepared according to reported literature procedure. AuCl·SMe_2 was purchased from Sigma Aldrich and TCI Chemicals and used as received. THF-d_8 and C_6D_6 were dried and distilled over potassium under argon and subsequently stored inside the GloveBox for the use of it. NMR spectra were recorded with Bruker NanoBay 300 MHz NMR spectrometer. ^{1}H and ^{13}C{^{1}H} NMR spectra were referenced to the peaks of residual protons of the deuterated solvent (^{1}H) and the deuterated solvent itself (^{13}C{^{1}H}), respectively. ^{31}P spectra were referenced to the peaks of H_3PO_4. Due to the poor solubility of our synthesized compounds we were not able to obtained well resolved ^{13}C{^{1}H} NMR spectra and were able to assigned few resonances based on ^{1}H-^{13}C{^{1}H} 2D NMR (HSQC). UV/Vis spectra were acquired using a Jasco V-670 spectrometer using quartz cells with a path length of 0.1 cm. Elemental analysis was performed on a Leco CHN-900 analyzer. Melting points were determined in closed NMR tubes under argon atmosphere and were uncorrected.

Experimental Details and Analytical Data

Synthesis of 4

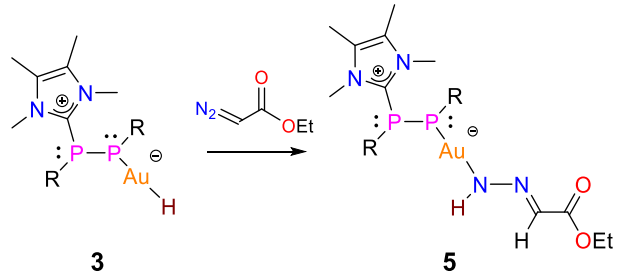


3 **4**

6 µL (0.049 mmol) of dimethyl acetylenedicarboxylate was added to a 25 mL Schlenk flask containing suspension of **3** (0.048 g, 0.047 mmol) in 5 mL of toluene at −78 °C. Then the reaction mixture was brought to room temperature over 12 hrs. The resulting yellow reaction mixture was dried under vacuum and subsequently washed with 5 mL of hexane to get pure **4** as a yellow powder. Yield: 0.045 g (81 %). Single crystals suitable for X-ray diffraction study were grown from saturated benzene solution at room temperature. **M.P.:** > 160 °C (turned black). **^{1}H NMR (300 MHz, THF-D_8, 298 K)**: δ = 0.94 (s, 3H, Mes-CH_3), 1.13 (s, 3H, NHC^{Me4}-CCH_3), 1.29 (s, 3H, Mes-CH_3), 1.44 (s, 3H, NHC^{Me4}-CCH_3), 1.49 (s, 3H, Mes-

CH_3), 1.98 (s, 6H, Mes-CH_3), 2.02 (s, 6H, Mes-CH_3), 2.19 (s, 3H, Mes-CH_3), 2.25 (s, 3H, Mes-CH_3), 2.30 (s, 3H, Mes-CH_3), 2.31 (s, 3H, Mes-CH_3), 2.37 (s, 3H, OCH_3), 2.50 (s, 3H, Mes-CH_3), 3.58 (s, 3H, merged with THF-d_8 resonance, N-CH_3), 3.59 (s, 3H, N-CH_3), 3.67 (s, 3H, OCH_3), 6.11-6.18 (m, 1H, Ar–*H*), 6.41 (s, 1H, Ar–*H*), 6.52 (s, 1H, Ar–*H*), 6.59 (s, 1H, Ar–*H*), 6.70 (br, 1H, Ar–*H*), 6.79 (br, 2H, Ar–*H*), 6.90 (s, 2H, Ar–*H*), 6.93 (s, 2H, Ar–*H*), 6.97 (s, 1H, vinyl–*H*), 7.08-7.25 (m, 3H, Ar–*H*). **^{13}C{^{1}H} NMR (75.43 MHz, THF-D$_8$, 298 K, selected resonances assigned based on ^{1}H-^{13}C{^{1}H} 2D NMR (HSQC) spectrum):** δ = 8.70 (1C, C-*C*H$_3$ of NHC^{Me_4}), 8.98 (1C, C-*C*H$_3$ of NHC^{Me_4}), 32.70 (1C, OCH$_3$), 32.95 (1C, N-*C*H$_3$), 36.42 (1C, N-*C*H$_3$), 50.45 (1C, O-*C*H$_3$), 126.11 (2C, *C*-CH$_3$ of NHC^{Me_4}), 133.03 (C=*C*-H) ppm. **^{31}P NMR (121.5 MHz, THF-D$_8$, 298 K):** δ = −31.4 (d, $^1J_{(^{31}P,^{31}P)}$ = 491 Hz), −6.8 (d, $^1J_{(^{31}P,^{31}P)}$ = 491 Hz) ppm. **IR (KBr, cm^{-1}):** ῡ (cm^{-1}) = 1716 (s), 1681 (vs), 1642 (w), 1611 (m), 1428 (s), 1314 (m), 1206 (vs), 1163 (vs), 1024 (s), 842 (m), 801 (m), 746 (m), 730 (m). **UV/Vis (THF):** $\lambda_{max}(\epsilon)$ = 403(3176), 329(8907) nm (Lmol^{-1}cm^{-1}). **Elemental Analysis:** Calcd. for ($C_{61}H_{69}AuN_2O_4P_2$): C, 63.54; H, 6.03; N, 2.43. Found: C, 62.89; H, 6.46; N, 2.53.

Synthesis of 5

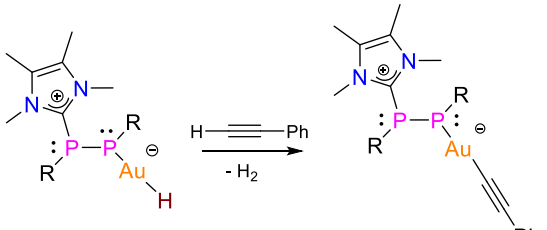


3 **5**

5 µL (0.05 mmol) of ethyl diazoacetate was added to a 25 mL Schlenk flask containing suspension of **3** (0.050 g, 0.05 mmol) in 7 mL of toluene at −78 °C. Then the reaction mixture was brought to room temperature over 12 hrs. The resulting yellow reaction mixture was dried under vacuum and subsequently washed with about 5 mL of hexane to get pure **6** as a yellow powder. Yield: 0.050 g (90%). Single crystals suitable for X-ray diffraction study were grown from saturated toluene solution at room temperature. **M.P.:** > 150 °C (turned black). **^{1}H NMR (300 MHz, THF-D$_8$, 298 K):** δ = 0.96 (s, 3H, Mes-CH_3), 1.22 (t, $^3J_{(^1H,^1H)}$= 7 Hz, 3H, CH_2CH_3), 1.36 (s, 3H, Mes-CH_3), 1.44 (s, 3H, Mes-CH_3), 1.46 (s, 3H, Mes-CH_3), 1.96 (s, 6H, NHC^{Me_4}-CCH_3,), 2.02 (s, 3H, Mes-CH_3), 2.15 (s, 3H, Mes-CH_3), 2.23 (s, 3H, Mes-CH_3), 2.26 (s, 3H, Mes-CH_3), 2.31 (br, 6H, Mes-CH_3), 2.42 (s, 3H, N-CH_3), 2.46 (s, 3H, Mes-CH_3), 2.49 (s, 3H, Mes-CH_3), 3.42 (s, 3H, N-CH_3), 4.03-4.07 (m, 2H, CH_2CH_3), 6.16 (s, 1H, N=C–*H*), 6.46 (br, 1H, Ar–*H*), 6.48 (s, 1H, Ar–*H*), 6.54-6.61 (m, 4H, Ar–*H*), 6.73 (br, 1H, N–*H,* full width at half maximum 14.7 Hz), 6.80 (s, 2H, Ar–*H*), 6.92-6.99 (m, 4H, Ar–*H*), 7.15 (br, 1H, Ar–*H*), 7.28 (s, 1H, Ar–*H*) ppm. **^{13}C{^{1}H} NMR (75.43**

MHz, THF-D_8, 298 K, selected resonances assigned based on ^{1}H-^{13}C{^{1}H} 2D NMR (HSQC) spectrum): δ = 8.9 (1C, C-*C*H_3 of NHC^{Me4}), 9.4 (1C, C-*C*H_3 of NHC^{Me4}), 33.42 (1C, N-*C*H_3), 35.75 (1C, N-*C*H_3), 58.05 (1C, *C*H_2), 116.2 (1C, N=*C*H), 167.42(1C, *C*=O) ppm. **^{31}P NMR (121.5 MHz, THF-D_8, 298 K):** δ = −39.4 (d, $^{1}J_{(^{31}P,^{31}P)}$ = 477 Hz), −5.5 (d, $^{1}J_{(^{31}P,^{31}P)}$ = 477 Hz) ppm. **IR (KBr, cm^{-1}):** ῡ (cm^{-1}) = 2020 (s), 1664 (s, br), 11605 (m), 1509 (m), 1234(vw), 1116 (m), 1050 (m), 842(vs), 800 (vs), 742 (vs), **UV/Vis (THF):** $\lambda_{max}(\epsilon)$ = 400(1861), 333(13127) nm (Lmol^{-1}cm^{-1}). **Elemental Analysis:** Calcd. for ($C_{59}H_{69}AuN_4O_2P_2$)**:** C, 62.98; H, 6.18; N, 4.98; **Found:** C, 61.56; H, 6.16; N, 4.40.

Synthesis of 6



3 **6**

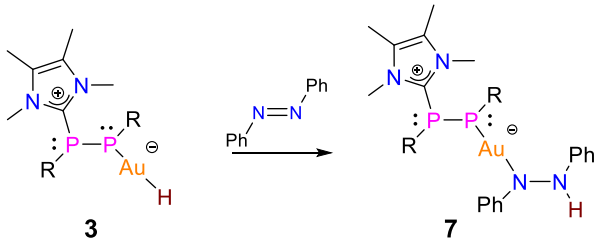
6 µL (0.05 mmol) of phenyl acetylene was added to a 25 mL Schlenk flask containing suspension of **3** (0.050 g, 0.05 mmol) in 5 mL of toluene at −78 °C. Then the reaction mixture was brought to room temperature over 12 hrs. The resulting yellow reaction mixture was dried under vacuum and subsequently washed with about 5 mL of hexane to get pure **6** as a yellow powder. Yield: 0.046 g (85%). Single crystals suitable for X-ray diffraction study were grown from saturated benzene solution at room temperature. When the same reaction was carried out at room temperature we were obtained compound **6** along with substantial amount of unidentified side product. **M.P.:** > 160 °C (turned black). **^{1}H NMR (300 MHz, C_6D_6, 298 K):** δ = 1.08 (s, 3H, Mes-C*H*$_3$), 1.19 (s, 3H, NHC^{Me4}-CC*H*$_3$), 1.23 (s, 3H, Mes-C*H*$_3$), 1.38 (s, 3H, NHC^{Me4}-CC*H*$_3$), 1.44 (s, 3H, Mes-C*H*$_3$), 1.97 (s, 3H, Mes-C*H*$_3$), 1.98 (s, 3H, N-C*H*$_3$), 2.07-2.10 (m, 6H, Mes-C*H*$_3$), 2.30 (s, 3H, Mes-C*H*$_3$), 2.35 (s,3H, Mes-C*H*$_3$), 2.45 (s, 6H, Mes-C*H*$_3$), 2.53 (s, 3H, Mes-C*H*$_3$), 2.77 (s, 3H, Mes-C*H*$_3$), 3.31 (s, 3H, N-C*H*$_3$), 6.25 (s, 1H, Ar–*H*), 6.54 (s,1H, Ar–*H*), 6.75-6.82 (m, 5H, Ar–*H,*), 6.90-6.94 (m, 2H, Ar–*H*), 6.99-7.10 (m, 6H, Ar–*H*), 7.20 (s, 1H, Ar–*H*), 7.21 (s, 1H, Ar–*H*), 7.67 (br,1H, Ar–*H*), 7.69 (br, 1H, Ar–*H*) ppm. **^{13}C{^{1}H} NMR (75.43 MHz, C_6D_6, 298 K, selected resonances assigned based on ^{1}H-^{13}C{^{1}H} 2D NMR (HSQC) spectrum):** δ = 8.7 (1C, C-*C*H_3 of NHC^{Me4}), 8.8 (1C, C-*C*H_3 of NHC^{Me4}), 101.0 (1C, Au-*C*), 101.1 (1C, C≡*C*-Ph), 155.8 (1C, N-*C*-N) ppm. **^{31}P NMR (121.5 MHz, C_6D_6, 298 K):** δ = −26.6 (d, $^{1}J_{(^{31}P,^{31}P)}$ = 460 Hz), 4.3 (d, $^{1}J_{(^{31}P,^{31}P)}$ = 460 Hz) ppm. **IR (KBr, cm^{-1}):** ῡ (cm^{-1}) = 2727 (w), 2100 (s), 1948 (vw), 1872 (vw), 1717(vw), 1637 (s), 1606 (s), 1483 (s), 1438

(vs), 1379(s), 1212 (ms), 1180 (ms), 1065 (w), 1025 (w), 843 (vs), 807 (s), 755 (vs), 695 (vs). **UV/Vis (THF):** $\lambda_{max}(\epsilon)$ = 404(5266) nm ($Lmol^{-1}cm^{-1}$). **Elemental Analysis:** Calcd. for ($C_{63}H_{67}AuN_2P_2$): C, 68.10; H, 6.08; N, 2.52. Found: C, 67.88; H, 6.57; N, 2.58.

Reaction of 1a with phenyl acetylene

About 5 mL of toluene was added to a Schlenk flask containing 0.052 g (0.088 mmol) of **1a** and 10 μL (0.088 mmol) of phenyl acetylene at room temperature. The reaction mixture was allowed to stir for overnight at room temperature. ^{1}H NMR spectrum of the crude reaction showed compound **1a** was not reacted with phenyl acetylene. Even after heating at 80 °C for 5 hrs there was no indication of any product formation.

Synthesis of 7



3 **7**

0.011g (0.057 mmol) of azobenzene was added to a 25 mL Schlenk flask containing suspension of **3** (0.057 g, 0.057 mmol) in 5 mL of toluene at −78 °C. Then the reaction mixture was brought to room temperature over 12 hrs. The resulting yellow reaction mixture was dried under vacuum and subsequently washed with 5 mL of cold hexane to get pure **7** as a yellow powder. Yield: 0.060 g (90%). Single crystals suitable for X-ray diffraction study were grown from saturated benzene solution at room temperature. **M.P.:** > 130 °C (turned black). **^{1}H NMR (300 MHz, THF-D$_8$, 298 K):** δ = 0.89 (s, 3H, Mes-CH_3), 0.96 (s, 3H, Mes-CH_3), 1.21 (s, 3H, Mes-CH_3), 1.29 (s, 3H, Mes-CH_3), 1.30 (s, 3H, Mes-CH_3), 1.50 (s, 3H, Mes-CH_3), 1.96 (s, 6H, N-CH_3 & Mes-CH_3), 2.04 (s, 3H, N-CH_3), 2.24 (s, 3H, Mes-CH_3), 2.33 (s, 3H, Mes-CH_3), 2.36 (s, 6H, Mes-CH_3), 2.44 (s, 3H, Mes-CH_3), 2.49 (s, 3H, N-CH_3), 3.04 (s, 3H, N-CH_3), 5.46 (s, 1H, N–*H*), 6.12 (t, 1H, Ar–*H*), 6.18 (s, 1H, Ar–*H*), 6.36 (br, 1H, Ar–*H*), 6.45 (s, 1H, Ar–*H*), 6.47 (s, 2H, Ar–*H*), 6.55 (s, 1H, Ar–*H*), 6.61 (s, 1H, Ar–*H*), 6.67 (s, 1H, Ar–*H*), 6.74 (br, 3H, Ar–*H*), 6.84-7.02 (m, 10H, Ar–*H*), 7.02 (s, 1H, Ar–*H*), 7.22 (t, 1H, Ar–*H*) ppm. **^{13}C{^{1}H} NMR (75.43 MHz, THF-D$_8$, 298 K, selected resonances assigned based on ^{1}H-^{13}C{^{1}H} 2D NMR (HSQC) spectrum):** δ = 8.7 (1C, C-*C*H$_3$ of NHC^{Me4}), 8.8 (1C, C-*C*H$_3$ of NHC^{Me4}), 33.1 (N-*C*H$_3$), 35.7 (N-*C*H$_3$) ppm. **^{31}P NMR (121.5 MHz, THF-D$_8$, 298 K):** δ = −42.3 (d, $^1J_{(^{31}P,^{31}P)}$ = 493 Hz), −7.9 (d, $^1J_{(^{31}P,^{31}P)}$ = 493 Hz) ppm. **IR (KBr, cm^{-1}):** ῡ (cm^{-1}) = 3340 (m),

2897 (s, br), 1642 (w), 1552 (vw), 1456(vs), 1377 (s), 1303 (m), 1277 (w), 1247(w), 1163 (m), 1081(w), 1026 (m), 979 (m), 844 (s), 746 (s), 695 (vs). **UV/Vis (THF):** $\lambda_{max}(\epsilon)$ = 401(1753), 323(7265) nm ($Lmol^{-1}cm^{-1}$). Most likely due to the lower decomposition temperature we did not obtained satisfactory elemental analysis result of this compound.

Reaction of 1a with azobenzene

About 5 mL of toluene was added to a Schlenk flask containing 0.050 g (0.085 mmol) of **1a** and 0.016 g (0.088) of azobenzene at room temperature. The reaction mixture was allowed to stir for overnight at room temperature. ^{1}H NMR spectrum of the crude reaction showed compound **1a** was not reacted with phenyl acetylene. Even after heating at 80 °C for 5 hrs there was no indication of any product formation.

NMR Spectra

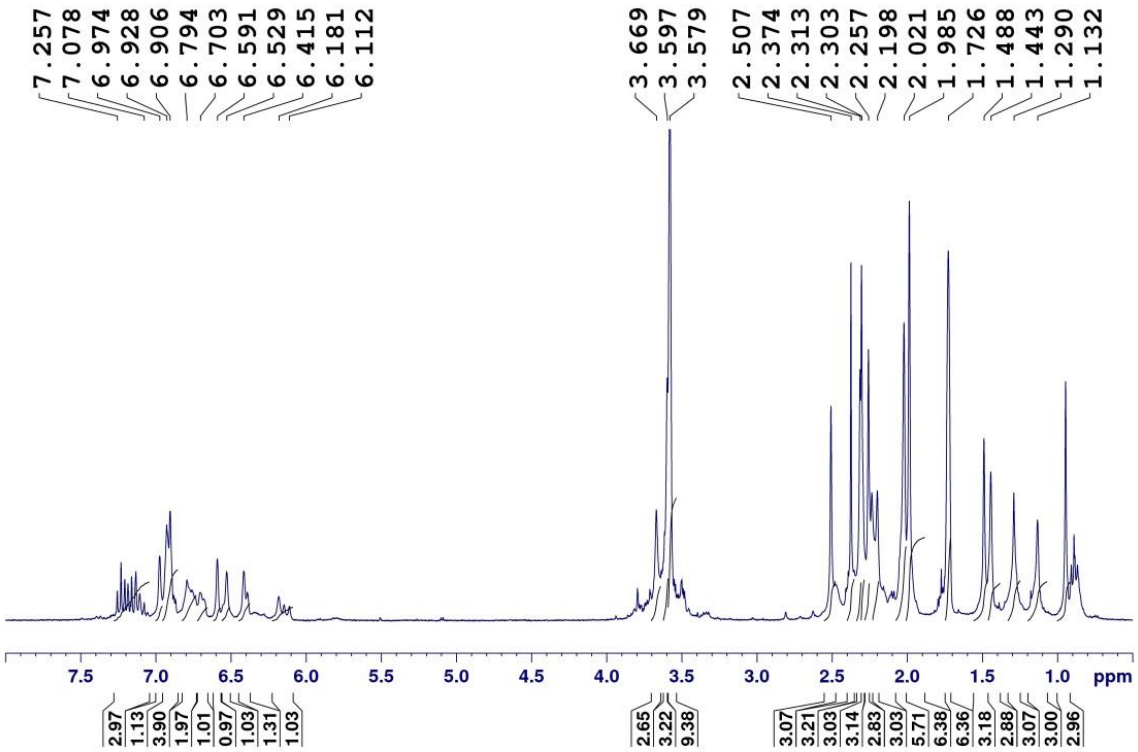


Fig. S1 ^{1}H NMR spectrum of **4** in THF-D_8 at room temperature (we integrate the residual protons of THF-D_8 to show the merging of three hydrogens of N-CH_3 at δ = 3.58 ppm).

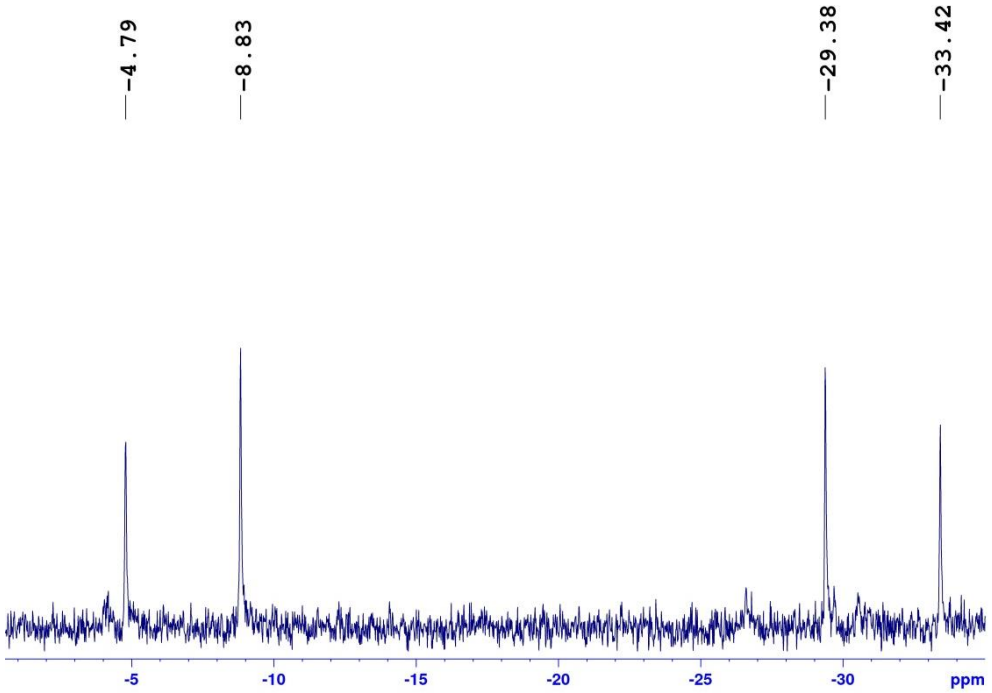


Fig. S2 ^{31}P NMR spectrum of **4** in THF-D_8 at room temperature.

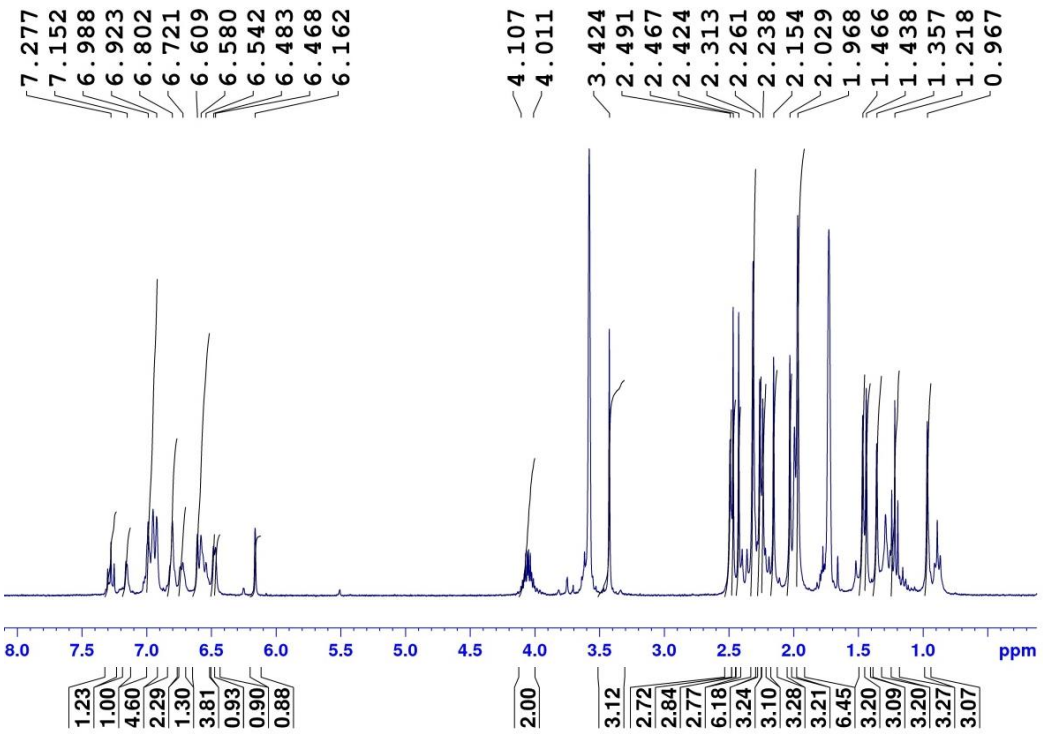


Fig. S3 ^{1}H NMR spectrum of **5** in THF-D_8 at room temperature.

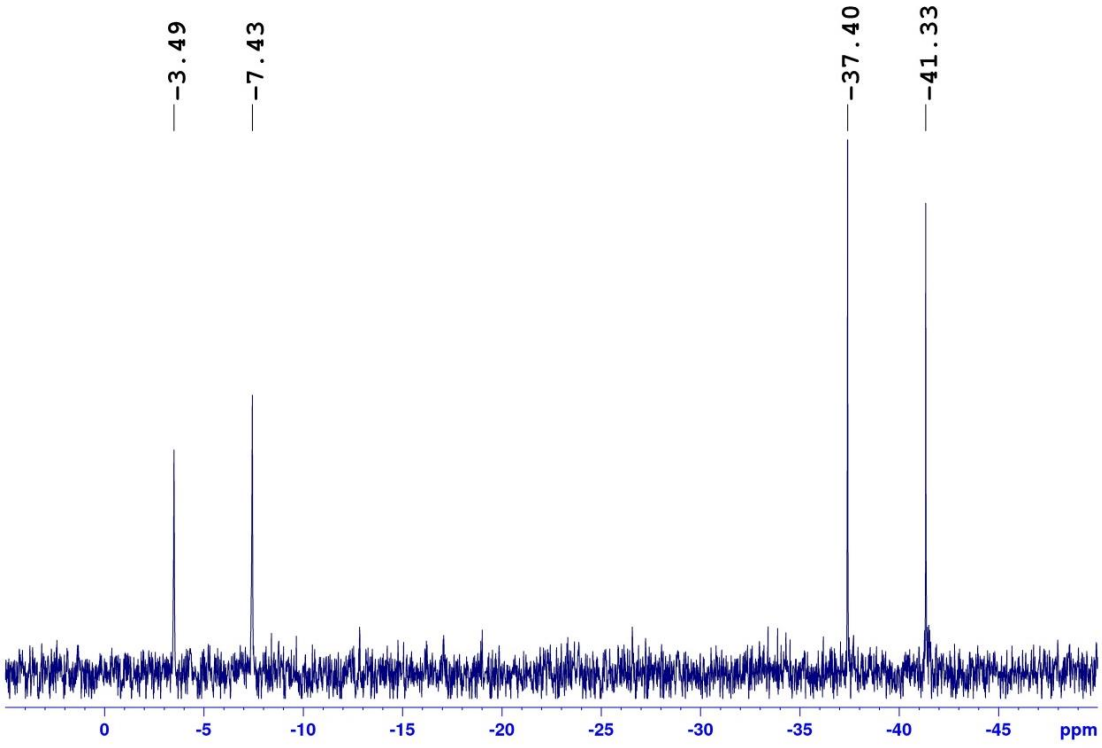


Fig. S4 ^{31}P NMR spectrum of **5** in THF-D_8 at room temperature.

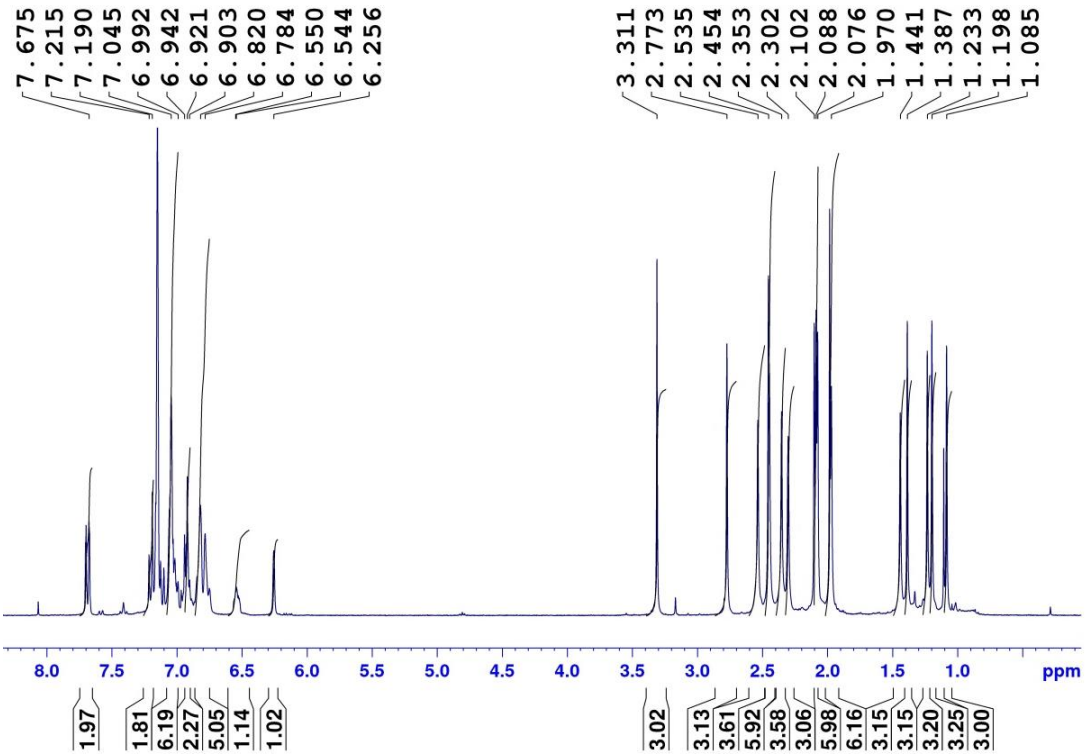


Fig. S5 ^{1}H NMR spectrum of **6** in benzene-D_6 at room temperature.

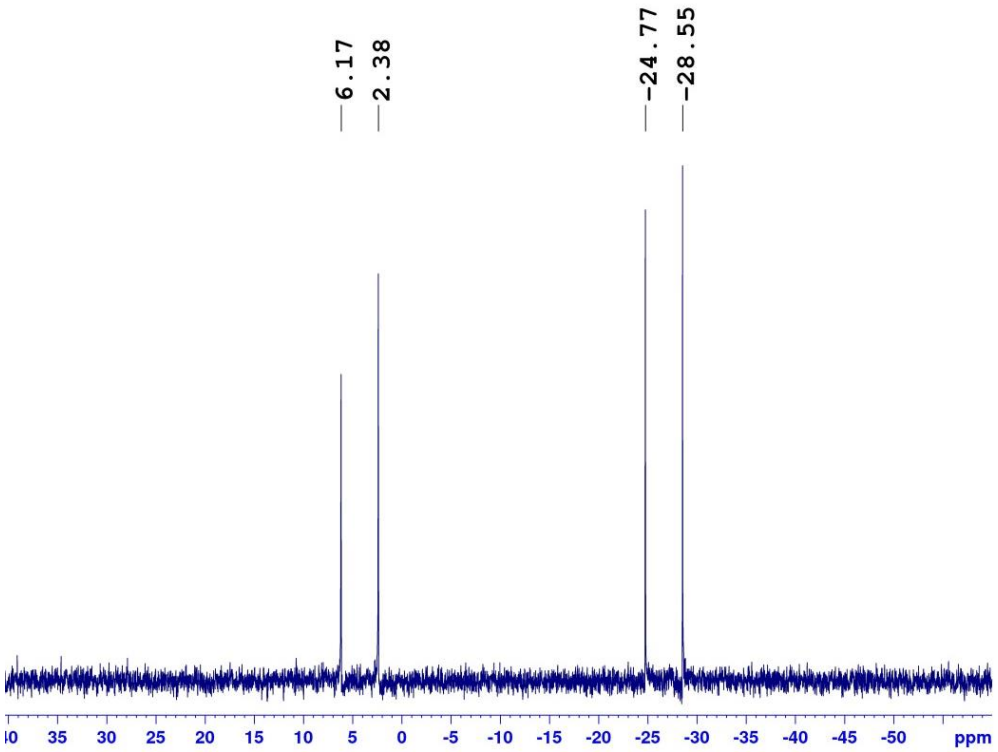


Fig. S6 ^{31}P NMR spectrum of **6** in benzene-D_6 at room temperature.

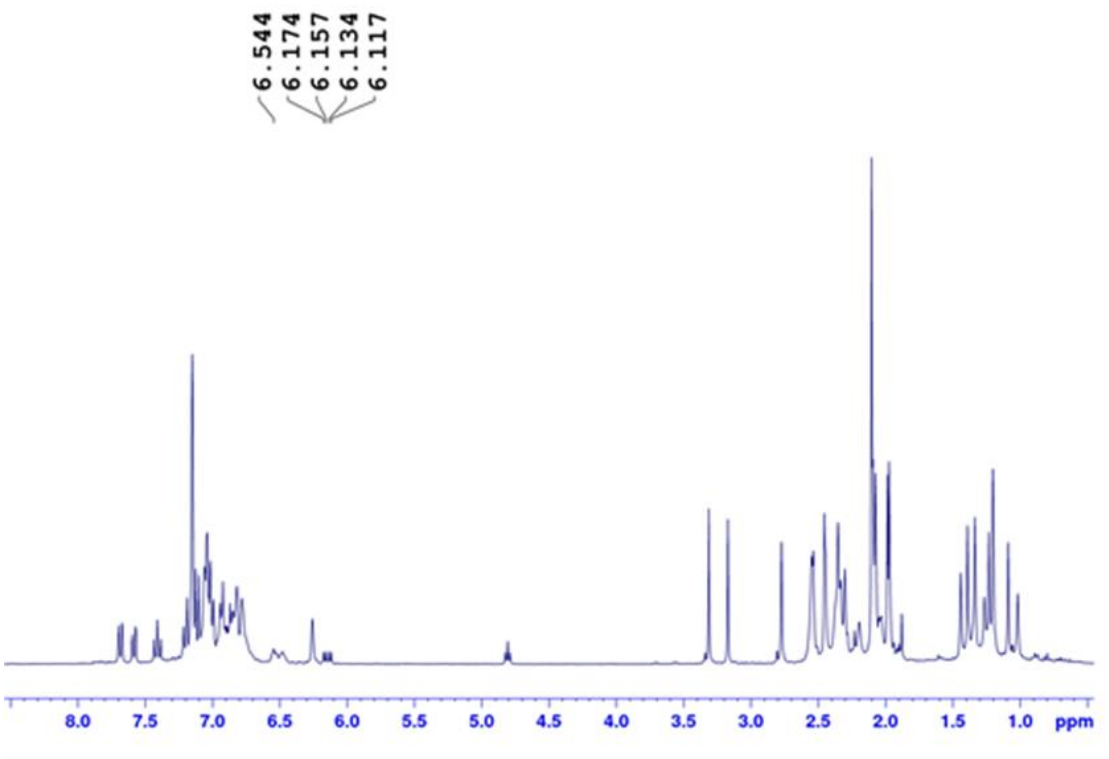


Fig. S7 ^{1}H NMR spectrum from the crude reactiin mixture of **3** and phenyl acetylene when the reaction was carried out at room temperature in benzene-D_6 at room temperature.

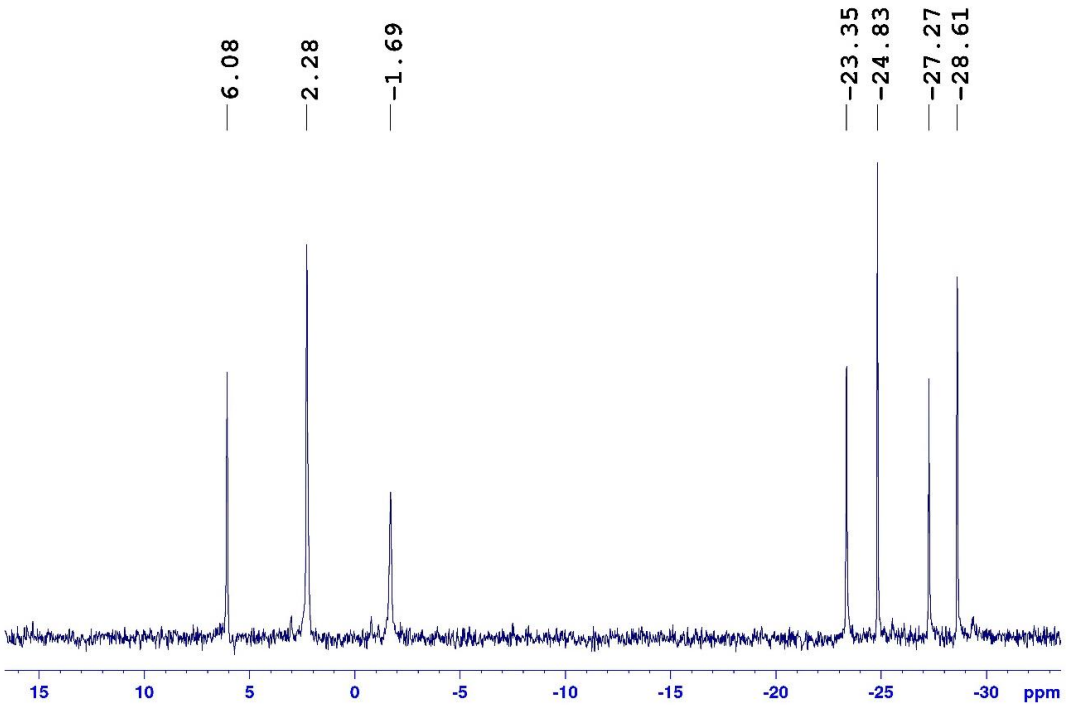


Fig. S8 ^{31}P NMR spectrum from the crude reactiin mixture of **3** and phenyl acetylene when the reaction was carried out at room temperature in benzene-D_6 at room temperature.

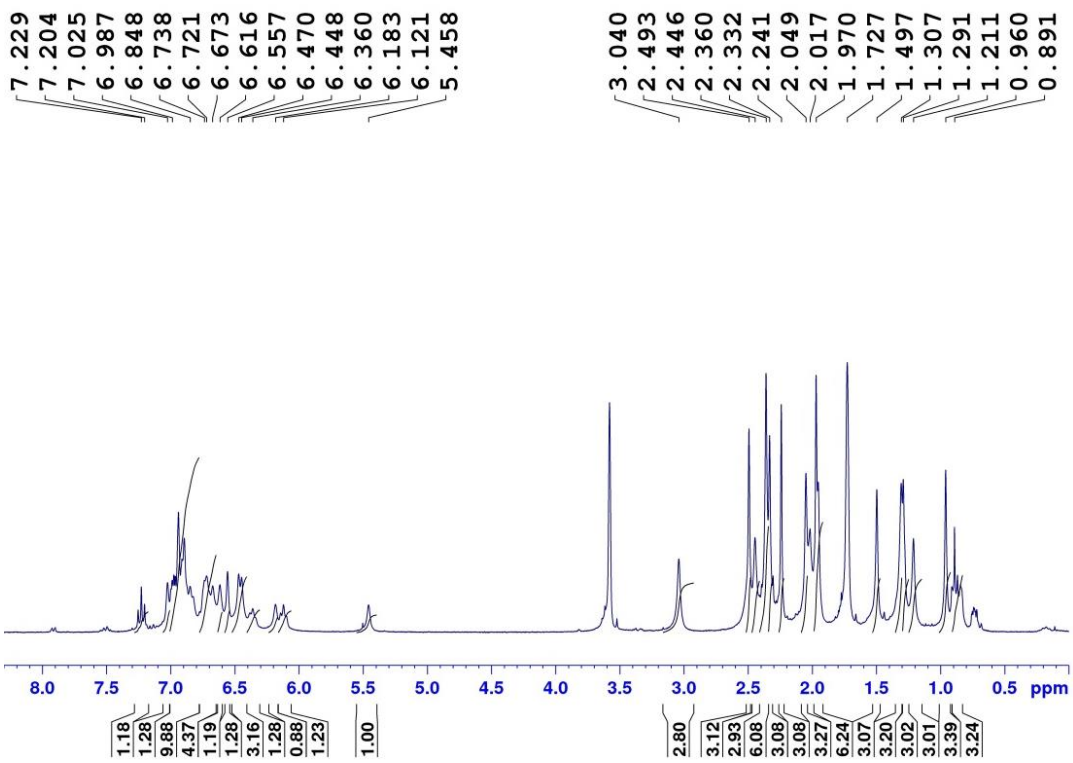


Fig. S9 ^{1}H NMR spectrum of **7** in THF-D_8 at room temperature.

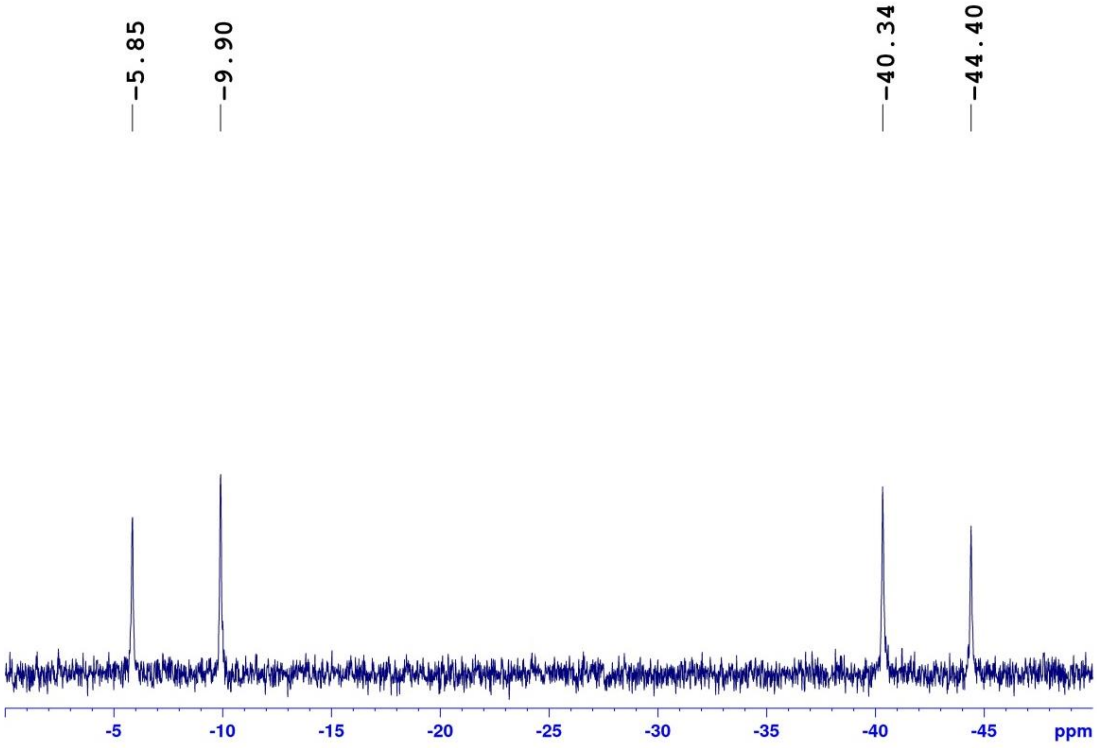


Fig. S10 ^{31}P NMR spectrum of **7** in THF-D_8 at room temperature.

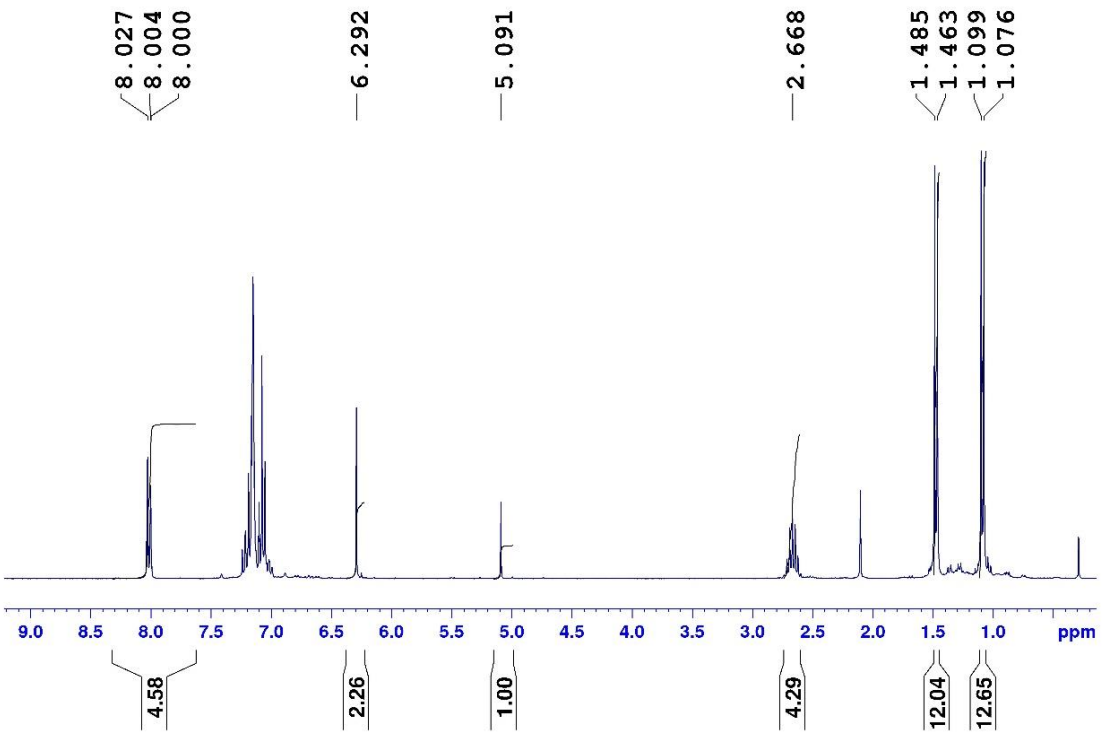


Fig. S11 ^{1}H NMR of 1:1 reation of **1a** with azobenzene in benzene-D_6 from crude reaction mixture at room temperature.

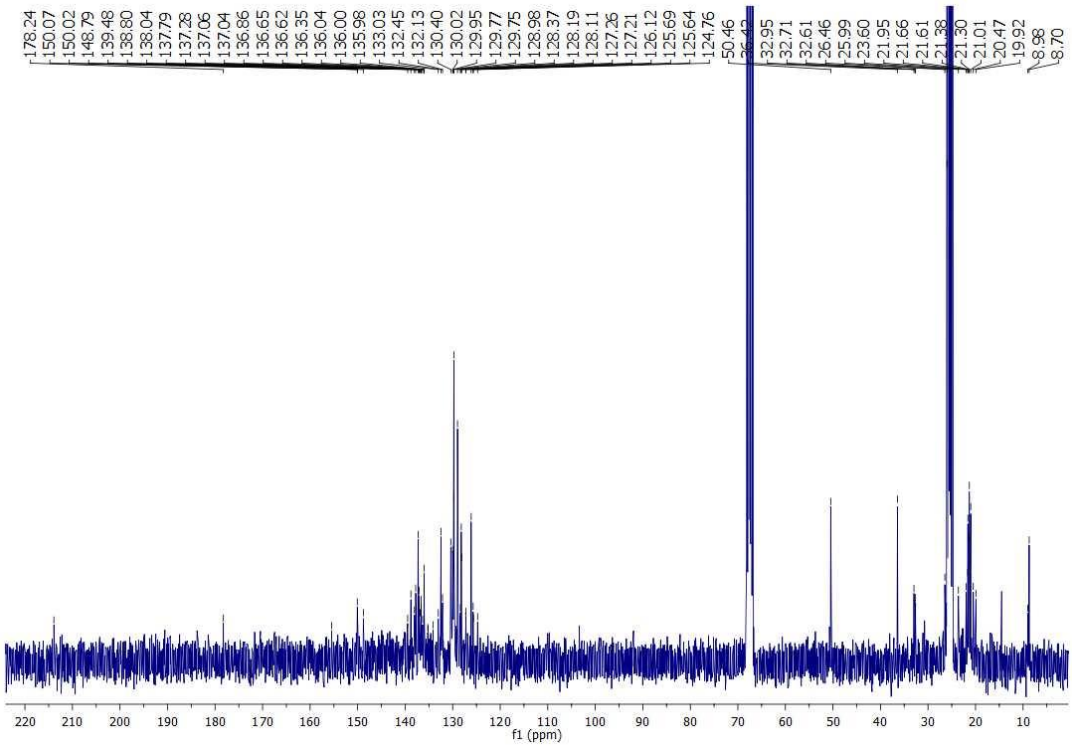


Fig. S12 $^{13}C\{^{1}H\}$ NMR spectrum of **4** in THF-D_8 at room temperature.

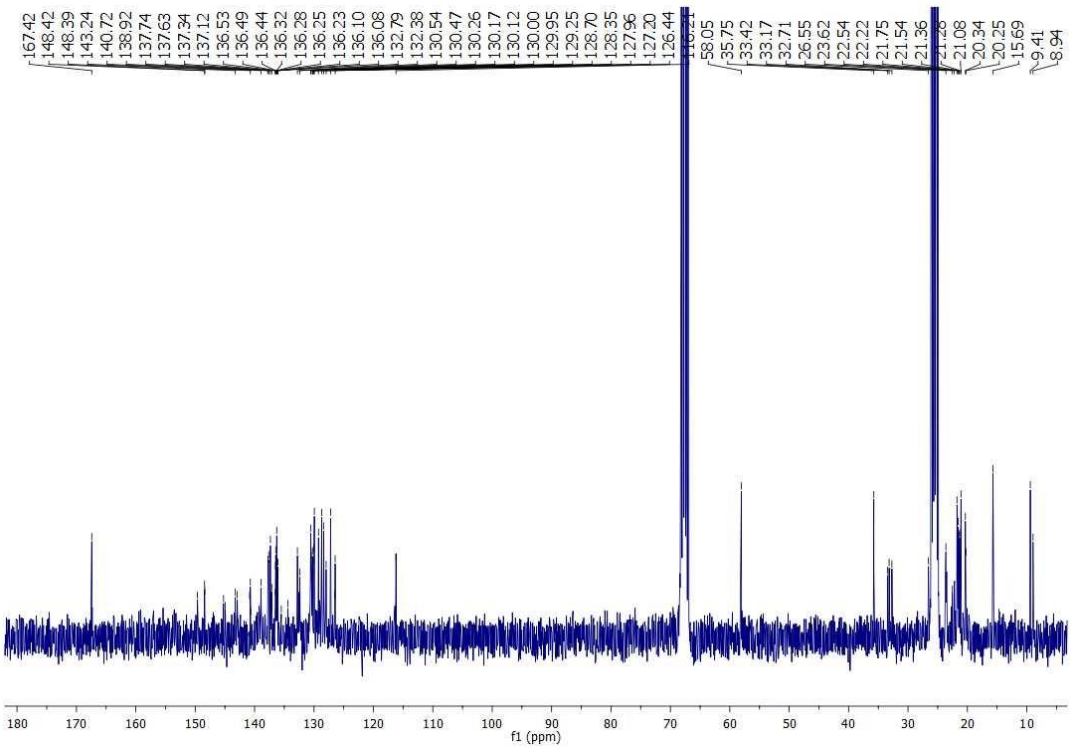


Fig. S13 $^{13}C\{^{1}H\}$ NMR spectrum of **5** in THF-D_8 at room temperature.

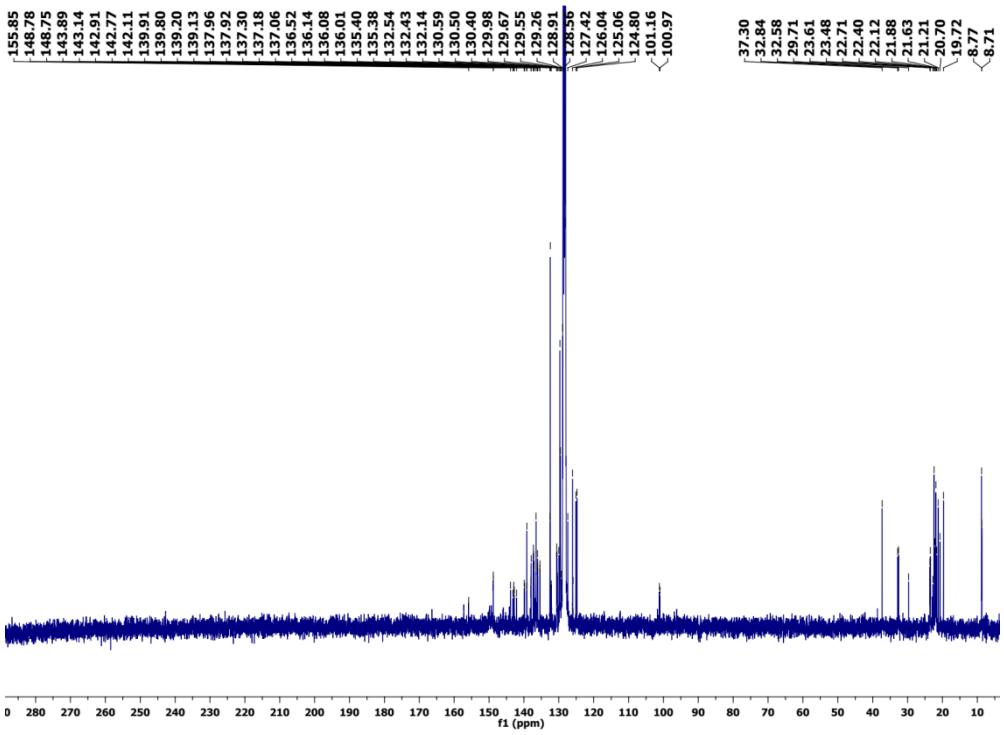


Fig. S14 $^{13}C\{^{1}H\}$ NMR spectrum of **6** in benzene-D_6 at room temperature.

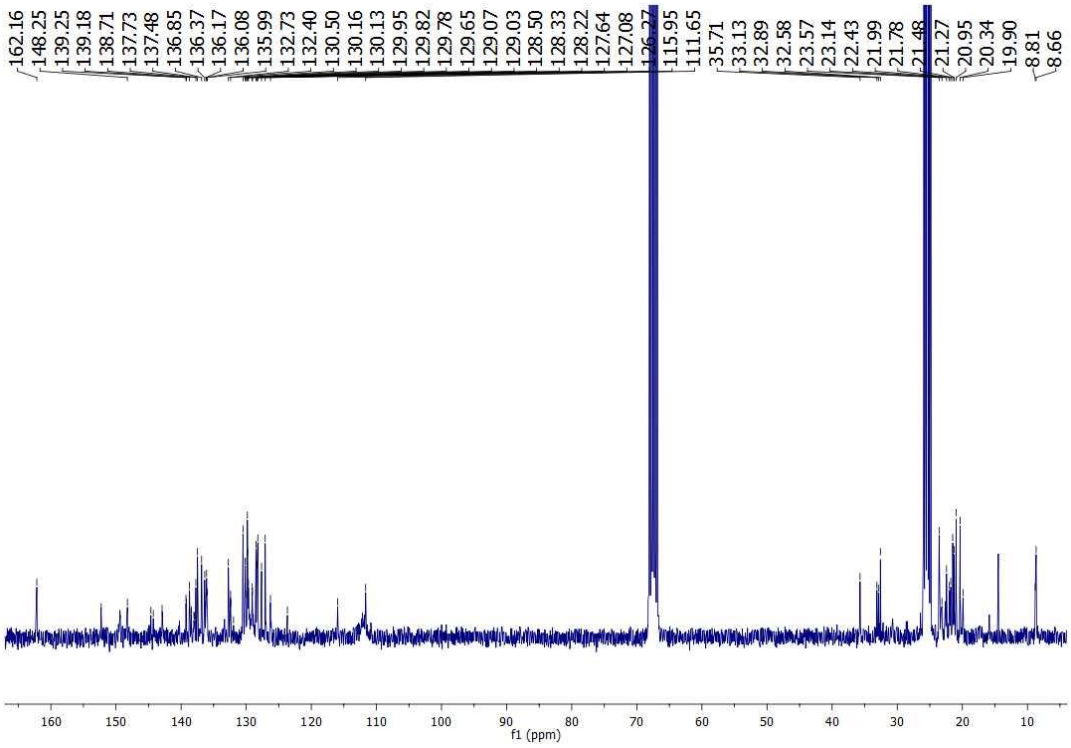


Fig. S15 $^{13}C\{^{1}H\}$ NMR spectrum of **7** in THF-D_8 at room temperature.

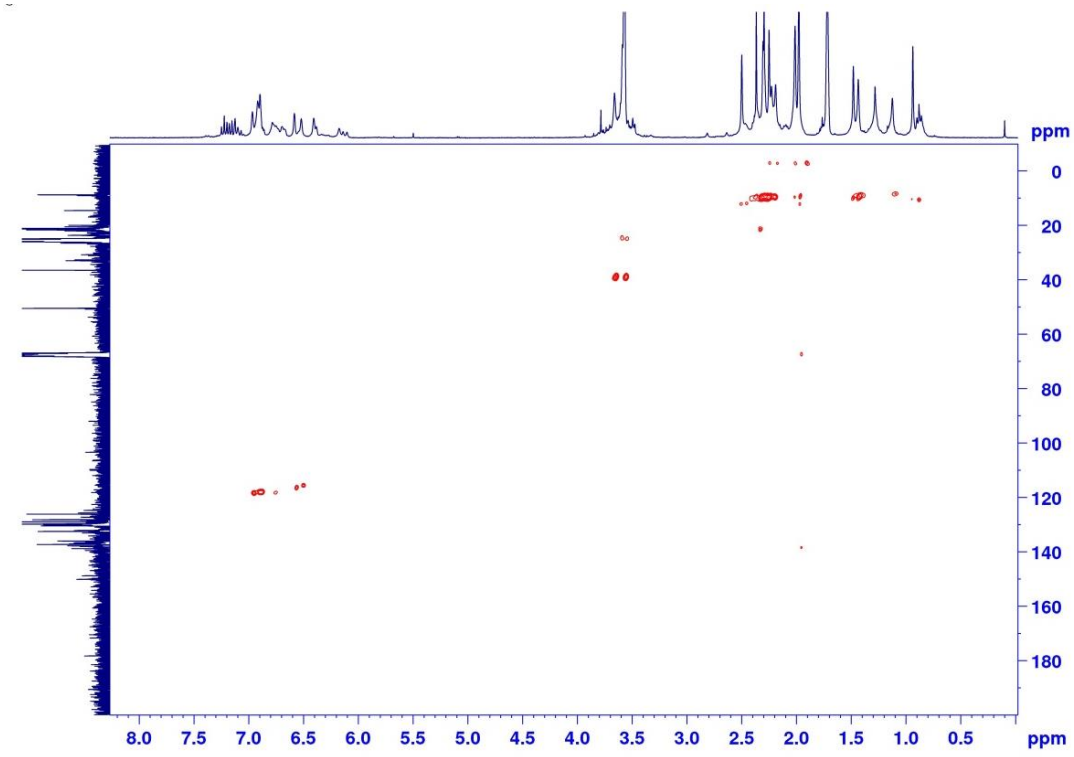


Fig 16 ^{1}H-$^{13}C\{^{1}H\}$ HSQC NMR spectrum of **4** in THF-D_8 at room temperature.

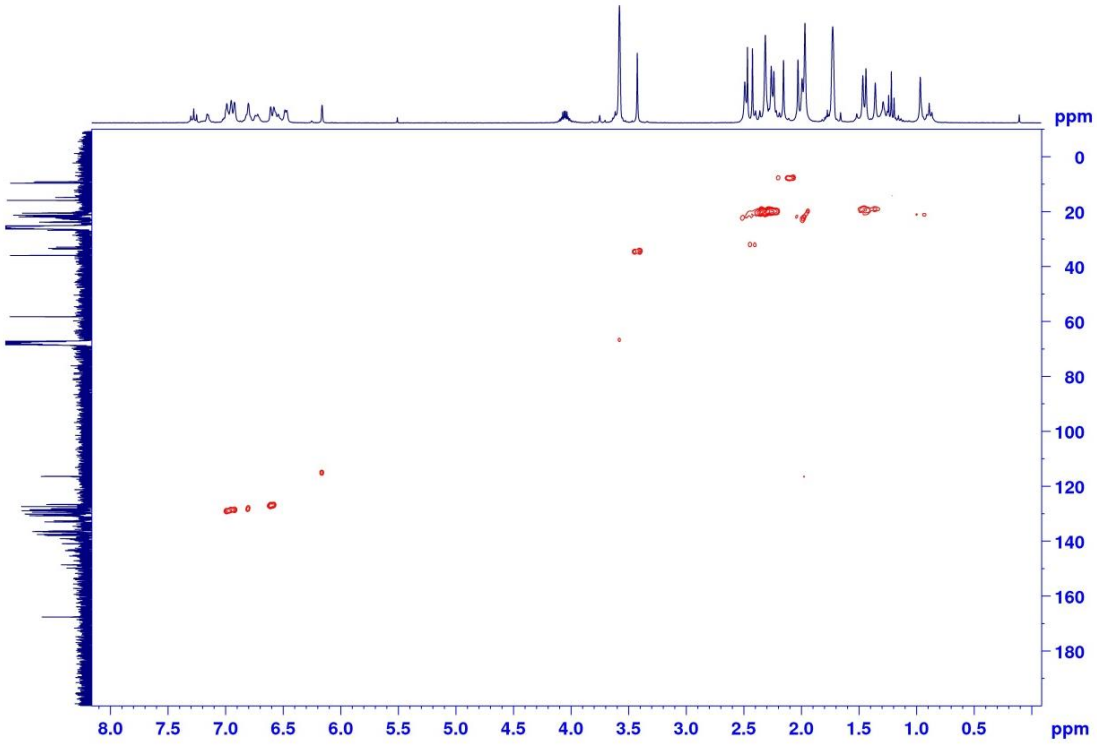


Fig 17 ^{1}H-^{13}C{^{1}H} HSQC NMR spectrum of **5** in THF-D_8 at room temperature.

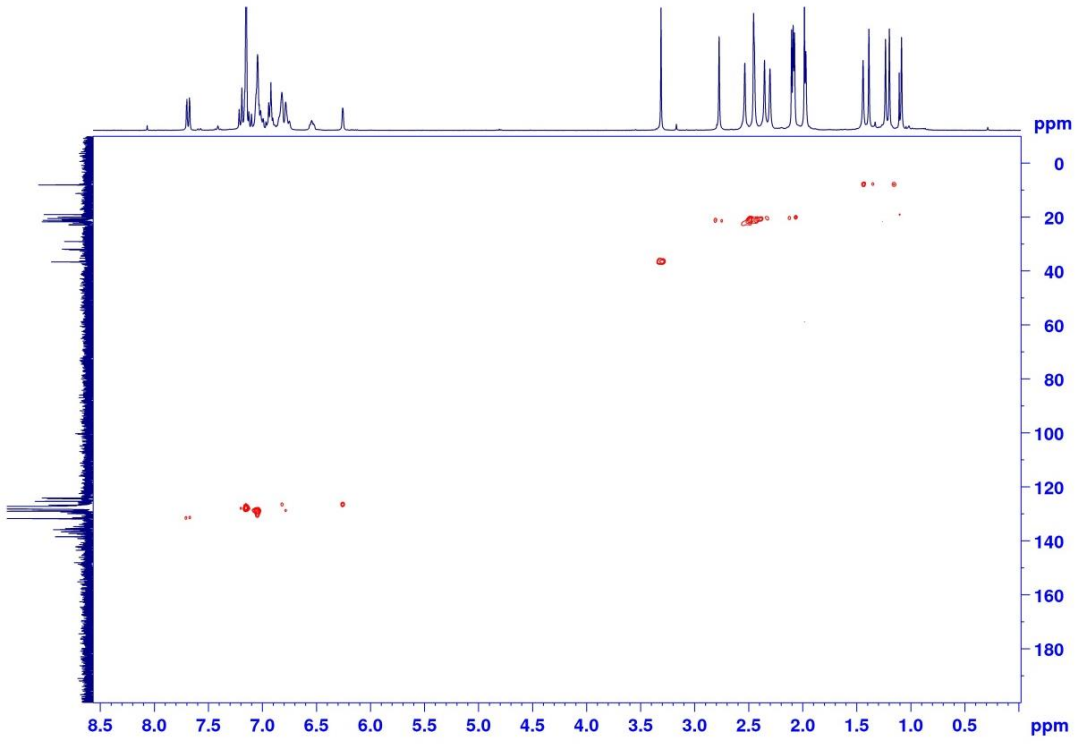


Fig 18 ^{1}H-^{13}C{^{1}H} HSQC NMR spectrum of **6** in benzene-D_6 at room temperature.

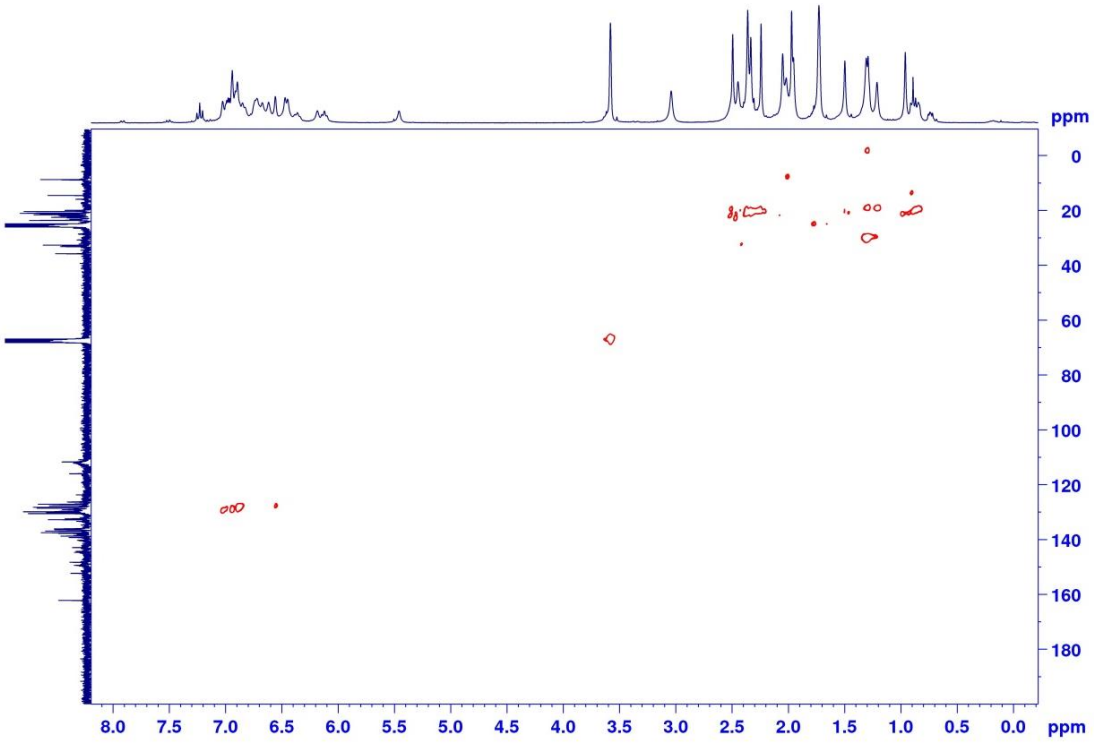


Fig 19 ^{1}H-$^{13}C\{^{1}H\}$ HSQC NMR spectrum of **7** in THF-D_8 at room temperature.

UV/Vis Spectra

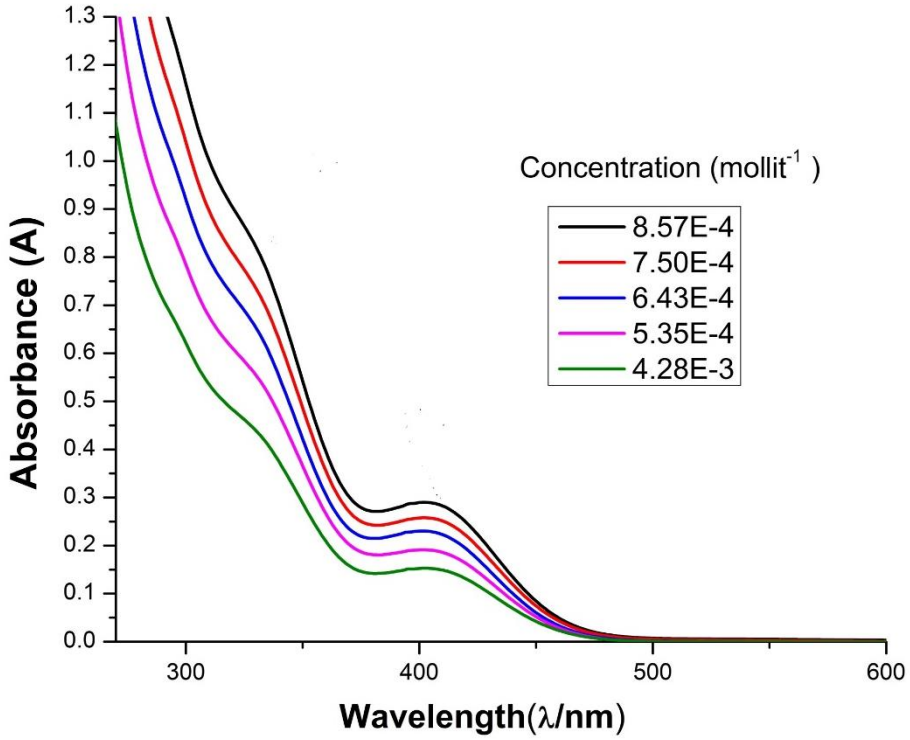


Fig. S20 UV/Vis spectra of **4** in THF at room temperature.

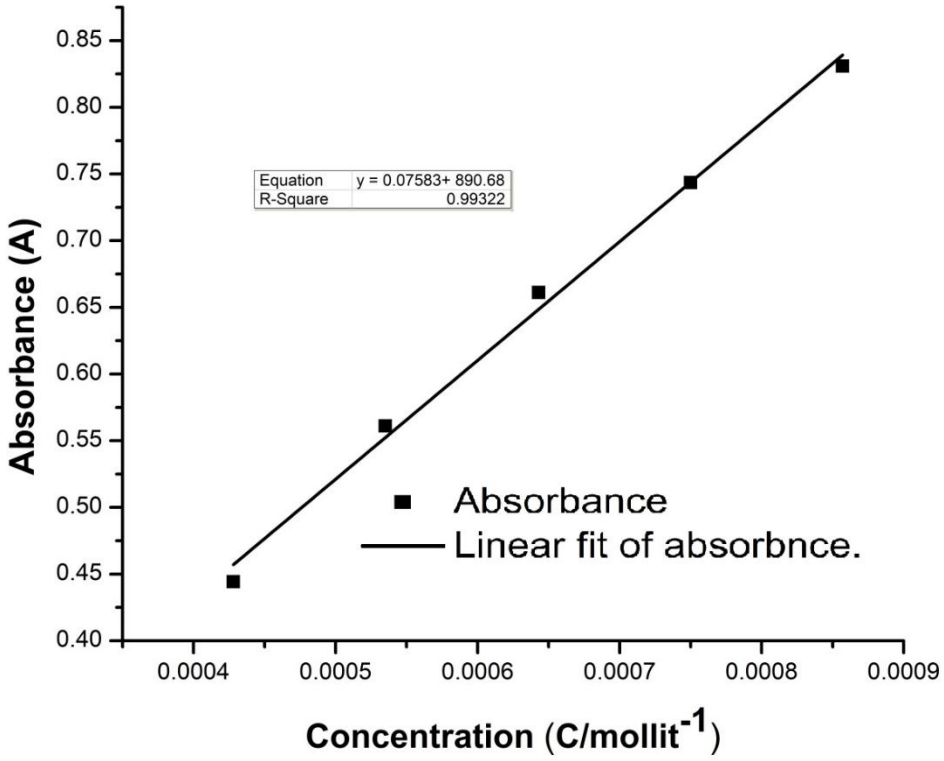


Fig. S21 Linear regression of **4** at 403 nm.

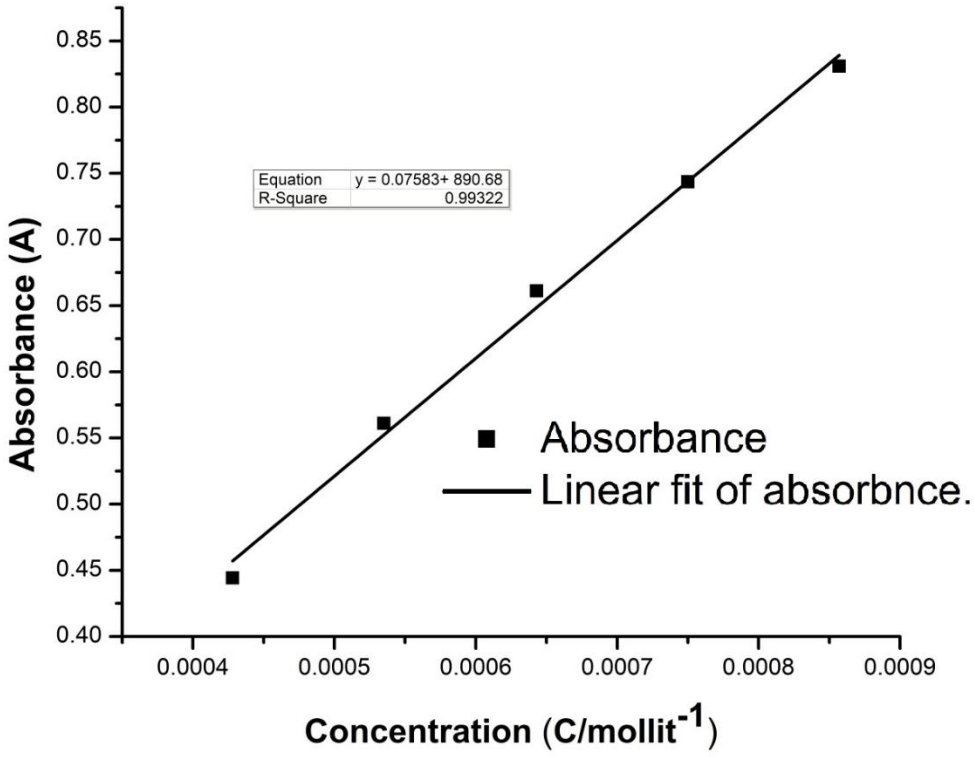


Fig. S22 Linear regression of **4** at 329 nm.

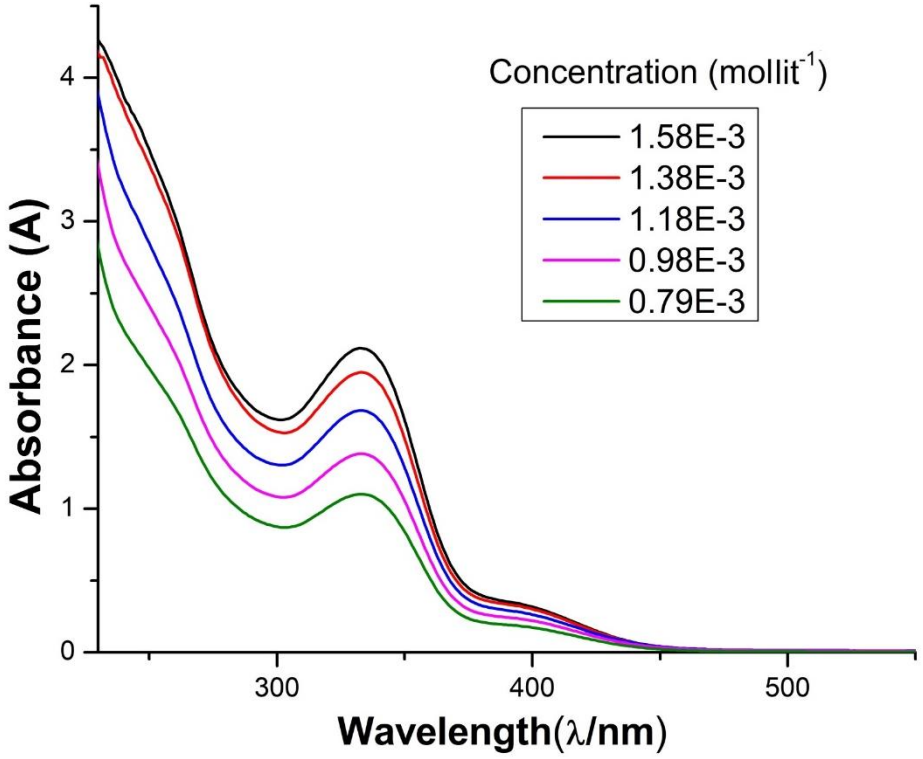


Fig. S23 UV/Vis spectra of **5** in THF at room temperature.

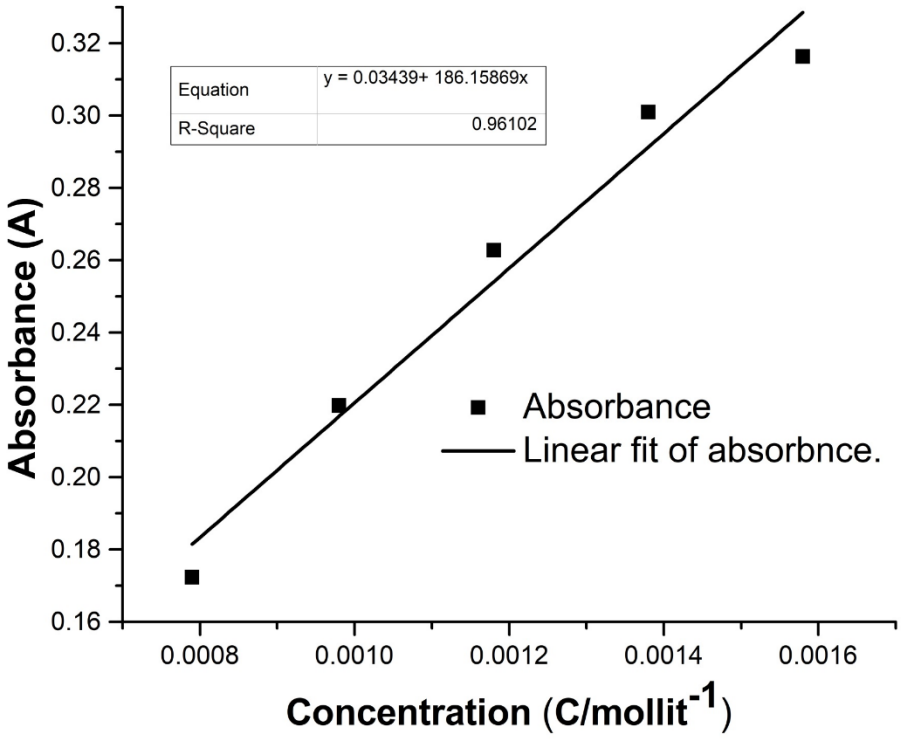


Fig. S24 Linear regression of **5** at 400 nm.

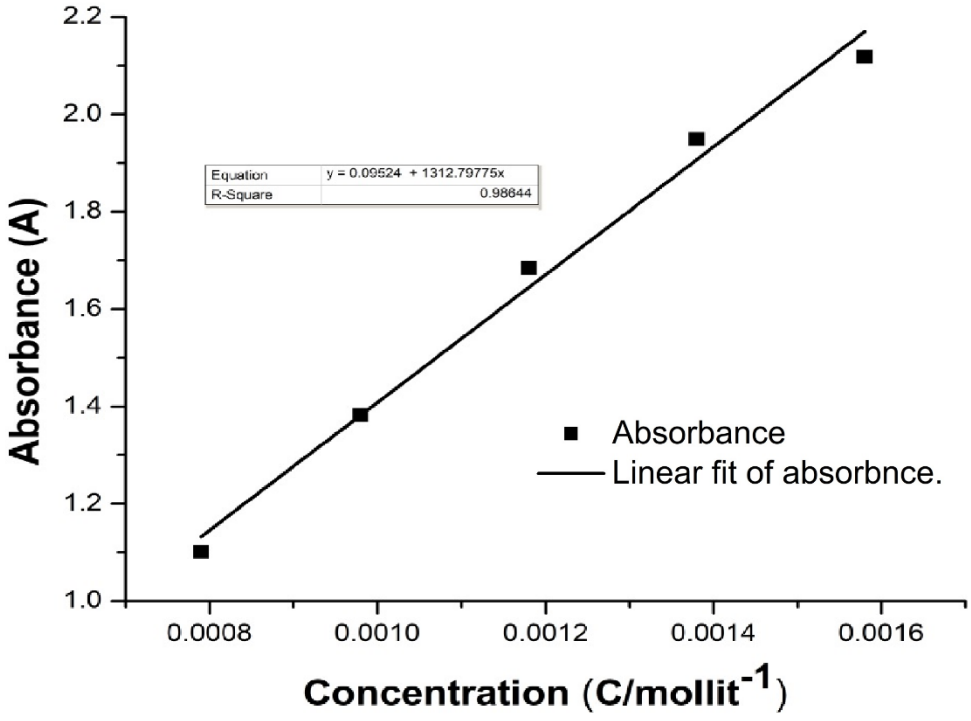


Fig. S25 Linear regression of **5** at 333 nm.

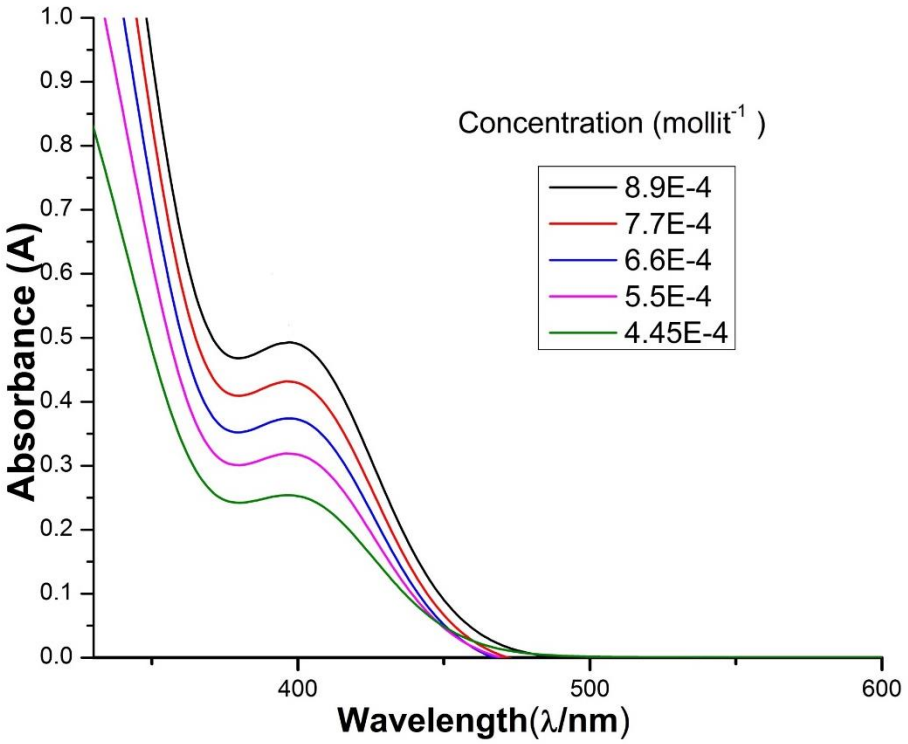


Fig. S26 UV/Vis spectra of **6** in THF at room temperature.

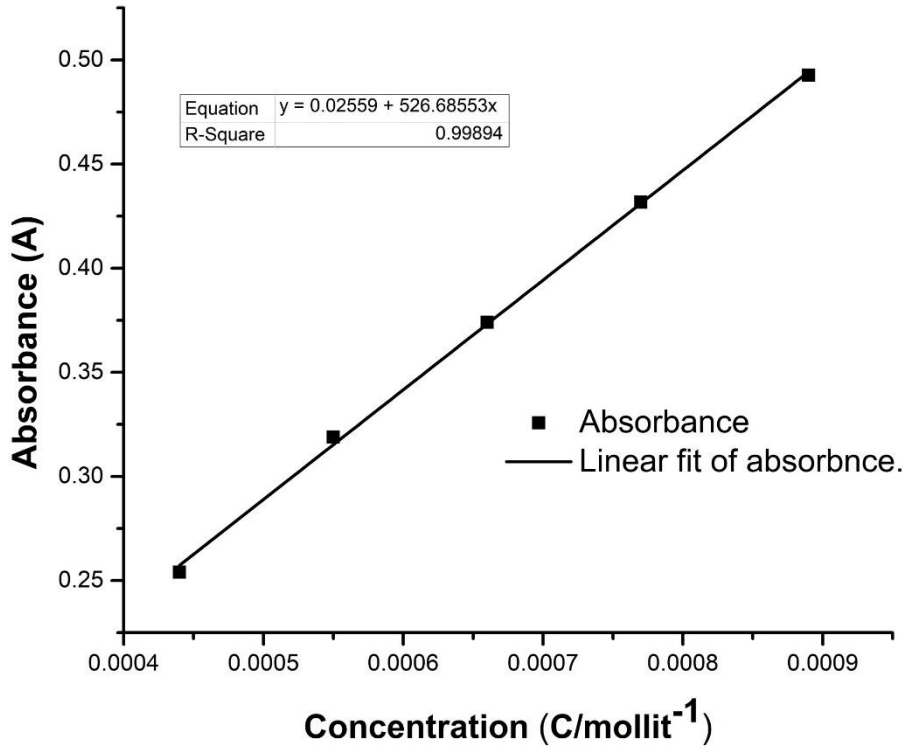


Fig. S27 Linear regression of **6** at 404 nm.

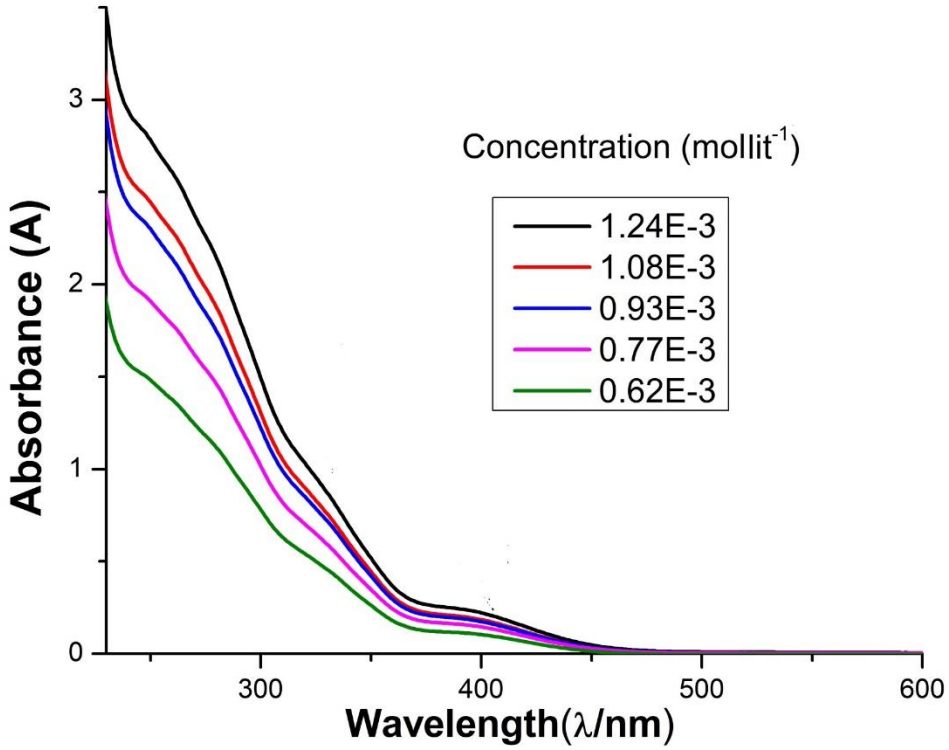


Fig. S28 UV/Vis spectra of **7** in THF at room temperature.

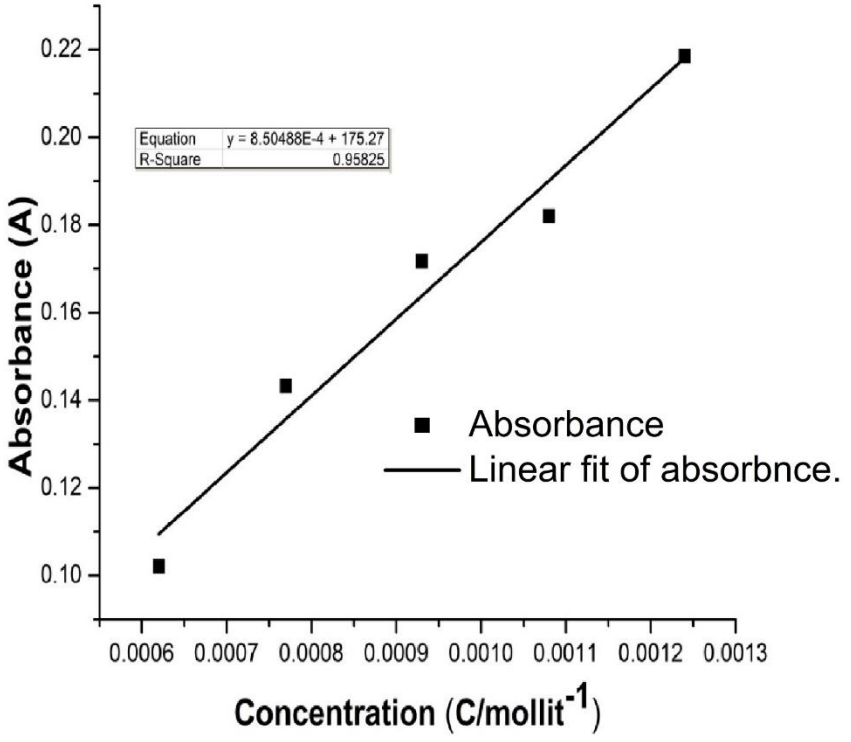


Fig. S29 Linear regression of **7** at 401nm.

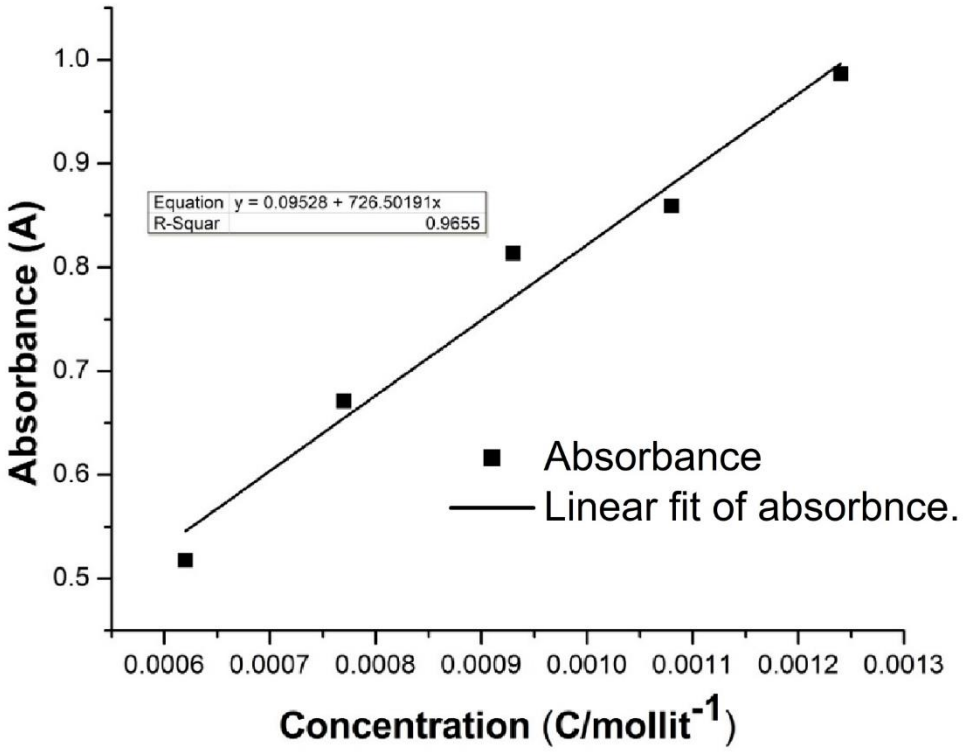


Fig. S30 Linear regression of **7** at 323 nm.

Crystallographic Details

Single crystal X-ray data of **4**, **5**, and **7** were collected at 120 K and **6** was collected at 293 K using a Rigaku XtaLAB AFC12 (RINC): Kappa single diffractometer with graphite-monochromated Mo Kα radiation, λ = 0.71073 Å. The unit cell parameters and the data reduction was obtained with the CrysAlisPro software from Rigaku Oxford Diffraction.[S3] A multi-scan absorption correction was applied to the collected reflections during data processing with SCALE3 ABSPACK also integrated in the CrysAlisPro software.[S4] The structure was solved by SHELXT[S4] structure solution program using Intrinsic phasing and refined by full matrix least-squares method based on F^2 using SHELXL[S5] refinement programme in the Olex-2 software.[S6] All non-hydrogen-atoms were refined with anisotropic displacement parameters. Hydrogens were placed in geometrically calculated positions or found in the Fourier difference map and include in the refinement process using riding model. The program Diamond (version 3.2k) is used for creating the crystallographic figures.[S7]

Table S1. Crystal data and structure refinement for **4** (CCDC: 1989684)

Identification code	AJ0690-1
Empirical formula	$C_{61}H_{69}AuN_2O_4P_2$
Formula weight	1153.08
Temperature/K	119.99(10)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	12.2527(3)
b/Å	18.7361(5)
c/Å	25.0944(7)
α/°	90
β/°	94.729(2)
γ/°	90
Volume/Å^3	5741.3(3)
Z	4
ρ_{calc}g/cm^3	1.334
μ/mm^{-1}	2.664
F(000)	2360.0
Crystal size/mm^3	0.13 × 0.12 × 0.11
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.196 to 50.054
Index ranges	-14 ≤ h ≤ 14, -22 ≤ k ≤ 22, -27 ≤ l ≤ 29
Reflections collected	71185
Independent reflections	10139 [R_{int} = 0.0515, R_{sigma} = 0.0350]
Data/restraints/parameters	10139/0/649
Goodness-of-fit on F^2	1.046
Final R indexes [I>=2σ (I)]	R_1 = 0.0445, wR_2 = 0.0941
Final R indexes [all data]	R_1 = 0.0552, wR_2 = 0.0979
Largest diff. peak/hole / e Å^{-3}	2.58/-1.85

Table S2. Crystal data and structure refinement for **5** (CCDC: 1989686)

Identification code	AJ0737
Empirical formula	$C_{59}H_{69}AuN_4O_2P_2$
Formula weight	1125.08
Temperature/K	119.97(10)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	18.5661(6)
b/Å	16.4929(5)
c/Å	18.7879(7)
α/°	90
β/°	109.411(4)
γ/°	90
Volume/Å^3	5426.0(3)
Z	4
ρ_{calc}g/cm^3	1.377
μ/mm^{-1}	2.815
F(000)	2304.0
Crystal size/mm^3	0.13 × 0.12 × 0.11
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.092 to 58.002
Index ranges	-23 ≤ h ≤ 24, -22 ≤ k ≤ 17, -25 ≤ l ≤ 20
Reflections collected	73725
Independent reflections	12845 [R_{int} = 0.1026, R_{sigma} = 0.0765]
Data/restraints/parameters	12845/439/588
Goodness-of-fit on F^2	1.062
Final R indexes [I>=2σ (I)]	R_1 = 0.0673, wR_2 = 0.1674
Final R indexes [all data]	R_1 = 0.0918, wR_2 = 0.1768
Largest diff. peak/hole / e Å^{-3}	2.07/-2.26

Table S3. Crystal data and structure refinement for **6** (CCDC: 1989685)

Identification code	AJ0664
Empirical formula	$C_{63}H_{67}AuN_2P_2$
Formula weight	1111.09
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	17.3820(9)
b/Å	17.2777(7)
c/Å	20.8054(11)
α/°	90
β/°	112.320(6)
γ/°	90
Volume/Å^3	5780.2(5)
Z	4
ρ_{calc}g/cm^3	1.277
μ/mm^{-1}	2.638
F(000)	2272.0
Crystal size/mm^3	0.14 × 0.13 × 0.12
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.066 to 50
Index ranges	-17 ≤ h ≤ 20, -20 ≤ k ≤ 19, -24 ≤ l ≤ 24
Reflections collected	47511
Independent reflections	10163 [R_{int} = 0.0845, R_{sigma} = 0.0782]
Data/restraints/parameters	10163/1/617
Goodness-of-fit on F^2	1.024
Final R indexes [I>=2σ (I)]	R_1 = 0.0543, wR_2 = 0.1268
Final R indexes [all data]	R_1 = 0.0857, wR_2 = 0.1383
Largest diff. peak/hole / e Å^{-3}	1.65/-1.02

Table S4. Crystal data and structure refinement for **7** (CCDC: 1989689)

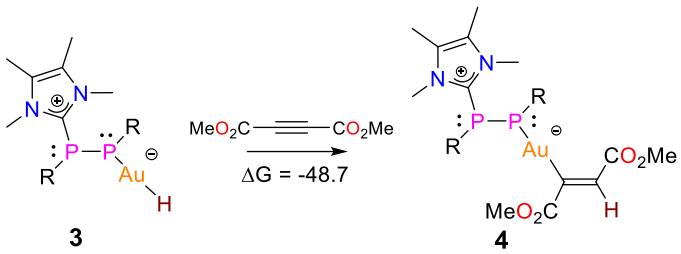
Identification code	AJ0721-1
Empirical formula	$C_{146}H_{158}Au_2N_8P_4$
Formula weight	2542.61
Temperature/K	120.02(10)
Crystal system	triclinic
Space group	P-1
a/Å	11.8644(2)
b/Å	21.3145(4)
c/Å	26.4459(6)
α/°	80.844(2)
β/°	81.813(2)
γ/°	86.997(2)
Volume/Å^3	6532.2(2)
Z	2
ρ_{calc}g/cm^3	1.293
μ/mm^{-1}	2.345
F(000)	2616.0
Crystal size/mm^3	0.13 × 0.12 × 0.11
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.61 to 58.046
Index ranges	-16 ≤ h ≤ 15, -28 ≤ k ≤ 28, -35 ≤ l ≤ 35
Reflections collected	113322
Independent reflections	30284 [R_{int} = 0.0608, R_{sigma} = 0.0777]
Data/restraints/parameters	30284/0/1473
Goodness-of-fit on F^2	1.032
Final R indexes [I>=2σ (I)]	R_1 = 0.0438, wR_2 = 0.0749
Final R indexes [all data]	R_1 = 0.0729, wR_2 = 0.0803
Largest diff. peak/hole / e Å^{-3}	0.70/-0.68

Computational Details

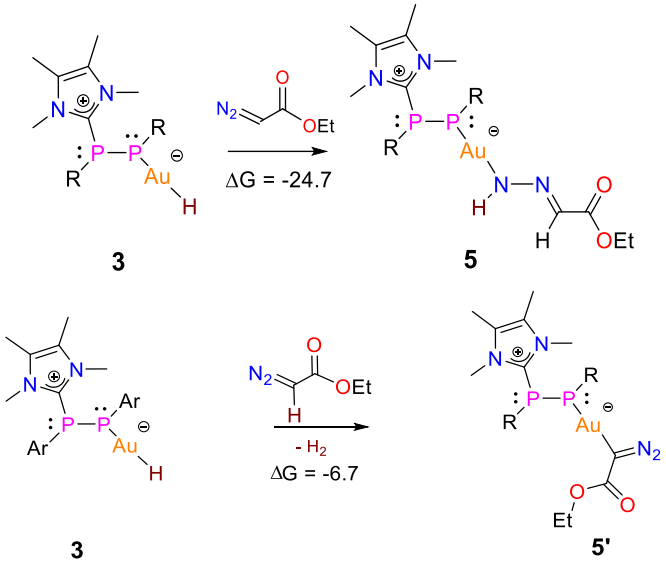
Gaussian 16 Rev B.01 and GaussView 5.0 package programs were used for all the calculations and visualizations for the considered structures, respectively.[S8,S9] Initially, all the geometries adopted from their X-ray structures were optimized using B3LYP functional with Grimme's D3 empirical dispersion correction.[S10-S13] The basis set of 6-31G(d,p) was chosen for the lighter atoms, H, C, N, O, and P, whereas LANL2DZ basis set was used for the Au atom. Selected bond lengths and angles of optimized and X-ray structures were compared and R^2 values (for selected bond lengths) were given to validate performance of the level of theory used herein (Figure S5). The stationary points were characterized as minima by harmonic vibrational frequency analysis. In the literature, the basis sets of SDD for Au and 6-31G(d,p) for lighter atoms with dispersion correction (D3) included DFT methods also show satisfying thermochemistry results for Au containing systems.[S14-S16] In order to get more accurate results for the electronic energies, we have performed single point frequency calculations for the optimized structures using M06-2X-D3 functional in combination with 6-31G(d,p) (for H, C, N, O, and P atoms) and SDD (for Au) basis sets.[S17,S18] Truhlar's SMD solvation model (Solvent = Toluene) was applied along with the corresponding single point calculations.[S19] Same strategy [optimization at B3LYP-D3/ LANL2DZ(Au)/ 6-31G(d,p)(H, C, N, O, and P) and thermochemistry at M06-2X-D3/SDD(Au)/ 6-31G(d,p)(H, C, N, O, and P)/SMD = Toluene] was applied to obtain possible reaction mechanisms for **3-Xyl** + **EDA** and **3-Xyl** + **DMDA** using simplified model systems [R = 2,6-Me_2-C_6H_3 (Xyl) instead of 2,6-Mes_2-C_6H_3]. To confirm the relationships between the local minimums and transition states, the intrinsic reaction coordinate (IRC) was employed.[S20] ΔG energies are given in kcal mol^{-1}.

Table S5. Selected bond lengths and angles, and R^2 values for bond lengths for comparison of theoretical and experimental results.

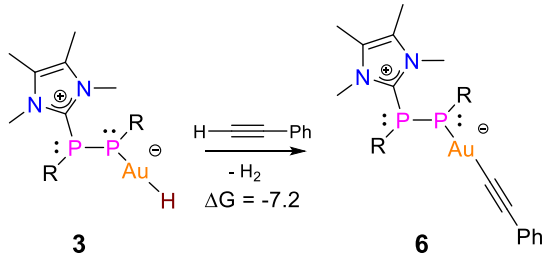
4			**5**		
	Exp.	**Theor.**		**Exp.**	**Theor.**
P1–P2	2.193	2.211	**P1–P2**	2.217	2.235
P1–Au1	2.307	2.378	**P1–Au1**	2.261	2.321
Au1–C56	2.069	2.080	**Au1–N3**	1.991	2.114
P1-C(Phenyl)	1.874	1.881	**N3–N4**	1.217	1.306
P2-C(NHC)	1.846	1.853	**P1-C(Phenyl)**	1.872	1.883
P2-C6(Phenyl)	1.865	1.878	**P2-C(NHC)**	1.834	1.852
N1(NHC)-C(NHC)	1.342	1.353	**P2-C6(Phenyl)**	1.873	1.877
N2(NHC)-C(NHC)	1.357	1.356	**N1(NHC)-C(NHC)**	1.350	1.357
C-C (back bond NHC)	1.351	1.367	**N2(NHC)-C(NHC)**	1.347	1.355
P2–P1–Au1	112.17	110.34	**C-C (back bond NHC)**	1.340	1.368
P1–Au1–C56	170.7	170.7	**P2–P1–Au1**	110.54	107.11
Au1-P1-P2-C(NHC)	35.0	35.0	**P1–Au1–N3**	168.0	172.4
			Au1-P1-P2-C(NHC)	-33.4	-35.9
R^2 for bond lengths		0.9980	**R^2 for bond lengths**		0.9878
6			**7**		
	Exp.	**Theor.**		**Exp.**	**Theor.**
P1–P2	2.206	2.229	**P1–P2**	2.205	2.230
P1–Au1	2.297	2.379	**P1–Au1**	2.263	2.330
Au1–C1	2.153	2.016	**Au1–N3**	2.067	2.103
C1-C2	1.139	1.228	**N3–N4**	1.414	1.402
P1-C(Phenyl)	1.868	1.884	**P1-C(Phenyl)**	1.873	1.881
P2-C(NHC)	1.837	1.860	**P2-C(NHC)**	1.844	1.846
P2-C6(Phenyl)	1.861	1.874	**P2-C6(Phenyl)**	1.872	1.876
N1(NHC)-C(NHC)	1.334	1.357	**N1(NHC)-C(NHC)**	1.349	1.355
N2(NHC)-C(NHC)	1.361	1.355	**N2(NHC)-C(NHC)**	1.349	1.354
C-C (back bond NHC)	1.352	1.368	**C-C (back bond NHC)**	1.371	1.369
P2–P1–Au1	108.43	104.01	**P2–P1–Au1**	114.26	110.6
P1–Au1–C1	171.5	172.0	**Au1-P1-P2-C(NHC)**	37.1	-34.0
Au1-P1-P2-C(NHC)	-31.7	-28.7			
R^2 for bond lengths		0.9762	**R^2 for bond lengths**		0.9983



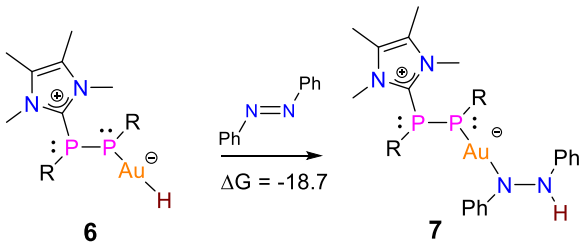
Scheme S1 Relative energy for the reaction of **3** with dimethyl acetylenedicarboxylate at the M06-2X-D3/6-31G(d,p)(SDD)//B3LYP-D3/6-31G(d,p)(LANL2DZ) level of theory.



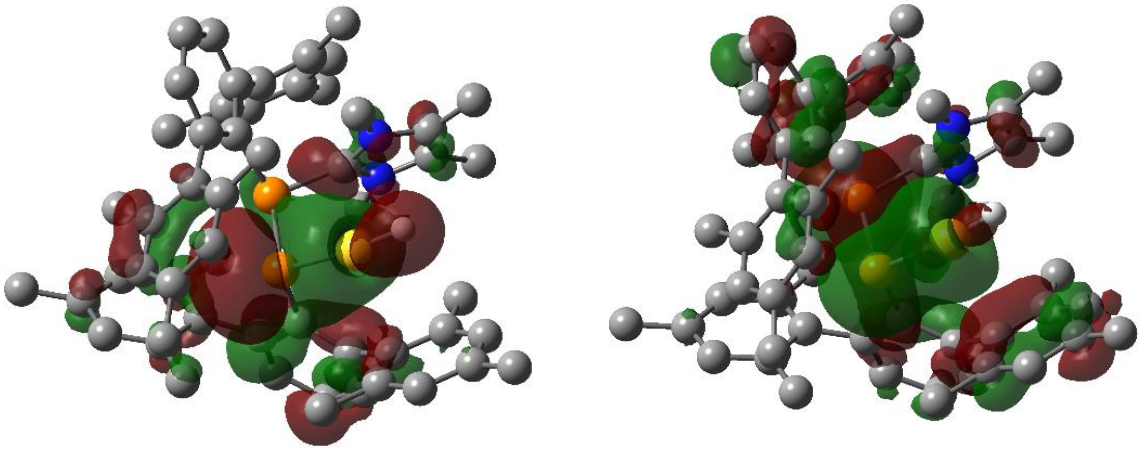
Scheme S2 Relative energy for the reactions of **3** with ethyl diazoacetate at the M06-2X-D3/6-31G(d,p)(SDD)//B3LYP-D3/6-31G(d,p)(LANL2DZ) level of theory.



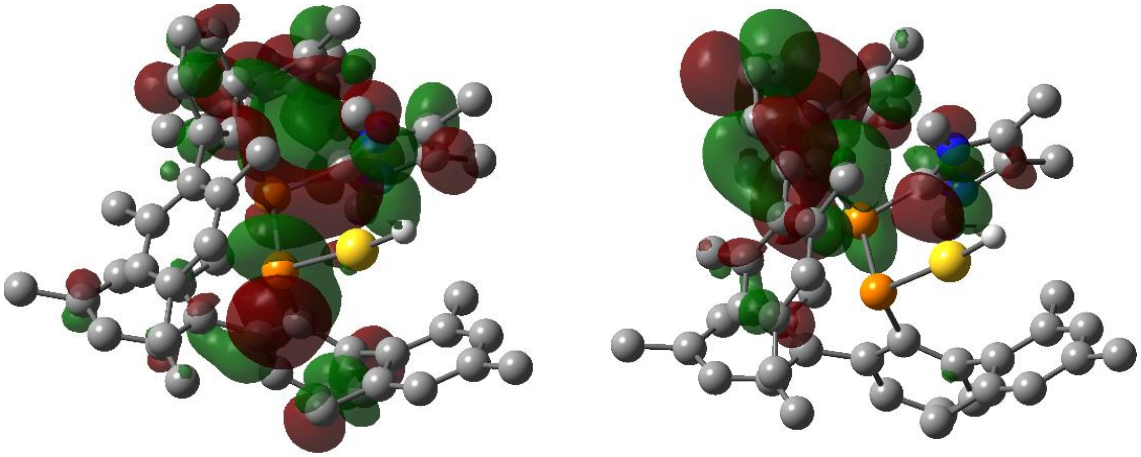
Scheme S3 Relative energy for the reaction of **3** with phenyl acetylene at the M06-2X-D3/6-31G(d,p)(SDD)//B3LYP-D3/6-31G(d,p)(LANL2DZ) level of theory.



Scheme S4 Relative energy for the reaction of **3** with azobenzene at the M06-2X-D3/6-31G(d,p)(SDD)//B3LYP-D3/6-31G(d,p)(LANL2DZ) level of theory.



HOMO **HOMO-1**



LUMO **LUMO+1**

Fig. S31 Frontier molecular orbitals of **3** (isovalue = 0.02 and hydrogen atoms except for Au-H are omitted for better clarity).

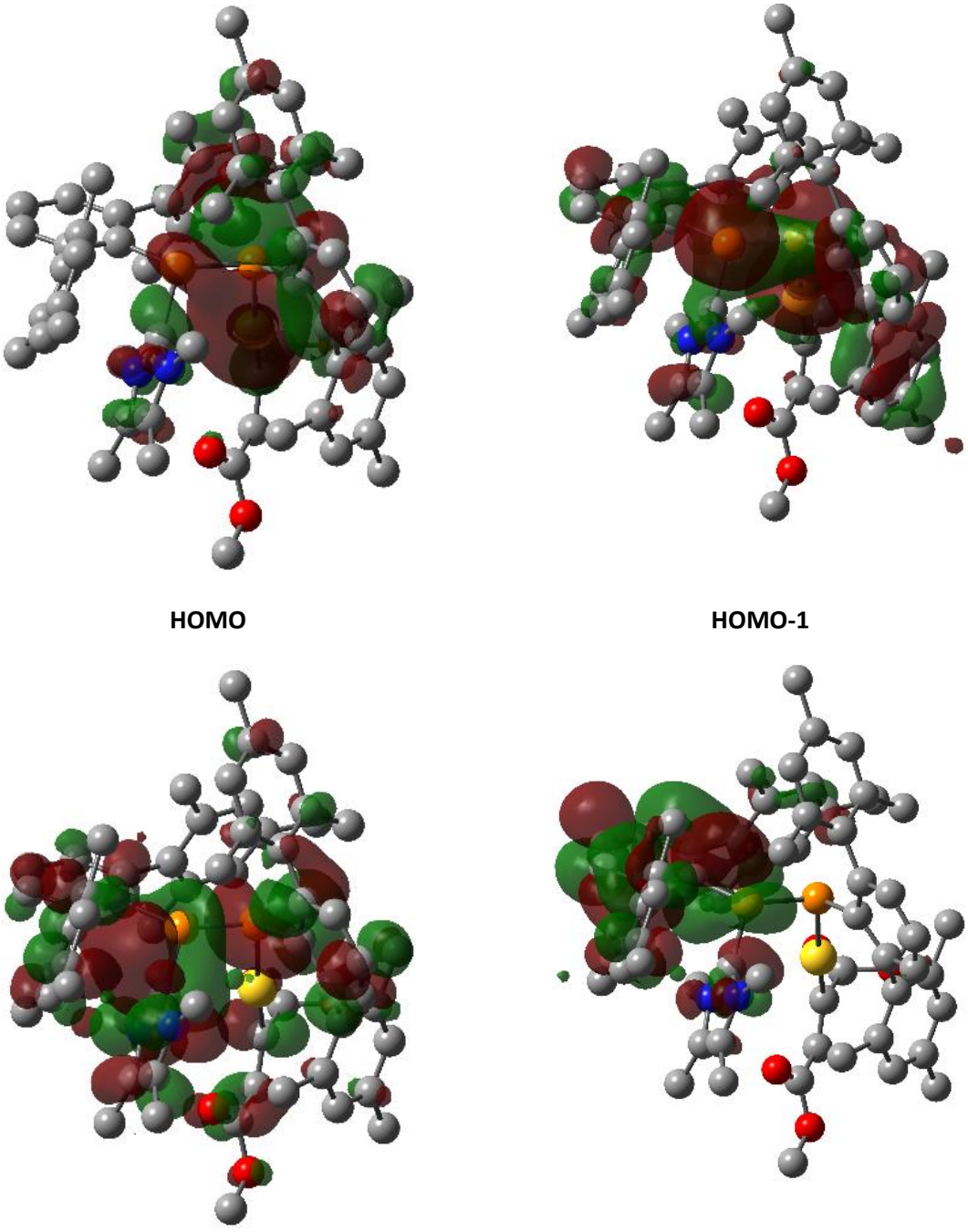
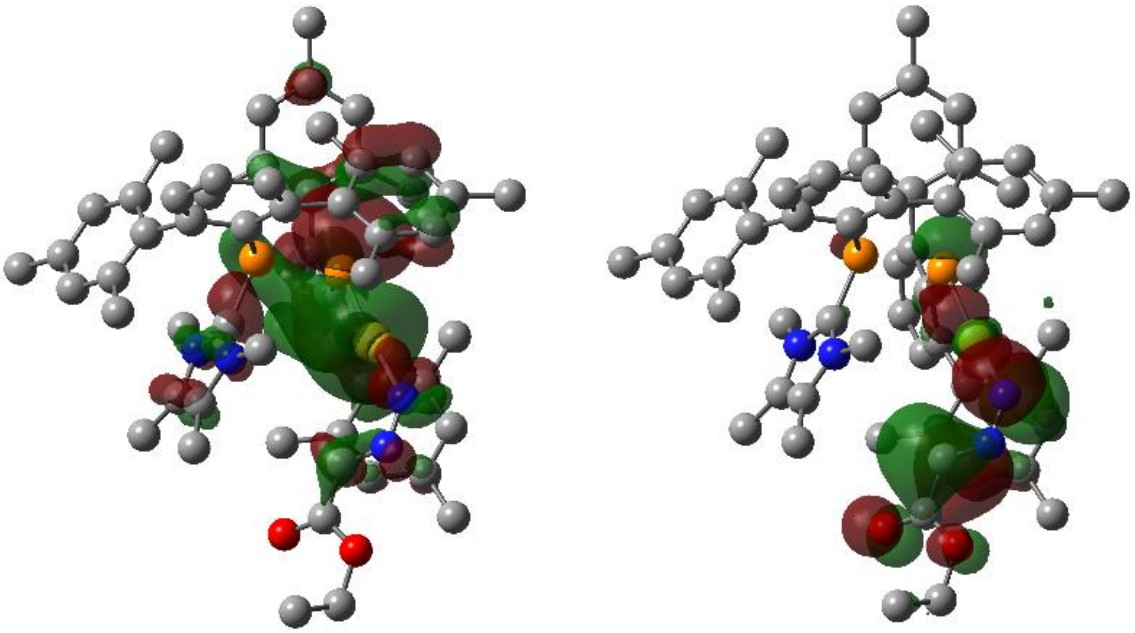
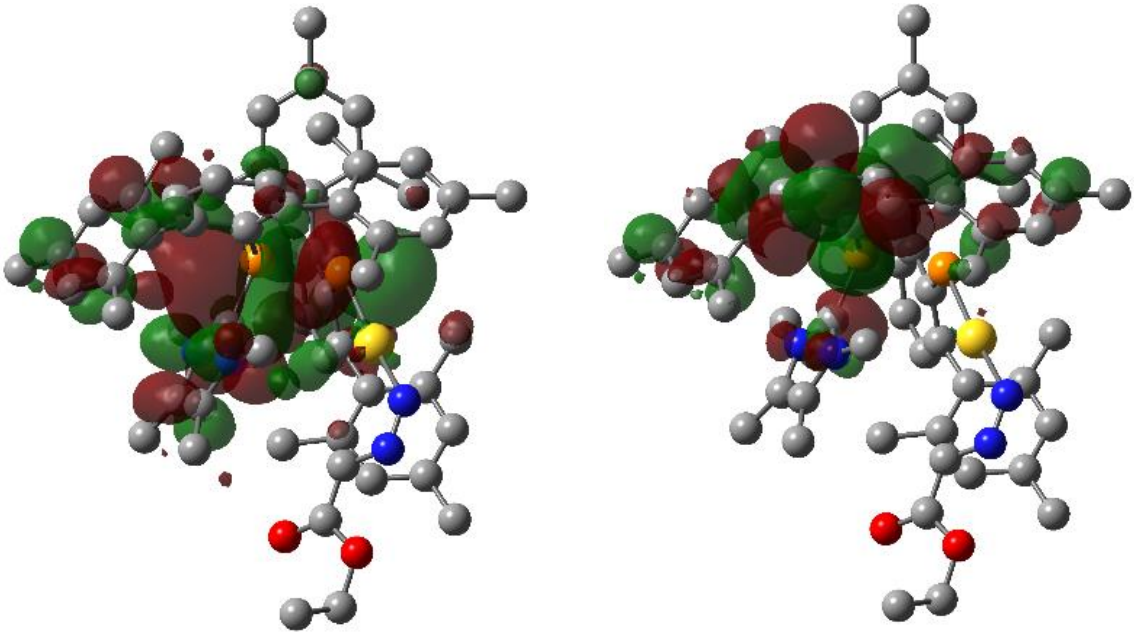


Fig. S32 Frontier molecular orbitals of **4** (isovalue = 0.02 and hydrogen atoms are omitted for better clarity).



HOMO **HOMO-1**



LUMO **LUMO+1**

Fig. S33 Frontier molecular orbitals of **5** (isovalue = 0.02 and hydrogen atoms are omitted for better clarity).

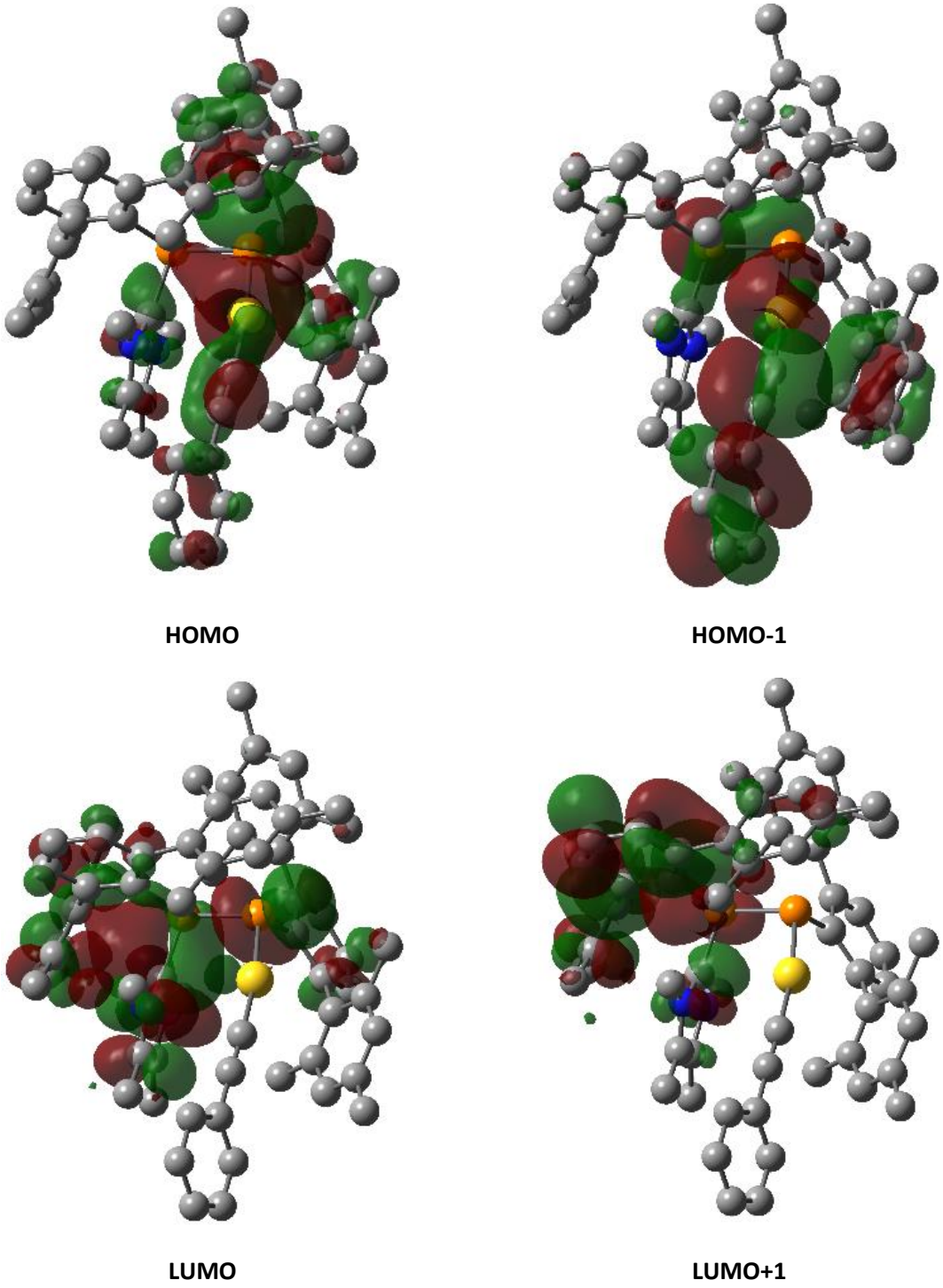
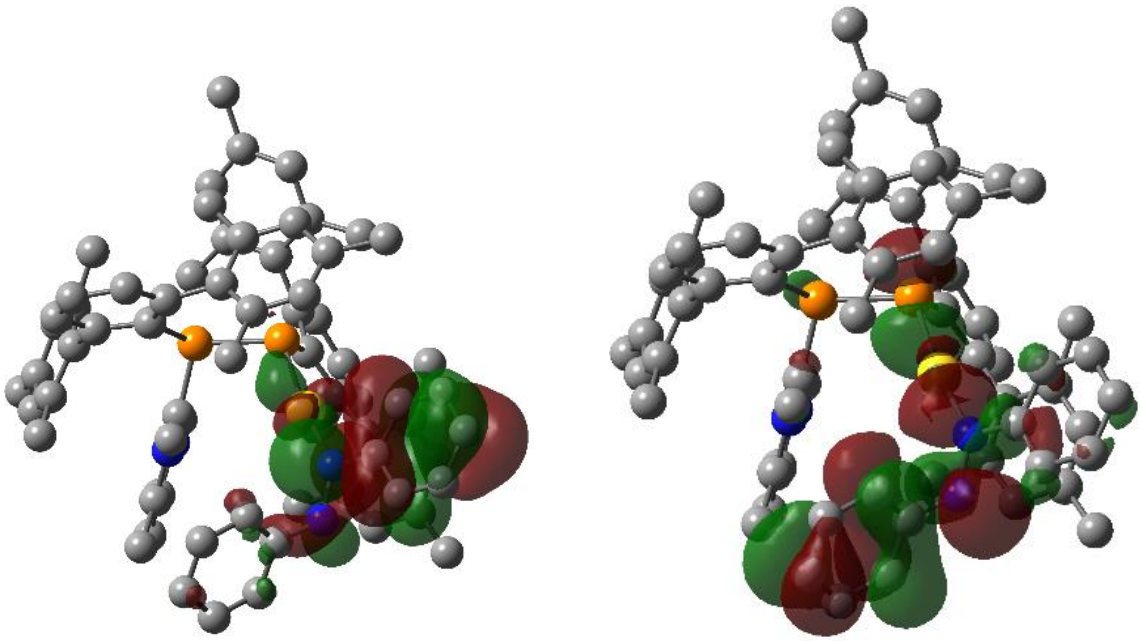
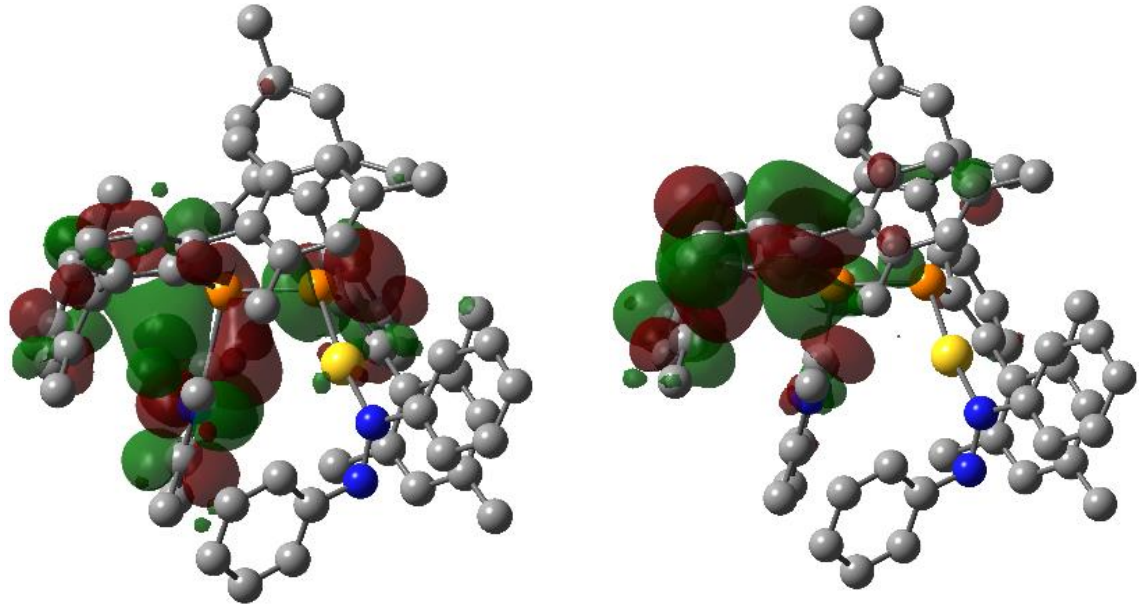


Fig. S34 Frontier molecular orbitals of **6** (isovalue = 0.02 and hydrogen atoms are omitted for better clarity).



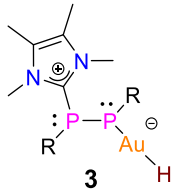
HOMO **HOMO-1**



LUMO **LUMO+1**

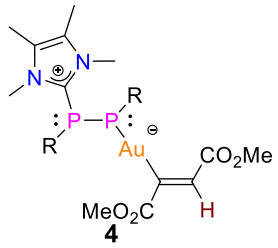
Fig. S35 Frontier molecular orbitals of **7** (isovalue = 0.02 and hydrogen atoms are omitted for better clarity).

Summary of frontier molecular orbitals of 3-7



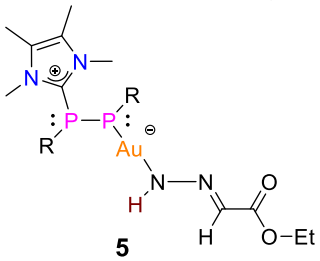
3

HOMO comes mainly from the Au−H *σ*-bond and nonbonding electrons of Au-coordinated P atom.
HOMO-1 concentrated over Au-P bond and P–P unit which correspond to the *s*-type lone pairs.
LUMO is mainly localized over the NHC-P unit and Au-coordinated P atom.



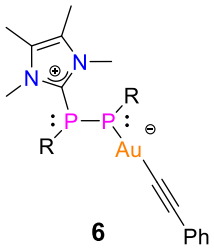
4

HOMO comes mainly from the Au−C *σ*-bond and nonbonding electrons of Au-Coordinated P atom.
HOMO-1 is concentrated over Au-P bond and P–P unit which correspond to the *s*-type lone pairs.



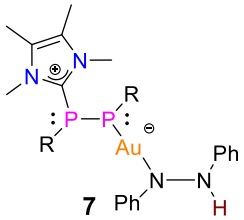
5

HOMO is mostly composed of nonbonding electrons of Au-coordinated P atom and Au-N bond.
HOMO-1 is mostly distributed on Au-P and Au-N bonds.
LUMO is mostly located over NHC-Au moiety.



6

HOMO is mostly composed of nonbonding electrons of Au-coordinated P atom, Au-C, and C-C *π*-bonds.
HOMO-1 is predominantly localized over Au-P bond, P-P unit, and *π*-bonding orbitals of ethynylbenzyl moiety.
LUMO is mainly dominated by NHC-P unit and Au-coordinated P atom.



7

HOMO is situated over Au-N bond and across the N-N bond.
HOMO-1 is mainly delocalized through both Au-N and NHC-Au bonds.
LUMO is mainly localized over the NHC-P unit and Au-coordinated P atom.

Proposed reaction mechanism for the formation of 4 from 3 and DMDA

The formation of *Z*-alkene isomer **4** can be envisaged to proceed by two different pathways: (i) a concerted *syn*-addition of the Au-H moiety to the C-C triple bond of DMDA followed by the rearrangement to **4** and (ii) a stepwise reaction through initial hydride transfer from Au-H to C-centre of the C-C triple bond of DMDA to yield an intermediate and then subsequent intramolecular reorientation of the remaining quasi-dicoordinate carbon atom of DMDA towards the Au-centre. Truncated model systems based on R = 2,6-Me_2-C_6H_3 (Xyl) instead of 2,6-Mes_2-C_6H_3 were considered for the modelling of the reaction mechanisms.

The optimization of the anticipated transition state for *syn*-addition results in **TS1**, which shows a dominating coordination of the hydrogen end of the Au(I) hydride to one of the alkyne C atoms (d_{CH} = 1.680 Å for **TS1**; 1.619 Å for **3-Xyl**) and a relatively weaker interaction of the Au-centre with the other (d_{AuC} = 1.672 Å). According to the calculated internal reaction coordinate **TS1** relaxes to *Z*-**4-Xyl** (Fig. S36), which resembles the proposed mechanism of the reaction of (C_5Me_5)Rh(PMe_3)H_2 with different internal alkynes as described by Jones *et al*.[S21] A saddle point of the potential energy surface (at point 33 of the IRC plot, circled in red in Fig. S37) on the way to product *Z*-**4-Xyl** could not be optimized to an additional intermediate at this level of theory, which received further support by a reverse IRC calculation back to **TS1**.[S22] The Gibbs energy barrier for the process corresponding to **TS1** is determined to $\Delta G^{\neq}$ = 12.3 kcal mol^{-1} and thus in line with a reaction proceeding a low temperature. Overall, the formation of the final product *Z*-**4-Xyl** turns out to be decidedly exergonic by ΔG = −47.1 kcal mol^{-1}.

We also considered the (step-wise) formation of the first unobserved *E*-alkene and then its isomerization: the hydride transfer from the Au(I) hydride to **DMDA** may yields the hypothetical intermediate **Int1**, which is lower in energy than **3-Xyl+DMDA** by ΔG = −19.3 kcal mol^{-1} (Fig. S38). The formation of the C-Au bond in *E*-**4-Xyl** occurs via the transition state **TS2** associated to a negligible energy barrier of $\Delta G^{\neq}$ = 2.2 kcal mol^{-1}. Then we tried the isomerization of *E*-**4-Xyl** to *Z*-**4-Xyl** considering the rotation about C=C double bond. However, we were not able to find any TS structures by considering the Au-C-C-H dihedral angle in the range of 85–110° and the C–C bond length in the range of 1.400–1.550 Å.

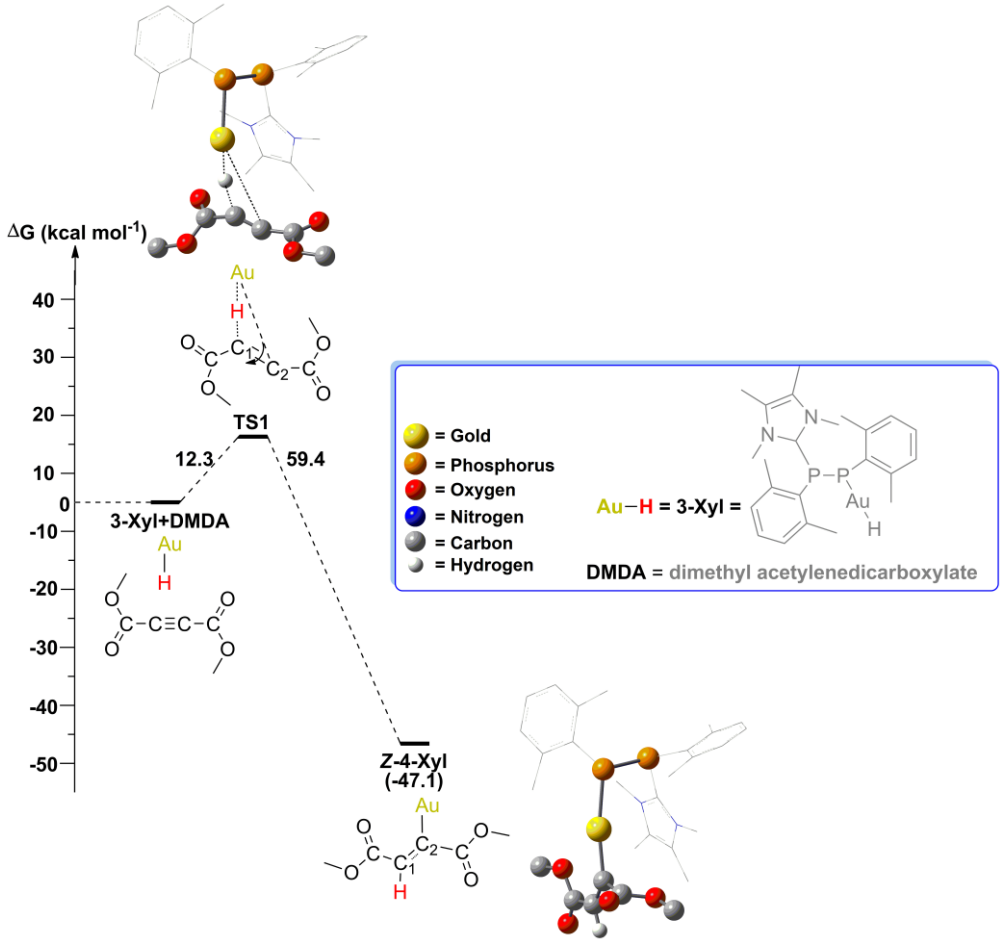


Fig. S36 Proposed reaction mechanism for the formation of *Z*-**4-Xyl** considering concerted pathway. Energy barriers are on the dashed lines. Relative energies are given in parentheses.

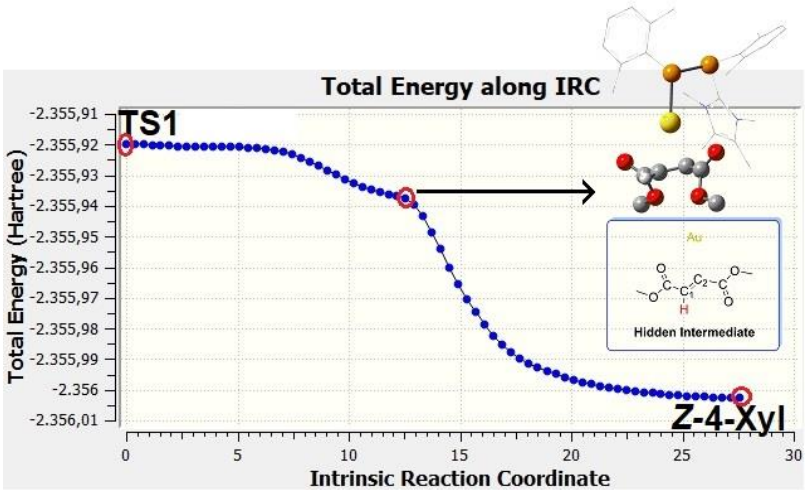


Fig. S37 The IRC plot for **TS1**.

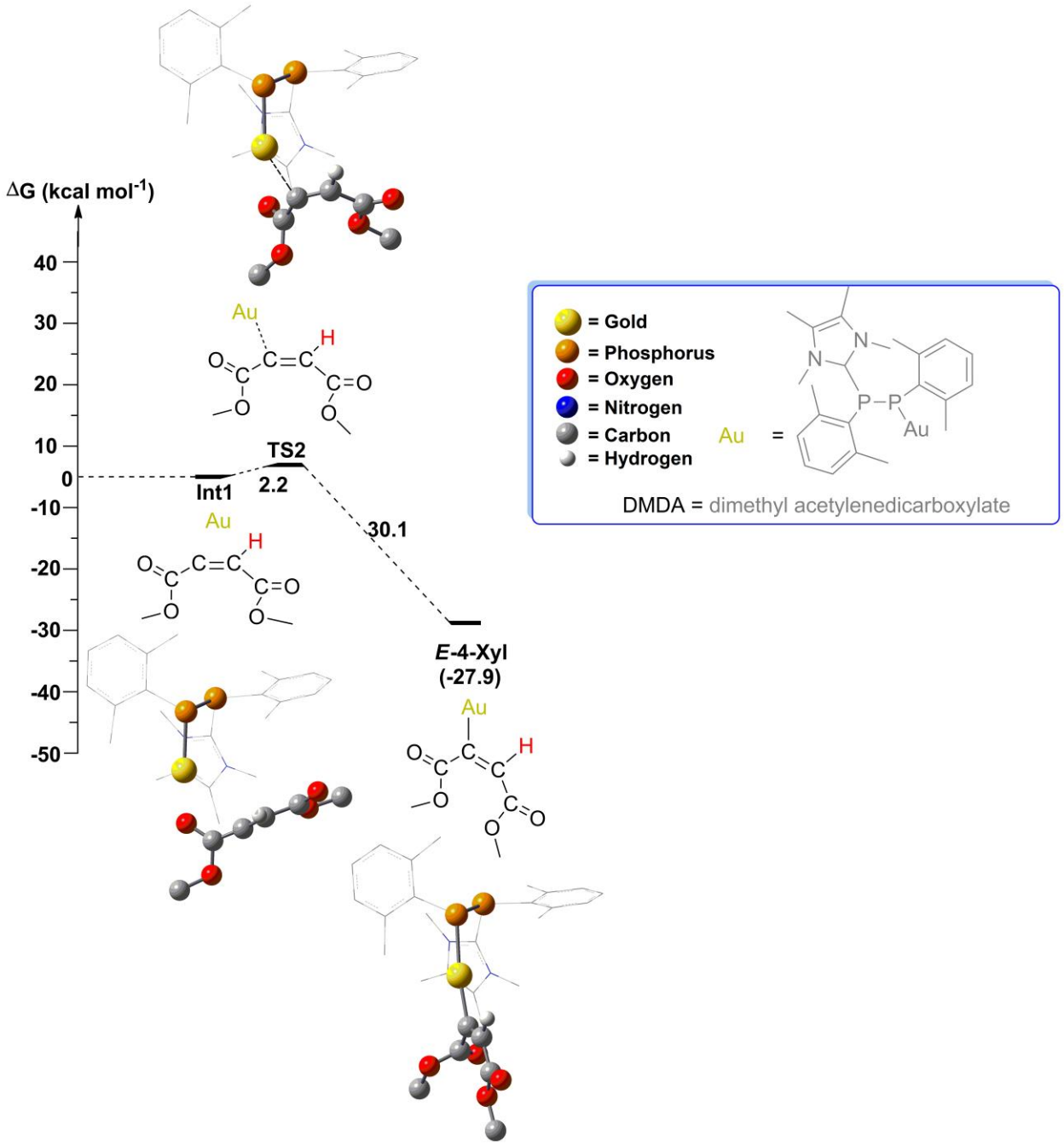


Fig. S38 Proposed reaction mechanism for the formation of *E*-**4-Xyl** via **Int1**. Energy barriers are on the dashed lines. Relative energies are given in parentheses.

Proposed reaction mechanism for the formation of 5 and 5' (dehydrogenative product) from 3 and EDA

The formation mechanism of **5** from the reaction of **3** with **EDA** was elucidated by DFT calculations on truncated model systems with R = 2,6-Me_2-C_6H_3 (Xyl) instead of 2,6-Mes_2-C_6H_3. The HOMO of EDA is mainly localized at the *α*-carbon atom and the terminal nitrogen atom (N1). Possible pathways via interaction of Au-H moiety with the *α*-carbon atom of EDA to form **5-Xyl** (Fig. S39) as well as the unobserved dehydrogenative coupling product **5'-Xyl** (Fig. S40) can be excluded on the basis of relatively high energy barriers as compared to the reaction mechanism through end-on nitrogen insertion across the Au-H bond (Fig. S41).

In the first step of the formation **5-Xyl** via the interaction of Au-H moiety with the *α*-carbon atom, the hydrogen abstraction from Au-H moiety of **3-Xyl** with the *α*-carbon atom of EDA and coordination of N1 to Au-center occur in a synchronous concerted manner to yield the intermediate **Int2** via **TS3** by an energy barrier of $\Delta G^{\neq}$ = 22.0 kcal mol^{-1} (Fig. S39). The second step is associated with the [1,3]-H shift from *α*-carbon atom to N1 atom to form intermediate **Int3** via **TS4** ($\Delta G^{\neq}$ = 33.5 kcal mol^{-1}). Then the formation of **5-Xyl** a rotational isomer of **Int3** can be considered with the overall energy of $\Delta G = -27.1$ kcal mol^{-1}. On the other hand, in the first step of the formation **5-Xyl** via end-on nitrogen insertion across the Au-H bond to terminal N1 atom occurred in a concerted fashion to yield intermediate **Int4** via **TS5** with energy barrier $\Delta G^{\neq}$ = 16.1 kcal mol^{-1} (Fig. S40). Then the second step is about inversion of N2-center to form **5-Xyl** with $\Delta G^{\neq}$ = 23.3 kcal mol^{-1} via **TS6**. The formation of dehydrogenative coupling product **5'-Xyl** occurred in a concerted manner via **TS7** with energy barrier $\Delta G^{\neq}$ = 30.0 kcal mol^{-1} (Fig. S41).

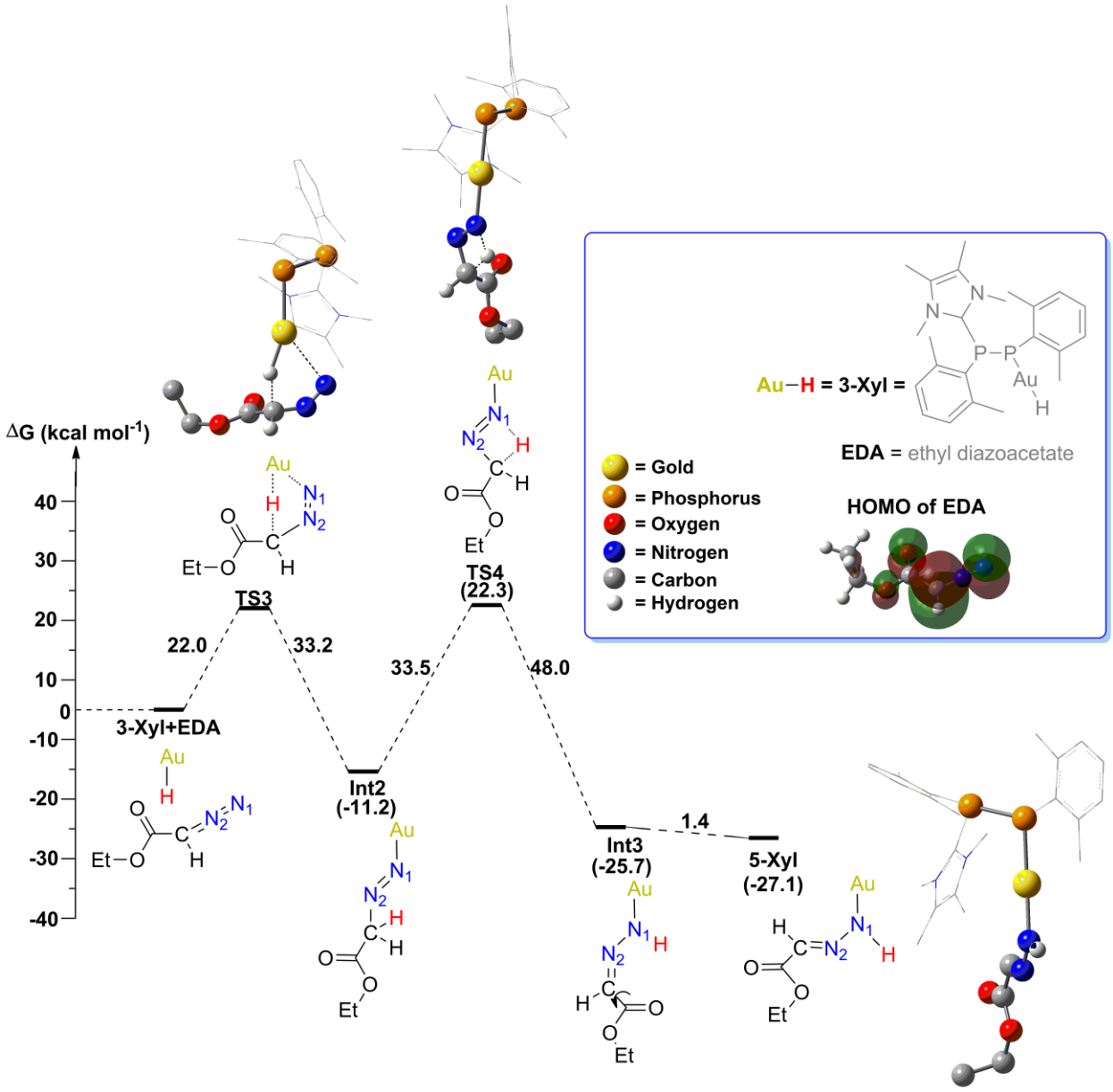


Fig. S39 Proposed reaction mechanisms for **3-Xyl** + **EDA** for the formation of **5-Xyl** considering the interaction of α-C of EDA with H of Au-H moiety. Energy barriers are on the dashed lines. Relative energies are given in parentheses.

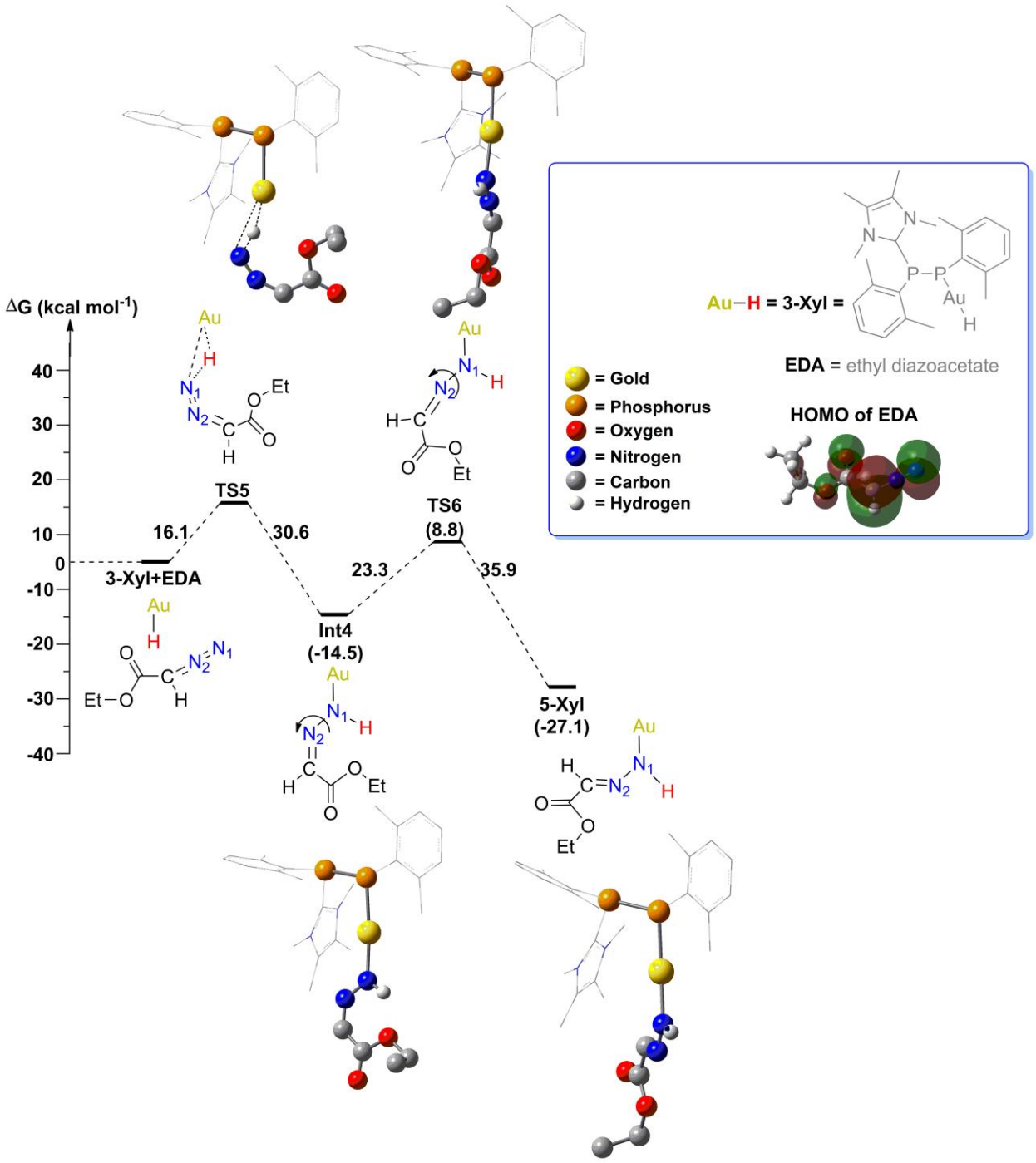


Fig. S40 Proposed reaction mechanisms for **3-Xyl** + **EDA** for the formation of **5-Xyl** considering the insertion of end-on nitrogen of EDA across Au-H moiety. Energy barriers are on the dashed lines. Relative energies are given in parentheses.

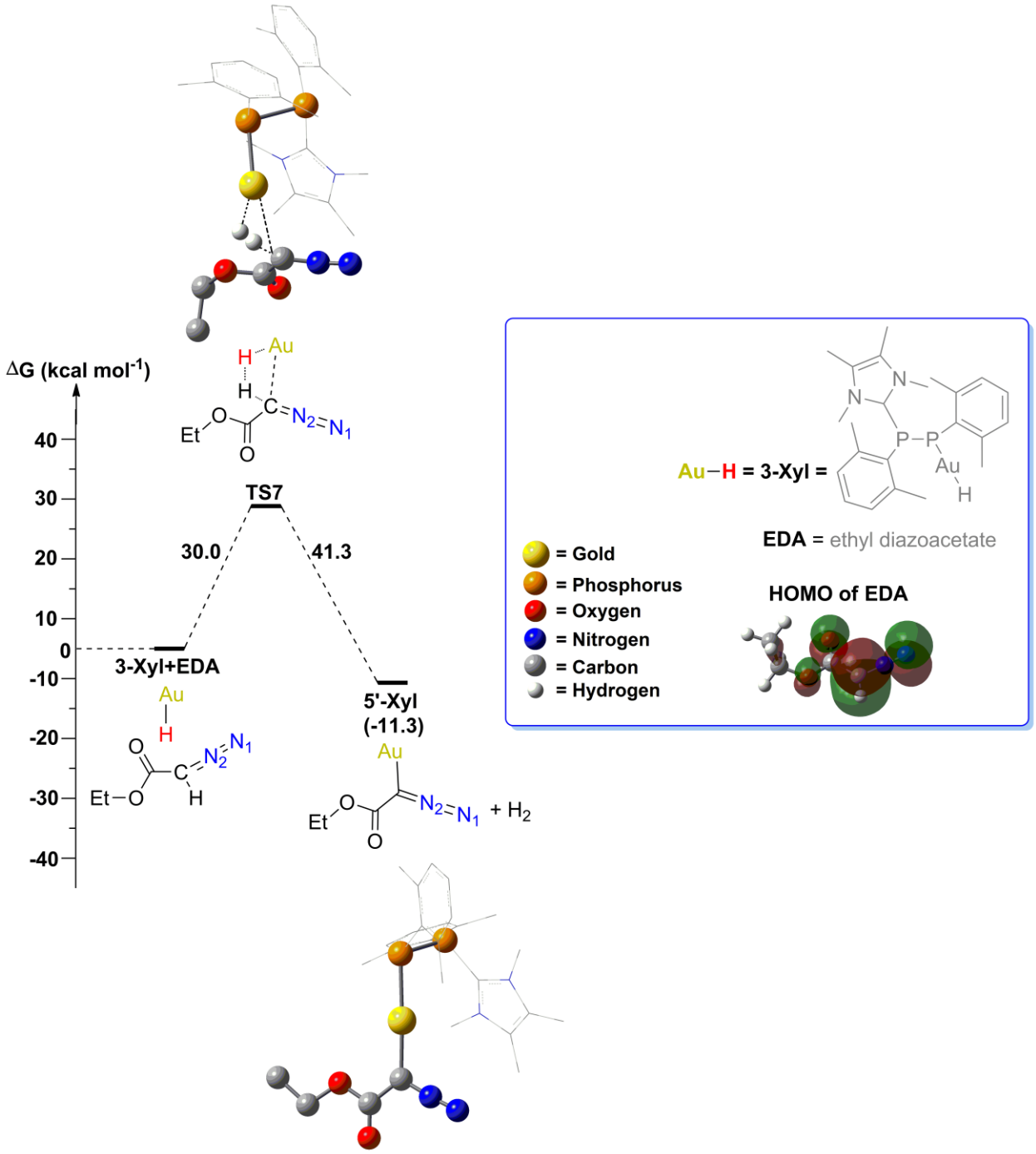


Fig. S41 Proposed reaction mechanisms for **3-Xyl** + **EDA** for the formation of **5'-Xyl**. Energy barriers are on the dashed lines. Relative energies are given in parentheses.

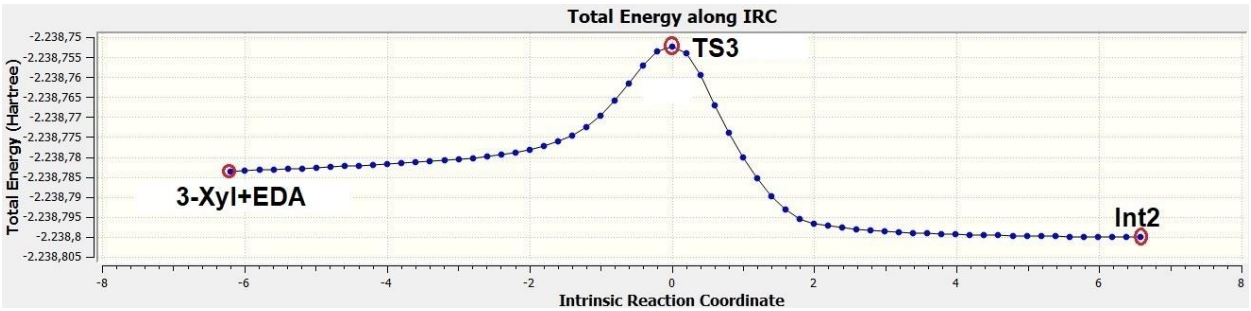


Fig. S42 The IRC plot for **TS3**.

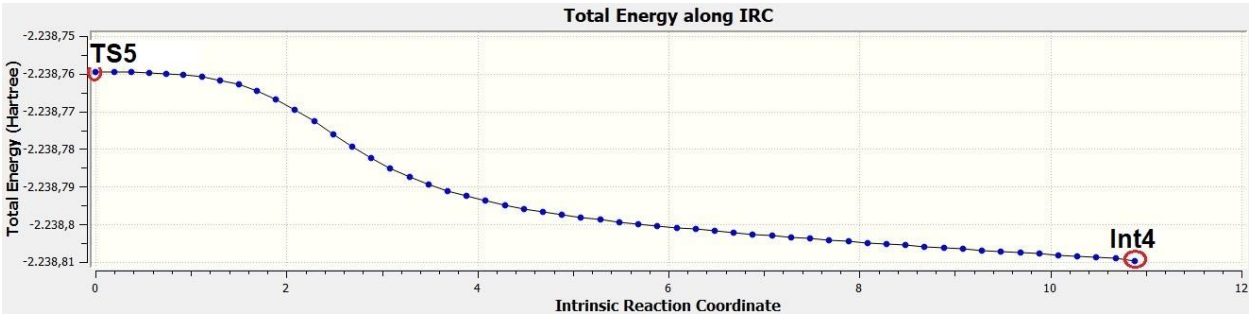


Fig. S43 The IRC plot for **TS5**.

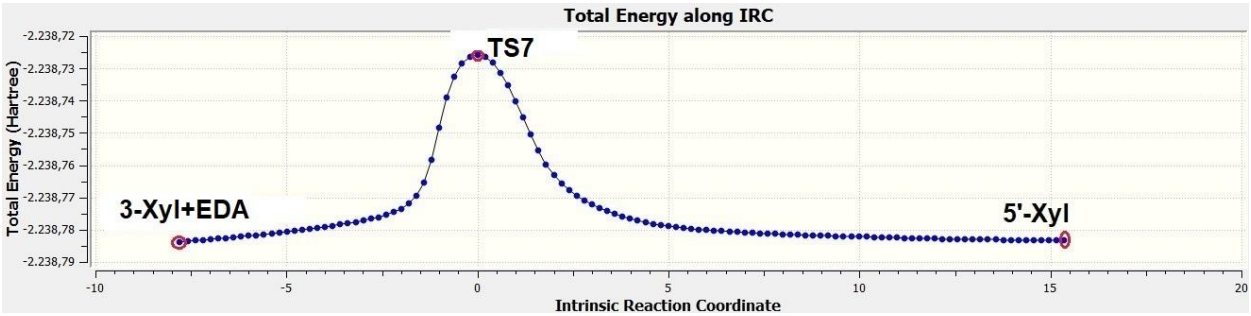


Fig. S44 The IRC plot for **TS7**.

Table S6. Cartesian coordinates and energy values of **3**

Au	2.39749600	-0.47328000	-1.11418100
P	0.78205000	0.91347500	0.06290100
P	-1.18020200	-0.12424800	-0.08043600
N	-0.21688900	-2.70254500	-1.17383800
N	-0.75331300	-2.70168600	0.92283000
C	2.05367100	0.22057400	2.58227400
C	-1.70448900	0.90071000	-2.80094700
C	0.01289100	1.53670600	2.76822300
C	-0.71739200	-1.92079900	-0.18695500
C	0.94314400	0.84117700	1.93800700
C	3.52885400	-1.70560100	1.87831700
C	0.08469600	-3.96642400	-0.68218100
C	-2.05717100	0.03790900	-1.73163200
C	0.03487100	-2.32582800	-2.56120200
H	-0.23921600	-1.28864300	-2.70368000
H	-0.56461100	-2.95834500	-3.22229300
C	-0.26641800	-3.97357700	0.63877400
C	0.60811300	1.79543600	-3.37110400
C	4.72655000	-2.17967400	1.33875900
H	4.90478100	-3.25330900	1.31115000
C	-3.23366400	-0.75862700	-1.85938900
C	0.69364500	-5.01963100	-1.54350400
H	0.05316500	-5.26132200	-2.40070400
H	0.84989200	-5.93710100	-0.97141100
H	1.66526800	-4.69256600	-1.93207900
C	3.27271700	-0.31955000	1.89428800
C	-0.62533400	1.93298800	-2.70807100
C	-1.02377500	2.51564900	2.28875500
C	5.43558700	0.05754900	0.86939500
H	6.17754600	0.74992700	0.47607800
C	0.11659600	1.45783500	4.16638200
H	-0.60280300	2.00573800	4.76942500
C	-0.59812300	3.78665800	1.83079600
C	4.24720700	0.57236900	1.39577200
C	-3.73055600	-2.95891500	-0.67679300
C	-1.55002200	4.77946300	1.58257100
H	-1.20992500	5.75461800	1.23809900
C	2.12227500	0.17418400	3.98450700
H	2.98139700	-0.31083300	4.44076000
C	2.50504200	-2.67901900	2.41121900

H	1.52478800	-2.46521000	1.97932200
H	2.39810600	-2.61271600	3.50112500
H	2.77449400	-3.70989500	2.15795900
C	-3.31839300	3.31321300	2.24210100
H	-4.37700500	3.12534300	2.41122400
C	-3.80329900	-1.55383200	-0.71815100
C	0.08719000	4.07362400	-1.82988600
H	-0.12957800	4.96891100	-1.25116300
C	0.86268400	4.10770000	1.63185200
H	1.47126000	3.76180900	2.47344600
H	1.01445600	5.18576200	1.51540700
H	1.23984300	3.61066900	0.73081600
C	-2.40008500	2.29349100	2.52123800
C	0.93413500	0.63759800	-4.28955300
H	1.64324500	-0.04673200	-3.80836700
H	1.40839100	1.00500300	-5.20728700
H	0.04662500	0.06986800	-4.58058300
C	-3.16602600	-3.78090400	-1.81469600
H	-3.97494900	-4.30429100	-2.34080100
H	-2.47312200	-4.54454700	-1.44539000
H	-2.64864100	-3.16608300	-2.55104000
C	4.01488000	2.06501600	1.38795900
H	3.31759800	2.34325500	0.58751400
H	4.95049300	2.60636900	1.21380700
H	3.58150900	2.41728900	2.32952600
C	-1.26200900	-2.26404000	2.22545300
H	-0.72711400	-1.37258900	2.55652600
H	-1.09959800	-3.06330200	2.94742100
H	-2.32933200	-2.05349800	2.14630200
C	1.59223900	2.77117000	-3.16508600
H	2.56415400	2.63679500	-3.63562900
C	-2.91688200	4.56287700	1.76860200
C	-0.90786400	3.11055700	-1.97860900
C	-0.18589800	-5.06355500	1.65359300
H	0.47186800	-4.79275500	2.48748600
H	0.21740800	-5.96964800	1.19527900
H	-1.17356200	-5.30785000	2.06301000
C	-2.91490000	0.98067100	3.06709000
H	-2.71949600	0.17150600	2.35874200
H	-3.99541400	1.02593400	3.23526600
H	-2.43798700	0.70801400	4.01361700
C	-3.55493000	0.03071600	-4.13644200

H	-4.11858400	0.02044100	-5.06535900
C	-5.01753600	-1.58153600	1.38387900
H	-5.54924100	-1.04398000	2.16632900
C	-3.94965900	-0.76292500	-3.06216800
H	-4.83767400	-1.38525900	-3.13554900
C	1.14477100	0.75440600	4.78339300
H	1.21430900	0.71054500	5.86715300
C	-2.45758500	0.87064500	-3.98667000
H	-2.16523700	1.53839400	-4.79229900
C	-4.50600100	-0.86408000	0.30225800
C	5.69016500	-1.31410000	0.81853400
C	1.36445000	3.89583900	-2.37310800
C	-4.73297300	0.62507700	0.20993200
H	-3.80138400	1.18371300	0.33583100
H	-5.42825400	0.96436400	0.98334600
H	-5.14133400	0.90223700	-0.76824600
C	-2.26356200	3.32656300	-1.35054300
H	-3.07580100	2.98310600	-1.99942200
H	-2.42289900	4.38414100	-1.12600700
H	-2.34876300	2.78753400	-0.40102500
C	-4.24336800	-3.64051600	0.43738900
H	-4.16074700	-4.72591600	0.46923800
C	-3.92646000	5.63286900	1.42937000
H	-3.53389600	6.63589800	1.63154600
H	-4.85396700	5.50925400	1.99926400
H	-4.19147800	5.59744500	0.36337200
C	-4.87186800	-2.97185700	1.48656000
C	-5.38433000	-3.71173300	2.69989600
H	-4.73584400	-3.54266400	3.57018400
H	-5.42806700	-4.79192000	2.52540200
H	-6.38853300	-3.37329900	2.98036000
C	2.46633100	4.88839500	-2.08916800
H	2.08018100	5.91170100	-2.01597800
H	3.24045700	4.86836100	-2.86378900
H	2.95426800	4.65639400	-1.13264700
C	6.94469200	-1.84686600	0.16989300
H	7.24471500	-2.81013500	0.59821600
H	7.78347300	-1.14988900	0.27836800
H	6.78280200	-2.00037700	-0.90533500
H	1.09876900	-2.43666600	-2.77622600
H	3.40935900	-1.36491200	-2.06227000

Zero-point correction= 1.037585 (Hartree/Particle)
Thermal correction to Energy= 1.099027
Thermal correction to Enthalpy= 1.099971
Thermal correction to Gibbs Free Energy= 0.944571
Sum of electronic and zero-point Energies= -3059.757268
Sum of electronic and thermal Energies= -3059.695826
Sum of electronic and thermal Enthalpies= -3059.694882
Sum of electronic and thermal Free Energies= -3059.850282

Table S7. Cartesian coordinates and energy values of **4**

Au	-1.96602400	-0.28717400	-0.38244400
P	1.75505400	0.16643800	-0.18701100
P	0.08928200	-1.17072500	0.42382700
N	1.34214200	2.70533500	0.92271900
N	0.30612000	2.61257300	-0.97546900
C	2.20472200	0.08367200	-2.00944800
O	-5.06176500	3.43705500	-0.35457700
O	-2.87298100	2.89824900	-0.45115300
C	1.06402400	1.88532600	-0.12159000
C	0.76062100	-1.94875100	-2.66637300
C	1.27685600	-3.08590700	-2.00324700
C	1.69968800	-0.82534700	-2.97589000
C	0.79043600	3.96227500	0.70872800
C	-0.34415800	2.12919600	-2.18957800
H	-0.00052600	2.71008100	-3.05016600
H	-1.42255800	2.22247000	-2.05773000
H	-0.09194500	1.08653200	-2.33201600
C	-0.66731000	-0.35449500	3.12381900
C	0.31728800	-0.93983200	2.27693000
C	0.13282600	3.90200800	-0.48846600
C	4.40095600	4.03960300	-0.42585000
H	4.20641900	5.11008700	-0.38334300
C	-1.17757000	-0.83586100	-3.94922800
H	-0.47372600	-0.02624700	-4.15215100
H	-2.07639800	-0.42432300	-3.48016900
H	-1.48873700	-1.24714700	-4.91787500
C	-1.42148300	-2.99049200	-2.71594000
H	-2.47144300	-2.93643400	-2.99217200
C	1.48435900	-1.48100900	2.89556000
C	-3.83635900	0.16833400	-1.17284700
C	2.47857800	-2.38380300	2.21690000

C	-2.07616300	-0.02250700	2.72480100
O	-5.12502300	-1.76282600	-0.78585900
C	3.83341800	-2.00224800	2.08181800
C	3.73288000	3.27023800	-1.38944800
C	2.15693100	2.33788500	2.08183700
H	1.85805700	1.35702200	2.45023000
H	1.98930100	3.07188900	2.86943500
H	3.21198700	2.32866400	1.80249500
O	-4.38875700	-1.40592200	-2.89622800
C	-0.94882400	-4.07873400	-1.98392600
C	-0.58215900	-1.93234100	-3.09124200
C	5.31967900	-0.15020800	-0.74396900
H	4.51151800	-0.81234700	-0.41975900
H	6.20281900	-0.38820400	-0.14400000
H	5.53501000	-0.39834400	-1.78932300
C	3.22564300	0.99772400	-2.40665800
C	0.41603100	-4.13353700	-1.67991300
H	0.81424300	-4.99697300	-1.15047800
C	3.95168300	1.87985300	-1.43175900
C	5.32295900	3.47698300	0.45705700
C	-2.52810200	1.30573700	2.62858000
C	2.73617600	-3.16854200	-1.62490200
H	3.38624600	-2.76194500	-2.40668700
H	3.03019800	-4.20385000	-1.43339600
H	2.93830800	-2.61143700	-0.70313100
C	0.68735500	-4.20677600	2.07034800
H	0.21866300	-3.80731900	2.97395500
H	0.65878100	-5.30034100	2.12020300
H	0.07459300	-3.88953800	1.21762200
C	5.60338200	2.10999000	0.33018300
H	6.35868800	1.66070600	0.97167900
C	4.94442900	1.30501700	-0.60064100
C	2.15114300	-0.73768000	-4.30391100
H	1.74467700	-1.44094900	-5.02513700
C	-3.00896300	-1.08319200	2.59748900
C	-4.04069300	2.57623900	-0.63083800
C	2.85811000	3.97860200	-2.39960400
H	2.34042900	4.83020900	-1.94743900
H	2.11727700	3.31416500	-2.84477800
H	3.47087900	4.36787800	-3.22353900
C	2.10328400	-3.71267500	1.90136800
C	4.31781900	-0.61877700	2.45366900

H	3.88411600	0.12867200	1.78449900
H	5.40685500	-0.55298800	2.36768200
H	4.04419000	-0.34022900	3.47564300
C	6.00208200	4.30762200	1.52077700
H	5.91657400	5.37925600	1.31186400
H	7.06721000	4.06220500	1.60164700
H	5.55675900	4.12729400	2.50874900
C	-4.34624400	-0.79139500	2.33503400
H	-5.04516100	-1.61183500	2.19232300
C	4.76062300	-2.92323900	1.57940800
H	5.79696400	-2.61194100	1.46314000
C	0.93212900	5.08707600	1.67704500
H	0.44803100	4.85782500	2.63437900
H	0.45863600	5.98597300	1.27536200
H	1.98508600	5.32120800	1.87395500
C	3.63773000	1.05568800	-3.74282300
H	4.41169000	1.76770300	-4.01704800
C	-0.39811600	-0.17416100	4.49089300
H	-1.16323900	0.29082600	5.10695300
C	4.40011900	-4.22678900	1.23592700
C	-1.89325500	-5.15569600	-1.50509800
H	-2.28458100	-4.90738300	-0.50878000
H	-1.39514300	-6.12876200	-1.42570500
H	-2.75306100	-5.26540900	-2.17574000
C	3.09214500	0.20462800	-4.69997800
H	3.42020500	0.25539800	-5.73462900
C	-2.57152800	-2.52588300	2.69149900
H	-2.00565200	-2.82013600	1.79939000
H	-3.43726000	-3.19145600	2.76849100
H	-1.92285800	-2.70199400	3.55620300
C	-0.63985500	4.93418300	-1.23427700
H	-0.22963600	5.08827000	-2.23978400
H	-0.60178900	5.89056000	-0.70657000
H	-1.68561100	4.62774300	-1.32367300
C	1.70663400	-1.28837100	4.26814800
H	2.59730200	-1.72245300	4.71473300
C	-4.47406900	-1.03984600	-1.73519300
C	-1.58846300	2.48667200	2.67675200
H	-1.99097400	3.28970700	3.30748000
H	-1.47242200	2.88883300	1.66468200
H	-0.60147300	2.21598600	3.05851700
C	3.06888100	-4.60267000	1.42249100

H	2.76782800	-5.62209200	1.18702100
C	0.79369000	-0.60393100	5.06316700
H	0.98202100	-0.46070800	6.12401300
C	-3.88461200	1.55277000	2.38244200
H	-4.21868400	2.58398500	2.28936400
C	-4.55829100	1.30719100	-1.15009300
H	-5.60211800	1.34070100	-1.46253000
C	-4.80590200	0.52348100	2.21028700
C	5.40468400	-5.18839800	0.64803400
H	5.36907900	-5.16790800	-0.45008300
H	5.20453400	-6.22012200	0.95871600
H	6.42849900	-4.93602300	0.94534000
C	-4.67022400	4.71733600	0.14636100
H	-5.59876300	5.24334300	0.37357500
H	-4.09752100	5.27196200	-0.60506200
H	-4.05737200	4.61549600	1.04725900
C	-5.62283200	-3.03486200	-1.22333200
H	-6.12683100	-3.46578400	-0.35687400
H	-4.79751500	-3.67974000	-1.54172700
H	-6.32212100	-2.91801800	-2.05655500
C	-6.25072700	0.80453500	1.87390200
H	-6.61010500	0.09408400	1.12120000
H	-6.37246500	1.81302200	1.46586900
H	-6.89930300	0.71242500	2.75587500

Zero-point correction= 1.162654 (Hartree/Particle)
Thermal correction to Energy= 1.235251
Thermal correction to Enthalpy= 1.236195
Thermal correction to Gibbs Free Energy= 1.058959
Sum of electronic and zero-point Energies= -3592.615102
Sum of electronic and thermal Energies= -3592.542505
Sum of electronic and thermal Enthalpies= -3592.541561
Sum of electronic and thermal Free Energies= -3592.718796

Table S8. Cartesian coordinates and energy values of **5**

Au	-1.48665400	-1.38982900	0.61532900
P	0.69514000	-1.36592500	-0.20642800
P	1.50743900	0.68675200	0.14409600
N	-0.01340100	2.56804300	-1.25632900
N	-0.95886600	2.23298800	0.66283400
C	1.87086700	0.19874600	3.04240000

C	-0.37498700	-1.30879400	-2.94139900
C	1.91501700	1.08239900	1.93309900
C	0.09287000	1.85620700	-0.10751900
C	0.76560700	-1.28917000	-2.08672000
C	0.92871700	2.49446200	-2.37583700
H	1.86640200	2.97748400	-2.09750600
H	0.48924000	3.00744600	-3.23037400
H	1.10830000	1.45379800	-2.64589700
C	1.57409500	-1.26488800	2.94445500
C	-1.78909600	-1.56490800	-2.50818200
C	2.39431200	2.40978300	2.14121800
C	2.05503300	-1.32601800	-2.69688200
C	2.56970900	-3.98959900	-1.51289000
H	1.87818100	-3.89395800	-0.66636300
H	3.04498800	-4.97421300	-1.45138600
H	1.96996400	-3.95215900	-2.42647400
C	0.38539500	-1.82002100	3.45866000
C	-1.29153800	1.71997400	1.98903600
H	-0.65108400	0.87601900	2.21151000
H	-2.33122300	1.38806900	1.99355800
H	-1.14001500	2.50105200	2.73949400
C	1.83582000	4.48137300	0.77805200
C	2.66316200	3.36702600	1.01479000
C	2.57016700	-2.11173200	2.40484400
C	3.23131900	5.13069900	-1.12270300
C	-0.20482300	-1.19984600	-4.33160100
H	-1.09267500	-1.19997000	-4.95816600
C	-0.67953800	-1.00896200	4.16901700
H	-0.36928800	0.02063100	4.35922900
H	-0.91830300	-1.46453900	5.13784800
H	-1.60651900	-0.98384500	3.58296900
C	1.05675500	-1.13050800	-4.91121200
H	1.16643400	-1.05553900	-5.98994200
C	2.17592900	-1.23182500	-4.09192400
H	3.16901400	-1.27733300	-4.53095100
C	4.18747200	0.76749800	-2.50059800
H	3.83757300	0.75416900	-3.53704900
H	5.12707200	1.32775800	-2.47041400
H	3.45013300	1.32172000	-1.91450100
C	3.83644900	3.19191300	0.23951300
C	-2.44216300	0.86060700	-2.99078600
H	-1.39050300	1.09062000	-2.81794100

H	-3.05708800	1.57159700	-2.42799000
H	-2.63925300	1.02400500	-4.05951600
C	0.16370700	-3.19483700	3.30484500
H	-0.77260100	-3.61498000	3.66826000
C	-2.77084000	-0.55595800	-2.58022700
C	4.09348100	4.06965800	-0.81485200
H	4.99278000	3.92613200	-1.41025900
C	4.82172800	2.09607600	0.56777500
H	5.09088800	2.11420200	1.62982300
H	5.73706200	2.20299900	-0.02161200
H	4.40956400	1.10397800	0.36064600
C	3.50404500	6.02520400	-2.30918100
H	4.56521600	6.29169100	-2.37397800
H	2.92456800	6.95285800	-2.25686400
H	3.24205100	5.52451800	-3.25114600
C	2.70659700	2.85018700	3.43256200
H	3.05995600	3.86968100	3.56186800
C	3.34227100	-1.58943700	-1.96318700
C	3.89365500	-1.55942000	1.93289600
H	3.81097700	-1.14565500	0.92173500
H	4.64788200	-2.34916200	1.88398800
H	4.26458300	-0.76469000	2.58787600
C	4.37435900	-0.62291100	-1.93565900
C	2.11954100	5.32784300	-0.30374400
H	1.46087500	6.17391100	-0.49293600
C	2.31648300	-3.47797200	2.29359700
H	3.07917200	-4.11970200	1.85713900
C	-4.09457200	-0.85695100	-2.24962100
H	-4.82966900	-0.05573600	-2.26600800
C	-3.50857200	-3.13792100	-1.83251800
H	-3.79105000	-4.14755500	-1.53995300
N	-3.36936200	-1.46866900	1.57526700
H	-3.60620700	-2.25051100	2.17876600
C	-4.48151900	-2.13496000	-1.84552300
C	-1.11529100	3.41156500	-1.20265300
C	0.68618700	4.84273900	1.69205200
H	0.34880700	3.99428800	2.28730700
H	-0.16493200	5.23214500	1.12499300
H	0.99468800	5.62497400	2.39813900
C	3.60332900	-2.89001200	-1.46670400
C	2.20951700	0.68030100	4.31874100
H	2.16812000	-0.01559500	5.15191200

C	-2.17476200	-2.88126300	-2.16314500
C	-1.16518000	-4.00360900	-2.09949600
H	-0.49462100	-4.00147500	-2.96539800
H	-1.66504600	-4.97664300	-2.05422400
H	-0.53538300	-3.91418200	-1.20513200
C	1.09837300	-4.03336200	2.69816000
C	5.60821600	-0.95105900	-1.36119400
H	6.38925300	-0.19380200	-1.33113100
C	5.87002100	-2.21837800	-0.83863300
C	2.59879200	1.99762100	4.52769800
H	2.84865800	2.34699000	5.52571900
C	-1.71400700	3.20070300	0.00925600
C	4.85709200	-3.17547800	-0.91799900
H	5.04622700	-4.17997300	-0.54308100
N	-4.42605000	-0.72225800	1.39470800
C	-5.89432100	-2.38806500	-1.38146400
H	-6.06072400	-1.90516200	-0.40957300
H	-6.09953300	-3.45819700	-1.26976100
H	-6.62865100	-1.97071800	-2.08132300
C	0.79920700	-5.49434100	2.46229700
H	0.07035200	-5.88091300	3.18300700
H	1.70462100	-6.10822300	2.52816400
H	0.37735700	-5.64226400	1.45896100
C	-4.33705700	0.32951900	0.61238000
H	-3.41551400	0.56919600	0.07863200
C	-1.50747400	4.32208700	-2.31603700
H	-0.70137600	5.01894500	-2.57495400
H	-2.38183600	4.90718300	-2.02232500
H	-1.77906600	3.75997800	-3.21760700
C	-2.93865700	3.82074900	0.59402300
H	-3.83256100	3.23747800	0.34183500
H	-3.07480000	4.82831800	0.18992300
H	-2.86249400	3.90778100	1.68194200
C	7.19024900	-2.53511100	-0.17814500
H	7.99702400	-1.90126400	-0.56227700
H	7.47694500	-3.58152200	-0.33190000
H	7.13454900	-2.37005600	0.90687700
O	-5.41512500	2.06658100	-0.55062600
O	-6.65996200	0.72884300	0.80338100
C	-5.48387400	1.11839800	0.24238500
C	-7.82127400	1.49356000	0.43734000
H	-8.66315500	0.83153000	0.65922500

H	-7.79974600	1.70011400	-0.63713300
C	-7.91113700	2.78896600	1.23467700
H	-7.88621200	2.57950600	2.30949300
H	-8.84522600	3.31515000	1.00372300
H	-7.07087900	3.44031200	0.97986000

Zero-point correction= 1.153476 (Hartree/Particle)
Thermal correction to Energy= 1.224539
Thermal correction to Enthalpy= 1.225483
Thermal correction to Gibbs Free Energy= 1.050227
Sum of electronic and zero-point Energies= -3475.489724
Sum of electronic and thermal Energies= -3475.418661
Sum of electronic and thermal Enthalpies= -3475.417717
Sum of electronic and thermal Free Energies= -3475.592972

Table S9. Cartesian coordinates and energy values of **5'**

Au	-1.95071500	-0.32268000	-0.38380200
P	-0.15962000	1.01964700	0.34801000
P	1.71736400	-0.06341200	-0.18222700
N	1.61438500	-2.59335000	1.01073400
N	0.59895100	-2.71005900	-0.89648400
C	1.53799200	0.81069700	-3.00481600
C	-0.92369200	0.29919200	3.07287900
C	2.16821500	0.02846600	-2.00165200
C	1.27535200	-1.86389000	-0.08160300
C	0.02027900	0.94045800	2.21807400
C	2.38137200	-2.07778800	2.14801600
H	3.40994300	-1.88783600	1.83781900
H	2.36814300	-2.82403200	2.94127200
H	1.92586900	-1.15959800	2.52043100
C	0.45570100	1.80673200	-2.72666400
C	-2.23906800	-0.29567500	2.65345900
C	3.31781200	-0.73742300	-2.35571500
C	1.07295400	1.68184500	2.83261100
C	-0.07558700	4.20231000	1.84996200
H	-0.63312000	3.70119900	1.04982200
H	-0.26983500	5.27725200	1.77557500
H	-0.47942100	3.84356900	2.80171900
C	-0.88453500	1.58884100	-3.10511900
C	-0.00389700	-2.39456100	-2.18703200
H	0.08046700	-1.33161000	-2.36912000

H	-1.05928800	-2.66669100	-2.16805900
H	0.51010600	-2.94721100	-2.97847300
C	4.15259300	-2.85234300	-1.21429900
C	4.16177300	-1.44999100	-1.33645900
C	0.82618600	3.02815800	-2.11986200
C	5.75324300	-2.71865700	0.63039300
C	-0.70615500	0.27981600	4.46101900
H	-1.43792500	-0.22309800	5.08777700
C	-1.34418900	0.38836300	-3.90674500
H	-0.51408300	-0.23580700	-4.24566000
H	-1.88854100	0.72017800	-4.79932200
H	-2.03119000	-0.23329500	-3.32049000
C	0.39051700	0.90759300	5.03980100
H	0.53849900	0.88220100	6.11622600
C	1.25292000	1.63148800	4.22333900
H	2.06014100	2.21166300	4.66289400
C	4.01741400	1.20108800	2.48833600
H	3.70071500	0.90119300	3.49160200
H	5.10652300	1.31082500	2.49646200
H	3.76980400	0.38060500	1.80926100
C	5.04806900	-0.68721500	-0.53429900
C	-1.28533400	-2.61757300	3.00477500
H	-0.40380600	-2.33131100	2.42783600
H	-1.53669200	-3.65420700	2.75734200
H	-1.00171900	-2.57920300	4.06454100
C	-1.85088800	2.52899800	-2.72673700
H	-2.89443900	2.31954300	-2.95222400
C	-2.43637300	-1.69161700	2.69332500
C	5.81783600	-1.33223400	0.43414000
H	6.49060300	-0.73948400	1.05052100
C	5.18673600	0.80196500	-0.73812500
H	5.34720900	1.04306100	-1.79477000
H	6.02725400	1.19942200	-0.16161200
H	4.28742000	1.33871700	-0.42196100
C	6.55780800	-3.37849600	1.72564600
H	7.59349700	-3.01929800	1.73248200
H	6.57869800	-4.46725500	1.61112500
H	6.13674900	-3.15678600	2.71552000
C	3.74008400	-0.79260200	-3.68917800
H	4.61410700	-1.39062500	-3.93308700
C	1.95429800	2.66970800	2.11811700
C	2.26755600	3.32630900	-1.78366000

H	2.55714300	2.85484100	-0.83784300
H	2.42132700	4.40098700	-1.65519400
H	2.95405300	2.96715800	-2.55703400
C	3.35179500	2.47988900	2.03186600
C	4.92880600	-3.45929700	-0.21530600
H	4.89681000	-4.54310000	-0.11493700
C	-0.16261900	3.95849600	-1.80325300
H	0.12707800	4.88804100	-1.31796800
C	-3.70008100	-2.21990000	2.41956200
H	-3.83361000	-3.29997000	2.42624900
C	-4.58874500	-0.01830000	2.12120500
H	-5.42607500	0.63937000	1.89596000
C	-4.79301300	-1.40074900	2.12575500
C	1.15913700	-3.90152900	0.88250000
C	3.37951900	-3.74710300	-2.15789900
H	2.64888000	-3.19335500	-2.74742300
H	2.86113700	-4.54297800	-1.61307400
H	4.06376700	-4.23130100	-2.86676100
C	1.40014700	3.91165100	1.72054100
C	2.00239400	0.73149900	-4.32839700
H	1.50291500	1.33673500	-5.07964900
C	-3.33722500	0.55017600	2.37516100
C	-3.17373500	2.05014400	2.29934800
H	-2.55002300	2.43880100	3.11067800
H	-4.14589800	2.55242700	2.34041200
H	-2.69334600	2.33775700	1.35504100
C	-1.51469400	3.70258200	-2.05061900
C	4.15156600	3.49850800	1.49858200
H	5.22503700	3.33586300	1.42358100
C	3.61742100	4.71536900	1.07341500
C	3.07521200	-0.07844200	-4.68256800
H	3.41183900	-0.12647400	-5.71453100
C	0.51130400	-3.97203900	-0.31960400
C	2.24042300	4.90404100	1.20881700
H	1.80385500	5.85579500	0.91095200
C	-6.14372500	-1.98881400	1.79366000
H	-6.27572900	-2.07385500	0.70838400
H	-6.95641100	-1.35802500	2.17293300
H	-6.26128800	-2.98920500	2.22456300
C	-2.58383000	4.66038100	-1.58237300
H	-3.37872400	4.77760100	-2.32783300
H	-2.17107500	5.65156700	-1.36562500

H	-3.05635100	4.28969600	-0.66332500
C	1.37701200	-4.94642200	1.92389200
H	2.44384400	-5.10507000	2.12147600
H	0.95383000	-5.89684900	1.59091300
H	0.88964100	-4.68058800	2.86948200
C	-0.17692200	-5.10620900	-1.00013300
H	-1.23809600	-4.89050200	-1.16696900
H	-0.10959200	-6.01030300	-0.39064400
H	0.28164800	-5.32146300	-1.97339600
C	4.49051200	5.77978300	0.45380400
H	5.52929400	5.69867100	0.79222100
H	4.13139700	6.78657200	0.69524100
H	4.49630500	5.69164300	-0.64156700
C	-3.59841600	-1.37689400	-1.11953800
N	-3.55548600	-2.67054600	-1.15904500
N	-3.42135800	-3.81187800	-1.17171800
C	-4.91023400	-0.79704200	-1.36192200
O	-4.85476300	0.56611800	-1.26747600
O	-5.95858000	-1.39034300	-1.59000500
C	-6.12058800	1.23884100	-1.30905000
C	-5.85242100	2.70215100	-1.00520600
H	-6.79367600	0.78754300	-0.57093600
H	-6.58067000	1.10106800	-2.29472200
H	-6.79072000	3.26828000	-0.99539000
H	-5.36902400	2.80550000	-0.02775000
H	-5.18952400	3.14145600	-1.75694800

Zero-point correction= 1.129291 (Hartree/Particle)
Thermal correction to Energy= 1.199453
Thermal correction to Enthalpy= 1.200397
Thermal correction to Gibbs Free Energy= 1.027585
Sum of electronic and zero-point Energies= -3474.294375
Sum of electronic and thermal Energies= -3474.224214
Sum of electronic and thermal Enthalpies= -3474.223270
Sum of electronic and thermal Free Energies= -3474.396082

Table S10. Cartesian coordinates and energy values of **6**

Au	-1.69987200	-0.95378700	0.40837000
P	1.52218300	0.71576800	0.11233900
P	0.60981700	-1.32478500	-0.02513400
N	-0.98340700	2.28685100	0.29977400

N	0.04174300	2.35636900	-1.60477400
C	0.91773800	-1.61902500	-1.86067700
C	1.38759100	-0.90069900	3.09680800
C	1.68358400	0.56630300	3.06249300
C	0.13716100	-1.41094300	3.49496200
C	0.13642900	1.87178100	-0.34070200
C	-0.12740900	-1.86549500	-2.80051300
C	2.26043000	-1.75074100	-2.32419400
C	1.82908700	1.31077000	1.86347000
C	2.52155300	-1.95512400	-3.68825500
H	3.55563000	-2.05660100	-4.00722600
C	2.44246000	-1.78808800	2.78040900
C	-0.99639000	-0.54549100	4.00419500
H	-0.67679300	0.47441700	4.23134900
H	-1.41069000	-0.97358300	4.92475900
H	-1.81254600	-0.49729500	3.27401700
C	1.49249700	-2.08985000	-4.61329100
H	1.71091700	-2.25772200	-5.66465300
C	-3.58502900	-0.37454800	0.82834800
C	3.47534700	-1.84922400	-1.44303300
C	-1.58218900	-2.02640500	-2.46855500
C	-1.33283200	2.07723700	1.70224100
H	-0.63631200	1.37429700	2.13880300
H	-2.33873600	1.66161800	1.76222000
H	-1.27479700	3.03125200	2.23435500
C	-1.80435700	2.99357400	-0.56846600
C	2.68352000	3.45161400	0.72799900
C	-0.07772000	-2.79356300	3.41879600
H	-1.06139300	-3.18121900	3.67675700
C	2.31163600	2.64973600	1.94441700
C	4.35813900	0.38810100	-2.31047500
H	4.08151900	0.19303300	-3.35125500
H	5.29194900	0.95894500	-2.31072200
H	3.57868500	1.02196400	-1.87888200
C	-3.15314600	3.47478700	-0.15311800
H	-3.79311500	2.62222700	0.10759600
H	-3.63035300	4.02590800	-0.96673300
H	-3.09891800	4.13738400	0.71882200
C	0.18106100	-2.07891400	-4.15422000
H	-0.63820100	-2.26185300	-4.84456100
C	-1.14939000	3.05777000	-1.76820000
C	4.50608400	-0.88507300	-1.50814900

C	3.82045400	-1.26872300	2.44845800
H	3.87371800	-0.93036100	1.40798100
H	4.56906500	-2.05726500	2.55961200
H	4.10652700	-0.42548000	3.08531700
C	4.84731000	2.11510500	0.63091000
H	5.02216500	2.26076000	1.70260100
H	5.81259400	2.14107000	0.11669600
H	4.43625500	1.10883400	0.50917400
C	2.52747300	3.24145400	3.19466200
H	2.88755500	4.26628100	3.22922600
C	0.64672500	4.98980800	0.98236200
H	0.40004500	4.35916000	1.83652100
H	-0.21480800	5.01307800	0.30587600
H	0.78908500	6.01056000	1.35907600
C	1.92069400	1.19785500	4.29466900
H	1.80063400	0.60949100	5.20007500
C	-2.52047200	-1.05911100	-2.88641800
C	2.19572600	-3.15870000	2.75562300
H	3.00664100	-3.83429000	2.49189000
C	1.06594200	2.17394700	-2.63684800
H	1.99720500	2.63785300	-2.30943000
H	0.72379000	2.65289700	-3.55333500
H	1.22416900	1.11082900	-2.82677700
C	0.92370200	-3.67813000	3.02036600
C	2.31261900	2.52954400	4.37217200
H	2.48382900	2.99777300	5.33761700
C	3.69456200	-3.04821000	-0.72143700
C	-2.03833700	-3.21217200	-1.85191200
C	2.65920200	-4.14563400	-0.67410400
H	1.83918300	-3.86625600	-0.00243300
H	3.09598900	-5.07960800	-0.30573800
H	2.22209400	-4.33392800	-1.65986500
C	1.89234900	4.51909900	0.26409700
C	3.91364900	3.16597000	0.08197500
C	-2.06690300	0.20589400	-3.57345400
H	-1.22641000	0.64893000	-3.03496200
H	-2.87788800	0.94047300	-3.61110400
H	-1.72799100	0.02106600	-4.60057400
C	4.90884500	-3.23360800	-0.05495300
H	5.06888700	-4.16162500	0.49128400
C	0.64503800	-5.15325900	2.85831100
H	-0.20604300	-5.47511200	3.46800900

H	1.51421500	-5.76170500	3.13355700
H	0.40441000	-5.38555800	1.81185400
C	4.26874900	3.88422000	-1.05959600
H	5.21091800	3.65425700	-1.55293600
C	5.70017700	-1.10853700	-0.81137700
H	6.48203800	-0.35289000	-0.85683600
C	-1.07395200	-4.28278900	-1.39694500
H	-0.28063000	-4.45891000	-2.13024300
H	-1.59545200	-5.22853100	-1.21706600
H	-0.58663900	-3.99071600	-0.45757900
C	-3.87736300	-1.25765200	-2.62712500
H	-4.58876100	-0.48731700	-2.91984700
C	-4.34200500	-2.40000800	-1.97236200
C	-1.53689000	3.72989300	-3.04228800
H	-0.81772400	4.50966700	-3.32176100
H	-2.51371100	4.20532400	-2.92661100
H	-1.60970200	3.02061600	-3.87396700
C	-3.40807300	-3.37498800	-1.61726900
H	-3.74976400	-4.28005300	-1.11883600
C	3.45216800	4.89663200	-1.58240200
C	5.92156700	-2.27223900	-0.07380600
C	2.28025200	5.20782100	-0.89570900
H	1.64964100	6.01932800	-1.25586300
C	-5.98799300	0.73562700	1.01002100
C	-4.69692300	0.13345400	0.95380700
C	-6.70912100	0.98132400	-0.17962500
H	-6.26461100	0.68743100	-1.12620100
C	7.19615000	-2.47099500	0.71048300
H	7.07112400	-2.13885300	1.75057100
H	8.02714200	-1.89851800	0.28392100
H	7.49009000	-3.52627200	0.74120400
C	-7.96540200	1.58170700	-0.14201800
H	-8.50456100	1.75851300	-1.06969100
C	-8.53479900	1.95398100	1.07934500
H	-9.51555500	2.42133000	1.10717400
C	3.84169900	5.62070100	-2.84972300
H	4.89300200	5.93068600	-2.82596800
H	3.22951500	6.51459500	-3.00833600
H	3.71947400	4.97410300	-3.72903200
C	-6.57664800	1.11564800	2.23456700
H	-6.03375800	0.92788900	3.15644700
C	-5.79710100	-2.53561700	-1.59878800

H	-5.98776700	-2.00508700	-0.65712200
H	-6.08479700	-3.58321900	-1.45769000
H	-6.45458400	-2.10009100	-2.36052300
C	-7.83321200	1.71682500	2.26501900
H	-8.26945100	2.00021000	3.21984000

Zero-point correction= 1.134213 (Hartree/Particle)
Thermal correction to Energy= 1.203439
Thermal correction to Enthalpy= 1.204383
Thermal correction to Gibbs Free Energy= 1.032114
Sum of electronic and zero-point Energies= -3366.783862
Sum of electronic and thermal Energies= -3366.714636
Sum of electronic and thermal Enthalpies= -3366.713692
Sum of electronic and thermal Free Energies= -3366.885961

Table S11. Cartesian coordinates and energy values of **7**

Au	1.73976800	-0.34531400	-0.02197900
P	-0.37417100	-1.29261000	0.22900600
P	-1.96435100	0.21324700	-0.19412500
N	3.72859500	0.23734000	-0.38343200
N	4.19852400	1.42847200	0.18914700
H	4.06827800	1.46078000	1.19527500
N	-1.60213200	2.36776300	1.56551500
N	-0.37756900	2.67945600	-0.19435300
C	-0.79869800	-1.57284900	2.04016100
C	-0.70268500	-1.22823200	-3.00579100
C	-1.54589900	0.00373900	-3.11401100
C	1.56477200	-0.97740700	2.97601600
C	0.10989700	-1.32973200	3.11112700
C	3.85831700	-1.69272100	2.63592100
H	4.56444100	-2.46266700	2.33478400
C	0.68525800	-1.20736500	-3.24408700
C	2.03394000	0.29936700	3.33907900
C	-2.16790300	0.64113100	-2.00964200
C	-1.34937500	-2.45718800	-2.73459600
C	2.49505800	-1.99037500	2.63996000
C	-1.25124800	1.81715000	0.37790600
C	4.72895400	-0.66021300	-0.72887200
C	-0.19408000	3.79015600	0.62178800
C	4.34107600	-0.42547100	2.97688000
C	0.81074700	-3.58780500	-2.70317600

C	-1.78893500	0.48876500	-4.41020300
H	-1.29851100	-0.01145600	-5.24042200
C	1.44871400	0.02589700	-3.67741000
H	1.96590100	-0.16351900	-4.62619800
H	2.21409200	0.27760000	-2.93536900
H	0.80626100	0.89678500	-3.82176100
C	0.31193100	2.47066900	-1.46514100
H	0.51403300	1.40878600	-1.57635300
H	1.26739500	2.99216400	-1.44800900
H	-0.30080300	2.81902500	-2.29984800
C	-2.63575100	1.56569400	-4.64490700
H	-2.80143800	1.92575400	-5.65656200
C	-2.59669600	-4.02903700	0.72543600
C	1.41910400	-2.38747200	-3.06635000
H	2.49845600	-2.35146900	-3.19366700
C	-2.97609500	-2.81700700	1.35391400
C	-2.04329900	-2.19578200	2.35820900
C	-3.30325600	2.14742900	-3.57018700
H	-4.01174400	2.95476500	-3.73501200
C	-0.58415900	-3.61337000	-2.59205700
H	-1.08662800	-4.55003100	-2.35913000
C	2.03484800	-3.36895000	2.23103400
H	1.27673000	-3.76656500	2.91383900
H	2.87550200	-4.06856900	2.19883000
H	1.58608000	-3.34470100	1.23009800
C	-3.10048800	1.69138200	-2.26234300
C	-2.84960700	-2.53038900	-2.57839000
H	-3.15898900	-2.23712000	-1.56912000
H	-3.20461000	-3.55366500	-2.72646500
H	-3.36872500	-1.87701600	-3.28695500
C	-2.40893200	-2.39467000	3.69841500
H	-3.35844500	-2.87944000	3.90948300
C	3.41108500	0.55347100	3.33803500
H	3.76383000	1.54234000	3.62993700
C	-0.29972900	-1.54547200	4.43788300
H	0.41239800	-1.34387100	5.23390300
C	-1.22293900	-4.62847000	0.90491300
H	-0.49949500	-4.11697300	0.25862600
H	-1.22293600	-5.69031900	0.63794100
H	-0.86527300	-4.53161200	1.93396200
C	-1.56234000	-2.03951900	4.74297600
H	-1.85835800	-2.20345900	5.77572900

C	-3.52126500	-4.70351700	-0.07690600
H	-3.21900400	-5.63605000	-0.55031300
C	-5.03988100	1.56316200	-0.66904300
C	-5.40082400	0.21646800	-1.24788800
H	-5.44549900	0.25649100	-2.34177800
H	-6.37217300	-0.12139500	-0.87478900
H	-4.66408300	-0.54849600	-0.98665700
C	-4.29814800	-2.34292400	1.19192700
C	-3.94644300	2.30527800	-1.18186600
C	1.06189900	1.40184700	3.68430200
H	0.34974100	1.53870300	2.86645500
H	1.58111800	2.35241900	3.84656300
H	0.47886200	1.17235700	4.58445000
C	3.84893600	2.69686100	-1.86157700
H	3.73729900	1.76894100	-2.40893100
C	6.09254200	-0.29169100	-0.83147500
H	6.37372900	0.73294200	-0.61468700
C	-0.96869100	3.59467800	1.73273100
C	0.69052400	4.92497000	0.23682000
H	1.74070600	4.62134700	0.18108000
H	0.61216500	5.73072300	0.97103000
H	0.41091800	5.33141300	-0.74200700
C	-5.18338100	-3.04506100	0.36476000
H	-6.19363600	-2.66178300	0.23524100
C	4.07770300	2.63118400	-0.47135200
C	5.81886300	-0.12827100	2.90822600
H	6.40264800	-0.87586500	3.45844200
H	6.05318800	0.85808800	3.32370000
H	6.16232500	-0.14894700	1.86628000
C	-3.73287500	3.62205100	-0.72772500
C	4.24752600	3.84127300	0.23973100
H	4.44080500	3.80440100	1.31042100
C	-5.80979800	2.10511400	0.36142900
H	-6.64210700	1.52540700	0.75505600
C	1.63646100	-4.81704700	-2.40819000
H	1.12305100	-5.73541500	-2.71533400
H	1.83003200	-4.89740200	-1.32959000
H	2.60914400	-4.78064500	-2.91013500
C	-2.54837800	1.77225800	2.51117600
H	-3.56443000	1.87775100	2.12652900
H	-2.45827800	2.29036800	3.46523300
H	-2.31087500	0.71887000	2.66090200

C	4.40243700	-2.00797500	-1.02213200
H	3.36916000	-2.33004500	-0.92990400
C	-2.73954700	4.55812800	-1.38024500
H	-1.95040400	4.02887700	-1.91299100
H	-2.27726400	5.22165200	-0.64285600
H	-3.24809900	5.19344300	-2.11742600
C	-4.79184400	-1.08822000	1.87662500
H	-4.58788800	-1.09028200	2.95137900
H	-5.87122800	-0.97004500	1.73886500
H	-4.30366200	-0.20608500	1.45378000
C	-5.54505100	3.37223200	0.89687500
C	-4.51676300	4.11999900	0.32347400
H	-4.32702100	5.12962500	0.68427100
C	-5.76893400	-4.93658400	-1.21367900
H	-5.61074300	-4.62153800	-2.25447100
H	-6.81358400	-4.72148100	-0.96358100
H	-5.62724400	-6.02268600	-1.17961500
C	-1.16015500	4.44848200	2.94026000
H	-2.21562500	4.70513300	3.09007500
H	-0.60131600	5.38053300	2.82957200
H	-0.79786300	3.95162600	3.84873500
C	5.37872500	-2.92062900	-1.40853400
H	5.08317000	-3.94648200	-1.62215800
C	-4.81514500	-4.22300800	-0.28623700
C	3.78454100	3.93202800	-2.50437100
H	3.60588500	3.95712500	-3.57723900
C	-6.35538700	3.90422800	2.05562600
H	-7.42525800	3.70962400	1.91836500
H	-6.22125500	4.98387900	2.18006900
H	-6.06186800	3.42348400	2.99869700
C	7.06030700	-1.22125100	-1.21048500
H	8.09761800	-0.89875200	-1.27940400
C	6.72285200	-2.54408600	-1.50683500
H	7.48318000	-3.26158900	-1.80237500
C	3.95449400	5.12853600	-1.79950900
H	3.91286500	6.08552300	-2.31134300
C	4.19909500	5.06549100	-0.42278100
H	4.34368300	5.98157300	0.14607400

Zero-point correction=	1.237163 (Hartree/Particle)
Thermal correction to Energy=	1.309931
Thermal correction to Enthalpy=	1.310875

Thermal correction to Gibbs Free Energy= 1.131562
Sum of electronic and zero-point Energies= -3632.157694
Sum of electronic and thermal Energies= -3632.084926
Sum of electronic and thermal Enthalpies= -3632.083982
Sum of electronic and thermal Free Energies= -3632.263295

Table S12. Cartesian coordinates and energy values of **dimethyl acetylenedicarboxylate (DMAD)**

O	-2.75241400	0.72272400	0.00160400
O	-2.46433500	-1.52925200	-0.00263700
C	0.59752100	0.09227500	-0.00051800
O	2.75245900	-0.72272000	0.00164400
O	2.46426300	1.52924200	-0.00265800
C	-2.01670300	-0.40285600	-0.00073100
C	2.01669000	0.40281800	-0.00063100
C	-0.59752200	-0.09237900	-0.00055100
C	-4.17893300	0.51308300	0.00172700
H	-4.61591300	1.51137100	0.00364600
H	-4.48128400	-0.04617600	0.89134300
H	-4.48189900	-0.04302800	-0.88964900
C	4.17896800	-0.51299000	0.00168500
H	4.61600300	-1.51125400	0.00359200
H	4.48133200	0.04629900	0.89127700
H	4.48184900	0.04312700	-0.88971600

Zero-point correction= 0.117130 (Hartree/Particle)
Thermal correction to Energy= 0.127480
Thermal correction to Enthalpy= 0.128424
Thermal correction to Gibbs Free Energy= 0.080629
Sum of electronic and zero-point Energies= -532.754394
Sum of electronic and thermal Energies= -532.744044
Sum of electronic and thermal Enthalpies= -532.743100
Sum of electronic and thermal Free Energies= -532.790894

Table S13. Cartesian coordinates and energy values of **ethyl diazoacetate (EDA)**

N	2.82536900	-1.23372700	0.07022300
N	2.21570100	-0.27408900	0.11860500
C	1.49746600	0.81631900	0.17052300
H	2.00613600	1.73920300	0.40732100
O	-0.64354200	1.77250800	-0.04849600
O	-0.37084100	-0.47336200	-0.36180000

C	0.06143100	0.78242100	-0.08368800
C	-1.78978900	-0.61639200	-0.61399000
H	-1.86655600	-1.54914000	-1.17805400
H	-2.12378400	0.21454200	-1.24154400
C	-2.57784000	-0.67697700	0.68580700
H	-2.20803900	-1.48617100	1.32402600
H	-3.63731100	-0.85951400	0.47258000
H	-2.49047600	0.27039700	1.22433200

Zero-point correction= 0.106721 (Hartree/Particle)
Thermal correction to Energy= 0.114698
Thermal correction to Enthalpy= 0.115643
Thermal correction to Gibbs Free Energy= 0.073971
Sum of electronic and zero-point Energies= -415.670504
Sum of electronic and thermal Energies= -415.662527
Sum of electronic and thermal Enthalpies= -415.661582
Sum of electronic and thermal Free Energies= -415.703254

Table S14. Cartesian coordinates and energy values of **phenyl acetylene**

C	3.23332700	0.00000700	-0.00008900
C	2.02341300	-0.00030900	-0.00000400
H	4.29963800	0.00087300	0.00042000
C	0.59380700	-0.00015500	0.00001100
C	-0.11931700	1.21346500	0.00000400
C	-0.11961500	-1.21360800	0.00000300
C	-1.51209900	1.20903700	0.00000100
H	0.42947200	2.15021900	0.00000200
C	-1.51238500	-1.20883500	0.00000100
H	0.42895500	-2.15049000	0.00000200
C	-2.21265900	0.00018900	0.00000200
H	-2.05256100	2.15171900	0.00000100
H	-2.05309000	-2.15137900	0.00000200
H	-3.29924600	0.00031200	0.00000100

Zero-point correction= 0.110552 (Hartree/Particle)
Thermal correction to Energy= 0.116869
Thermal correction to Enthalpy= 0.117813
Thermal correction to Gibbs Free Energy= 0.080265
Sum of electronic and zero-point Energies= -308.162025
Sum of electronic and thermal Energies= -308.155708
Sum of electronic and thermal Enthalpies= -308.154764

Sum of electronic and thermal Free Energies= -308.192312

Table S15. Cartesian coordinates and energy values of **azobenzene**

N	0.50900800	-0.37154500	-0.00001400
N	-0.50900800	0.37154500	-0.00001400
C	-0.23152800	1.76194100	-0.00001900
C	-1.35713400	2.59655000	-0.00003700
C	1.05760600	2.32402800	0.00005400
C	-1.20359300	3.98213100	-0.00004300
H	-2.33966600	2.13424000	-0.00006300
C	1.20359300	3.70612000	0.00005800
H	1.91667100	1.66252800	0.00009000
C	0.07660300	4.53903500	-0.00000400
H	-2.07934400	4.62509400	-0.00008300
H	2.19878500	4.14304600	0.00011300
H	0.20051900	5.61866700	-0.00001400
C	0.23152800	-1.76194100	-0.00001900
C	1.35713400	-2.59655000	-0.00003700
C	-1.05760600	-2.32402800	0.00005400
C	1.20359300	-3.98213100	-0.00004300
H	2.33966600	-2.13424000	-0.00006300
C	-1.20359300	-3.70612000	0.00005800
H	-1.91667100	-1.66252800	0.00009000
C	-0.07660300	-4.53903500	-0.00000400
H	2.07934400	-4.62509400	-0.00008300
H	-2.19878500	-4.14304600	0.00011300
H	-0.20051900	-5.61866700	-0.00001400

Zero-point correction= 0.192742 (Hartree/Particle)
Thermal correction to Energy= 0.203235
Thermal correction to Enthalpy= 0.204179
Thermal correction to Gibbs Free Energy= 0.156458
Sum of electronic and zero-point Energies= -572.346866
Sum of electronic and thermal Energies= -572.336373
Sum of electronic and thermal Enthalpies= -572.335428
Sum of electronic and thermal Free Energies= -572.383149

Table S16. Cartesian coordinates and energy values of **3-Xyl+EDA**

Au	0.98794300	-1.26392800	-0.13779700
P	-1.39033500	-0.93786600	-0.69753700

P	-1.94123100	0.67505300	0.81954300
N	0.55194000	2.02306500	1.00889400
N	-0.37638200	2.41638100	-0.91001900
C	-0.53974400	1.74481700	0.25571300
C	0.84345100	1.43884600	2.31686500
H	-0.08722400	1.06430600	2.74216700
H	1.26891900	2.20342100	2.96850500
H	1.54437500	0.60841200	2.20011500
C	-1.30878200	2.41722000	-2.03832800
H	-1.98923600	3.27034000	-1.97268000
H	-1.87313700	1.48669600	-2.03064900
H	-0.73557400	2.47041600	-2.96419300
N	4.04755500	-0.19865600	3.27704600
H	2.56916300	-1.51278000	0.12587100
C	1.41825000	2.85864900	0.31601500
C	0.82486800	3.11985400	-0.89040000
N	4.61718400	-0.58328300	2.37025000
C	5.26922500	-1.02355700	1.33226100
H	5.49293400	-2.07911000	1.29301100
C	2.73886500	3.29109200	0.86025300
H	2.64224900	3.72218600	1.86238500
H	3.17366300	4.05732000	0.21521100
H	3.45134800	2.45934800	0.90075700
C	1.29292900	3.95292500	-2.03691100
H	1.46746600	3.34822600	-2.93411900
H	2.23583300	4.43944500	-1.78184100
H	0.57151900	4.73521800	-2.29739600
O	5.18551800	1.08761600	0.23067000
O	6.14416100	-0.72480300	-0.76805300
C	5.50202400	-0.09272600	0.23794300
C	6.37653600	0.04606000	-1.96936300
H	7.26488800	-0.40869100	-2.41453900
H	6.60030300	1.07818600	-1.68907300
C	5.18087900	-0.02787800	-2.90710500
H	4.94767900	-1.06578300	-3.15960600
H	5.40215400	0.51397800	-3.83332500
H	4.29995900	0.41998300	-2.44142700
C	-2.21520000	-2.51517200	-0.11979700
C	-2.76382700	-3.31658700	-1.16203100
C	-2.28065100	-2.99667800	1.21514900
C	-3.40324700	-4.52234900	-0.85036000
C	-2.94260900	-4.20417100	1.48117200

C	-3.51152000	-4.96259300	0.46457300
H	-3.81854900	-5.12102100	-1.65740400
H	-2.99286600	-4.55636700	2.50865000
H	-4.01849700	-5.89617400	0.69272400
C	-3.39981800	1.76143500	0.31832000
C	-4.55570900	1.23636600	-0.31594000
C	-3.41872800	3.11482700	0.75973700
C	-5.63189200	2.08821600	-0.59915900
C	-4.51567000	3.92917800	0.44804000
C	-5.61122700	3.43301000	-0.24836500
H	-6.50456400	1.67374200	-1.09688300
H	-4.51059200	4.96350900	0.78336300
H	-6.45437400	4.07685200	-0.48135400
C	-2.64868400	-2.94508400	-2.62697400
H	-3.03973600	-1.94517000	-2.83779200
H	-1.60509500	-2.94317400	-2.96174900
H	-3.19332900	-3.66534800	-3.24498300
C	-1.63422100	-2.29023800	2.38317300
H	-0.62613500	-1.94940200	2.12198200
H	-2.19550400	-1.40658300	2.70427200
H	-1.55966400	-2.96597200	3.24033400
C	-4.71639300	-0.22217000	-0.67708200
H	-5.74862900	-0.42423200	-0.97518900
H	-4.06048300	-0.51503400	-1.49987400
H	-4.47976900	-0.88518300	0.16027800
C	-2.32967900	3.73765500	1.61154400
H	-1.98162900	3.04926000	2.38835400
H	-1.45258700	4.05012300	1.03353900
H	-2.71536200	4.63081800	2.11064100

Zero-point correction= 0.598971 (Hartree/Particle)
Thermal correction to Energy= 0.640540
Thermal correction to Enthalpy= 0.641484
Thermal correction to Gibbs Free Energy= 0.521333
Sum of electronic and zero-point Energies= -2237.691278
Sum of electronic and thermal Energies= -2237.649709
Sum of electronic and thermal Enthalpies= -2237.648765
Sum of electronic and thermal Free Energies= -2237.768916

Table S17. Cartesian coordinates and energy values of **Int2**

Au	-0.90081800	-1.20322900	-0.63891400

P	1.14846600	-0.92052100	0.61444900
P	1.97083100	0.79501100	-0.68932300
N	-0.45452000	1.88016900	-1.70296400
N	-0.26976100	2.29974300	0.41522300
C	0.35754800	1.70778000	-0.63162100
C	-0.26095500	1.31018900	-3.03754000
H	0.73350700	0.86892700	-3.08607200
H	-0.34838600	2.10250700	-3.78507300
H	-1.02473400	0.54194500	-3.20003600
C	0.22219900	2.36064500	1.79159300
H	0.72038900	3.31583700	1.97917200
H	0.91760900	1.54114100	1.95849700
H	-0.62415000	2.24353700	2.46874600
N	-2.56493100	-0.84406900	-1.92561400
H	-3.30853100	-1.99780500	0.13729800
C	-1.60874700	2.55351900	-1.32975600
C	-1.48629800	2.83498900	0.00415400
N	-3.75742800	-0.90800500	-1.63997100
C	-4.16994000	-1.48972900	-0.33344300
H	-4.97956600	-2.20592300	-0.49857200
C	-2.74305800	2.77924100	-2.27084400
H	-2.43020400	3.31971800	-3.17099600
H	-3.52527800	3.36098000	-1.78093300
H	-3.17744400	1.82005000	-2.57217900
C	-2.44024800	3.49996400	0.93869300
H	-2.95523900	2.76011600	1.56034100
H	-3.20693700	4.02792300	0.36882400
H	-1.94162900	4.22936500	1.58473100
O	-4.22924700	0.74483400	0.62675900
O	-5.57121200	-0.87897400	1.46464000
C	-4.64133900	-0.39723100	0.60957300
C	-6.05308600	0.02419500	2.48693500
H	-7.06622000	-0.32280000	2.70391700
H	-6.09725500	1.03431500	2.07290800
C	-5.17053200	-0.02869900	3.72527300
H	-5.10160300	-1.04991400	4.11080100
H	-5.58974800	0.60858900	4.51126200
H	-4.16245000	0.32643800	3.49566700
C	2.21706100	-2.41506100	0.26449000
C	2.51774200	-3.20609800	1.41074000
C	2.68407800	-2.84916200	-1.00531700
C	3.30864000	-4.35328400	1.27628500

C	3.48256300	-3.99902700	-1.08900200
C	3.80655200	-4.74509100	0.03813500
H	3.53089900	-4.94509200	2.16072800
H	3.84037800	-4.31569100	-2.06559500
H	4.42609800	-5.63336900	-0.04998000
C	3.06926100	1.99608800	0.25742100
C	4.02644200	1.54826300	1.20444400
C	3.07236600	3.36835700	-0.12109600
C	4.85823700	2.48216400	1.83650000
C	3.92016800	4.26502900	0.54288100
C	4.79350500	3.83766200	1.53606000
H	5.57688900	2.12496000	2.56947300
H	3.90443600	5.31201300	0.25021500
H	5.44409100	4.54630600	2.04045300
C	1.97630000	-2.89026100	2.79115800
H	2.22810600	-1.87753400	3.11979800
H	0.88322900	-2.96130900	2.82280800
H	2.37532400	-3.59722700	3.52471500
C	2.33837400	-2.15505300	-2.30128300
H	1.27464400	-1.89464100	-2.33447500
H	2.89810000	-1.22453000	-2.44024500
H	2.55965100	-2.80729100	-3.15111000
C	4.23458000	0.09183700	1.55017800
H	5.16527600	-0.03220200	2.11052500
H	3.41786800	-0.30403400	2.15842100
H	4.29969800	-0.54220800	0.66112400
C	2.24527600	3.93123300	-1.26071200
H	2.23134900	3.25681000	-2.12286700
H	1.20404400	4.13017100	-0.98330600
H	2.67300800	4.88120100	-1.59296500

Zero-point correction= 0.604829 (Hartree/Particle)
Thermal correction to Energy= 0.645937
Thermal correction to Enthalpy= 0.646881
Thermal correction to Gibbs Free Energy= 0.528711
Sum of electronic and zero-point Energies= -2237.710534
Sum of electronic and thermal Energies= -2237.669426
Sum of electronic and thermal Enthalpies= -2237.668482
Sum of electronic and thermal Free Energies= -2237.786652

Table S18. Cartesian coordinates and energy values of **Int3**

Au	0.61429700	-1.26810700	-0.43964000
P	-1.70871800	-0.87369300	-0.62590600
P	-1.86382200	0.85595800	0.89960200
N	0.81913700	1.77814400	0.96112200
N	-0.09203400	2.25441000	-0.94615400
C	-0.33432400	1.67750600	0.25535500
C	1.06401400	1.20980100	2.28429700
H	0.10831700	0.93247200	2.72705600
H	1.56326300	1.95031000	2.91203100
H	1.69340300	0.32150200	2.19008800
C	-1.04358600	2.37724200	-2.05102000
H	-1.82320800	1.62785100	-1.93655900
H	-0.51775500	2.19281400	-2.98813900
H	-1.48772300	3.37634200	-2.06304900
N	2.68536400	-1.36323900	-0.32896500
H	5.34507700	-1.24299800	-2.18953900
C	1.80630700	2.38046400	0.19246300
C	1.22654400	2.69690000	-1.00718500
N	3.46621000	-1.37070600	-1.37605500
C	4.77257900	-1.15371800	-1.27382900
H	3.18172400	-1.18678300	0.54900300
C	3.20996600	2.53663000	0.67353700
H	3.26087700	3.11982800	1.60002000
H	3.80651900	3.05649200	-0.07819400
H	3.67727500	1.56066800	0.85460000
C	1.80500500	3.34330100	-2.22128900
H	1.84389200	2.64776500	-3.06723100
H	2.82667800	3.66828600	-2.01834400
H	1.22931300	4.22205400	-2.53159400
O	4.96141400	-0.54707100	1.03848200
O	6.81518700	-0.64682100	-0.28242800
C	5.46930300	-0.77419900	-0.07234800
C	7.61598100	-0.27186100	0.85025800
H	8.59854800	-0.71165600	0.65625700
H	7.19455600	-0.71711400	1.75515700
C	7.71535100	1.24201700	0.99065400
H	8.08952800	1.69425300	0.06704300
H	8.40126000	1.50269300	1.80442900
H	6.73474800	1.66752400	1.21927500
C	-2.58651700	-2.32745500	0.16173600
C	-3.39337800	-3.08459200	-0.73488700
C	-2.47617100	-2.75530100	1.51150100

C	-4.10992500	-4.18910200	-0.25881600
C	-3.22074900	-3.86201000	1.94459400
C	-4.04315300	-4.57070500	1.07683700
H	-4.72296200	-4.75715600	-0.95381200
H	-3.13460300	-4.17567400	2.98189800
H	-4.61103400	-5.42555000	1.43356700
C	-3.16750200	2.12483700	0.42628300
C	-4.43843800	1.73189800	-0.06685400
C	-2.95158900	3.49481500	0.74714200
C	-5.39696000	2.71212100	-0.35631200
C	-3.93902000	4.43854300	0.43471400
C	-5.14736400	4.06197400	-0.13985900
H	-6.36088400	2.39636000	-0.74653000
H	-3.75692900	5.48304700	0.67498200
H	-5.90159700	4.80721100	-0.37520700
C	-3.47515300	-2.78778300	-2.21946200
H	-2.50583600	-2.92716500	-2.71125000
H	-4.18942600	-3.46217500	-2.70075800
H	-3.78276100	-1.75947200	-2.42981400
C	-1.55866400	-2.10583000	2.52038200
H	-0.57901900	-1.89543500	2.07739800
H	-1.95344500	-1.15559400	2.89394100
H	-1.41273900	-2.76703900	3.37936400
C	-4.84406700	0.28932800	-0.26166000
H	-5.92953100	0.21598400	-0.37005700
H	-4.38677900	-0.14574000	-1.15333000
H	-4.55610900	-0.34360800	0.58278800
C	-1.72754800	4.00975700	1.47980600
H	-1.42628200	3.33647800	2.28869800
H	-0.85776200	4.15137400	0.82868900
H	-1.94913800	4.98170900	1.92893200

Zero-point correction= 0.605709 (Hartree/Particle)
Thermal correction to Energy= 0.645872
Thermal correction to Enthalpy= 0.646816
Thermal correction to Gibbs Free Energy= 0.532179
Sum of electronic and zero-point Energies= -2237.732368
Sum of electronic and thermal Energies= -2237.692205
Sum of electronic and thermal Enthalpies= -2237.691261
Sum of electronic and thermal Free Energies= -2237.805897

Table S19. Cartesian coordinates and energy values of **Int4**

Au	0.96192400	-0.57317400	-0.80636500
P	-1.28879300	-0.90219600	-1.43100500
P	-2.47980800	0.51714800	-0.14874800
N	-1.73661600	-0.08961900	2.49550600
N	-0.40079800	1.44165400	1.73967200
C	-2.01643400	2.80281700	-1.94626400
C	-1.53467500	-3.39006900	0.12704900
C	-2.60003100	2.27773800	-0.76202400
C	-1.49156800	0.70482800	1.41655400
C	-2.12108100	-2.45360800	-0.76768200
C	-2.83308100	-1.04957000	2.63062400
H	-3.54467300	-0.88044400	1.82406200
H	-3.32252900	-0.90393700	3.59604000
H	-2.45815800	-2.07235800	2.55513300
C	-3.48205200	3.09884000	-0.00015100
C	-3.41558400	-2.73196000	-1.29510200
C	0.29466000	2.41794700	0.89574500
H	1.32660300	2.07992500	0.74317400
H	0.27978200	3.39269900	1.39139100
H	-0.22143000	2.49931500	-0.05389700
C	-2.25425700	-4.53885300	0.49086200
H	-1.79491100	-5.24923200	1.17381100
C	-3.52882900	-4.79030400	-0.00536000
H	-4.06630600	-5.68726100	0.29008700
C	-4.09803900	-3.88875200	-0.89685200
H	-5.08607800	-4.08282900	-1.30628300
C	-3.73628300	4.41144600	-0.41309900
H	-4.40459100	5.02844800	0.18156000
N	2.92880600	-0.10995000	-0.31495600
H	3.73552100	-0.60348500	-0.69680300
C	-0.77575100	0.12173700	3.47823500
C	-2.31589200	4.12110800	-2.32230900
H	-1.86355200	4.51588200	-3.22773200
C	-3.16108000	4.92616300	-1.56910100
H	-3.37263800	5.94444100	-1.88249700
C	0.06710900	1.08798400	2.99932500
N	3.22403100	0.84724700	0.52883700
C	4.44752800	1.18447900	0.89575900
H	4.51261300	2.01291900	1.59378400
C	-0.76586300	-0.62765900	4.76868500
H	-1.66148400	-0.42717300	5.36833700

H	0.10149400	-0.33546800	5.36291100
H	-0.70906600	-1.70973200	4.60739700
C	1.29904400	1.69163300	3.58541900
H	2.16286100	1.49645800	2.94043700
H	1.49949000	1.26282800	4.56891800
H	1.20196000	2.77637600	3.70676500
O	6.81202000	1.05761000	0.95611100
O	5.68266900	-0.40801500	-0.36836900
C	5.74720900	0.64155800	0.52355600
C	6.94548700	-0.97746100	-0.77327700
H	6.70494000	-2.00294400	-1.06712600
H	7.61654100	-0.99454400	0.08867700
C	7.56461900	-0.20109500	-1.92712400
H	6.87458700	-0.14604900	-2.77477500
H	8.48309900	-0.69560300	-2.26247600
H	7.81549500	0.81309700	-1.60800900
C	-1.06787200	2.03848100	-2.84053100
H	-1.55348700	1.18759500	-3.32545700
H	-0.67648200	2.69605300	-3.62109700
H	-0.21150700	1.63166600	-2.29245500
C	-4.17477800	2.62161100	1.25907700
H	-4.69670700	1.67245500	1.09840400
H	-3.47294200	2.46443700	2.08688900
H	-4.90721700	3.36149800	1.59229700
C	-0.15176900	-3.24459300	0.72337500
H	0.62946600	-3.30997200	-0.04061600
H	-0.00726500	-2.28031000	1.21957600
H	0.03149900	-4.03894800	1.45369100
C	-4.10764300	-1.82524400	-2.28981200
H	-4.40326600	-0.87182500	-1.83668000
H	-3.45523300	-1.58154200	-3.13329900
H	-5.01347500	-2.30328000	-2.67382100

Zero-point correction= 0.604709 (Hartree/Particle)
Thermal correction to Energy= 0.645725
Thermal correction to Enthalpy= 0.646669
Thermal correction to Gibbs Free Energy= 0.530227
Sum of electronic and zero-point Energies= -2237.717553
Sum of electronic and thermal Energies= -2237.676537
Sum of electronic and thermal Enthalpies= -2237.675593
Sum of electronic and thermal Free Energies= -2237.792035

Table S20. Cartesian coordinates and energy values of **5-Xyl**

Au	0.42601100	-0.82327200	-1.59941400
P	-1.83407700	-1.04454700	-0.93342800
P	-2.20590000	0.54360000	0.61090500
N	0.00308000	0.44097000	2.33910900
N	0.38643200	1.95187300	0.83303400
C	-3.07776600	2.49006000	-1.41822700
C	-1.25977300	-3.41185700	0.71787100
C	-2.92253000	2.13499900	-0.05096200
C	-0.54805600	1.06465000	1.26070600
C	-2.21564200	-2.50180300	0.19054000
C	-0.65008900	-0.57826700	3.16168900
H	-1.71513900	-0.57879400	2.93397300
H	-0.49391400	-0.34337100	4.21611200
H	-0.24462400	-1.56745400	2.93997100
C	-3.46517800	2.98846300	0.95424900
C	-3.59800300	-2.74255100	0.44010400
C	0.31716100	2.77436600	-0.37331900
H	-0.72063600	2.98505800	-0.61236900
H	0.79154900	2.24324300	-1.20396600
H	0.83892400	3.71399500	-0.18984400
C	-1.69692100	-4.49685200	1.49297000
H	-0.95664700	-5.18571400	1.89195100
C	-3.04513100	-4.71103000	1.75565200
H	-3.35950100	-5.55866400	2.35842600
C	-3.98545800	-3.83608400	1.22461900
H	-5.04394300	-4.00216200	1.40798100
C	-4.13352900	4.15947600	0.58070700
H	-4.53691400	4.80458800	1.35650400
N	2.36653500	-0.57648700	-2.35484800
H	2.52277200	-0.64409400	-3.35413500
C	1.30104600	0.89162700	2.55202800
C	-3.76905600	3.66860800	-1.73909300
H	-3.88398100	3.93336300	-2.78661700
C	-4.29525600	4.49955100	-0.75797500
H	-4.82426000	5.40723600	-1.03410800
C	1.53810600	1.85319900	1.60684100
N	3.50862200	-0.40982200	-1.73989500
C	3.53969400	-0.30298900	-0.43470300
H	2.62948500	-0.35868800	0.16667100
C	2.21094600	0.34592700	3.60422800
H	2.19045900	0.94502000	4.52241600

H	3.23144700	0.31865400	3.21071800
H	1.93824800	-0.67868100	3.86874000
C	2.75750600	2.67644400	1.36192500
H	3.03696900	2.66186700	0.30454400
H	3.59712700	2.25354600	1.91454200
H	2.61451700	3.71987400	1.66878900
O	4.81059200	0.10728200	1.51584000
O	5.89603600	-0.12950700	-0.46421700
C	4.77076700	-0.09309700	0.29647100
C	7.14220100	0.07763600	0.22213500
H	7.88387400	-0.44180800	-0.39123700
H	7.09647200	-0.39220300	1.20799600
C	7.47677500	1.55866400	0.34528700
H	7.47452600	2.03967100	-0.63755400
H	8.47023800	1.68633100	0.78960900
H	6.74729600	2.06074300	0.98581200
C	-2.52457000	1.68800100	-2.57317200
H	-3.08730400	0.76476500	-2.73639900
H	-2.56506400	2.27782100	-3.49312200
H	-1.48519600	1.38573000	-2.41462400
C	-3.34824500	2.69354500	2.43513600
H	-3.74401300	1.70333000	2.68262600
H	-2.30826600	2.71538800	2.78150500
H	-3.89968100	3.43828500	3.01506000
C	0.23179500	-3.30729900	0.48793400
H	0.49546700	-3.47646100	-0.56136100
H	0.63097300	-2.32145400	0.74494200
H	0.76213300	-4.05513500	1.08513700
C	-4.69782400	-1.86302800	-0.11504700
H	-4.70856000	-0.87226800	0.35445000
H	-4.57791600	-1.69868400	-1.18995100
H	-5.67564000	-2.32030500	0.06204200

Zero-point correction= 0.605668 (Hartree/Particle)
Thermal correction to Energy= 0.646671
Thermal correction to Enthalpy= 0.647615
Thermal correction to Gibbs Free Energy= 0.531138
Sum of electronic and zero-point Energies= -2237.737483
Sum of electronic and thermal Energies= -2237.696480
Sum of electronic and thermal Enthalpies= -2237.695536
Sum of electronic and thermal Free Energies= -2237.812013

Table S21. Cartesian coordinates and energy values of **5'-Xyl**

Au	-1.32860300	-0.25070200	-0.60343300
P	0.36729900	1.36754400	-1.10082400
P	2.21508300	0.58269300	-0.09781400
N	1.44395200	-0.06674700	2.52983900
N	1.32955300	-1.85489100	1.30818500
C	2.96986000	-1.06586400	-2.41698400
C	-0.68056500	3.31521000	0.82972900
C	3.26187700	-0.58186800	-1.11373000
C	1.64230200	-0.53438000	1.26860500
C	0.29977900	2.98531900	-0.14578900
C	1.64882700	1.31254900	2.97172600
H	2.26314200	1.82710000	2.23359400
H	2.15453000	1.30932200	3.93908800
H	0.69327300	1.83432700	3.05564800
C	4.52012700	-0.89791200	-0.52188100
C	1.24804100	3.98005000	-0.52342700
C	1.34015900	-2.76604300	0.16217500
H	0.91854300	-2.25319300	-0.70062000
H	0.70967700	-3.62253300	0.39191900
H	2.35701700	-3.09358700	-0.06138900
C	-0.66262000	4.58725900	1.42168900
H	-1.41696400	4.82773100	2.16675300
C	0.28723600	5.54149500	1.07418400
H	0.28126200	6.52017900	1.54627700
C	1.23102700	5.23366900	0.10140700
H	1.96505800	5.97842300	-0.19566800
C	5.43164500	-1.70002000	-1.21857500
H	6.38363100	-1.93967400	-0.75250200
C	0.97676900	-1.08404200	3.35494700
C	3.92525800	-1.85272400	-3.07784000
H	3.69356900	-2.22084200	-4.07341800
C	5.14303800	-2.17626300	-2.49230800
H	5.86239300	-2.79102900	-3.02572600
C	0.91188300	-2.21512800	2.58724000
C	0.63730600	-0.86040400	4.79099200
H	1.51118000	-0.55521800	5.37841300
H	0.24787100	-1.77955100	5.23141800
H	-0.12934600	-0.08668400	4.90783600
C	0.47950100	-3.59912700	2.94369700
H	-0.41034500	-3.90041500	2.37915300

H	0.23519900	-3.64913200	4.00634800
H	1.27011700	-4.33267800	2.75095700
C	-2.76246200	-1.73011700	-0.27594800
N	-2.37160000	-2.91210600	0.08525200
N	-1.95529600	-3.93665400	0.39935700
C	-4.21451900	-1.58102000	-0.37041100
O	-4.54847400	-0.31036400	-0.74307800
O	-5.05367800	-2.44265000	-0.15398500
C	-5.95787100	-0.06490700	-0.88163100
C	-6.12994500	1.37740000	-1.32339400
H	-6.45565300	-0.25958800	0.07495000
H	-6.37701200	-0.76601000	-1.61144500
H	-7.19349600	1.60825400	-1.44391400
H	-5.71044900	2.06589000	-0.58352400
H	-5.62790400	1.55478700	-2.27906500
C	1.67999500	-0.80101000	-3.15816700
H	1.57986100	0.24942000	-3.44383900
H	1.63906400	-1.40616200	-4.06770600
H	0.79188200	-1.03717600	-2.56340900
C	4.93671100	-0.40742600	0.84981800
H	4.80880400	0.67527900	0.94812000
H	4.35369600	-0.87079300	1.65488500
H	5.98742000	-0.64655100	1.03392000
C	-1.77878200	2.37631400	1.27874200
H	-2.47263900	2.13503300	0.46703700
H	-1.39004600	1.41699400	1.63503600
H	-2.35996200	2.83168100	2.08662600
C	2.29074500	3.75334900	-1.59641500
H	3.06592300	3.04850300	-1.27320800
H	1.84645000	3.33588000	-2.50481600
H	2.78717200	4.69466200	-1.84958300

Zero-point correction= 0.582117 (Hartree/Particle)
Thermal correction to Energy= 0.622054
Thermal correction to Enthalpy= 0.622998
Thermal correction to Gibbs Free Energy= 0.508413
Sum of electronic and zero-point Energies= -2236.543498
Sum of electronic and thermal Energies= -2236.503561
Sum of electronic and thermal Enthalpies= -2236.502617
Sum of electronic and thermal Free Energies= -2236.617202

Table S22. Cartesian coordinates and energy values of **H_2**

H	0.00000000	0.00000000	0.37139700
H	0.00000000	0.00000000	-0.37139700

Zero-point correction= 0.010205 (Hartree/Particle)
Thermal correction to Energy= 0.012566
Thermal correction to Enthalpy= 0.013510
Thermal correction to Gibbs Free Energy= -0.001282
Sum of electronic and zero-point Energies= -1.156666
Sum of electronic and thermal Energies= -1.154306
Sum of electronic and thermal Enthalpies= -1.153362
Sum of electronic and thermal Free Energies= -1.168154

Table S23. Cartesian coordinates and energy values of **3-Xyl+DMDA**

Au	-0.02708100	0.81470800	-2.05707200
P	2.33272000	-0.73315800	0.56726400
P	1.58918000	-0.94635100	-1.52343300
N	0.15067400	-0.98122400	2.34950300
N	0.42172600	1.11082100	1.85230800
C	3.57473500	0.63021600	0.88182200
O	-6.22929700	-0.76834700	0.92082800
O	-4.20628800	-1.58216200	1.54061400
C	0.91152600	-0.13048700	1.60922600
C	4.10882600	1.52333300	-0.08569600
C	-0.81426300	-0.27516600	3.06004000
C	0.86924000	2.34725100	1.20864400
H	1.67525400	2.81173500	1.78170700
H	0.01738800	3.02118900	1.12547800
H	1.21049800	2.11470300	0.20206300
C	-0.43326500	-3.01538400	-1.09523000
C	0.93984300	-2.69221500	-1.26602700
C	-0.63493300	1.04704700	2.75672200
C	1.88922400	-3.75228000	-1.32439500
C	-3.88981000	1.55110200	0.07623200
O	-3.67302900	3.09618300	-1.61243600
C	0.29355300	-2.43630500	2.40325200
H	-0.53791100	-2.91667900	1.88392500
H	0.31638700	-2.76030600	3.44609400
H	1.22402200	-2.71195300	1.90915700
O	-2.54900800	3.46249500	0.32582600
C	4.09714600	0.65812800	2.20842800

C	5.11034400	2.42638900	0.30163100
H	5.50937600	3.10707400	-0.44539300
C	-4.89524300	-0.70775400	1.05021100
C	-1.82707300	-0.94569600	3.92675200
H	-2.53070800	-1.53253000	3.32678200
H	-2.40297300	-0.19564900	4.47238100
H	-1.36209100	-1.60703100	4.66601900
C	5.08749800	1.58844300	2.54621300
H	5.46966500	1.60136200	3.56365800
C	-0.81641500	-4.35977300	-0.97010500
H	-1.87025600	-4.59425000	-0.84011600
C	5.59510700	2.47377200	1.60286800
H	6.36875100	3.18594200	1.87586600
C	-1.36290600	2.25748200	3.23914700
H	-0.67717000	2.98117800	3.69405700
H	-2.09365300	1.97173700	3.99845900
H	-1.89475000	2.75808200	2.42342500
C	1.46201200	-5.07988200	-1.18881000
H	2.19954100	-5.87740400	-1.23441300
C	-3.28442400	2.79332000	-0.37775600
C	0.11797200	-5.38935000	-1.01069700
H	-0.20006500	-6.42405400	-0.91266300
C	-4.37550100	0.53806600	0.52762600
H	-0.96873200	2.05705600	-2.50171900
C	-6.83971900	-1.98084300	1.40495000
H	-7.90665800	-1.85752800	1.22501000
H	-6.63938900	-2.11056700	2.47115400
H	-6.45274600	-2.84505600	0.86030600
C	-3.04744600	4.25933500	-2.20096800
H	-3.57489200	4.41980400	-3.13993400
H	-1.99308500	4.03854200	-2.38268800
H	-3.15227500	5.12118100	-1.53894400
C	3.63852400	-0.28493400	3.30176000
H	4.32068900	-0.23420500	4.15473600
H	2.63693300	-0.03891500	3.67467100
H	3.60326400	-1.32146200	2.95154600
C	3.66758800	1.57678500	-1.52919800
H	3.85280500	0.63474500	-2.05148600
H	2.59525500	1.77554900	-1.63434300
H	4.20214700	2.37110100	-2.05710500
C	3.36823800	-3.50971900	-1.52967900
H	3.82150200	-3.01486100	-0.66298300

H	3.89309700	-4.45722200	-1.68535800
H	3.55132500	-2.85790100	-2.38858800
C	-1.53691400	-1.98279300	-1.04228200
H	-1.29857800	-1.15233100	-0.37293400
H	-1.71617800	-1.53354300	-2.02526600
H	-2.47149900	-2.43789300	-0.70078300

Zero-point correction= 0.609226 (Hartree/Particle)
Thermal correction to Energy= 0.652387
Thermal correction to Enthalpy= 0.653331
Thermal correction to Gibbs Free Energy= 0.529744
Sum of electronic and zero-point Energies= -2354.779649
Sum of electronic and thermal Energies= -2354.736488
Sum of electronic and thermal Enthalpies= -2354.735544
Sum of electronic and thermal Free Energies= -2354.859130

Table S24. Cartesian coordinates and energy values of *Z*-**4-Xyl**

Au	-1.03369400	-0.26739700	-1.04865000
P	2.14456600	0.03309300	0.58606500
P	1.28058900	-0.96581100	-1.23161600
N	0.08091500	-0.15299600	2.45424500
N	0.01958500	1.84115400	1.60720400
C	3.15387700	1.55728400	0.21537100
O	-3.38266700	-1.65123000	0.73726500
O	-5.39061200	-0.75407600	1.23263000
C	0.70421300	0.66935800	1.56500000
C	3.18292000	2.26869700	-1.01485500
C	-1.02906400	0.47696200	3.00274800
C	0.23022000	3.01763400	0.76565400
H	0.15901500	3.91437300	1.38477000
H	-0.53730500	3.04382000	-0.01203400
H	1.22024900	2.97526900	0.32540500
C	0.74545900	-3.76683100	-0.64116400
C	1.71302500	-2.73460200	-0.78002100
C	-1.06711500	1.73507400	2.47012300
C	3.09286500	-3.08505800	-0.72241800
C	-2.87369400	0.68787800	-0.96398100
O	-2.59461100	3.03831800	-1.17161900
C	0.42883700	-1.55110400	2.69628600
H	-0.14345300	-2.20152000	2.03059400
H	0.21258600	-1.79897000	3.73604000

H	1.49053200	-1.69244300	2.49434700
O	-3.20096800	1.89395300	-3.02515000
C	4.05628000	1.92751300	1.25483900
C	4.11680000	3.30378000	-1.17759400
H	4.13502500	3.84298100	-2.12086700
C	-4.33275300	-0.68006500	0.62923800
C	-1.94342300	-0.19441200	3.97110100
H	-2.37650100	-1.10321400	3.54237700
H	-2.76819600	0.47127200	4.23016800
H	-1.43136400	-0.46761600	4.90118400
C	4.95868800	2.97613100	1.04626400
H	5.63867900	3.25291000	1.84737700
C	1.16662100	-5.07632000	-0.36854700
H	0.41526600	-5.85441400	-0.25853600
C	5.00114200	3.65697000	-0.16597200
H	5.71371200	4.46276300	-0.31797100
C	-2.05946600	2.83588200	2.64181800
H	-1.59655800	3.75423200	3.02060700
H	-2.83182800	2.53665700	3.35229600
H	-2.54961700	3.06436600	1.68905400
C	3.46572600	-4.40535600	-0.44072600
H	4.52344300	-4.65210900	-0.39085900
C	-2.92542600	1.88466300	-1.84418000
C	2.51352500	-5.39965800	-0.24839100
H	2.81760500	-6.42054800	-0.03402300
C	-4.00401700	0.44323300	-0.26700200
H	-4.85959300	1.11429700	-0.35597000
C	-3.79396900	-2.79478900	1.49627900
H	-2.95501600	-3.49073700	1.46352300
H	-4.68299000	-3.25347000	1.05535200
H	-4.02989100	-2.52225500	2.52936900
C	-2.61433800	4.22563100	-1.98234200
H	-2.32197300	5.04242100	-1.32071500
H	-3.61475400	4.40339300	-2.38451000
H	-1.91448400	4.13887000	-2.81756400
C	4.08239300	1.23873200	2.60392200
H	4.87249000	1.66162000	3.23027000
H	3.13702200	1.35488000	3.14640000
H	4.25889900	0.16291800	2.50680100
C	2.24466400	2.00887700	-2.17125100
H	2.53076600	1.11735600	-2.73590100
H	1.21323300	1.84135400	-1.84853300

H	2.25022100	2.86195200	-2.85591700
C	4.20526100	-2.09361200	-0.98643600
H	4.36631400	-1.41254800	-0.14262400
H	5.14818000	-2.61895100	-1.16434100
H	3.98502600	-1.47009900	-1.85857900
C	-0.74064300	-3.54879200	-0.81094700
H	-1.14301200	-2.79632600	-0.12557500
H	-0.98879800	-3.19672200	-1.81811700
H	-1.28269200	-4.48566700	-0.64876000

Zero-point correction= 0.614387 (Hartree/Particle)
Thermal correction to Energy= 0.656381
Thermal correction to Enthalpy= 0.657325
Thermal correction to Gibbs Free Energy= 0.538185
Sum of electronic and zero-point Energies= -2354.857981
Sum of electronic and thermal Energies= -2354.815987
Sum of electronic and thermal Enthalpies= -2354.815043
Sum of electronic and thermal Free Energies= -2354.934183

Table S25. Cartesian coordinates and energy values of **Int1**

Au	-0.00630800	-1.44749300	-0.87408800
P	1.31601200	1.67330800	0.33588400
P	1.45927500	0.26722500	-1.44337300
N	1.55112900	-0.04859900	2.53639600
N	-0.55694700	0.18881800	2.08389100
C	0.03223200	3.01888800	0.17683600
O	-4.53503400	0.86816200	-0.06011800
O	-4.78505700	1.34017600	-2.25609300
C	0.67946100	0.61980800	1.72972700
C	-0.91675000	3.16149200	-0.87132200
C	0.86485900	-0.93640000	3.35625600
C	-1.84074600	0.59360600	1.50391300
H	-1.68028700	1.41830200	0.82054000
H	-2.50216500	0.92551900	2.30659300
H	-2.31228400	-0.23603800	0.96881700
C	3.82265700	-1.38139100	-0.80519300
C	3.28418200	-0.13358900	-1.22242900
C	-0.46461200	-0.79021400	3.06501800
C	4.18314900	0.90075100	-1.61498100
C	-3.32551700	-1.57181700	-0.73536600
O	-3.51816100	-3.67003500	0.21232300

C	3.00709900	0.09709700	2.54405700
H	3.48317700	-0.76514200	2.07281200
H	3.35219100	0.19280100	3.57566100
H	3.27171100	0.99032000	1.98041300
O	-1.41835500	-2.86893200	-0.17881900
C	0.13662500	4.03965800	1.16773100
C	-1.71470600	4.31641700	-0.90716600
H	-2.43158100	4.42278200	-1.71630300
C	-4.42494400	0.56634900	-1.38561500
C	1.55641600	-1.83304200	4.32791900
H	2.26812600	-2.49907800	3.82780700
H	0.82563100	-2.45723100	4.84477900
H	2.10726000	-1.26798700	5.08877100
C	-0.69696100	5.16062900	1.09524000
H	-0.61097800	5.92940000	1.85854700
C	5.21534300	-1.54277900	-0.74279200
H	5.61614400	-2.50089700	-0.42150300
C	-1.61374800	5.30860600	0.06047200
H	-2.24623700	6.19031400	0.00928900
C	-1.66013700	-1.53078000	3.56364600
H	-2.43141900	-0.85681500	3.95004800
H	-1.37485400	-2.20937700	4.36957500
H	-2.10346000	-2.12744800	2.75822100
C	5.56578900	0.69390300	-1.52919300
H	6.23599000	1.49646200	-1.82602000
C	-2.70220800	-2.68392600	-0.31545600
C	6.08729800	-0.51666700	-1.08908900
H	7.16199600	-0.66611600	-1.03228200
C	-3.82375800	-0.76111400	-1.65360800
H	-3.83608000	-0.99741100	-2.72255000
C	-5.14753000	2.13303500	0.21383600
H	-6.10538200	2.22398600	-0.30413900
H	-4.49968300	2.95645300	-0.10169900
H	-5.29391400	2.16432000	1.29486900
C	-3.03764100	-5.00279100	0.04267300
H	-3.77565000	-5.64596900	0.52710100
H	-2.05836500	-5.14377300	0.50690900
H	-2.97134400	-5.26964100	-1.02038600
C	1.10931200	3.97010300	2.32621800
H	1.11316300	4.91458400	2.87685600
H	0.84359400	3.17910400	3.03893600
H	2.13002000	3.76502800	1.98926100

C	-1.15244400	2.13905200	-1.95927900
H	-0.33849100	2.12296600	-2.68955200
H	-1.23732200	1.12134800	-1.56613200
H	-2.08409200	2.35821000	-2.48691400
C	3.71404000	2.24112900	-2.13983700
H	3.23599900	2.84534000	-1.36010100
H	4.56141900	2.81491200	-2.52574800
H	2.97919900	2.12434000	-2.94200600
C	2.98993100	-2.58798400	-0.42939500
H	2.27116600	-2.37253000	0.36800700
H	2.40224400	-2.95733300	-1.27583800
H	3.63703000	-3.40443200	-0.09462000

Zero-point correction= 0.612366 (Hartree/Particle)
Thermal correction to Energy= 0.654163
Thermal correction to Enthalpy= 0.655107
Thermal correction to Gibbs Free Energy= 0.534835
Sum of electronic and zero-point Energies= -2354.812453
Sum of electronic and thermal Energies= -2354.770656
Sum of electronic and thermal Enthalpies= -2354.769711
Sum of electronic and thermal Free Energies= -2354.889984

Table S26. Cartesian coordinates and energy values of *E*-**4-Xyl**

Au	-0.98369400	-0.48955000	-1.00197300
P	2.49477500	0.66119400	-0.14675200
P	1.34858000	-0.59814100	-1.60282500
N	2.00621000	-0.41072600	2.40965500
N	0.51930000	1.11570900	2.01023500
C	2.45627800	2.50819900	-0.42976200
O	-5.74806000	0.55417200	-0.13654400
O	-6.04295800	0.84532900	-2.35725700
C	1.61008500	0.50610800	1.48395900
C	1.78378700	3.18695600	-1.48129100
C	1.15137500	-0.38936500	3.50658400
C	-0.30424700	2.15054200	1.37782800
H	0.03278300	2.29803800	0.35826200
H	-0.19726500	3.08885700	1.92958700
H	-1.34539400	1.81886000	1.37783700
C	1.74442100	-3.26501200	-0.44739500
C	2.27472700	-2.18453800	-1.20365800
C	0.21622700	0.57815800	3.25663200

C	3.56918000	-2.32608500	-1.78179900
C	-3.00486900	-0.16358800	-0.62956800
O	-3.97479100	-1.52746500	1.02861300
C	3.15378700	-1.31207000	2.29635000
H	2.82129000	-2.33193000	2.09162300
H	3.72503200	-1.28649000	3.22670400
H	3.77689900	-0.97791000	1.46821100
O	-3.11934500	0.45454900	1.68939200
C	3.30491300	3.25094200	0.44255000
C	1.95931400	4.57243700	-1.61624800
H	1.43887300	5.08341700	-2.42141900
C	-5.31047800	0.56905300	-1.42447000
C	1.32199000	-1.30014700	4.67653700
H	1.29649700	-2.35355200	4.37643900
H	0.51595200	-1.14025700	5.39462500
H	2.27019600	-1.12715300	5.19893200
C	3.43438200	4.63402600	0.27184500
H	4.07901100	5.18802400	0.94906300
C	2.51616100	-4.42258300	-0.26283100
H	2.09892900	-5.24388700	0.31478200
C	2.76808200	5.29849300	-0.75102600
H	2.88321600	6.37124500	-0.87706700
C	-0.94976100	1.04093000	4.06465600
H	-0.88687300	2.11338700	4.28109000
H	-0.97759700	0.51198700	5.01950400
H	-1.88800000	0.85446900	3.53134100
C	4.30622700	-3.49764500	-1.56390200
H	5.29365200	-3.58780100	-2.00947000
C	-3.38679400	-0.33408200	0.78951900
C	3.79102600	-4.54295800	-0.80611200
H	4.37071200	-5.44898400	-0.65132000
C	-3.87519900	0.23919400	-1.57776900
H	-3.54951700	0.35696200	-2.60688000
C	-7.13379500	0.86826600	0.03502400
H	-7.76534000	0.13541500	-0.47513300
H	-7.36030300	1.85979400	-0.36618600
H	-7.31374300	0.84265600	1.11047000
C	-4.33611200	-1.77890000	2.39042600
H	-4.80869200	-2.76159400	2.39359300
H	-5.03456400	-1.01959200	2.75238400
H	-3.45344800	-1.78293100	3.03717500
C	4.09611800	2.61653000	1.56743900

H	4.79966700	3.33904200	1.98943300
H	3.45474800	2.27244300	2.38771700
H	4.66521500	1.74766500	1.22083700
C	0.86679900	2.51690200	-2.47774900
H	1.39498200	1.79159200	-3.10205400
H	0.05229500	1.96799900	-1.99278100
H	0.41357400	3.26471300	-3.13367400
C	4.20159700	-1.25418100	-2.64209500
H	4.46843300	-0.36684800	-2.05643100
H	5.11613100	-1.63087100	-3.10952000
H	3.51856500	-0.91572300	-3.42644000
C	0.36772400	-3.25998000	0.17974600
H	0.19309600	-2.37307300	0.79625100
H	-0.42395700	-3.26252600	-0.57646700
H	0.23144500	-4.14799500	0.80514800

Zero-point correction= 0.615698 (Hartree/Particle)
Thermal correction to Energy= 0.657947
Thermal correction to Enthalpy= 0.658891
Thermal correction to Gibbs Free Energy= 0.540389
Sum of electronic and zero-point Energies= -2354.859057
Sum of electronic and thermal Energies= -2354.816809
Sum of electronic and thermal Enthalpies= -2354.815864
Sum of electronic and thermal Free Energies= -2354.934367

Table S27. Cartesian coordinates and energy values of **TS1**

Au	-0.54479200	-0.92768800	-1.20545000
P	2.09843900	0.73247800	0.47030200
P	1.86793400	-0.63796600	-1.29665700
N	0.20489700	-0.08676000	2.36624800
N	-0.50166500	1.74613700	1.44803200
C	2.41902900	2.51378000	0.02348800
O	-4.53328800	-2.81915100	0.22386300
O	-2.67092900	-2.26684400	1.37835200
C	0.49551000	0.82495700	1.39878800
C	2.25414400	3.10337800	-1.25802100
C	-0.97879000	0.24832800	3.00978300
C	-0.70868700	2.85987200	0.52068600
H	-0.27905000	3.78298000	0.91829700
H	-1.78001100	2.97715400	0.35339200
H	-0.23483100	2.62219000	-0.42570900

C	2.40429700	-3.36531900	-0.38751400
C	2.90497700	-2.05735500	-0.63245900
C	-1.41563000	1.41492200	2.44631800
C	4.30628500	-1.83088800	-0.50328000
C	-4.26075400	0.31312500	-0.35609100
O	-5.37531300	1.68679200	-1.83436500
C	0.94281100	-1.32143500	2.61447600
H	0.44353400	-2.15353500	2.11318600
H	0.98374300	-1.50811600	3.68876300
H	1.95456800	-1.21876300	2.22235700
O	-4.11054100	2.65732400	-0.22019700
C	2.98792800	3.28736300	1.07666800
C	2.67077400	4.42862800	-1.45439300
H	2.54141900	4.87354400	-2.43734800
C	-3.52396900	-1.99472500	0.55607400
C	-1.58806100	-0.60633100	4.06911300
H	-1.89110800	-1.57189000	3.65201800
H	-2.47972200	-0.12110900	4.47017100
H	-0.90200100	-0.78207900	4.90538600
C	3.37304300	4.61071000	0.83291100
H	3.80057400	5.19246400	1.64515400
C	3.28272500	-4.37051300	0.04360200
H	2.88544100	-5.36453900	0.23329800
C	3.22664200	5.18104000	-0.42700500
H	3.53863500	6.20628400	-0.60526000
C	-2.61060600	2.25279800	2.75723400
H	-2.32002100	3.26583800	3.05980700
H	-3.16841400	1.80796600	3.58356600
H	-3.28062300	2.33808800	1.89516600
C	5.14287800	-2.86420800	-0.06333700
H	6.20780400	-2.66973800	0.03762900
C	-4.54285800	1.64438100	-0.76918100
C	4.63953900	-4.12769500	0.22369400
H	5.30064700	-4.92143100	0.56081100
C	-3.61418000	-0.73341000	-0.19473200
H	-2.21406400	-0.93858200	-1.10097400
C	-4.54990700	-4.07873200	0.91737700
H	-5.40789700	-4.61853600	0.51782500
H	-4.66123300	-3.92499900	1.99388700
H	-3.62582800	-4.63112500	0.73021900
C	-5.69919300	3.00283400	-2.30514500
H	-6.37150500	2.85179600	-3.14969400

H	-4.79911100	3.53456600	-2.62524100
H	-6.19211100	3.58536700	-1.52217400
C	3.19349600	2.74609300	2.47680600
H	3.71006600	3.48416100	3.09640300
H	2.24538200	2.50917100	2.97355700
H	3.78411800	1.82473100	2.47291800
C	1.62877200	2.40516000	-2.44427200
H	2.31424800	1.68631800	-2.90167000
H	0.73270000	1.83473300	-2.18032700
H	1.34690300	3.13909700	-3.20462300
C	4.96091800	-0.51105300	-0.84970600
H	4.76114500	0.26201300	-0.09867200
H	6.04648500	-0.63057300	-0.91369400
H	4.59676100	-0.12324000	-1.80622400
C	0.96198400	-3.77026300	-0.59561700
H	0.26611200	-3.19651200	0.02619300
H	0.64016600	-3.61658400	-1.63074600
H	0.82926700	-4.83070200	-0.36056600

Zero-point correction= 0.608309 (Hartree/Particle)
Thermal correction to Energy= 0.651172
Thermal correction to Enthalpy= 0.652116
Thermal correction to Gibbs Free Energy= 0.530814
Sum of electronic and zero-point Energies= -2354.762001
Sum of electronic and thermal Energies= -2354.719137
Sum of electronic and thermal Enthalpies= -2354.718193
Sum of electronic and thermal Free Energies= -2354.839496

Table S28. Cartesian coordinates and energy values of **TS2**

Au	-0.43470800	-1.19438300	-0.84513500
P	1.81252400	1.44762900	0.15404500
P	1.49563900	-0.06726600	-1.51211000
N	1.73075300	-0.12305400	2.47960700
N	-0.28148600	0.55199400	2.03844600
C	0.88005700	3.05601000	-0.02089700
O	-4.62769800	0.43622500	0.03539900
O	-4.98711000	1.79079100	-1.73849300
C	1.00856600	0.66296900	1.63496300
C	-0.00222000	3.41367100	-1.07587000
C	0.88792800	-0.76882000	3.37742800
C	-1.45751600	1.18648500	1.43844000

H	-1.14662700	1.80162100	0.60196000
H	-1.94051700	1.82328100	2.18474300
H	-2.15190000	0.41894600	1.09378400
C	3.23967100	-2.28914100	-0.64691800
C	3.10943200	-0.98676300	-1.20377300
C	-0.38190700	-0.34478600	3.09421200
C	4.28069500	-0.32754900	-1.67991400
C	-3.03157000	-1.26770900	-1.62192700
O	-4.26972700	-2.72164000	-0.24173500
C	3.18239400	-0.30913800	2.45566600
H	3.43667200	-1.28939900	2.04726900
H	3.57323600	-0.21604400	3.47108500
H	3.62067900	0.45640700	1.81743000
O	-2.18799200	-2.08613500	0.40655000
C	1.22209500	4.03061000	0.96207100
C	-0.52303400	4.71662000	-1.10815800
H	-1.20214200	4.98117300	-1.91345300
C	-4.44820700	0.80144300	-1.27354600
C	1.38881500	-1.72850600	4.40448900
H	1.93238600	-2.56253900	3.94736300
H	0.55051600	-2.14672900	4.96412600
H	2.06113600	-1.24757200	5.12462200
C	0.66484900	5.31178700	0.88839800
H	0.92775800	6.04310600	1.64802200
C	4.51553800	-2.86357400	-0.53520800
H	4.60387600	-3.85960800	-0.10860900
C	-0.20273600	5.66031500	-0.14052500
H	-0.62408200	6.66026900	-0.18951700
C	-1.69963900	-0.75283200	3.66052000
H	-2.27506000	0.10570000	4.02321100
H	-1.55640200	-1.43740100	4.49857400
H	-2.28700100	-1.26531500	2.88974900
C	5.53261900	-0.94012600	-1.54023100
H	6.41491100	-0.41970700	-1.90380300
C	-3.15337800	-1.98548900	-0.42821300
C	5.65878400	-2.19840500	-0.96440500
H	6.63510200	-2.66532900	-0.86758100
C	-3.54391600	-0.09570800	-2.02737200
H	-3.32056500	0.30828700	-3.01413300
C	-5.56827700	1.23925700	0.75247400
H	-6.55626800	1.19496800	0.28542300
H	-5.25222000	2.28640300	0.78348000

H	-5.61065800	0.82307800	1.76056400
C	-4.21551400	-3.72808200	0.77267400
H	-5.11370100	-4.33280200	0.63605100
H	-4.21986200	-3.28484900	1.77354300
H	-3.32093300	-4.34808100	0.66606200
C	2.17299600	3.75133900	2.10738100
H	2.38288200	4.67186400	2.65837300
H	1.76245000	3.03046700	2.82471500
H	3.12453800	3.34127300	1.75288500
C	-0.44481600	2.47686700	-2.17578900
H	0.38334500	2.18686300	-2.82793500
H	-0.87757800	1.54827000	-1.79036600
H	-1.20943800	2.95676400	-2.79130800
C	4.24469200	1.02716500	-2.35461100
H	3.99357700	1.82979500	-1.65144100
H	5.22193300	1.26187700	-2.78607500
H	3.49544300	1.06053700	-3.15110100
C	2.08016300	-3.13599800	-0.16840800
H	1.47168200	-2.62842400	0.58625400
H	1.39842000	-3.39180900	-0.98566800
H	2.44987500	-4.07252500	0.26052300

Zero-point correction= 0.613315 (Hartree/Particle)
Thermal correction to Energy= 0.655561
Thermal correction to Enthalpy= 0.656505
Thermal correction to Gibbs Free Energy= 0.535276
Sum of electronic and zero-point Energies= -2354.808378
Sum of electronic and thermal Energies= -2354.766132
Sum of electronic and thermal Enthalpies= -2354.765188
Sum of electronic and thermal Free Energies= -2354.886417

Table S29. Cartesian coordinates and energy values of **TS3**

Au	-1.04532500	-1.23106000	-0.16203200
P	1.28222400	-0.92177500	0.59066200
P	2.04789000	0.79041300	-0.70889500
N	-0.30225600	1.96958500	-1.76562700
N	-0.24008100	2.23737700	0.38286900
C	0.43949800	1.70512900	-0.66281200
C	-0.00939400	1.51968400	-3.12495200
H	1.00729700	1.12972500	-3.14882600
H	-0.09717600	2.36271600	-3.81407600
H	-0.71570500	0.73439500	-3.40183000

C	0.15722800	2.18702100	1.78912800
H	0.44775200	3.18333900	2.13413900
H	0.99206300	1.49993900	1.90280700
H	-0.68173100	1.81733300	2.38073600
N	-2.74668000	-0.33292200	-2.27795700
H	-2.74781600	-1.55113400	-0.12181900
C	-1.45755500	2.65716500	-1.41802300
C	-1.41664800	2.83210900	-0.06130600
N	-3.78464800	-0.58533100	-1.79960000
C	-4.25064500	-1.17630300	-0.66244300
H	-4.77739900	-2.11226200	-0.82137100
C	-2.49393400	3.04735800	-2.41736600
H	-2.10447200	3.75810000	-3.15585100
H	-3.34087700	3.51309200	-1.91143200
H	-2.86875500	2.16770100	-2.94937400
C	-2.41719700	3.44218500	0.86239200
H	-3.02696000	2.66700200	1.33911100
H	-3.09849700	4.08458200	0.30132800
H	-1.94108400	4.05343100	1.63492200
O	-4.57541900	0.95419800	0.39778800
O	-5.47530900	-0.94291900	1.28618000
C	-4.78378400	-0.24746300	0.35168800
C	-5.91016800	-0.20949000	2.45167200
H	-6.81849200	-0.72297600	2.77689400
H	-6.15887600	0.81200500	2.15423300
C	-4.84494700	-0.22576300	3.53828900
H	-4.57769600	-1.25173600	3.80639700
H	-5.21748600	0.28106700	4.43516000
H	-3.94249400	0.29005000	3.19989400
C	2.20070600	-2.44236000	0.01011100
C	2.63550000	-3.31348100	1.05033900
C	2.42928900	-2.82661400	-1.33855400
C	3.33732500	-4.48200700	0.73163000
C	3.14611500	-4.00082700	-1.60974500
C	3.61240100	-4.82133200	-0.58906000
H	3.66658800	-5.13350700	1.53736500
H	3.32211900	-4.27770600	-2.64645400
H	4.16586900	-5.72721700	-0.82097800
C	3.15854100	1.95167900	0.27318200
C	4.19667300	1.41696900	1.08083800
C	3.10578300	3.36040500	0.07736300
C	5.03842300	2.28650800	1.78677200

C	3.96664000	4.18946500	0.80909000
C	4.90950300	3.66642300	1.68622300
H	5.81801300	1.85993600	2.41267800
H	3.90660200	5.26473000	0.65930900
H	5.56708800	4.32516000	2.24611500
C	2.32196900	-3.06283800	2.51169800
H	2.64059800	-2.07189300	2.84788400
H	1.24452400	-3.12008500	2.70538600
H	2.81144100	-3.81355100	3.13945000
C	1.89733800	-2.05331100	-2.52207600
H	0.86605900	-1.72950500	-2.34270000
H	2.48668000	-1.15458100	-2.73105800
H	1.91157500	-2.67811800	-3.42017200
C	4.48976500	-0.06259800	1.18466500
H	5.49864600	-0.21608700	1.57808500
H	3.78571600	-0.57369000	1.84455100
H	4.43497600	-0.56795800	0.21561900
C	2.22284100	4.04497400	-0.94920300
H	2.19394000	3.49021300	-1.89210000
H	1.18870700	4.18554000	-0.61686100
H	2.62213700	5.03880200	-1.16991200

Zero-point correction= 0.598209 (Hartree/Particle)
Thermal correction to Energy= 0.639376
Thermal correction to Enthalpy= 0.640321
Thermal correction to Gibbs Free Energy= 0.523085
Sum of electronic and zero-point Energies= -2237.658589
Sum of electronic and thermal Energies= -2237.617422
Sum of electronic and thermal Enthalpies= -2237.616478
Sum of electronic and thermal Free Energies= -2237.733714

Table S30. Cartesian coordinates and energy values of **TS4**

Au	-0.55034200	-1.42588000	0.67570400
P	1.75134500	-0.83813800	0.64208300
P	1.56691700	0.85082400	-0.91159800
N	-1.05399000	1.83457800	-0.39051200
N	0.27843500	2.32090100	1.24921800
C	0.22075900	1.69689600	0.04692000
C	-1.61425200	1.28679900	-1.63084800
H	-0.86391400	0.65563600	-2.10259500
H	-1.87482200	2.10905500	-2.30371100

H	-2.51170700	0.70648700	-1.40018300
C	1.45936100	2.43632300	2.10598200
H	2.12896800	1.60270700	1.90510900
H	1.14118700	2.38500500	3.14746400
H	1.97456500	3.38265000	1.92095700
N	-2.62111700	-1.81517900	0.67031800
H	-5.39883000	-1.75601000	1.51340800
C	-1.80797200	2.54403900	0.53284300
C	-0.96478300	2.85904100	1.56639200
N	-3.41260700	-0.98233200	1.17492000
C	-4.71810300	-1.46913800	0.71215900
H	-3.68367800	-2.41959200	0.18214600
C	-3.25439600	2.84050600	0.32314200
H	-3.40122300	3.53715300	-0.51112600
H	-3.67714500	3.29814700	1.21942900
H	-3.81617200	1.92751000	0.09805100
C	-1.22777900	3.59638200	2.83695400
H	-1.10719700	2.94994700	3.71382900
H	-2.25369000	3.96797500	2.84266000
H	-0.56032500	4.45655300	2.95891000
O	-4.70871900	0.18083800	-1.03508600
O	-6.59997300	-0.99300700	-0.57308400
C	-5.29544400	-0.65864900	-0.34172100
C	-7.23233900	-0.37886600	-1.70921400
H	-8.00247900	-1.09131100	-2.01922000
H	-6.50110300	-0.26659600	-2.51394400
C	-7.84592800	0.96769800	-1.34790300
H	-8.54412100	0.86444800	-0.51158600
H	-8.39294000	1.37714900	-2.20461900
H	-7.06272800	1.67624500	-1.06731200
C	2.60644500	-2.27358300	-0.20201200
C	3.52212700	-2.97798100	0.63108700
C	2.38946900	-2.73670000	-1.52708200
C	4.22803300	-4.07166200	0.11629300
C	3.12827900	-3.83047100	-2.00142500
C	4.04924500	-4.49149600	-1.19746500
H	4.92406700	-4.59955600	0.76311700
H	2.95918400	-4.17186000	-3.01952300
H	4.60964300	-5.33750000	-1.58562200
C	2.92741300	2.14537200	-0.76048200
C	4.27451600	1.81004800	-0.46695000
C	2.62243100	3.48379600	-1.13801300

C	5.24320500	2.82224200	-0.43346900
C	3.62459000	4.46160000	-1.08439800
C	4.92564600	4.14640800	-0.71123100
H	6.26823700	2.55161400	-0.19443100
H	3.37421200	5.48130100	-1.36606200
H	5.69096000	4.91630100	-0.67573700
C	3.74379200	-2.62851700	2.08969600
H	2.83098100	-2.76127500	2.68114300
H	4.51352700	-3.27583000	2.51995200
H	4.05554100	-1.58924600	2.23118700
C	1.36940200	-2.13686900	-2.46552400
H	0.41820400	-1.95895400	-1.95190900
H	1.69165200	-1.17568500	-2.87861100
H	1.18375700	-2.81313900	-3.30469500
C	4.74801300	0.39634000	-0.22070000
H	5.84024700	0.35625500	-0.24538400
H	4.42076300	0.01801900	0.75092700
H	4.37803400	-0.30462600	-0.97410000
C	1.26830700	3.92552600	-1.65759500
H	0.83232200	3.18515300	-2.33598200
H	0.54014200	4.11083600	-0.85978600
H	1.37327900	4.86035700	-2.21487700

Zero-point correction= 0.600103 (Hartree/Particle)
Thermal correction to Energy= 0.640757
Thermal correction to Enthalpy= 0.641701
Thermal correction to Gibbs Free Energy= 0.526420
Sum of electronic and zero-point Energies= -2237.655710
Sum of electronic and thermal Energies= -2237.615057
Sum of electronic and thermal Enthalpies= -2237.614112
Sum of electronic and thermal Free Energies= -2237.729393

Table S31. Cartesian coordinates and energy values of **TS5**

Au	-1.15354600	-0.22342800	-0.75537900
P	0.68096600	1.22878900	-1.27340900
P	2.40878700	0.32204400	-0.13602000
N	1.53909800	0.15602700	2.53404200
N	1.02435100	-1.69514100	1.52987700
C	2.97098000	-1.65596000	-2.24370300
C	-0.21282400	3.27872500	0.64250200
C	3.28710100	-1.09614800	-0.97683700

C	1.64783700	-0.50448700	1.34825000
C	0.71905400	2.86624800	-0.34844600
C	2.08244700	1.48047700	2.83961700
H	2.76650600	1.76856800	2.04308900
H	2.61572500	1.43954100	3.79174500
H	1.28067500	2.21958900	2.89485700
C	4.46054700	-1.53537800	-0.29664400
C	1.72629700	3.78357300	-0.76659100
C	0.82750700	-2.75840300	0.54025900
H	-0.24381300	-2.95249500	0.43608300
H	1.34383000	-3.66178900	0.87718400
H	1.24661100	-2.44630800	-0.40903900
C	-0.09645600	4.55988200	1.20382300
H	-0.81574400	4.86734500	1.95868800
C	0.90562300	5.44094600	0.81187500
H	0.97438500	6.42840100	1.25993600
C	1.80607400	5.04932400	-0.17174700
H	2.58272000	5.73557200	-0.49929500
C	5.26282300	-2.52757700	-0.87121000
H	6.15015500	-2.85855400	-0.33835000
N	-2.50548300	-2.59441000	0.45374900
H	-2.21942900	-1.62167300	-0.30379100
C	0.81584800	-0.60469300	3.44614300
C	3.81708000	-2.63816100	-2.78042900
H	3.56711500	-3.06323800	-3.74841400
C	4.94970300	-3.07948500	-2.10789200
H	5.58516900	-3.84372200	-2.54595700
C	0.49218600	-1.77329800	2.81118700
N	-3.66328500	-2.62931600	0.84035800
C	-4.85363100	-2.07781000	0.86324500
H	-5.61144700	-2.59795500	1.43714300
C	0.50791100	-0.12842600	4.82643500
H	1.41556000	0.02075800	5.42291200
H	-0.11096000	-0.86278100	5.34445900
H	-0.04163500	0.81908800	4.81362000
C	-0.30296000	-2.94964900	3.26855300
H	-1.17613900	-3.09216300	2.62216000
H	-0.65185200	-2.79520400	4.29110100
H	0.28989200	-3.87121000	3.25225300
O	-6.43498200	-0.42040600	0.28104100
O	-4.34182700	-0.29998300	-0.60716200
C	-5.30580500	-0.87485700	0.18178800

C	-4.75929300	0.85748600	-1.36261200
H	-3.83288200	1.40313100	-1.56116800
H	-5.41955800	1.46811100	-0.74137300
C	-5.44994700	0.46090600	-2.66015800
H	-4.80022200	-0.17913200	-3.26505300
H	-5.69312700	1.35579700	-3.24405800
H	-6.37815900	-0.07480700	-2.44797500
C	1.76189900	-1.27519500	-3.06652400
H	1.81074400	-0.24073400	-3.41699100
H	1.68404200	-1.92509900	-3.94190400
H	0.82656300	-1.36697600	-2.50408900
C	4.89879300	-0.97770200	1.04142500
H	4.93882100	0.11653300	1.03008100
H	4.22189100	-1.26478200	1.85500500
H	5.89246600	-1.35213800	1.30069200
C	-1.35660800	2.42427900	1.14322500
H	-2.09617400	2.23054800	0.36013500
H	-1.02533300	1.44286700	1.49644100
H	-1.87379300	2.92691000	1.96612900
C	2.73538400	3.45680300	-1.84633800
H	3.44228300	2.68341000	-1.52423900
H	2.24983400	3.08049100	-2.75160800
H	3.31542900	4.34688700	-2.10642800

Zero-point correction= 0.597060 (Hartree/Particle)
Thermal correction to Energy= 0.637724
Thermal correction to Enthalpy= 0.638669
Thermal correction to Gibbs Free Energy= 0.521884
Sum of electronic and zero-point Energies= -2237.668060
Sum of electronic and thermal Energies= -2237.627396
Sum of electronic and thermal Enthalpies= -2237.626451
Sum of electronic and thermal Free Energies= -2237.743237

Table S32. Cartesian coordinates and energy values of **TS6**

Au	0.53396400	-0.78027900	-1.40001900
P	-1.82798300	-0.83810000	-1.25486700
P	-2.35397000	0.67700300	0.32016900
N	-0.78288700	0.09954500	2.57897300
N	0.26832500	1.56793600	1.38068500
C	-2.36427400	2.90512800	-1.60414400
C	-1.83838200	-3.32894300	0.30918300

C	-2.59149900	2.42782000	-0.28494100
C	-0.87581700	0.83923700	1.43950000
C	-2.57542900	-2.30411000	-0.34442800
C	-1.78752300	-0.83950900	3.07969400
H	-2.72228600	-0.66561600	2.54852600
H	-1.93060300	-0.67731800	4.14977700
H	-1.47023000	-1.86901000	2.90101300
C	-3.17967700	3.30076400	0.67721700
C	-3.99431300	-2.41748900	-0.40896200
C	0.70063600	2.42538500	0.27669200
H	-0.16574400	2.74154100	-0.29530500
H	1.38891200	1.86867600	-0.36584500
H	1.19784700	3.30624300	0.68545600
C	-2.52512200	-4.40237300	0.89694400
H	-1.95148300	-5.18139100	1.39286300
C	-3.91195200	-4.49391100	0.85338200
H	-4.42153800	-5.33538100	1.31485900
C	-4.63586800	-3.50451100	0.19855200
H	-5.71923000	-3.57360000	0.14252000
C	-3.50695100	4.61169600	0.31374400
H	-3.94863300	5.26842000	1.05835800
N	2.61434800	-0.53769900	-1.49389900
H	3.11631400	-0.40858900	-2.37982800
C	0.43009400	0.33873600	3.21588600
C	-2.72355200	4.22461700	-1.91966400
H	-2.54608600	4.58204600	-2.93019700
C	-3.28741400	5.07634000	-0.97818500
H	-3.55404900	6.09393600	-1.24899300
C	1.09147500	1.26993200	2.46274600
N	3.36332000	-0.55438000	-0.46641700
C	4.11160000	-0.56550000	0.55784900
H	3.73901200	-0.73434500	1.58469700
C	0.82634700	-0.35179900	4.47807300
H	0.16114700	-0.09991800	5.31235100
H	1.83917300	-0.06100000	4.76079600
H	0.81668000	-1.44066600	4.36023800
C	2.42884000	1.90327100	2.65368900
H	3.10416700	1.65940400	1.82720400
H	2.89138300	1.53353100	3.57016200
H	2.35273400	2.99354700	2.73520700
O	6.29160500	-0.36436100	1.51757200
O	6.06603200	-0.21921200	-0.74330100

C	5.58145000	-0.38059700	0.52301700
C	7.48795000	-0.03571600	-0.85377600
H	7.73941700	-0.38963500	-1.85791800
H	7.99066400	-0.66384600	-0.11324800
C	7.88120600	1.42480500	-0.67188800
H	7.34668300	2.06301800	-1.38258900
H	8.95700700	1.55089400	-0.83777700
H	7.64868500	1.75391800	0.34384400
C	-1.73770500	2.08592000	-2.70819000
H	-2.39814200	1.28355900	-3.04826000
H	-1.50909500	2.72396900	-3.56612300
H	-0.80730900	1.60188000	-2.39461600
C	-3.47316600	2.88082700	2.10241200
H	-4.06692100	1.96181400	2.13868400
H	-2.55860000	2.69237300	2.67728600
H	-4.02619700	3.66703800	2.62300800
C	-0.32900200	-3.35724900	0.41059000
H	0.14330700	-3.47657300	-0.56975500
H	0.08236100	-2.43529100	0.83335200
H	-0.00602100	-4.19406700	1.03736800
C	-4.86597500	-1.40446800	-1.11940300
H	-4.88482300	-0.44161900	-0.59537400
H	-4.50456100	-1.20225700	-2.13185900
H	-5.89649000	-1.76620600	-1.18100000

Zero-point correction= 0.602581 (Hartree/Particle)
Thermal correction to Energy= 0.642257
Thermal correction to Enthalpy= 0.643201
Thermal correction to Gibbs Free Energy= 0.527857
Sum of electronic and zero-point Energies= -2237.680058
Sum of electronic and thermal Energies= -2237.640382
Sum of electronic and thermal Enthalpies= -2237.639438
Sum of electronic and thermal Free Energies= -2237.754782

Table S33. Cartesian coordinates and energy values of **TS7**

Au	0.62446500	-1.70146200	-0.03292900
P	-1.42143900	-0.73905100	-0.62747200
P	-1.64243700	1.07909400	0.78233500
N	0.98487700	1.82805000	1.53613000
N	0.72343200	2.07275600	-0.60243200
C	0.08921500	1.67698900	0.52855100

C	0.75194200	1.50812800	2.94741000
H	-0.27228400	1.15650700	3.05794000
H	0.89698200	2.40642400	3.55255100
H	1.45360800	0.73314800	3.26521000
C	0.17737900	2.06143800	-1.95942800
H	0.67119200	1.28433400	-2.54671400
H	0.34040900	3.03730000	-2.42180600
H	-0.88795600	1.85314200	-1.92062800
N	3.46926400	-0.57155800	3.12867400
C	2.18837400	2.31150400	1.04470500
C	2.02339700	2.46255100	-0.30855200
N	3.48258600	-0.75343900	1.98533400
C	3.37150800	-1.08196800	0.75305100
C	3.39022400	2.58976000	1.88757500
H	3.35554900	2.03769100	2.82762700
H	3.48343700	3.65878800	2.11211500
H	4.28268100	2.24809700	1.35597500
C	2.99778900	2.92503900	-1.33955800
H	2.87265100	3.98786900	-1.58045900
H	2.89384500	2.35585800	-2.26742500
H	4.01195900	2.75791700	-0.97316600
O	4.94086900	0.53941100	-0.10847300
O	4.04151200	-1.05811600	-1.45356200
C	4.19634200	-0.43856900	-0.23514400
C	4.86945300	-0.58475100	-2.52601100
H	4.94310400	0.50565100	-2.48036900
H	4.33589600	-0.87232200	-3.43703100
C	6.25737000	-1.21218900	-2.48468600
H	6.78548500	-0.90010500	-1.58052500
H	6.84293300	-0.89487300	-3.35492600
H	6.18852600	-2.30409800	-2.49483800
C	-2.63699100	-2.01669100	0.00460100
C	-3.31679200	-2.72993300	-1.02356900
C	-2.89224100	-2.35269700	1.36034500
C	-4.27256600	-3.69305800	-0.68095400
C	-3.86529800	-3.31948600	1.65354900
C	-4.56408200	-3.97802600	0.64894100
H	-4.78674500	-4.22881200	-1.47460800
H	-4.05936600	-3.56498000	2.69449500
H	-5.31396000	-4.72303400	0.89975700
C	-2.61921800	2.44264900	-0.07745100
C	-3.80490900	2.14249700	-0.79722900

C	-2.28759900	3.80873100	0.15033900
C	-4.53097700	3.18122600	-1.39513600
C	-3.04349900	4.81117500	-0.47119200
C	-4.14146900	4.50835100	-1.26762600
H	-5.42788100	2.93152500	-1.95570600
H	-2.77153100	5.84945100	-0.29928500
H	-4.71318800	5.30008800	-1.74276100
C	-3.01224800	-2.53958200	-2.49641300
H	-3.13170600	-1.50322400	-2.82637600
H	-1.97992200	-2.82266900	-2.73173900
H	-3.67301700	-3.16583900	-3.10248700
C	-2.13793500	-1.76119800	2.52796200
H	-1.06511000	-1.69889800	2.31442500
H	-2.47494500	-0.74988800	2.77536900
H	-2.27168500	-2.38362700	3.41709900
C	-4.37586700	0.74870900	-0.91713900
H	-5.42944500	0.79966900	-1.20481900
H	-3.85506100	0.15516300	-1.67189000
H	-4.32268700	0.19217600	0.02289400
C	-1.19916400	4.27708100	1.09676300
H	-1.18234900	3.68917700	2.01959600
H	-0.19539100	4.24056500	0.66044300
H	-1.38401600	5.31682500	1.37965200
H	2.41806200	-2.55523700	0.32367500
H	1.89435500	-3.18200300	0.08728500

Zero-point correction= 0.594943 (Hartree/Particle)
Thermal correction to Energy= 0.636136
Thermal correction to Enthalpy= 0.637081
Thermal correction to Gibbs Free Energy= 0.518620
Sum of electronic and zero-point Energies= -2237.644868
Sum of electronic and thermal Energies= -2237.603674
Sum of electronic and thermal Enthalpies= -2237.602730
Sum of electronic and thermal Free Energies= -2237.721191

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