Supporting Information

Materials and Methods

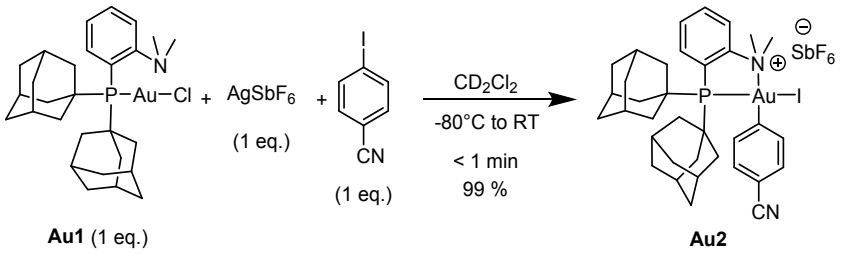
Unless otherwise stated, all reactions and manipulations were carried out under an atmosphere of dry argon using standard Schlenk techniques or in a glovebox under an inert atmosphere. Dry, oxygen-free solvents were employed. Melting points were determined with a Stuart SMP40 apparatus and are uncorrected. Solution ^{1}H, ^{13}C, ^{19}F and ^{31}P NMR spectra were recorded on Bruker Avance 300, 400 or 500 spectrometers at 298K unless otherwise stated. Chemical shifts (δ) are expressed with a positive sign, in parts per million. Chemical shifts (δ) are expressed with a positive sign, in parts per million. ^{1}H and ^{13}C chemical shifts are referenced internally to residual protio (^{1}H) or deutero (^{13}C) solvent, while ^{31}P and ^{19}F chemical shifts are relative to 85% H_3PO_4 and $CFCl_3$ respectively. The following abbreviations and their combinations are used: br, broad; s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet. GC-MS analyses were performed on a MS Perkin Elmer Clarus MS560, GC PerkinElmer Clarus 500 and Agilent HP6890. All commercial starting materials were used as received unless otherwise stated. 4-*Tert*-butyliodobenzene, 1-methylindole, 1,2-dimethylindole, 4-methylindole, 5-methylindole, 6-methylindole, 7-methylindole, 5-bromo-1-methylindole, 5-methoxyindole and methylindole-6-carboxylate were purchased from Fluorochem. Indole, 1-acetylindole, 1-bromo-4-iodobenzene, 1-iodo-4-nitrobenzene, 4-iodoacetophenone, 2-iodonaphthalene and 1-iodonaphthalene were purchased from Aldrich. 1-Benzylindole, 1-(*p*-toluenesulfonyl)indole and 2-iodoanisole were purchased from Alfa Aesar. 4-Iodoanisole and 4-iodobenzotrifluoride were purchased from Acros.

Experimental Procedures and analytical data

General Procedure for Oxidative Addition of Iodoarenes to the (P,N) Gold Complex

In a glovebox, a screw-cap NMR tube was charged with silver hexafluoroantimonate (8.0 mg, 0.023 mmol) in CD_2Cl_2 (0.3 mL). (MeDalphos)AuCl Complex **Au1** (15 mg, 0.023 mmol) was transferred into a small glass vial and dissolved in CD_2Cl_2 (0.3 mL). The iodoarene (0.023 mmol) was added to the solution of **Au1**. The prepared solution was loaded into a plastic syringe equipped with stainless steel needle. The syringe was closed by blocking the needle with a septum. Outside the glovebox, the NMR tube was cooled down to -80°C (Ethanol/N_2 cold bath). At this temperature, the solution of complex **Au1** and iodoarene was added. The tube was gently shaken and allowed to warm to RT. The formation of the gold(III) complex was confirmed by ^{1}H and ^{31}P NMR spectroscopy as well as high-resolution mass spectrometry (Electrospray ionization, positive mode). Iodine to chloride exchange reaction from aryl gold(III) complexes was systematically observed with all substrates. In the following examples, only the mass peak corresponding to the aryl gold(III) chloride derivatives is indicated.

Reaction of Complex Au1 with 4-Iodobenzonitrile (Au2)



^{1}H NMR (300 MHz, CD_2Cl_2): δ 7.88 (m, 3H), 7.69 (m, 1H), 7.48 (m, 4H), 3.46 (s, 6H), 2.05 (m, 18H), 1.67 (m, 12H). **^{31}P{^{1}H} NMR** (300 MHz, CD_2Cl_2): δ 78.7 (s). **HRMS (ESI$^+$)**: calculated for $[M^+] = C_{35}H_{44}N_2PClAu^+$: 755.26. Found: 755.2603.

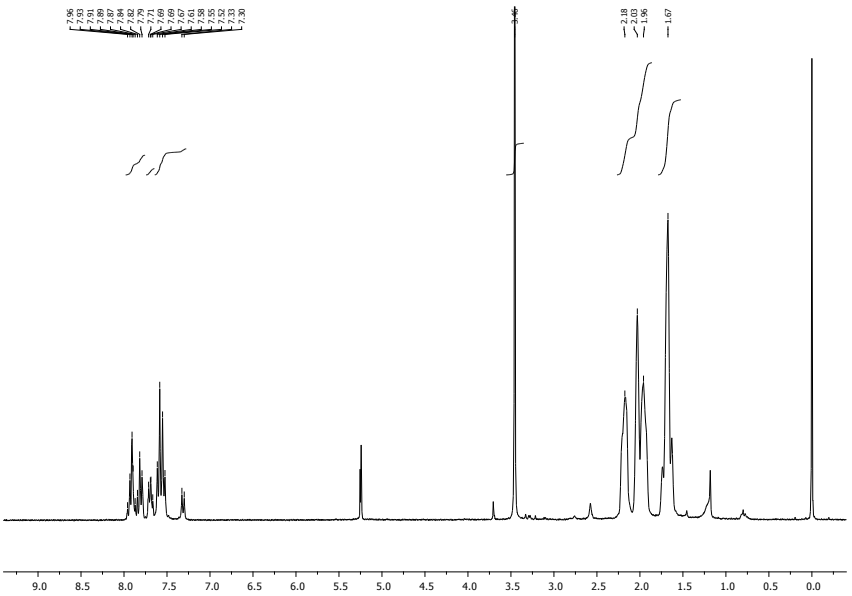


Figure S1. ^{1}H NMR spectrum of (**Au2**) in CD_2Cl_2.

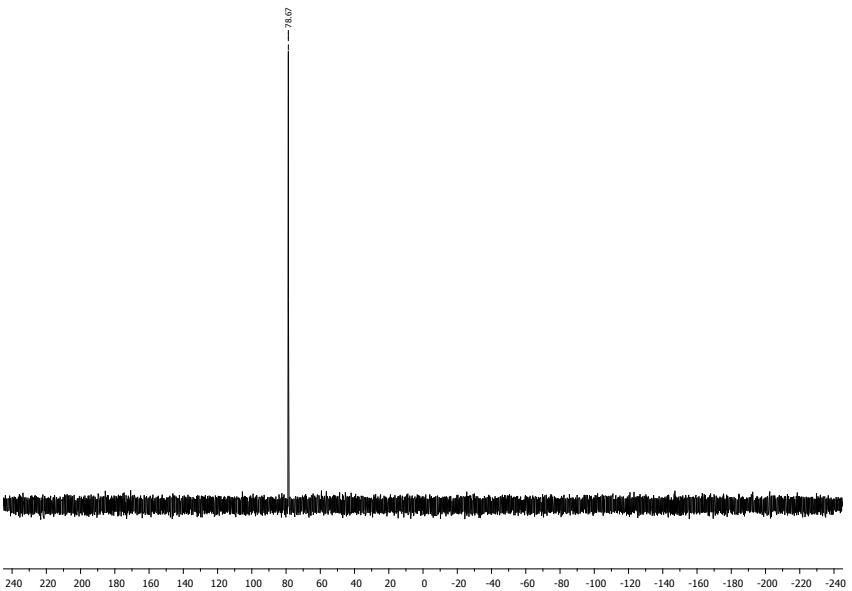
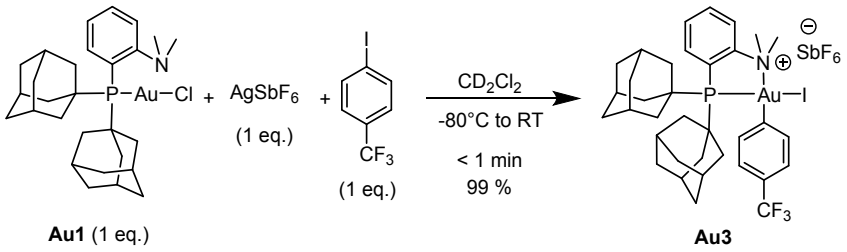


Figure S2. ^{31}P{^{1}H} NMR spectrum of (**Au2**) in CD_2Cl_2.

Reaction of Complex Au1 with 4-Iodobenzotrifluoride (Au3)



^{1}H NMR (300 MHz, CD_2Cl_2): δ 8.06 – 7.22 (m, 8H), 3.45 (s, 6H), 2.41 – 1.84 (m, 18H), 1.69 (m, 12H). **^{31}P{^{1}H} NMR** (300 MHz, CD_2Cl_2): δ 77.7 (s). **HRMS (ESI^{+})**: calculated for [M^{+}] = $C_{35}H_{44}NPF_3ClAu^{+}$: 798.25. Found: 798.2537.

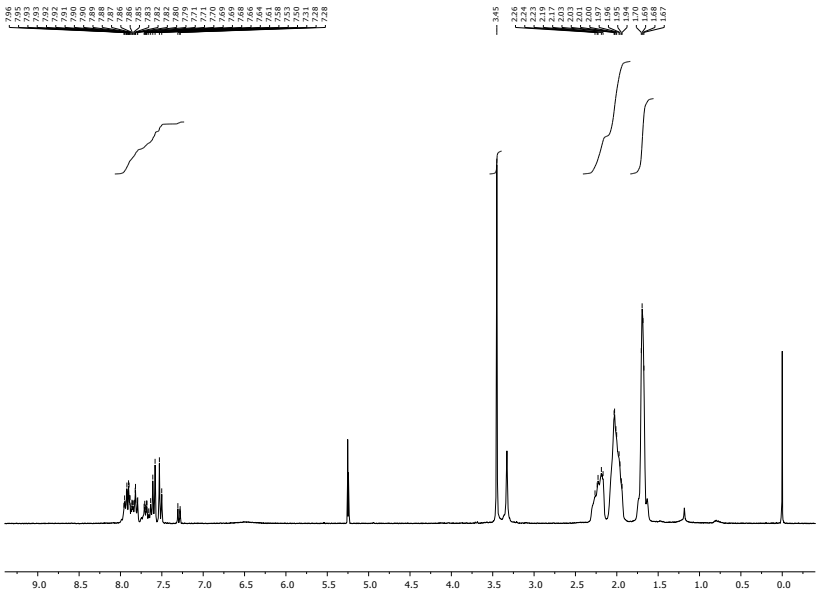


Figure S3. ^{1}H NMR spectrum of (**Au3**) in CD_2Cl_2.

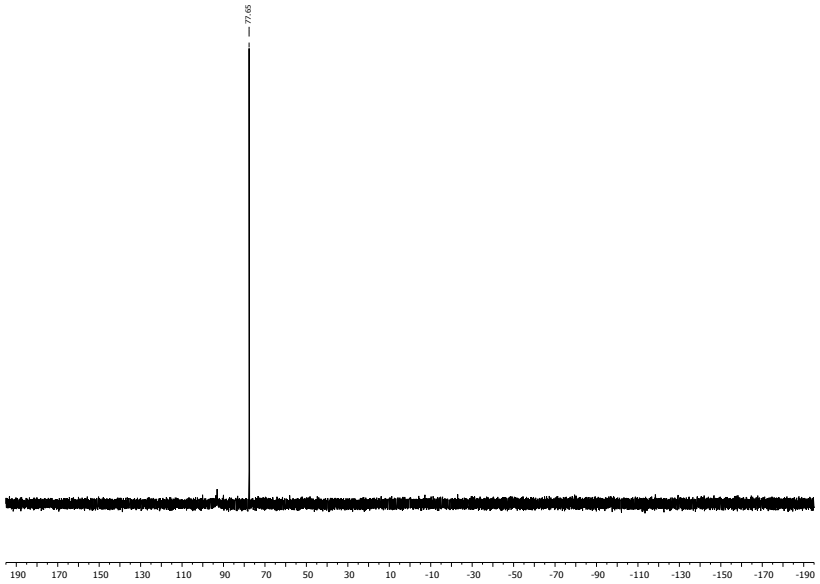
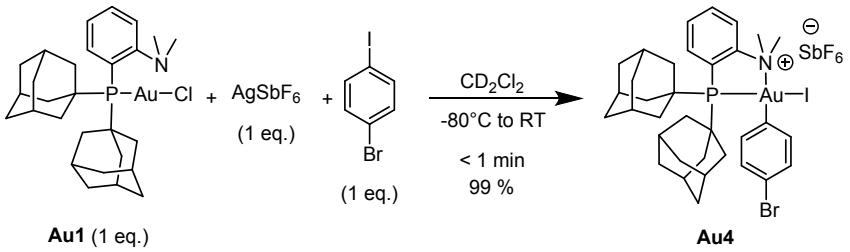


Figure S4. ^{31}P{^{1}H} NMR spectrum of (**Au3**) in CD_2Cl_2.

Reaction of Complex Au1 with *p*-Bromoiodobenzene (Au4)



^{1}H NMR (300 MHz, CD_2Cl_2): δ 8.03 – 7.79 (m, 3H), 7.79 – 7.14 (m, 5H), 3.50 (s, 6H), 2.54 – 1.89 (m, 18H), 1.71 (s, 12H). **^{31}P{^{1}H} NMR** (300 MHz, CD_2Cl_2): δ 74.7 (s). **HRMS (ESI^{+})**: calculated for [M^{+}] = $C_{34}H_{44}NPBrClAu^{+}$: 808.17. Found: 808.1742.

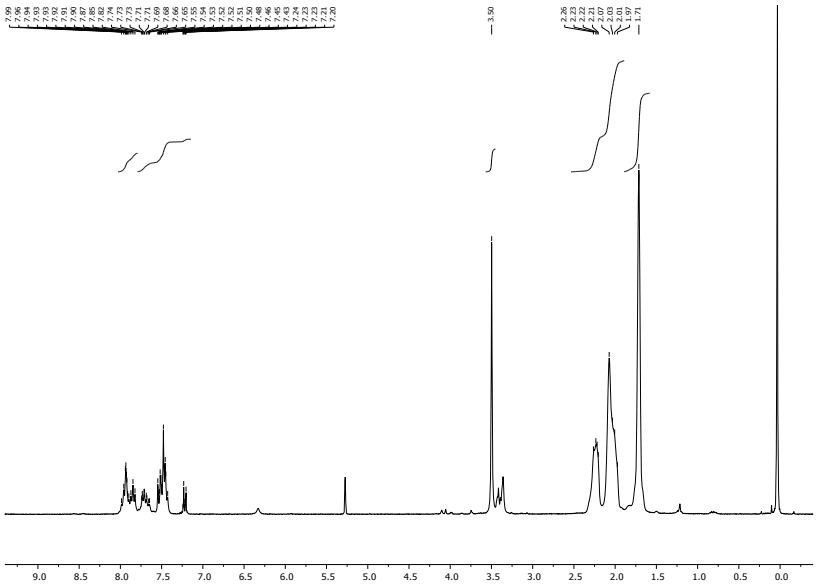


Figure S5. ^{1}H NMR spectrum of (**Au4**) in CD_2Cl_2.

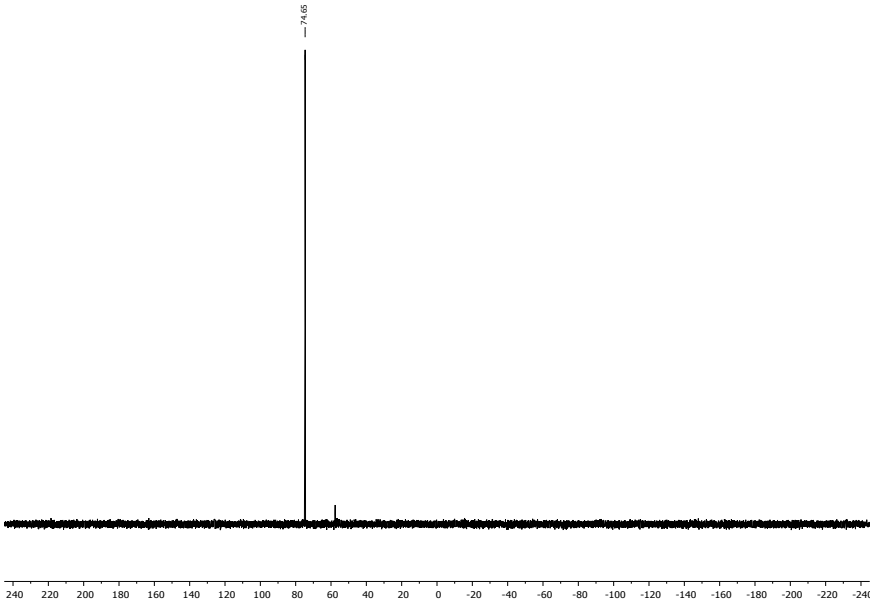
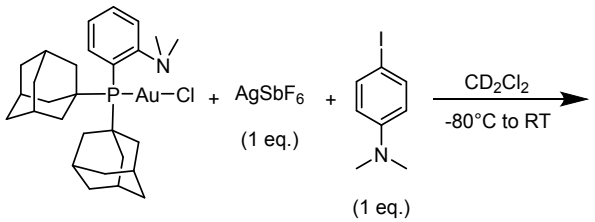


Figure S6. ^{31}P{^{1}H} NMR spectrum of (**Au4**) in CD_2Cl_2.

Reaction of Complex Au1 with 4-Iodo-*N*,*N*-dimethylaniline



Au1 (1 eq.)

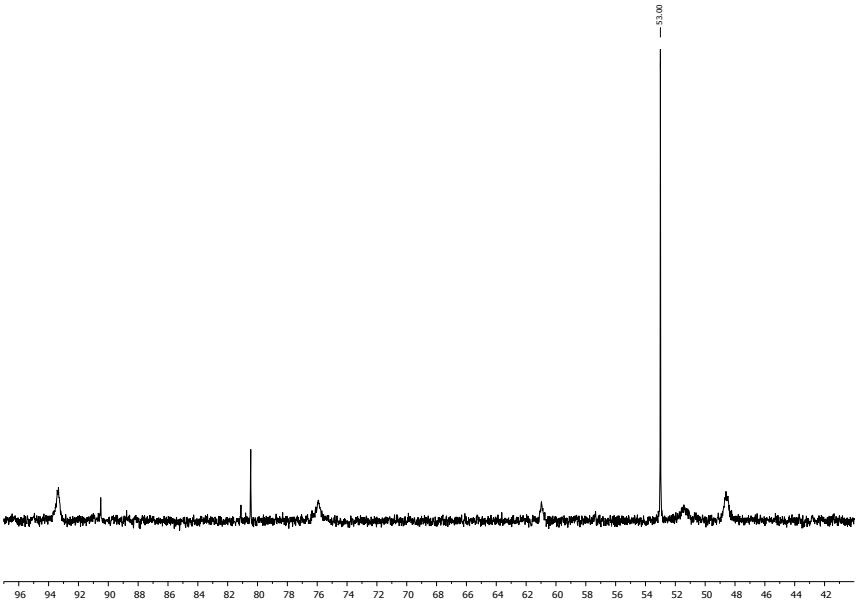
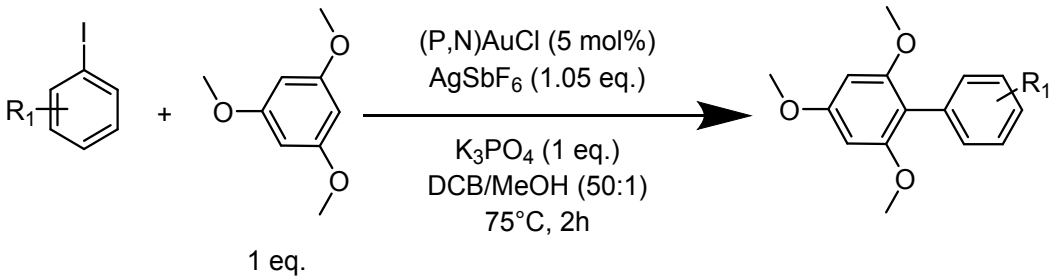


Figure S7. $^{31}P\{^{1}H\}$ NMR spectrum of the crude mixture.

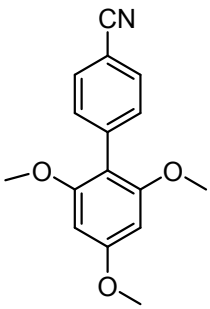
General procedure for gold-catalyzed direct arylation of 1,3,5–trimethoxybenzene with iodoarenes



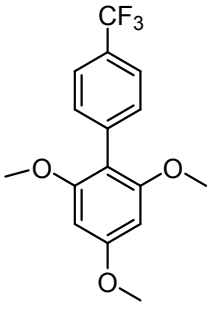
In a glovebox, a flame dried Schlenk equipped with a magnetic stirrer bar was charged with silver hexafluoroantimonate (130.0 mg, 0.38 mmol) and potassium phosphate tribasic (76.0 mg, 0.36 mmol) in *o*-dichlorobenzene (1.8 mL). The (P,N)AuCl complex **Au1** (12.0 mg, 0.018 mmol) was transferred into a small glass vial and dissolved in *o*-dichlorobenzene (1.8 mL). Iodoarene (0.36 mmol, 1 eq.), 1,3,5–trimethoxybenzene (0.36 mmol, 1 eq.) and methanol (72 µL) were added to the gold complex solution. This solution was loaded into a plastic syringe equipped with stainless steel needle. The syringe was closed by blocking the needle with a septum. Outside the glovebox, the Schlenk was cooled down to -10°C (Ethanol/N_2 cold bath). At this temperature, the solution of (P,N)AuCl complex, iodoarene and 1,3,5–trimethoxybenzene was added. The reaction mixture was then stirred at 75°C. After complete conversion, silver salts were filtrated, and the solvent evaporated. Isolated yields were determined after column chromatography (pentane/dichloromethane). The fractions containing the biaryl product were then concentrated under vacuum to yield the pure product.

Characterization of biaryl products

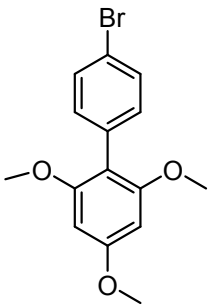
See A. Zeineddine, L. Estévez, S. Mallet-Ladeira, K. Miqueu, A. Amgoune, D. Bourissou, *Nat. Commun*. **2017**, *8*, 565.



2',4',6'-trimethoxybiphenyl-4-benzonitrile was prepared according to the general procedure described above using 4-iodobenzonitrile with 1,3,5–trimethoxybenzene, and purified by column chromatography (pentane/dichloromethane 100:0 to 95:5) to afford a white solid (65% isolated yield). Analytical data are consistent with that previously reported in the literature.[i] **^{1}H NMR** (300 MHz, CD_2Cl_2): δ 7.59 (d, *J* = 8.2 Hz, 2H), 7.39 (d, *J* = 8.2 Hz, 2H), 6.18 (s, 2H), 3.83 (s, 3H), 3.69 (s, 6H).



2',4',6'-trimethoxybiphenyl-4-benzotrifluoride was prepared according to the general procedure described above using 4-iodobenzotrifluoride with 1,3,5–trimethoxybenzene, and purified by column chromatography (pentane/dichloromethane 100:0 to 95:5) to afford a white solid (65% isolated yield). Analytical data are consistent with that previously reported in the literature.[i] **^{1}H NMR** (300 MHz, CD_2Cl_2): δ 7.57 (d, *J* = 8.3 Hz, 2H), 7.39 (d, *J* = 8.2 Hz, 2H), 6.19 (s, 2H), 3.81 (s, 3H), 3.67 (s, 6H).

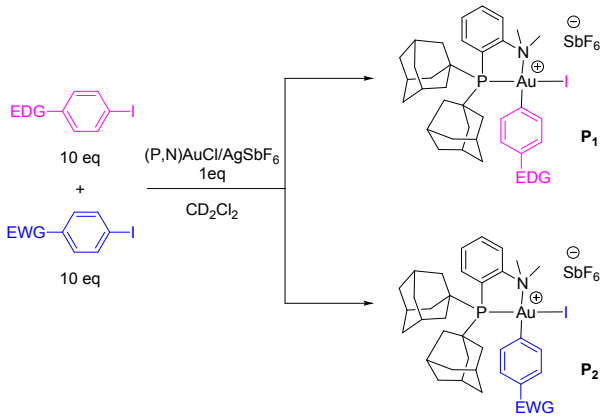


2',4',6'-trimethoxybiphenyl-4-bromobenzene was prepared according to the general procedure described above using 1-bromo-4-iodobenzene with 1,3,5–trimethoxybenzene, and purified by column chromatography (pentane/dichloromethane 100:0 to 95:5) to afford a white solid (65% isolated yield). Analytical data are consistent with that previously reported in the literature.[i] **^{1}H NMR** (300 MHz, $CDCl_3$): δ 7.47–7.37 (m, 2H), 7.17–7.08 (m, 2H), 6.14 (s, 2H), 3.79 (s, 3H), 3.65 (s, 6H).

Competition experiments

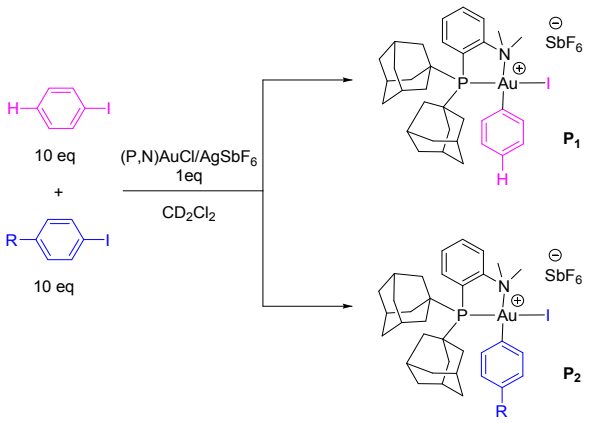
General procedure for competition experiments (oxidative addition step)

- Competition reactions between EDG and EWG *p*-substituted iodoarenes



In a glovebox, a screw-cap NMR tube was charged with $AgSbF_6$ (8.0 mg, 0.023 mmol) in CD_2Cl_2 (0.3 mL). Complex **Au1** (15 mg, 0.023 mmol) was transferred into a glass vial and dissolved in CD_2Cl_2 (0.3 mL). EDG *p*-substituted iodoarene (0.23 mmol) and EWG *p*-substituted iodoarene (0.23 mmol) were added to the solution of **Au1**. The prepared solution was loaded into a plastic syringe equipped with stainless steel needle. The syringe was closed by blocking the needle with a septum. Outside the glovebox, the NMR tube was cooled down to -80°C (Ethanol/N_2 cold bath). At this T, the solution of complex **Au1** and the two iodoarenes was added. The tube was gently shaken and allowed to warm to RT. The relative ratios of oxidative addition products $\mathbf{P_1}$ and $\mathbf{P_2}$ were determined by $^{31}P\{^1H\}$ NMR spectroscopy.

- Competition reactions between iodobenzene and *p*-substituted iodoarenes for Hammett correlation construction (oxidative addition)

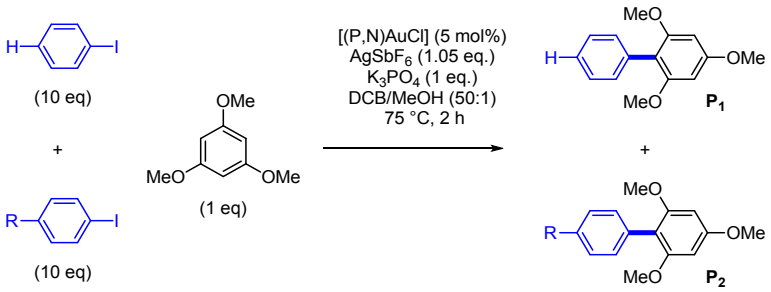


In a glovebox, a screw-cap NMR tube was charged with $AgSbF_6$ (8.0 mg, 0.023 mmol) in CD_2Cl_2 (0.3 mL). Complex **Au1** (15 mg, 0.023 mmol) was transferred into a glass vial and dissolved in CD_2Cl_2 (0.3 mL). Iodobenzene (0.23 mmol) and the corresponding *p*-substituted iodoarene (0.23 mmol) were added to the solution of **Au1**. The prepared solution was loaded into a plastic syringe equipped with stainless steel needle. The syringe was closed by blocking the needle with a septum. Outside the glovebox, the NMR tube was cooled down to -80°C (Ethanol/N_2 cold bath). At this T, the solution of complex **Au1** and the two iodoarenes was added. The tube was gently shaken and allowed to warm to RT. The relative ratios of oxidative addition products $\mathbf{P_1}$ and $\mathbf{P_2}$ were determined by $^{31}P\{^1H\}$ NMR spectroscopy.

	Ratio P_1 / P_2
R = CF_3	77 / 23
R = Br	70 / 30
R = Me	47 / 53
R = OMe	43 / 57

Table S1. Relative ratios of oxidative addition products $\mathbf{P_1}$ and $\mathbf{P_2}$ as obtained from competition experiments.

General procedure for competition experiments (catalytic cross-coupling)



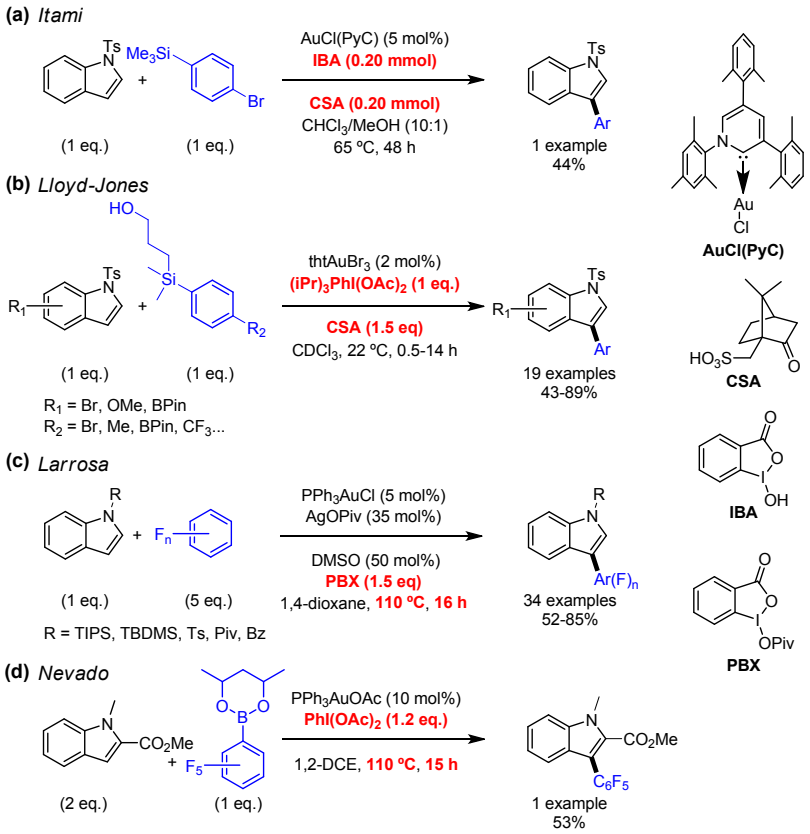
In a glovebox, a flame dried Schlenk equipped with a magnetic stirrer bar was charged with $AgSbF_6$ (130.0 mg, 0.38 mmol) and K_3PO_4 (76.0 mg, 0.36 mmol) in dichlorobenzene (1.8 mL). Complex **Au1** (12.0 mg, 0.018 mmol) was transferred into a small glass vial and dissolved in dichlorobenzene (1.8 mL). Iodobenzene (3.6 mmol, 10 eq), *p*-substituted iodoarene (3.6 mmol, 10 eq), 1,3,5–trimethoxybenzene (0.36 mmol, 1 eq) and methanol (72 µL) were added to the gold complex solution. This solution was loaded into a plastic syringe equipped with stainless steel needle. The syringe was closed by blocking the needle with a septum. Outside the glovebox, the Schlenk was cooled down to -10°C (Ethanol/N_2 cold bath). At this temperature, the solution of complex **Au1**, the two iodoarenes and 1,3,5–trimethoxybenzene was added. The reaction mixture was then stirred at 75°C. Yields were determined using calibrated GC-MS analysis vs. *n*-dodecane as internal standard.

	Yield P_1	Yield P_2
R = CF_3	83%	16%
R = Br	75%	24%
R = Me	46%	53%
R = OMe	45%	55%

Table S2. Yields in coupling products **P_1** and **P_2** as obtained from competition experiments.

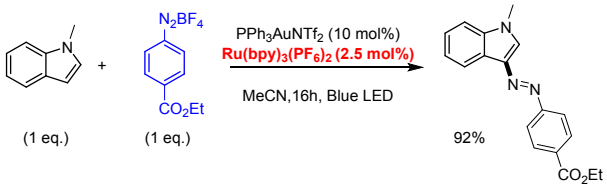
State of the art for Au-catalyzed arylation of indoles

A few examples have been reported for the gold-catalyzed oxidative arylation of indoles (Scheme S1), all of them resulting in C3 selectivity. In 2015, Itami and coworkers[ii] described the first, single example, of gold-mediated arylation of *N*-tosyl indole with *p*-bromo trimethylsilylbenzene (Scheme S1a). Later on, Lloyd-Jones *et al*.,[iii] reported the first room temperature, gold-mediated arylation of indoles (Scheme S1b).[iv] This methodology has been applied to arenes bearing a 3-hydroxypropyldimethylsilyl group. It works well with *N*-tosyl indoles, it tolerates electron-withdrawing as well as electron-donating groups on both partners and it does not require inert conditions. In 2015, Larrosa *et al*. reported a gold-catalyzed arylation of indoles via double C–H activation (Scheme S1c).[v] The reaction involves perfluorinated arenes and *N*-protected indoles and does not require prefunctionalization nor directing groups. In 2017, Nevado´s group[vi] described an isolated example of perfluoroarylation of an *N*-methyl indole with an aryl boronate (Scheme S1d). Despite these advances, the requirement for a stoichiometric oxidant to access the Au(I)/Au(III) cycle represents a limitation regarding functional group tolerance and requires the protection of the indole with an electron-withdrawing group (such as TIPS, Ts or Piv).



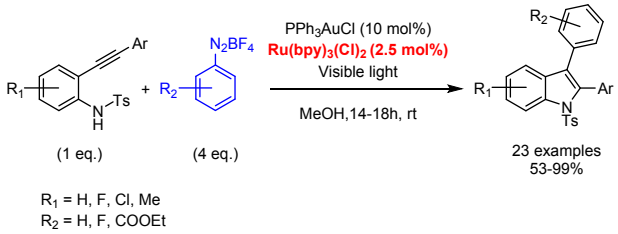
Scheme S1. Recently developed approaches for the direct gold-catalyzed C3 arylation of indoles.

It is also worth noting that the dual gold/photoredox route developed by Lee and coworkers[vii] for oxidant-free Au(I)/Au(III) catalytic cross-coupling does not work with very electron-rich arenes, such as 1,3,5-trimethoxybenzene. Moreover, the reaction does not proceed with *N*-methyl indole due to competing azo coupling (Scheme S2).



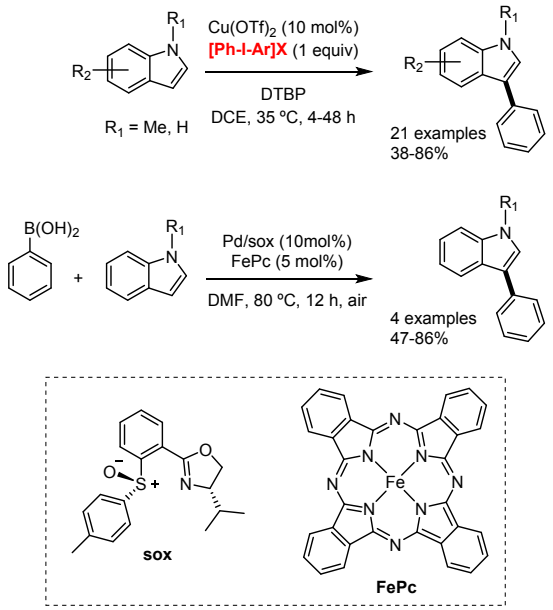
Scheme S2. Competing azo coupling in the gold/photoredox route developed by Lee.

C3-arylated indoles have been prepared through an intramolecular aminoarylation of alkynes catalyzed by a dual gold/photoredox system. N-tosylindoles are obtained in moderate to good yields under mild and base-free conditions.[viii] Gold-catalyzed cascade reactions starting from *ortho*-azido alkynyl arenes leading to substituted indoles have also been reported.[ix]



Scheme S3. Intramolecular arylation of alkynes for the synthesis of C3-arylindoles.

Other metals, such as Pd, Cu or Ir have also been shown to promote the C3 arylation of indoles, but they generally require high temperatures (140 ºC or more), long reaction times and inert conditions.[x] To the best of our knowledge, the methods for the C3 arylation of indoles under mild conditions (T <100 ºC) are limited to a Cu-catalyzed protocol with diaryliodonium salts (35 ºC)[xi] and a dual Pd/Fe-catalysed process with arylboronic acids (80 ºC) (Scheme S4).[xii] The Cu-catalyzed protocol works with a broad scope of substrates (21 examples), but requires the use of diaryliodonium salts that need to be synthesized for each particular arylation.

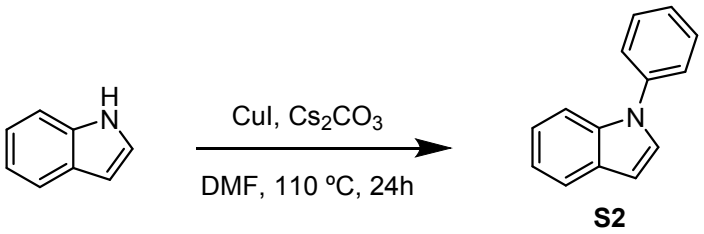


Scheme S4. Reported examples of metal-catalyzed C3 arylation of indoles under mild conditions.

Transition-metal-free processes have also been reported; however, some drawbacks, such as the need for highly reactive arylating agents (e.g., hypervalent iodine reagents[xiii] and diazonium salts[xiv]) and low regioselectivity due to aryne intermediates,[xv] limit their synthetic application.

Synthesis of the starting materials (numbered SX with respect to the deriving C3-arylated indole X).

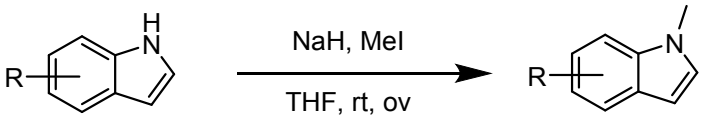
General Procedure for *N*-Phenylation of indoles[xvi]



S2

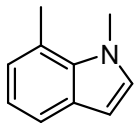
A mixture of indole (0.82 g, 7.0 mmol), iodobenzene (1.02 g, 5.0 mmol), CuI (191 mg, 1.0 mmol) and Cs_2CO_3 (3.26 g, 10 mmol) in DMF (10 mL) was vigorously stirred at 120 °C under nitrogen atmosphere for 16 h. After cooling the mixture to ambient temperature, the reaction mixture was diluted with EtOAc (40 mL) and washed with H_2O (2×30 mL). The aqueous phase was extracted with EtOAc (2×30 mL), and the combined organic phases were dried over Na_2SO_4. After filtration and evaporation of the solvents under vacuum, the crude product was purified by column chromatography on silica gel (pentane) to afford a yellowish oil (77% isolated yield). Analytical data are consistent with those previously reported in the literature.[xvi] **^{1}H NMR** (300 MHz, $CDCl_3$): δ 7.77-7.74 (m, 1H), 7.63-7.60 (m, 1H), 7.47-7.42 (m, 4H), 7.31-7.22 (m, 4H), 6.72 (d, *J* = 4.0 Hz, 1H).

General Procedure for *N*-methylation of indoles[xvii]



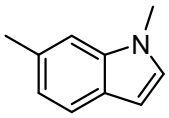
NaH (1.7–2.0 eq., 60 % dispersion in mineral oil) was added in four separate portions to a stirring solution of indole (1.0 eq.) in anhydrous THF at 0 ºC. The resulting mixture was allowed to warm to room temperature over 30 min, cooled to 0 ºC and MeI (1.04 eq.) was added dropwise over 5 min. The resulting mixture was allowed to warm to room temperature and stirred overnight. The reaction was quenched with H_2O (3 mL) and diluted with EtOAc (5 mL). The phases were separated and the aqueous phase was washed with EtOAc (3 x 10 mL), followed by washing of the combined organic phase with brine (1 x 20 mL). Combined organic phases were dried over $MgSO_4$, filtered and concentrated under vacuum. The crude product was purified by column chromatography using the specified eluent to afford products **S24**-**S30**.

Characterization of starting materials:



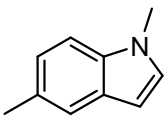
S24

1,7-dimethylindole (S24) was prepared according to the general procedure described above using iodomethane (247 µL, 3.97 mmol) with 7-methyl-1*H*-indole (500 mg, 3.8 mmol) and NaH (156 mg, 6.5 mmol) in THF (3.75 mL), and purified by column chromatography (pentane/dichloromethane 90:10 to 70:30) to afford a white solid (35% isolated yield). Analytical data are consistent with those previously reported in the literature.[xx] **^{1}H NMR** (300 MHz, CD_2Cl_2): δ 7.29 (d, *J* = 7.5 Hz, 1H), 6.83-6.74 (m, 3H), 6.28 (d, *J* = 3.1 Hz, 1H), 3.90 (s, 3H), 2.63 (s, 3H).



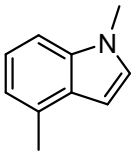
S25

1,6-dimethylindole (S25) was prepared according to the general procedure described above using iodomethane (247 µL, 3.97 mmol) with 6-methyl-1*H*-indole (500 mg, 3.8 mmol) and NaH (156 mg, 6.5 mmol) in THF (3.75 mL), and purified by column chromatography (pentane/dichloromethane 90:10 to 70:30) to afford a colorless oil (11% isolated yield). Analytical data are consistent with those previously reported in the literature.[xviii] **^{1}H NMR** (500 MHz, CD_2Cl_2): δ 7.38 (d, *J* = 8.0 Hz, 1H), 7.05 (s, 1H), 6.92 (d, *J* = 3.0 Hz, 1H), 6.84 (d, *J* = 8.0 Hz, 1H),
6.31 (d, *J* = 2.3 Hz, 1H), 3.66 (s, 3H), 2.40 (s, 3H).



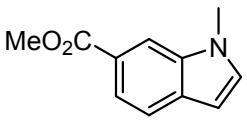
S26

1,5-dimethylindole (S26) was prepared according to the general procedure described above using iodomethane (247 µL, 3.97 mmol) with 5-methylindole (500 mg, 3.8 mmol) and NaH (156 mg, 6.5 mmol) in THF (3.75 mL), and purified by column chromatography (pentane/dichloromethane 90:10 to 70:30) to afford a colorless oil (39% isolated yield). Analytical data are consistent with those previously reported in the literature.[xix] **^{1}H NMR** (300 MHz, CD_2Cl_2): δ 7.32 (s, 1H), 7.17 (d, *J* = 8.5 Hz, 1H), 6.98 (m, 2H), 6.31 (d, *J* = 2.9 Hz, 1H), 3.70 (s, 3H), 2.37 (s, 3H).



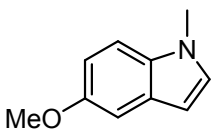
S27

1,4-dimethylindole (S27) was prepared according to the general procedure described above using iodomethane (247 µL, 3.97 mmol) with 4-methylindole (500 mg, 3.8 mmol) and NaH (156 mg, 6.5 mmol) in THF (3.75 mL), and purified by column chromatography (pentane/dichloromethane 90:10 to 70:30) to afford a yellow oil (42% isolated yield). Analytical data are consistent with those previously reported in the literature.[xx] **^{1}H NMR** (300 MHz, CD_2Cl_2): δ 7.03 (m, 3H), 6.79 (d, *J* = 6.9 Hz, 1H), 6.39 (d, *J* = 3.1 Hz, 1H), 3.68 (s, 3H), 2.44 (s, 3H).



S28

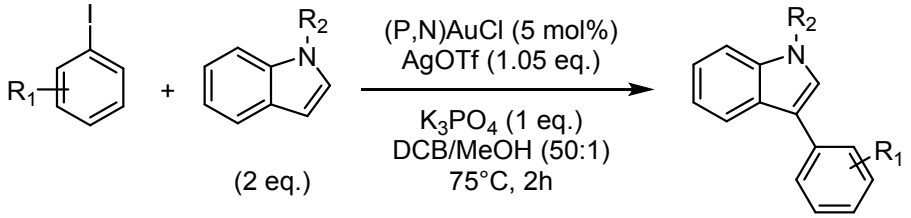
1-methyl-6-carboxyindole methyl ester (S28) was prepared according to the general procedure described above using iodomethane (247 µL, 3.97 mmol) with methylindole-6-carboxylate and NaH (156 mg, 6.5 mmol) in THF (3.75 mL), and purified by column chromatography (pentane/dichloromethane 90:10 to 70:30) to afford a yellow solid (43% isolated yield). Analytical data are consistent with those previously reported in the literature.[xviii] **^{1}H NMR** (300 MHz, CD_2Cl_2): δ 7.98 (s, 1H), 7.65 (d, *J* = 8.3 Hz, 1H), 7.51 (d, *J* = 8.3 Hz, 1H), 7.11 (d, *J* = 2.8 Hz, 1H), 6.41 (d, *J* = 2.5 Hz, 1H), 3.80 (s, 3H), 3.70 (s, 3H).



S30

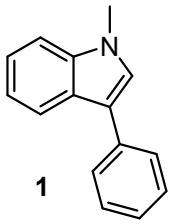
5-methoxy-1-methylindole (S30) was prepared according to the general procedure described above using iodomethane (247 µL, 3.97 mmol) with 5-methoxy-1*H*-indole and NaH (156 mg, 6.5 mmol) in THF (3.75 mL), and purified by column chromatography (pentane/dichloromethane 90:10 to 70:30) to afford a white solid (56% isolated yield). Analytical data are consistent with those previously reported in the literature.[xix] **^{1}H NMR** (300 MHz, CD_2Cl_2): δ 7.13 (d, *J* = 8.9 Hz, 1H), 6.99 – 6.91 (m, 2H), 6.75 (dd, *J* = 8.9, 2.4 Hz, 1H), 6.28 (d, *J* = 3.0 Hz, 1H), 3.73 (s, 3H), 3.67 (s, 3H).

General procedure for gold-catalyzed direct arylation of indoles with iodoarenes



In a glovebox, a flame dried Schlenk equipped with a magnetic stirrer bar was charged with silver trifluoromethanesulfonate (98.0 mg, 0.38 mmol) and potassium phosphate tribasic (76.0 mg, 0.36 mmol) in *o*-dichlorobenzene (1.8 mL). Complex **Au1** (12.0 mg, 0.018 mmol) was transferred into a small glass vial and dissolved in *o*-dichlorobenzene (1.8 mL). Iodoarene (0.36 mmol, 1 eq.), indole (0.72 mmol, 2 eq.) and methanol (72 µL) were added to the gold complex solution. This solution was loaded into a plastic syringe equipped with stainless steel needle. The syringe was closed by blocking the needle with a septum. Outside the glovebox, the Schlenk was cooled down to -10°C (Ethanol/N_2 cold bath). At this temperature, the solution of (P,N)AuCl complex, iodoarene and indole was added. The reaction mixture was then stirred at 75°C. After complete conversion, silver salts were filtrated, and the solvent evaporated. Isolated yields were determined after column chromatography (pentane/dichloromethane). The fractions containing the biaryl product were then concentrated under vacuum to yield the pure product. Known products were characterized by ^{1}H NMR and authenticated by comparison with literature data. New products were characterized by ^{1}H, ^{13}C NMR spectroscopy and mass spectrometry (electronic impact).

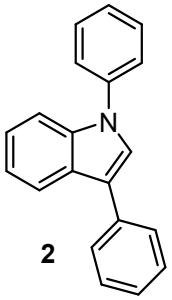
Characterization of biaryl products:



1

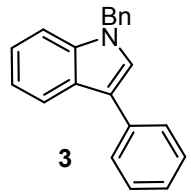
1-methyl-3-phenyl-1*H*-indole (1) was prepared according to the general procedure described above using iodobenzene with 1-methyl-1*H*-indole, and purified by column chromatography (pentane/dichloromethane 100:0 to 95:5) to afford a colorless oil (87% isolated yield). Analytical data are consistent with those previously reported in the literature.[xxi] **^{1}H NMR** (300 MHz, $CDCl_3$): δ 7.93 (d, *J* = 8.0 Hz, 1H), 7.64 (d, *J* = 7.7 Hz, 2H), 7.44-7.33 (m, 3H), 7.28-7.15 (m, 4H), 3.80 (s, 3H).

For NMR data of the C2-arylated product, see ref. xix. Comparison of the ^{1}H NMR spectra allows unambiguous identification of the C3-arylated product.



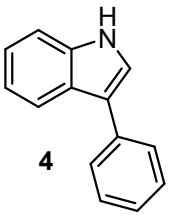
2

1,3-diphenyl-1*H*-indole (2) prepared according to the general procedure described above using iodobenzene with 1-phenyl-1*H*-indole, and purified by column chromatography (pentane/dichloromethane 90:10) to afford a yellow oil (31% isolated yield). Analytical data are consistent with those previously reported in the literature.[xxii] **^{1}H NMR** (300 MHz, $CDCl_3$): δ 8.01 (d, *J* = 7.7 Hz, 1H), 7.74 (d, *J* = 7.6 Hz, 2H), 7.64-7.47 (m, 8H), 7.42-7.24 (m, 4H).



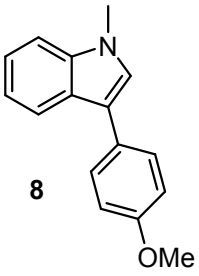
3

3-phenyl-1-benzyl-indole (3) was prepared according to the general procedure described above using iodobenzene with 1-benzyl-1*H*-indole, and purified by column chromatography (pentane/dichloromethane 95:5 to 90:10) to afford a light yellow solid (21% isolated yield). Analytical data are consistent with those previously reported in the literature.[xxiii] **^{1}H NMR** (300 MHz, CD_2Cl_2): 7.95 (d, *J* = 7.1 Hz, 1H), 7.67 (d, *J* = 7.5 Hz, 2H), 7.42 (t, *J* = 7.6 Hz, 2H), 7.37 – 7.24 (m, 6H), 7.24 – 7.13 (m, 4H), 5.33 (s, 2H).



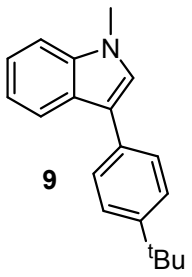
4

3-phenyl-1*H*-indole (4) was prepared according to the general procedure described above using iodobenzene with 1*H*-indole, and purified by column chromatography (pentane/dichloromethane 95:5 to 90:10) to afford a light yellow solid (30% isolated yield). Analytical data are consistent with those previously reported in the literature.[xi] **^{1}H NMR** (300 MHz, $CDCl_3$): δ 8.17 (br. s, 1H), 7.97 (d, *J* = 7.7 Hz, 1H), 7.69 (d, *J* = 7.5 Hz, 2H), 7.49-7.41 (m, 3H), 7.35-7.19 (m, 4H).



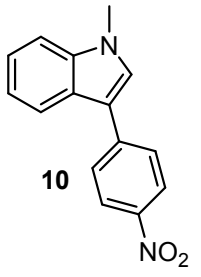
8

3-(4-methoxyphenyl)-1-methyl-1*H*-indole (8) was prepared according to the general procedure described above using 4-iodoanisole with 1-methyl-1*H*-indole, and purified by column chromatography (pentane/dichloromethane 85:15) to afford a white crystalline solid (37% isolated yield). Analytical data are consistent with those previously reported in the literature.[xxi] **^{1}H NMR** (300 MHz, $CDCl_3$): δ 7.91 (d, *J* = 8.0 Hz, 1H), 7.58 (d, *J* = 8.7 Hz, 2H), 7.37 (d, *J* = 8.3 Hz, 1H), 7.31-7.26 (m, 1H), 7.21-7.17 (m, 2H), 7.00 (d, *J* = 8.7 Hz, 2H), 3.87 (s, 3H), 3.84 (s, 3H).



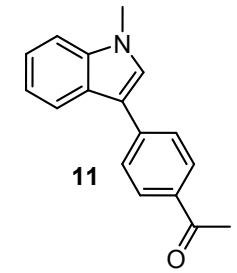
9

3-(4-(tert-butyl)phenyl)-1-methyl-1*H*-indole (9) prepared according to the general procedure described above using 4-tert-butyliodobenzene with 1-methyl-1*H*-indole, and purified by column chromatography (pentane/dichloromethane 90:10) to afford a yellow oil (31% isolated yield). **^{1}H NMR** (500 MHz, CD_2Cl_2): δ 7.84-7.80 (m, 1H), 7.52-7.48 (m, 2H), 7.40-7.35 (m, 2H), 7.29-7.27 (m, 1H), 7.18-7.14 (m, 2H), 7.10-7.04 (m, 1H), 3.73 (s, 3H), 1.28 (s, 9H). **^{13}C NMR** (500 MHz, CD_2Cl_2): δ 147.88 (Cq), 136.84 (Cq), 132.02 (Cq), 126.00 (CH), 125.76 (CH), 125.38 (Cq), 124.95 (CH), 121.04 (CH), 119.01 (CH), 118.95 (CH), 115.40 (Cq), 108.82 (CH), 33.64 (Cq), 32.04 (CH_3), 30.44 (CH_3). **MS** (m/z): Calcd. for $C_{19}H_{21}N$: 263.2. Found: 263.0.

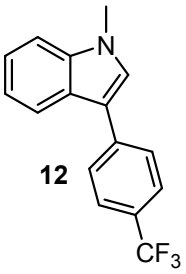


10

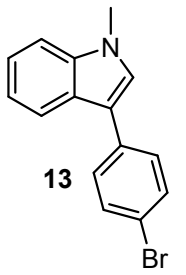
1-methyl-3-(4-nitrophenyl)-1*H*-indole (10) was prepared according to the general procedure described above using 1-iodo-4-nitrobenzene with 1-methyl-1*H*-indole, and purified by column chromatography (pentane/dichloromethane 90:10) to afford a yellow solid (52% isolated yield). Crystals suitable for X-ray diffraction analysis were obtained by layering a DCM solution with pentane. Analytical data are consistent with those previously reported in the literature.[xi] **Mp**: 152-155 ºC. **^{1}H NMR** (300 MHz, $CDCl_3$): δ 8.27 (d, *J* = 9.0 Hz, 2H), 7.96 (d, *J* = 7.9 Hz, 1H), 7.78 (d, *J* = 9.0 Hz, 2H), 7.43-7.26 (m, 4H), 3.88 (s, 3H).



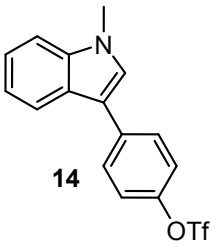
1-(4-(1-methyl-1*H*-indol-3-yl)phenyl)ethan-1-one (11) was prepared according to the general procedure described above using 4'-iodoacetophenone with 1-methyl-1*H*-indole, and purified by column chromatography (pentane/dichloromethane 80:20) to afford a yellow solid (71% isolated yield). Analytical data are consistent with those previously reported in the literature.[xxi] **^{1}H NMR** (300 MHz, $CDCl_3$): δ 7.96 (d, *J* = 8.3 Hz, 2H), 7.90 (d, *J* = 8.3 Hz, 1H), 7.68 (d, *J* = 8.3 Hz, 2H), 7.34-7.27 (m, 2H), 7.25-7.13 (m, 2H), 3.81 (s, 3H), 2.58 (s, 3H).



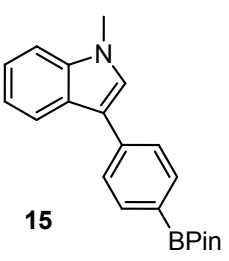
1-methyl-3-(4-(trifluoromethyl)phenyl)-1*H*-indole (12) was prepared according to the general procedure described above using 4-iodobenzotrifluoride with 1-methyl-1*H*-indole, and purified by column chromatography (pentane/dichloromethane 90:10) to afford a yellow solid (84% isolated yield). Analytical data are consistent with that previously reported in the literature.[xxiv] **^{1}H NMR** (300 MHz, CD_2Cl_2): δ 7.90 (d, *J* = 8.0 Hz, 1H), 7.75 (d, *J* = 8.3 Hz, 2H), 7.64 (d, *J* = 8.2 Hz, 2H), 7.37 (d, *J* = 8.1 Hz, 1H), 7.33 (s, 1H), 7.26 (t, *J* = 7.2 Hz, 1H), 7.18 (dd, *J* = 11.0, 4.0 Hz, 1H), 3.80 (s, 3H).



1-methyl-3-(4-bromo)-1*H*-indole (13) was prepared according to the general procedure described above using 1-bromo-4-iodobenzene with 1-methyl-1*H*-indole, and purified by column chromatography (pentane/dichloromethane 90:10) to afford a white solid (38% isolated yield). Crystals suitable for X-ray diffraction analysis were obtained by layering a DCM solution with pentane. Analytical data are consistent with those previously reported in the literature.[xxiv] **Mp**: 89-93 ºC. **^{1}H NMR** (300 MHz, CD_2Cl_2): δ 7.78 (d, *J* = 8.0 Hz, 1H), 7.46 (s, 4H), 7.30 (d, *J* = 8.2 Hz, 1H), 7.14 (m, 3H), 3.74 (s, 3H).

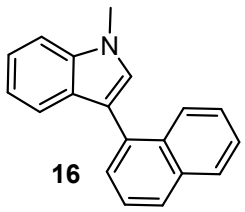


4-(1-methyl-1H-indol-3-yl)phenyl trifluoromethanesulfonate (14) was prepared according to the general procedure described above using 4-iodophenyl trifluoromethanesulfonate with 1-methyl-1*H*-indole, and purified by column chromatography (pentane/dichloromethane 80:20) to afford a yellow solid (71% isolated yield). **^{1}H NMR** (500 MHz, CD_2Cl_2): δ 7.80 (dt, *J* = 8.0, 1.0 Hz, 1H), 7.68–7.61 (m, 2H), 7.32 (dt, *J* = 8.3, 1.0 Hz, 1H), 7.28–7.24 (m, 2H), 7.23 (s, 1H), 7.21 (ddd, *J* = 8.2, 7.0, 1.2 Hz, 1H), 7.11 (ddd, *J* = 8.0, 7.0, 1.1 Hz, 1H), 3.76 (s, 3H). **^{13}C NMR** (500 MHz, CD_2Cl_2): δ 146.64 (Cq), 136.85 (Cq), 135.71 (Cq), 127.59 (CH), 126.58 (CH), 124.91 (Cq), 121.41 (CH), 120.84 (CH), 119.49 (CH), 118.99 (CF_3, q, *J* = 125.3 Hz), 118.49 (CH), 113.65 (Cq), 109.05 (CH), 32.14 (CH_3). **^{19}F NMR** (500 MHz, CD_2Cl_2): δ -73.20 (s). **MS** (m/z): Calcd. for $C_{16}H_{12}F_3NO_3S$: 355.1. Found: 355.0.



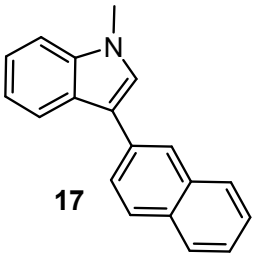
1-methyl-3-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-1H-indole (15) was prepared according to the general procedure described above using 4-iodophenylboronic acid pinacol ester with 1-methyl-1*H*-indole, and purified by column chromatography (pentane/dichloromethane 20:80) to afford a white solid (51% isolated yield). **^{1}H NMR** (500 MHz, CD_2Cl_2): δ 7.86 (dt, *J* = 8.0, 1.0 Hz, 1H), 7.75 – 7.70 (m, 2H), 7.61 – 7.57 (m, 2H), 7.30 (dt, *J* = 8.2, 1.0 Hz, 1H),

7.26 (s, 1H), 7.18 (ddd, J = 8.2, 7.0, 1.2 Hz, 1H), 7.09 (ddd, J = 8.1, 7.0, 1.1 Hz, 1H), 3.74 (s, 3H), 1.26 (s, 12H). **^{13}C NMR** (500 MHz, CD_2Cl_2): 137.83 (Cq), 136.91 (Cq), 134.38 (CH), 126.45 (CH), 125.32 (CH), 125.12 (Cq), 121.16 (CH), 119.21 (CH), 119.00 (CH), 115.25 (Cq), 108.89 (CH), 82.89 (Cq), 32.08 (CH_3), 23.92 (CH_3). **MS** (m/z): Calcd. for $C_{21}H_{24}BNO_2$: 333.2. Found: 333.1.



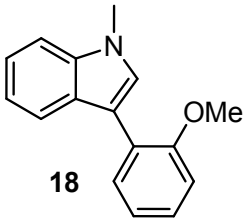
16

1-methyl-3-(naphthalen-1-yl)-1*H*-indole (16) was prepared according to the general procedure described above using 1-iodonaphthalene with 1-methyl-1*H*-indole, and purified by column chromatography (pentane/dichloromethane 95:5 to 90:10) to afford a yellow oil (37% isolated yield). **^{1}H NMR** (500 MHz, CD_2Cl_2): δ 8.03-7.98 (m, 1H), 7.86-7.82 (m, 1H), 7.77 (d, *J* = 8.0 Hz, 1H), 7.53-7.29 (m, 6H), 7.22-7.17 (m, 2H), 7.03-6.98 (m, 1H), 3.81 (s, 3H). **^{13}C NMR** (500 MHz, CD_2Cl_2): δ 137.06 (Cq), 134.10 (Cq), 133.09 (Cq), 132.47 (Cq), 128.46 (CH), 128.21 (CH), 128.00 (Cq), 127.59 (CH), 126.80 (CH), 126.46 (CH), 125.68 (CH), 125.62 (CH), 125.61 (CH), 121.84 (CH), 120.07 (CH), 119.49 (CH), 114.59 (C_q), 109.48 (CH), 32.82 (CH_3). **MS** (m/z): Calcd. for $C_{19}H_{15}N$: 257.1. Found: 257.3.



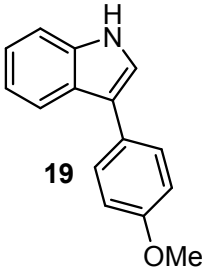
17

1-methyl-3-(naphthalen-2-yl)-1*H*-indole (17) was prepared according to the general procedure described above using 2-iodonaphthalene with 1-methyl-1*H*-indole, and purified by column chromatography (pentane/dichloromethane 95:5 to 90:10) to afford a yellow oil (34% isolated yield). Analytical data are consistent with those previously reported in the literature.[xxv] **^{1}H NMR** (300 MHz, CD_2Cl_2): δ 8.15 (s, 1H), 8.09 (d, *J* = 7.8 Hz, 1H), 7.94-7.78 (m, 4H), 7.55-7.19 (m, 6H), 3.79 (s, 3H).



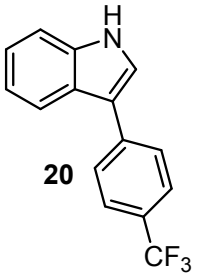
18

3-(2-methoxyphenyl)-1-methyl-*1H*-indole (18) was prepared according to the general procedure described above using 2-iodoanisole with 1-methyl-1*H*-indole, and purified by column chromatography (pentane/dichloromethane 95:5) to afford a white solid (50% isolated yield). Analytical data are consistent with those previously reported in the literature.[xxi] **^{1}H NMR** (300 MHz, $CDCl_3$): δ 7.80 (d, *J* = 8.0 Hz, 1H), 7.65 (dd, *J* = 7.4, 1.7 Hz, 1H), 7.40-7.37 (m, 1H), 7.36 (br. s, 1H), 7.32-7.23 (m, 2H), 7.17 (t, *J* = 7.5 Hz, 1H), 7.10-7.02 (m, 2H), 3.88 (s, 3H), 3.85 (s, 3H).



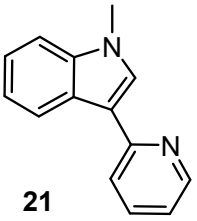
19

3-(4-methoxyphenyl)-1*H*-indole (19) was prepared according to the general procedure described above using 4-iodoanisole with 1*H*-indole, and purified by column chromatography (pentane/diethyl ether 80:20) to afford a white solid (33% isolated yield). Analytical data are consistent with that previously reported in the literature.[xiii,a] **^{1}H NMR** (300 MHz, CD_2Cl_2): δ 8.24 (br s, 1H), 7.78 (d, *J* = 8.2 Hz, 1H), 7.53 – 7.47 (m, 2H), 7.37 – 7.30 (m, 1H), 7.23 (d, *J* = 2.5 Hz, 1H), 7.10 (m, 2H), 6.95 – 6.87 (m, 2H), 3.75 (s, 3H).



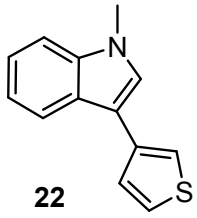
20

3-(4-(trifluoromethyl)phenyl)-1*H*-indole (20) was prepared according to the general procedure described above using 4-iodobenzotrifluoride with 1*H*-indole, and purified by column chromatography (pentane/diethyl ether 80:20) to afford a white solid (37% isolated yield). Analytical data are consistent with that previously reported in the literature.[xxvi] **^{1}H NMR** (300 MHz, CD_2Cl_2): δ 8.48 (br s, 1H), 7.85 (d, *J* = 7.8 Hz, 1H), 7.73 (m, 2H), 7.61 (m, 2H), 7.41 (m, 2H), 7.16 (m, 2H).



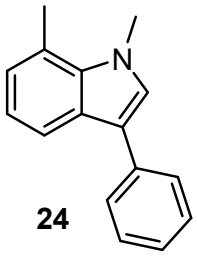
21

1-methyl-3-(pyridin-2-yl)-1*H*-indole (21) was prepared according to the general procedure described above using 2-iodopyridine with 1-methyl-1*H*-indole, and purified by column chromatography (pentane/dichloromethane 80:20) to afford a yellowish solid (16% isolated yield). Analytical data are consistent with that previously reported in the literature.[xxvii] **^{1}H NMR** (300 MHz, CD_2Cl_2): δ 8.62 – 8.48 (m, 1H), 8.27 – 8.15 (m, 1H), 7.70 – 7.55 (m, 3H), 7.36 – 7.10 (m, 3H), 7.07 – 6.96 (m, 1H), 3.79 (s, 3H).



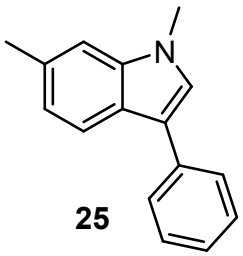
22

1-methyl-3-(thiophen-3-yl)-1*H*-indole (22) was prepared according to the general procedure described above using 3-iodothiophene with 1-methyl-1*H*-indole, and purified by column chromatography (pentane/dichloromethane 80:20) to afford a white solid (33% isolated yield). Analytical data are consistent with that previously reported in the literature.[xxi] **^{1}H NMR** (300 MHz, CD_2Cl_2) δ 7.81 (d, *J* = 7.9 Hz, 1H), 7.37 – 7.25 (m, 4H), 7.22 – 7.05 (m, 3H), 3.72 (s, 3H).



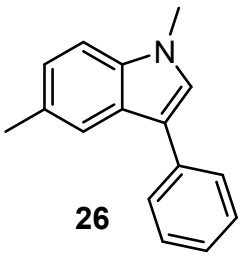
24

1,7-dimethyl-3-phenyl-1*H*-indole (24) was prepared according to the general procedure described above using iodobenzene with 1,7-dimethylindole, and purified by column chromatography (pentane/dichloromethane 95:5 to 90:10) to afford a light yellow solid (20% isolated yield). **^{1}H NMR** (500 MHz, CD_2Cl_2): 7.64 (d, *J* = 8.0 Hz, 1H), 7.53 (dd, *J* = 8.2, 1.2 Hz, 2H), 7.33 (t, *J* = 7.9 Hz, 2H), 7.17 (t, 1H), 7.05 (s, 1H), 6.92 (m, 1H), 6.86 (d, *J* = 7.1 Hz, 1H), 4.00 (s, 3H), 2.70 (s, 3H). **^{13}C NMR** (500 MHz, CD_2Cl_2): δ 135.55 (Cq), 135.01 (Cq), 127.98 (CH), 127.76 (CH), 126.62 (CH), 126.42 (Cq), 124.89 (CH), 123.80 (CH), 121.06 (Cq), 119.32 (CH), 116.94 (CH), 115.32 (Cq), 36.16(CH_3), 18.85 (CH_3). **MS** (m/z): Calcd. for $C_{16}H_{15}N$: 221.1. Found: 220.9.



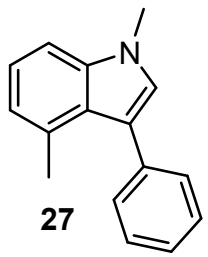
25

1,6-dimethyl-3-phenyl-1*H*-indole (25) was prepared according to the general procedure described above using iodobenzene with 1,6-dimethylindole, and purified by column chromatography (pentane/dichloromethane 95:5 to 90:10) to afford a yellow oil (20% isolated yield). **^{1}H NMR** (500 MHz, CD_2Cl_2): δ 7.71 (d, *J* = 8.2 Hz, 1H), 7.60 (d, *J* = 7.7 Hz, 2H), 7.37 (t, *J* = 7.6 Hz, 2H), 7.18 (m, 3H), 6.96 (d, *J* = 8.2 Hz, 1H), 3.69 (s, 3H), 2.42 (s, 3H). **^{13}C NMR** (500 MHz, CD_2Cl_2): δ 138.03 (Cq), 135.90 (Cq), 131.78 (Cq), 128.71 (CH), 126.90 (CH), 126.08 (CH), 125.46 (CH), 123.86 (Cq), 121.60 (CH), 119.34 (CH), 116.03 (Cq), 109.55 (CH), 32.69 (CH_3), 21.50 (CH_3). **MS** (m/z): Calcd. for $C_{16}H_{15}N$: 221.1. Found: 221.4.



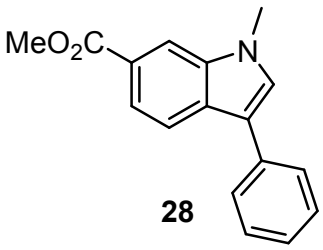
26

1,5-dimethyl-3-phenyl-1*H*-indole (26) was prepared according to the general procedure described above using iodobenzene with 1,5-dimethylindole, and purified by column chromatography (pentane/dichloromethane 95:5 to 90:10) to afford a yellow oil (25% isolated yield). Analytical data are consistent with those previously reported in the literature.[xxviii] **^{1}H NMR** (300 MHz, CD_2Cl_2): δ 7.63 (s, 1H), 7.56 (d, *J* = 7.6 Hz, 2H), 7.34 (t, *J* = 7.7 Hz, 2H), 7.18 (m, 3H), 7.01 (d, *J* = 8.4 Hz, 1H), 3.72 (s, 3H), 2.39 (s, 3H).



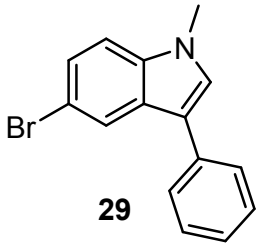
27

1,4-dimethyl-3-phenyl-1*H*-indole (27) was prepared according to the general procedure described above using iodobenzene with 1,4-dimethylindole, and purified by column chromatography (pentane/dichloromethane 95:5 to 90:10) to afford a light yellow oil (20% isolated yield). **^{1}H NMR** (500 MHz, CD_2Cl_2): δ 7.62 (s, 1H), 7.56 (dd, *J* = 8.1, 1.1 Hz, 2H), 7.34 (t, *J* = 8.0 Hz, 2H), 7.20 – 7.13 (m, 3H), 7.01 (d, *J* = 8.3 Hz, 1H), 3.72 (s, 3H), 2.38 (s, 3H). **^{13}C NMR** (500 MHz, CD_2Cl_2): δ 135.27 (Cq), 135.14 (Cq), 128.38 (Cq), 127.92 (CH), 126.26 (CH), 125.99 (CH), 125.41 (Cq), 124.68 (CH), 122.69 (CH), 118.52 (CH), 114.90 (Cq), 108.49 (CH), 32.04 (CH_3), 20.51 (CH_3). **MS** (m/z): Calcd. for $C_{16}H_{15}N$: 221.1. Found: 221.1.



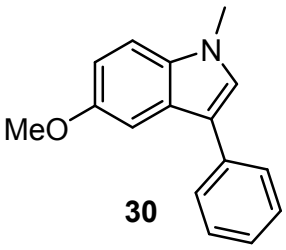
28

1-methyl-3-phenyl-6-carboxyindole methyl ester (28) was prepared according to the general procedure described above using iodobenzene with 1-methyl-6-carboxyindole methyl ester, and purified by column chromatography (pentane/dichloromethane 95:5 to 90:10) to afford a light yellow solid (30% isolated yield). Analytical data are consistent with those previously reported in the literature.[xxix] **^{1}H NMR** (300 MHz, CD_2Cl_2): δ 8.06 (dd, *J* = 1.5, 0.7 Hz, 1H), 7.86 (dd, *J* = 8.5, 0.7 Hz, 1H), 7.75 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.60–7.54 (m, 2H), 7.41–7.33 (m, 3H), 7.24–7.17 (m, 1H), 3.85 (s, 3H), 3.82 (s, 3H).



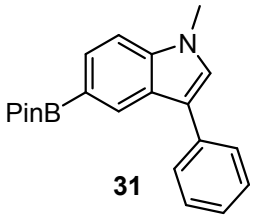
29

5-bromo-1-methyl-3-phenyl-1*H*-indole (29) was prepared according to the general procedure described above using iodobenzene with 5-bromo-1-methylindole, and purified by column chromatography (pentane/dichloromethane 95:5 to 90:10) to afford a brown oil (30% isolated yield). Analytical data are consistent with those previously reported in the literature.[xxx] **^{1}H NMR** (300 MHz, $CDCl_3$): δ 7.99 (d, *J* = 1.9 Hz, 1H), 7.55 (m, 1H), 7.53 (m, 1H), 7.39 (m, 2H), 7.30 (m, 1H), 7.24 (m, 1H), 7.16 (m, 2H), 3.75 (s, 3H).



30

5-methoxy-1-methyl-3-phenyl-1*H*-indole (30) was prepared according to the general procedure described above using iodobenzene with 5-methoxy-1-methylindole, and purified by column chromatography (pentane/dichloromethane 95:5 to 90:10) to afford a light yellow solid (30% isolated yield). Analytical data are consistent with those previously reported in the literature.[xxx] **^{1}H NMR** (300 MHz, CD_2Cl_2): δ 7.53 (d, *J* = 7.7 Hz, 2H), 7.33 (t, *J* = 7.6 Hz, 2H), 7.27 (d, *J* = 2.2 Hz, 1H), 7.16 (d, *J* = 8.6 Hz, 2H), 7.13 (s, 1H), 6.81 (dd, *J* = 8.9, 2.3 Hz, 1H), 3.74 (s, 3H), 3.67 (s, 3H).

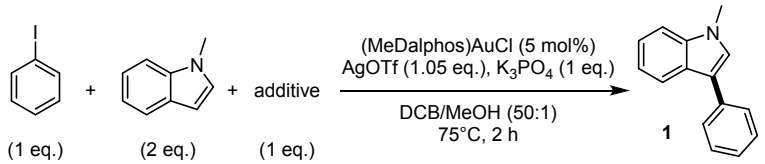


31

1-methyl-3-phenyl-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1*H*-indole (31) was prepared according to the general procedure described above using iodobenzene with 1-methylindole-5-boronic acid pinacol ester, and purified by column chromatography (pentane/dichloromethane 50:50 to 10:90) to afford a white oil (50% isolated yield). **^{1}H NMR** (500 MHz, CD_2Cl_2): δ 8.25 (t, *J* = 1.0 Hz, 1H), 7.62 – 7.55 (m, 3H), 7.40 – 7.34 (m, 2H), 7.30 (dd, *J* = 8.3, 0.8 Hz, 1H), 7.23 – 7.16 (m, 2H), 3.76 (s, 3H), 1.27 (s, 12H). **^{13}C NMR** (500 MHz, CD_2Cl_2): δ 139.39 (Cq), 135.46 (Cq), 128.70 (CH), 127.94 (CH), 127.30 (CH), 127.23 (CH), 126.80 (CH), 125.75 (CH), 116.99 (Cq), 108.95 (CH), 83.42 (Cq), 32.79 (CH_3), 29.68 (Cq), 24.68 (CH_3). **MS** (m/z): Calcd. for $C_{21}H_{24}BNO_2$: 333.2. Found: 333.1.

Functional group compatibility

The general procedure for gold-catalyzed direct arylation of indoles with iodoarenes was followed. The corresponding additive (1 eq.) was added in the Schlenk together with the silver trifluoromethanesulfonate and potassium phosphate tribasic.



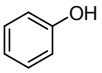
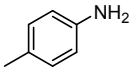
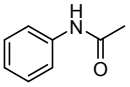
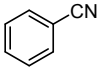
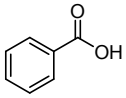
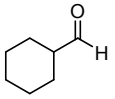
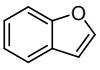
Entry	Additive	Yield of **1**	Additive remaining	SM remaining
1	None	99%	-	88%
2		87%	100%	102%
3		99%	77%	98%
4		0%	73%	200%
5		99%	74%	94%
6		99%	76%	99%
7		0%	0%	200%
8		24%*	0%	44%
9		20%	0%	0%
10		0%	0%	200%
11		98%	100%	88%
12		100%	99%	87%

Table S3. Study of functional group compatibility. Yields determined using calibrated GC-MS with *n*-dodecane as internal standard. *Yield determined using NMR with *n*-dodecane as internal standard

NMR spectra

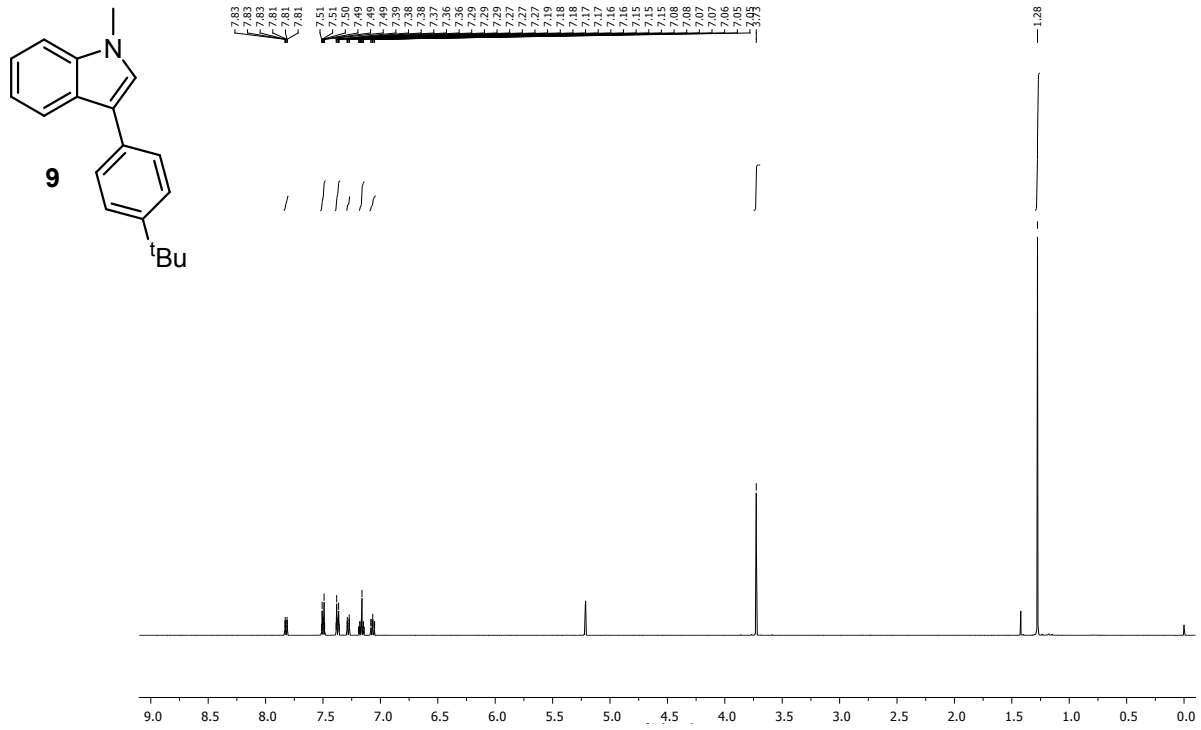


Figure S8. ^{1}H NMR spectrum of **9** in CD_2Cl_2.

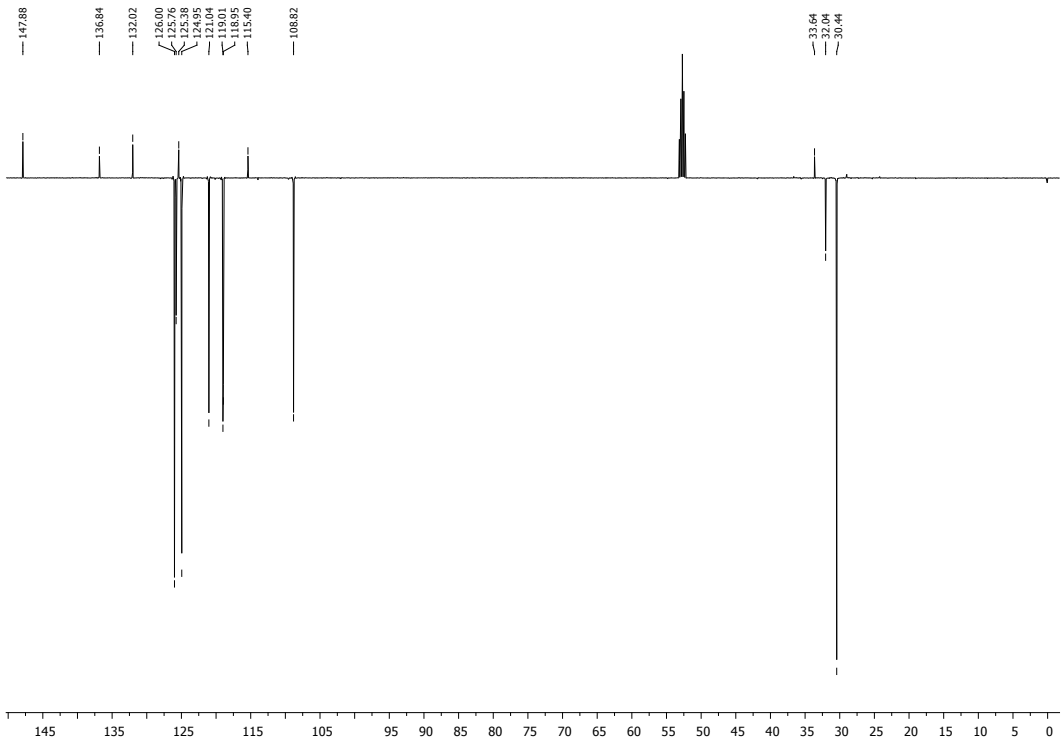


Figure S9. $^{13}C\{^{1}H\}$ NMR spectrum of **9** in CD_2Cl_2.

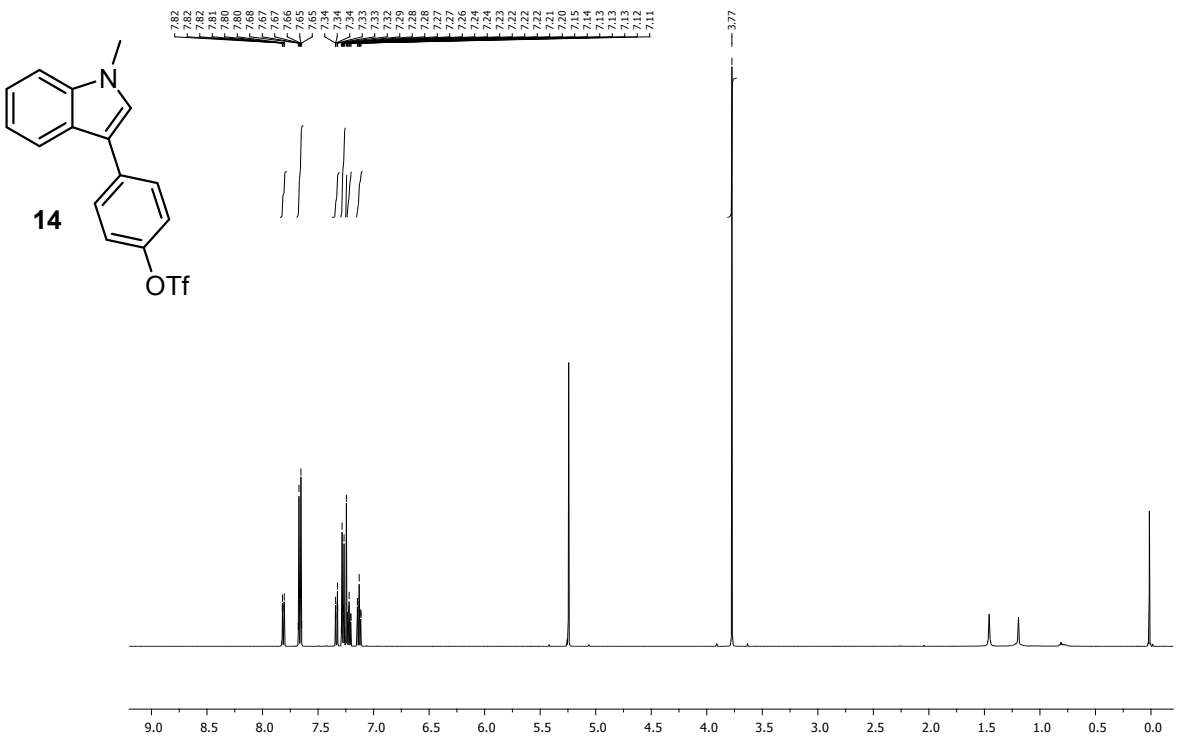


Figure S10. ^{1}H NMR spectrum of **14** in CD_2Cl_2.

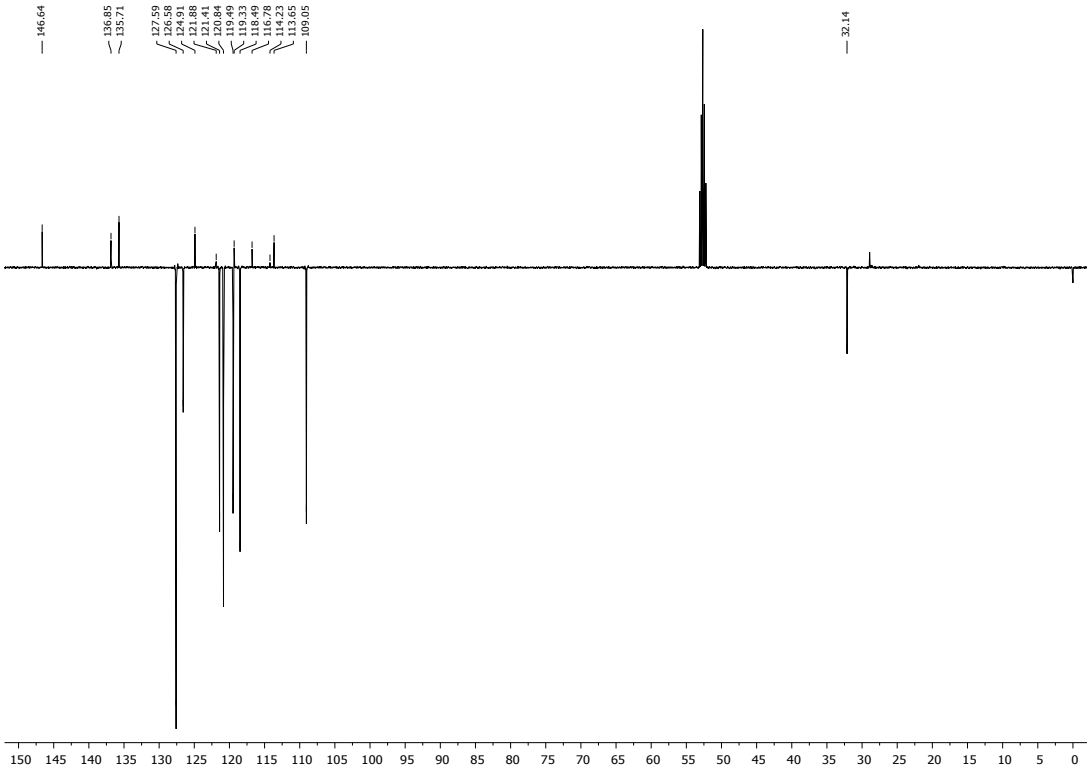


Figure S11. $^{13}C\{^{1}H\}$ NMR spectrum of **14** in CD_2Cl_2.

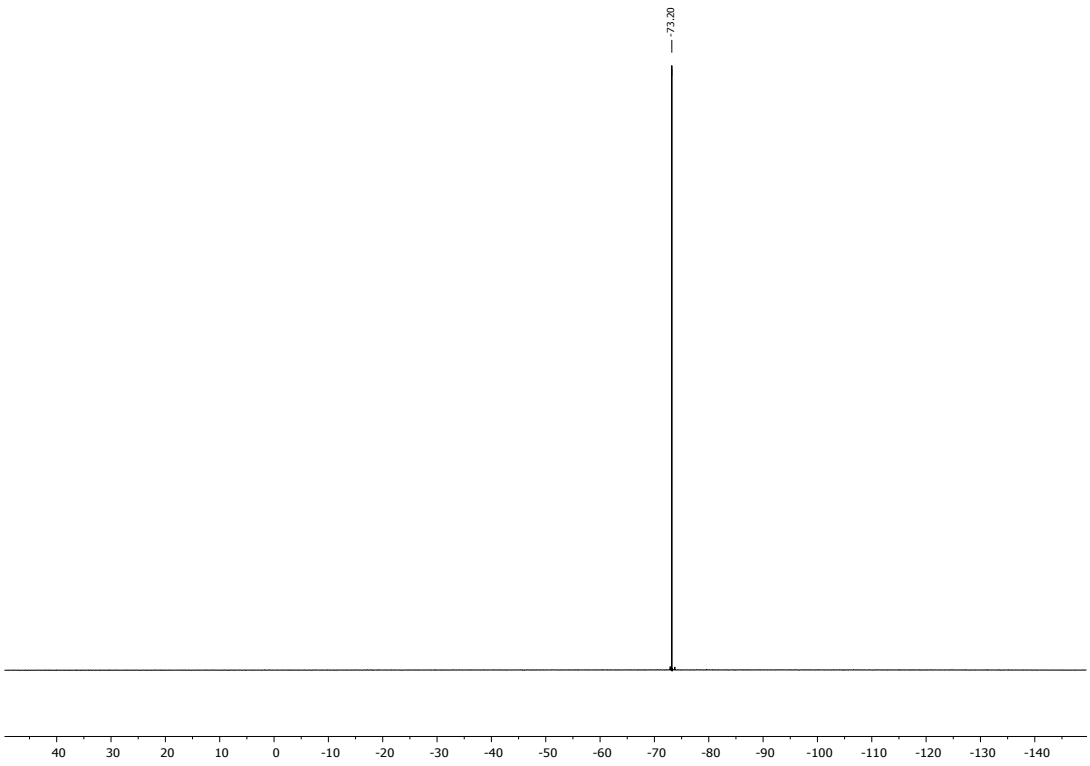


Figure S12. ^{19}F NMR spectrum of **14** in CD_2Cl_2.

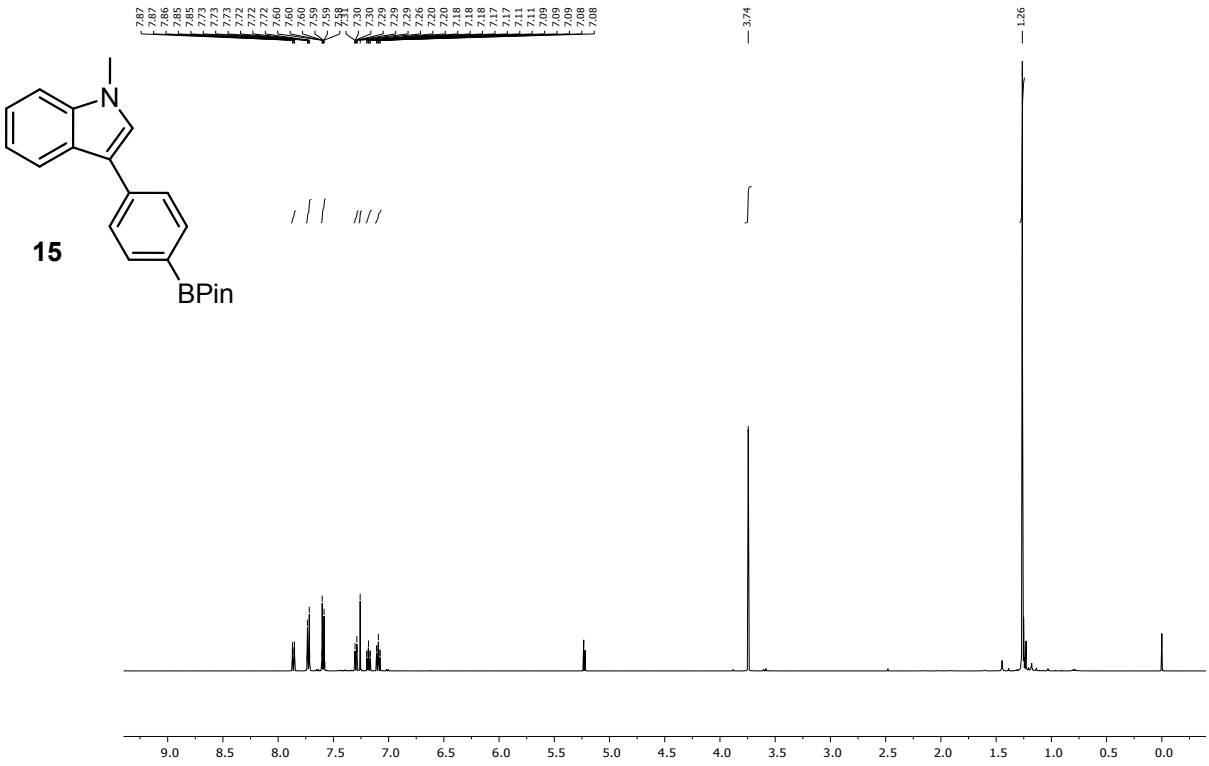


Figure S13. ^{1}H NMR spectrum of **15** in CD_2Cl_2.

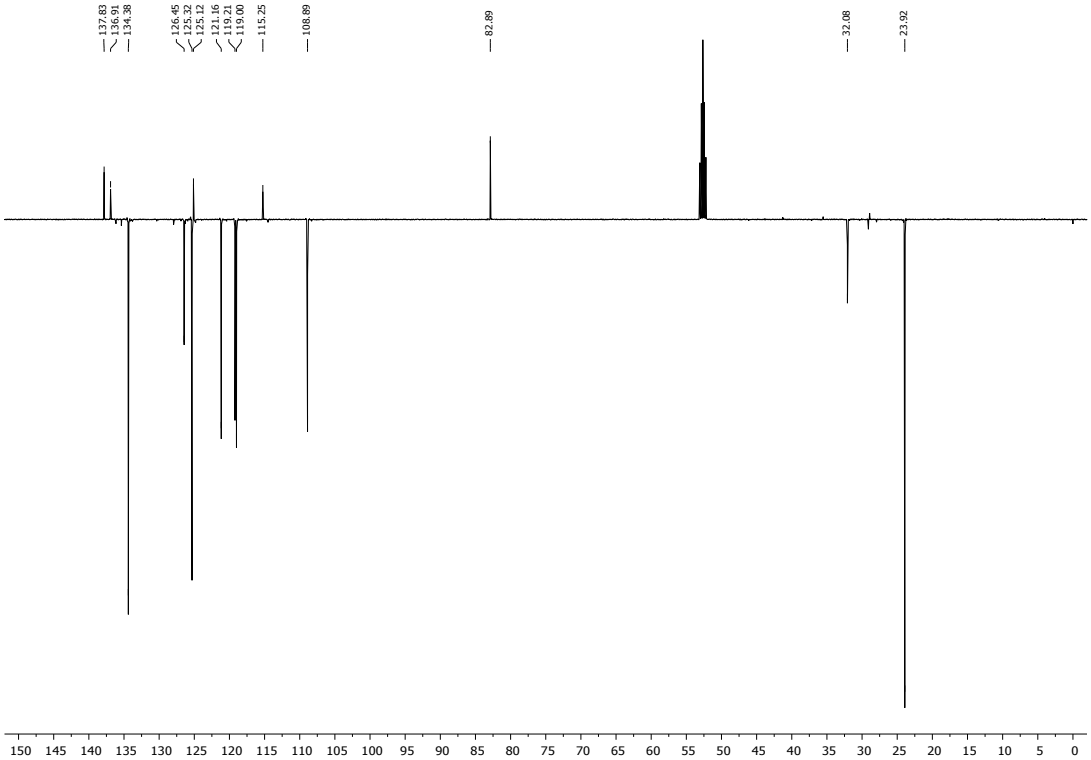


Figure S14. $^{13}C\{^{1}H\}$ NMR spectrum of **15** in CD_2Cl_2.

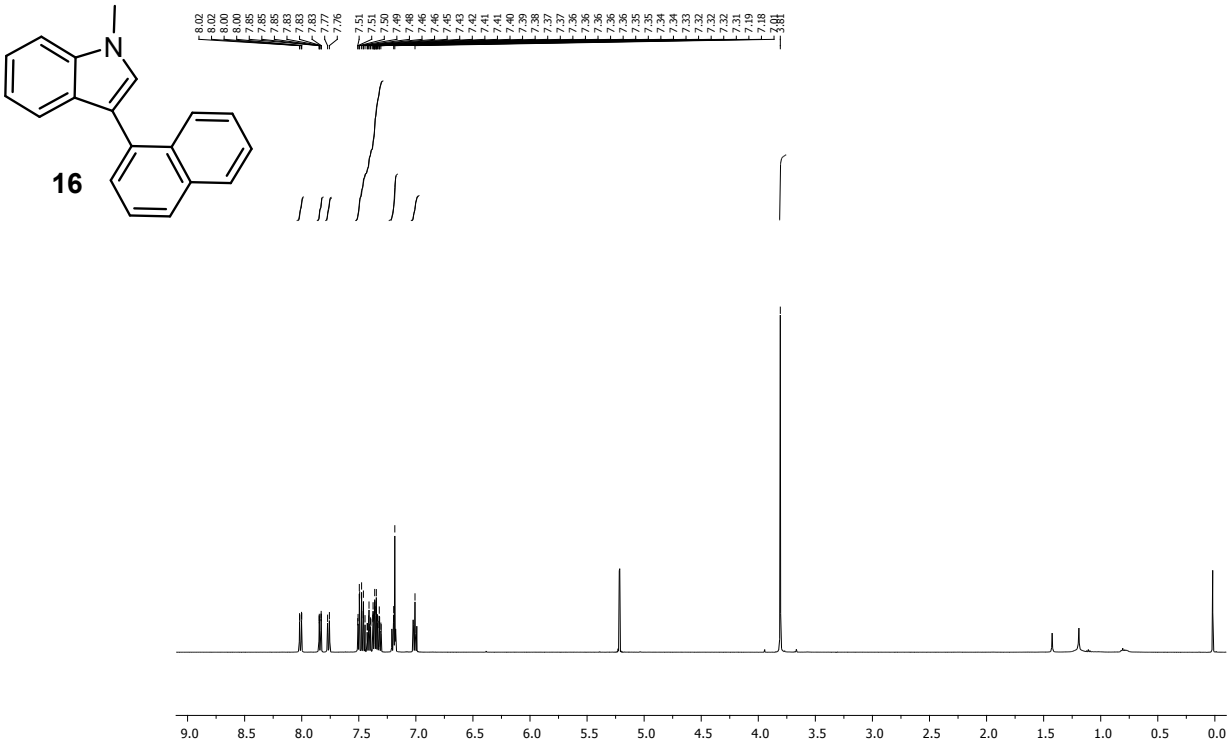


Figure S15. ^{1}H NMR spectrum of **16** in CD_2Cl_2.

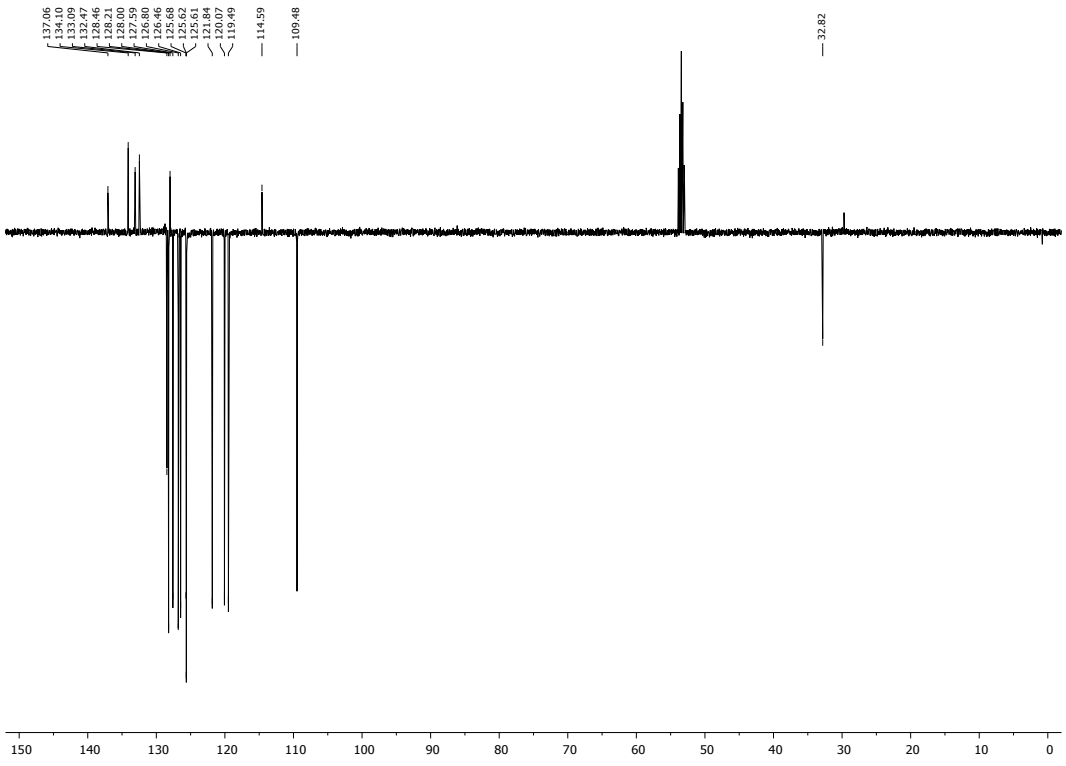


Figure S16. $^{13}C\{^{1}H\}$ NMR spectrum of **16** in CD_2Cl_2.

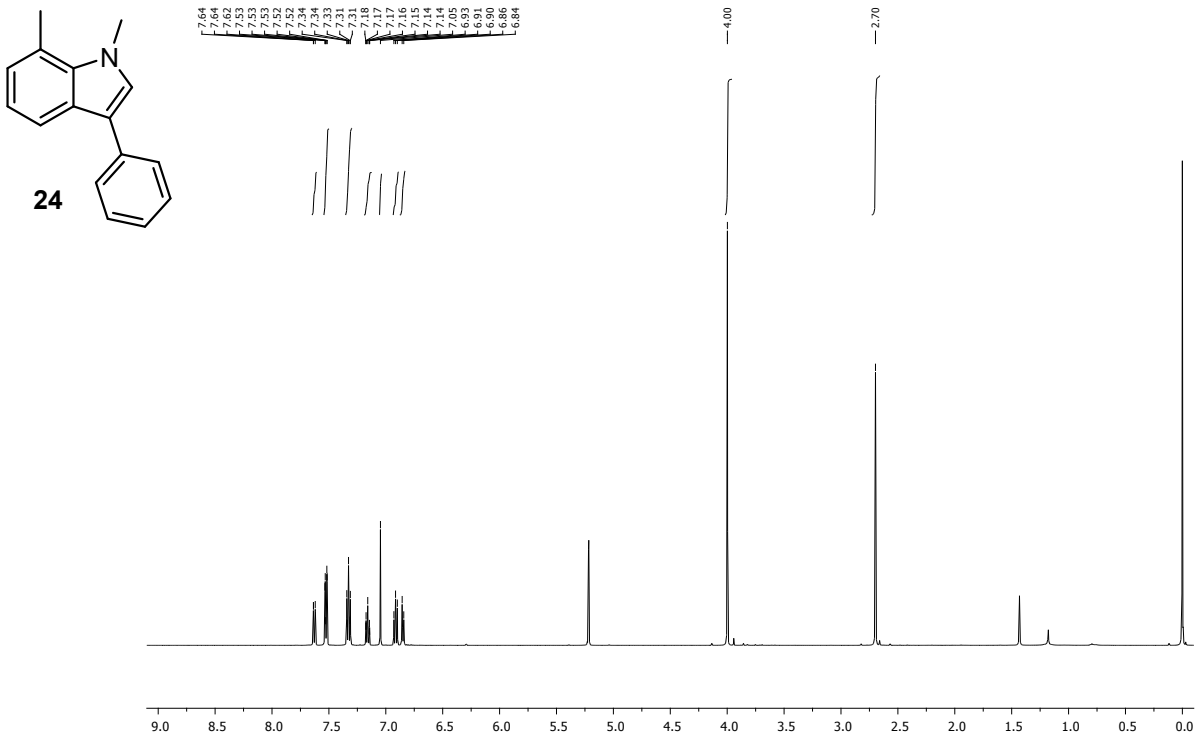


Figure S17. ^{1}H NMR spectrum of **24** in CD_2Cl_2.

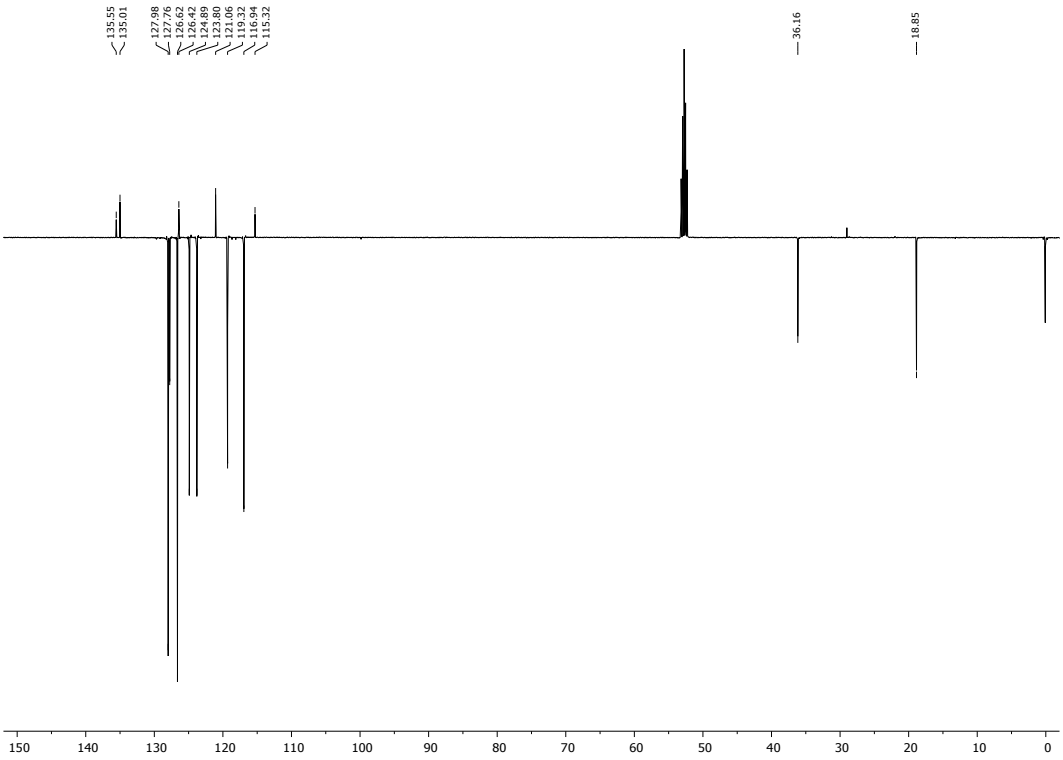


Figure S18. $^{13}C\{^{1}H\}$ NMR spectrum of **24** in CD_2Cl_2.

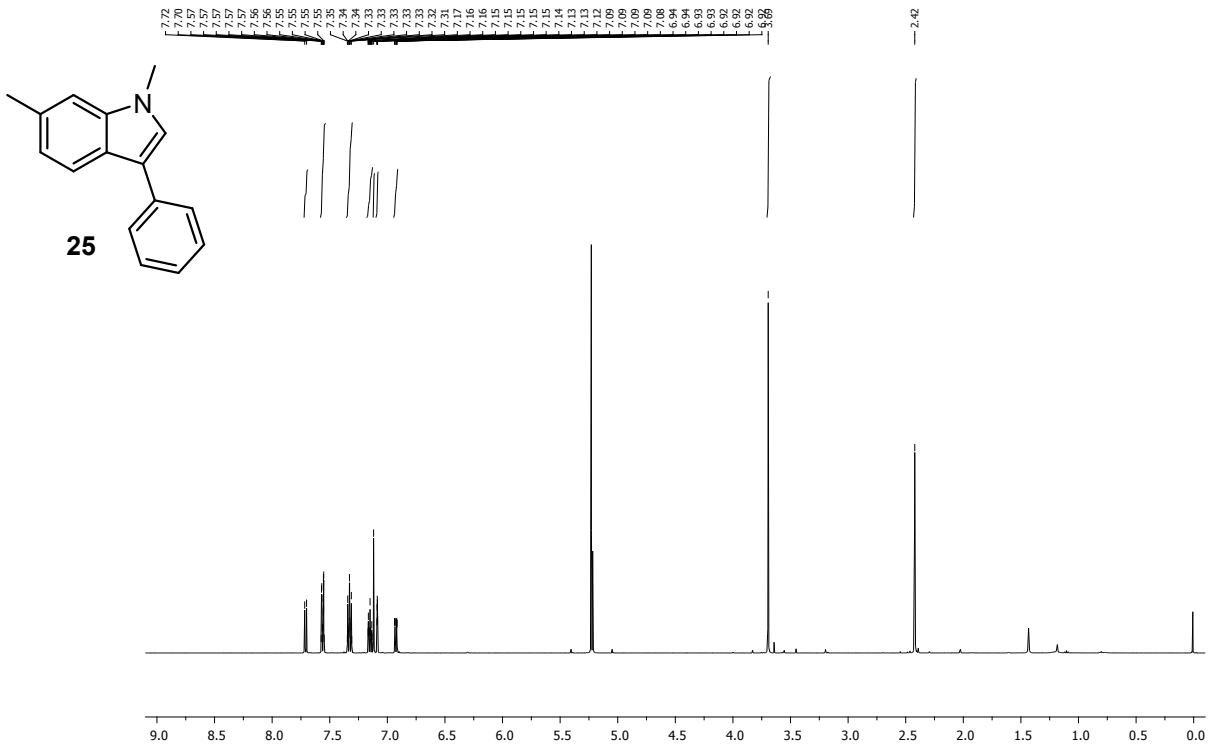


Figure S19. ^{1}H NMR spectrum of **25** in CD_2Cl_2.

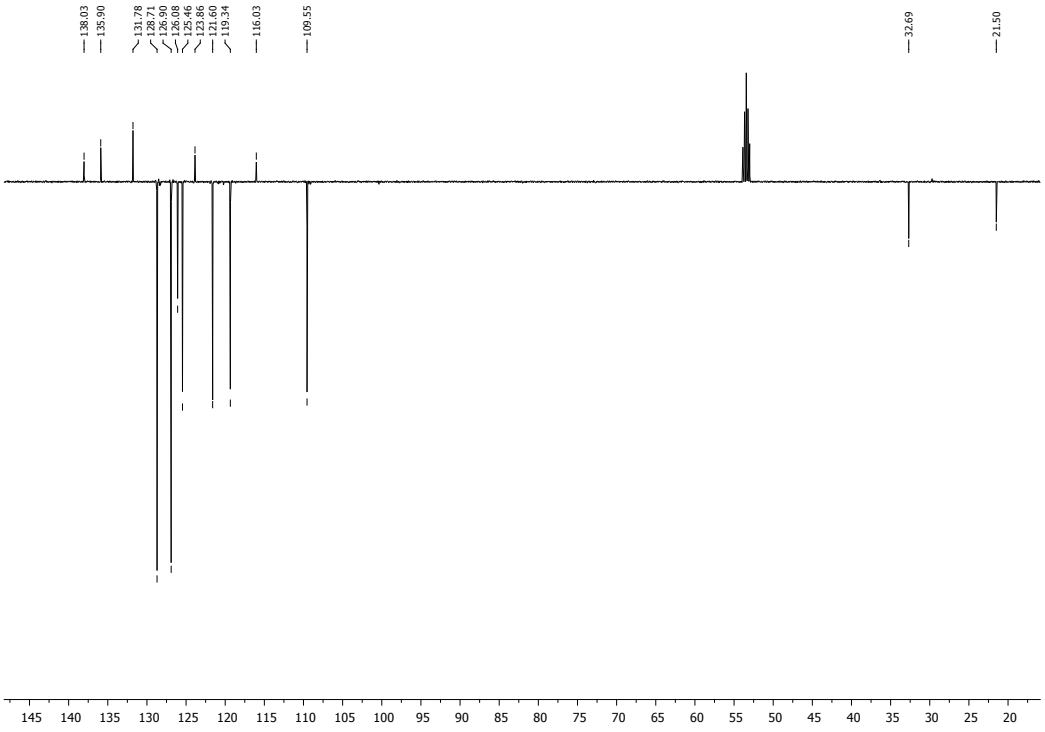


Figure S20. $^{13}C\{^{1}H\}$ NMR spectrum of **25** in CD_2Cl_2.

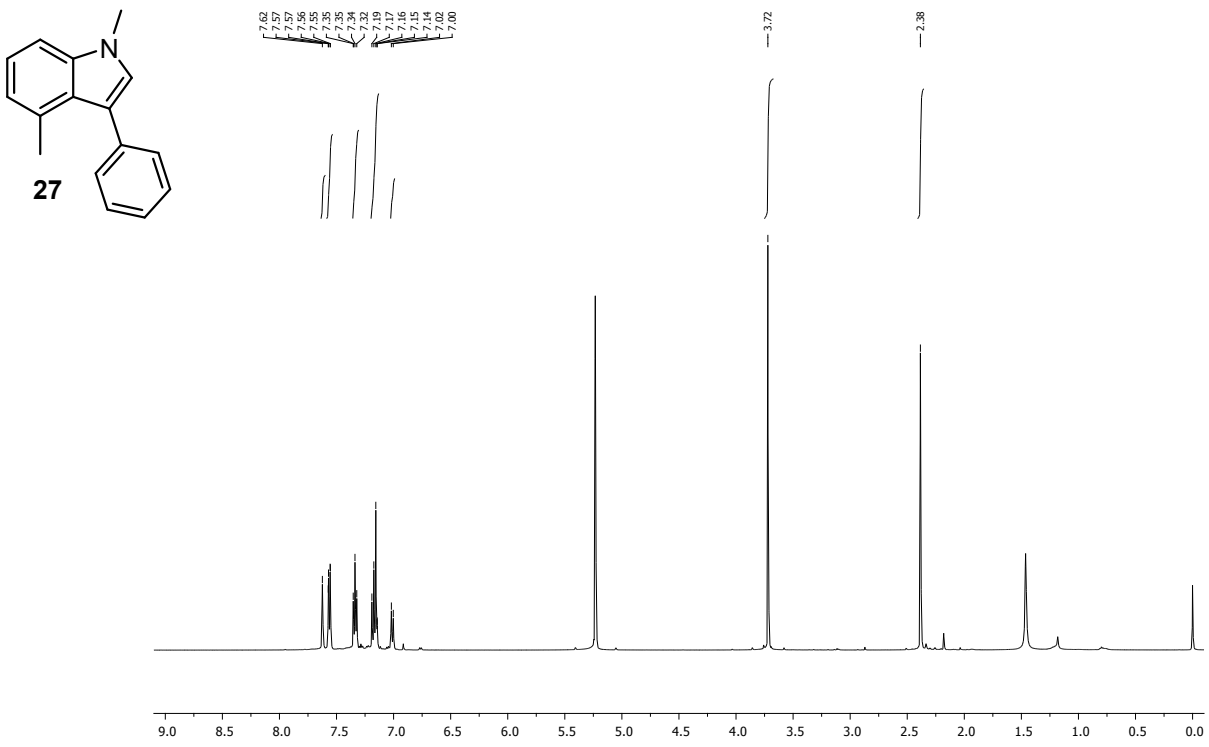


Figure S21. ^{1}H NMR spectrum of **27** in CD_2Cl_2.

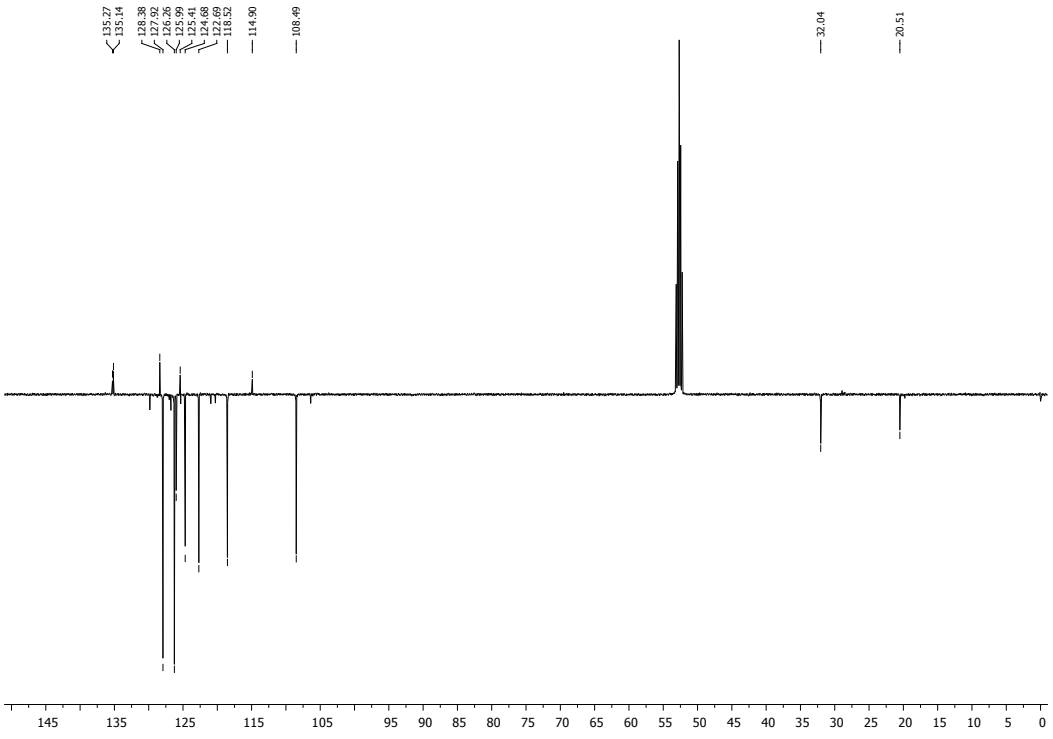


Figure S22. $^{13}C\{^{1}H\}$ NMR spectrum of **27** in CD_2Cl_2.

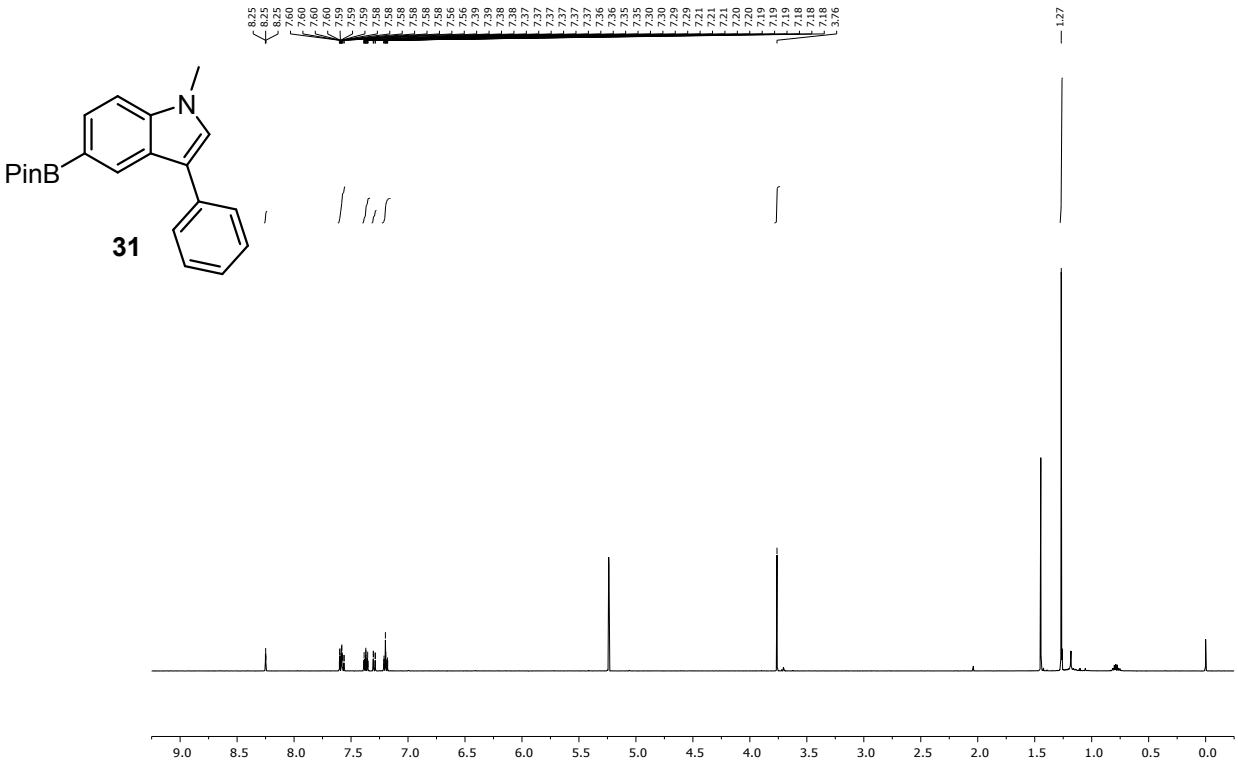


Figure S23. ^{1}H NMR spectrum of **31** in CD_2Cl_2.

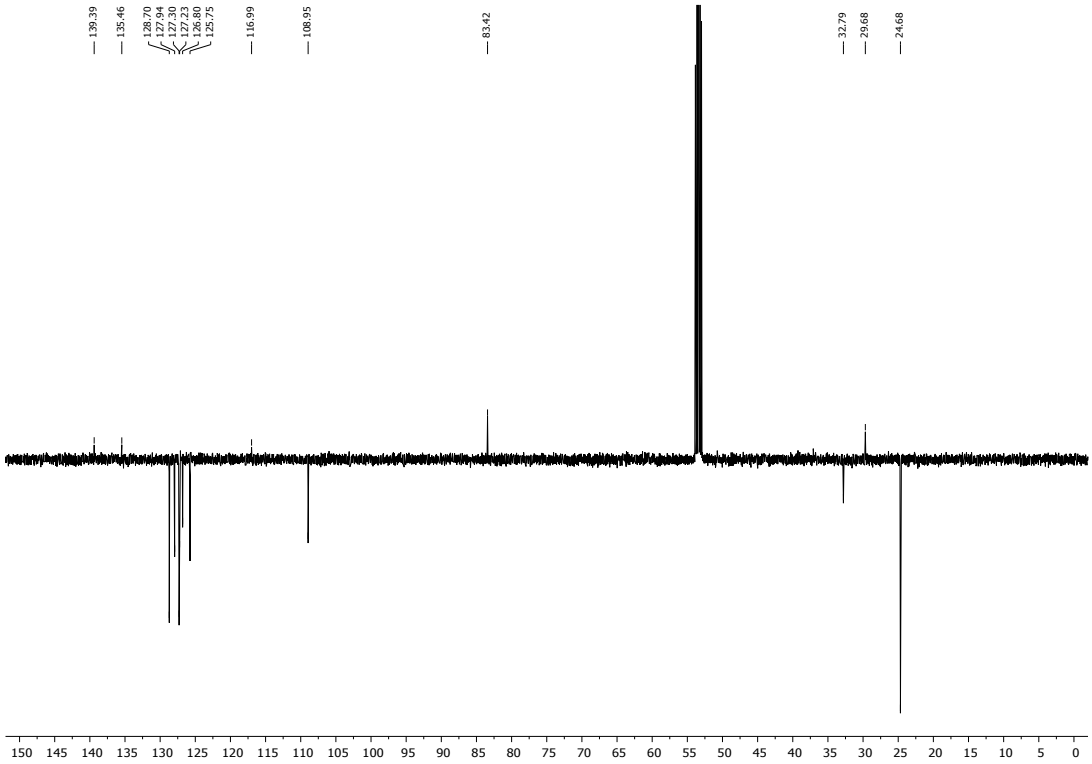


Figure S24. $^{13}C\{^{1}H\}$ NMR spectrum of **31** in CD_2Cl_2.

Crystallographic data collection and structure determination

The data were collected at low temperature (193 K) on a Bruker-AXS D8-Venture diffractometer equipped with a CMOS area detector, using MoKα radiation (λ = 0.71073 Å). Phi- and omega- scans were used. The data were integrated with SAINT, and an empirical absorption correction with SADABS was applied.[xxxi] The structures were solved using an intrinsic phasing method (SHELXT)[xxxii] and refined using the least-squares method on F^2[xxxiii]. All non-H atoms were refined with anisotropic displacement parameters. The H atoms were refined isotropically at calculated positions using a riding model.

CCDC-1894885 (**10**) and CCDC-1894886 (**13**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.a-c.uk/data_request/cif.

Selected data for **10:** $C_{15}H_{12}N_2O_2$, M = 252.27, orthorhombic, space group *Pbca*, a = 16.5065(10) Å, b = 7.0663(4) Å, c = 21.0475(15) Å, V = 2455.0(3) Å^3, Z = 8, crystal size 0.40 x 0.20 x 0.15 mm^3, 97445 reflections collected (3042 independent, R*int* = 0.0762), 173 parameters, $R1$ [I>2σ(I)] = 0.0552, *wR*2 [all data] = 0.1315, largest diff. peak and hole: 0.220 and –0.225 eÅ^{-3}.

Selected data for **13:** $C_{15}H_{12}BrN$, M = 286.17, orthorhombic, space group $P2_12_12_1$, a = 7.0113(7) Å, b = 10.6464(2) Å, c = 16.842(2) Å, V = 1257.2(2) Å^3, Z = 4, crystal size 0.40 x 0.05 x 0.02 mm^3, 29152 reflections collected (3131 independent, R*int* = 0.0544), 155 parameters, $R1$ [I>2σ(I)] = 0.0334, *wR*2 [all data] = 0.0683, largest diff. peak and hole: 0.409 and –0.447 eÅ^{-3}.

Computational Details

Calculations have been carried out with B97D Grimme's functional including dispersion,[xxxiv] as implemented in Gaussian 09.[xxxv] Gold, palladium and iodine atoms were described with the relativistic electron core potential SDD and the associated basis set.[xxxvi] The gold and palladium atoms have been augmented by a set of f polarization functions.[xxxvii] The 6-31G** basis set was employed for all other atoms. Full optimizations for all stationary points, *minima* and transition state structures involved in the oxidative addition (OA) of iodobenzene (PhI) to the metal were performed by taking into account solvent effects (dichloromethane, DCM) by means of the universal Solvation Model based on solute electron Density (SMD).[xxxviii] Profiles of the oxidative addition were computed: i) for the real gold cationic complexes (MeDalphos)Au^+ (**A**), (bipy)Au^+ (**B**)[xxxix] and *o*-carboranyl(P,P)Au^+ (**C**)[xl] without taking into account counter-anion, at the B97D(SMD-DCM)/SDD+f(Au), SDD(I), 6-31G**(other atoms) level of theory; iii) for model palladium complexes $(PPh_3)_2Pd$ (**D**) and chelate [1,2-$(Ph_2P)_2(C_6H_4)$]Pd (**E**) at the B97D(SMD-DCM)/SDD+f(Pd), SDD(I), 6-31G**(other atoms) level of theory to compare the impact of the metal on charge transfer at the transition state. Frequency calculations were undertaken at the same level of theory than optimization to confirm the nature of the stationary points, yielding one imaginary frequency for transition states (TS), corresponding to the expected process, and zero for *minima*. The connectivity of the transition states and their adjacent *minima* was confirmed by intrinsic reaction coordinate (IRC)[xli] calculations. All energies presented correspond to free energies in solution (electronic energies into brackets) and are given in kcal.mol^{-1}. All reported electronic energies (ΔE) were zero-point energy (ZPE) corrected and Gibbs free energies (ΔG) temperature corrected using unscaled density functional frequencies.

To further analyze the impact of the metal (gold *versus* palladium) on the oxidative addition process, Natural Bond Orbital[xlii] (NBO, 5.9 version)[xliii] analyses have been performed. Stabilizing interactions (ΔE(2) in kcal·mol^{-1}), determined at second order perturbation theory, have been computed to get insight on donor-acceptor interactions. Natural Localized Molecular Orbitals (NLMO) have also been determined. The optimized structures were subjected to an Atoms-In Molecules analysis (QTAIM analysis) using AIMAll software.[xliv] Bader charges have been calculated in order to determine the influence of the metal in the ligand→metal

charge transfer (CT) at the transition state of the OA process for gold and palladium complexes. Charge decomposition analysis (CDA) was carried out with the CDA 2.2 program of G. Frenking.[xlv] The orbital contributions to the charge distributions were divided into four parts: (i) the mixing of the occupied orbitals of the ligand and the unoccupied MOs of the metal fragment (Ligand ✂ M donation *d*), (ii) the mixing of the unoccupied orbitals of the ligand and the occupied MOs of the metal fragment (Ligand ✎ M back-donation *b*), (iii) the mixing of the occupied orbitals of the ligand and the occupied orbitals of the metal fragment (ligand ↔ M repulsive polarization *r*), and (iv) the mixing of the unoccupied orbitals of the ligand and the unoccupied orbitals of the metal fragment (residual term Δ).

Energy Decomposition Analysis[xlvi] was performed for all the transition states with Amsterdam Density Functional 2018.01 program package[xlvii] at ZORA-BP86-D3/TZ2P level of theory on the geometry optimized from Gaussian 09 at B97D(SDM-DCM)/SDD+f(M),SDD(I), 6-31G** level of theory. This analysis is based on the EDA method of Morokuma and the ETS partitioning scheme of Ziegler and Rauk. The term ΔE_{int} can be decomposed into different contributions: (i) electrostatic interaction energy between the fragments (ΔE_{elstat}), (ii) destabilizing Pauli repulsion from interactions between electrons on either fragment with the same spin (ΔE_{pauli}), (iii) stabilizing orbital interaction (ΔE_{orb}) and (iv) dispersion energy term (ΔE_{disp}).

$$\Delta E_{int} = \Delta E_{elestat} + \Delta E_{Pauli} + \Delta E_{orb} + \Delta E_{disp}$$

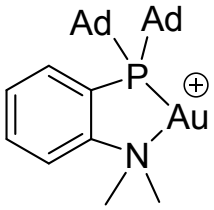
To further characterize the interaction between the substrate and metal fragments in the transition states, the Natural Orbital Chemical Valence (NOCV) approach was used.[xlviii] ETS-NOCV scheme combines charge rearrangement (NOCV) and bond energy analysis. It is a powerful tool to quantitatively analyze chemical bonds, combining the extended transition state (ETS) method for energy decomposition analysis combined with the natural orbitals for chemical valence (NOCV) theory. In this approach, the ΔE_{orb} term is decomposed into the contributions from different natural orbitals of chemical valence (NOCV) eigenvalues (λ_i) as follow:

$$\Delta E_{orb} = \sum_{k} \Delta E_{orb}^{k} = \sum_{k=1}^{M/2} v_k [- F_{-k,-k}^{TS} + F_{k,k}^{TS}]$$

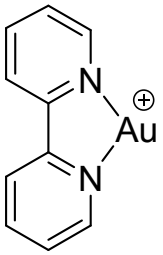
where $F^{TS}_{k,k}$ are diagonal Kohn-Sham matrix elements defined over NOCV with respect to the transition state (TS) density. The components ΔE^{k}_{orb} provide energetic estimation of $\Delta\rho^{k}$ and allow to characterize the importance of a particular electron flow channel for the bonding between considered molecular fragments. The color code used to analyze these densities are red (depletion) and blue (accumulation) and the direction of the charge flow is from red → blue. Hirshfeld charge analysis was also used to determine the magnitude of the charge transfer between the ligand (PhI) and the metal fragments.[xlix]

Scheme S5. Different complexes studied to analyze and compare the oxidative addition process of PhI to Au and Pd complexes.

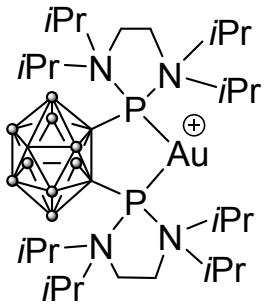
Real gold complexes



A



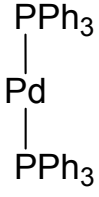
B



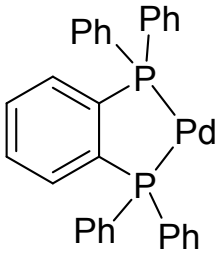
C

with ○ : B

Model Palladium complexes



D



E

Figure S25. Energy profile for the oxidative addition of PhI (ΔG and ΔE values into brackets in kcal·mol^{-1}) to the gold complex **A**, computed at the SMD(dichloromethane)-B97D/SDD+f(Au),SDD(I),6-31G**(other atoms) level of theory. Main geometrical parameters (distances in Å and bond angle in °).

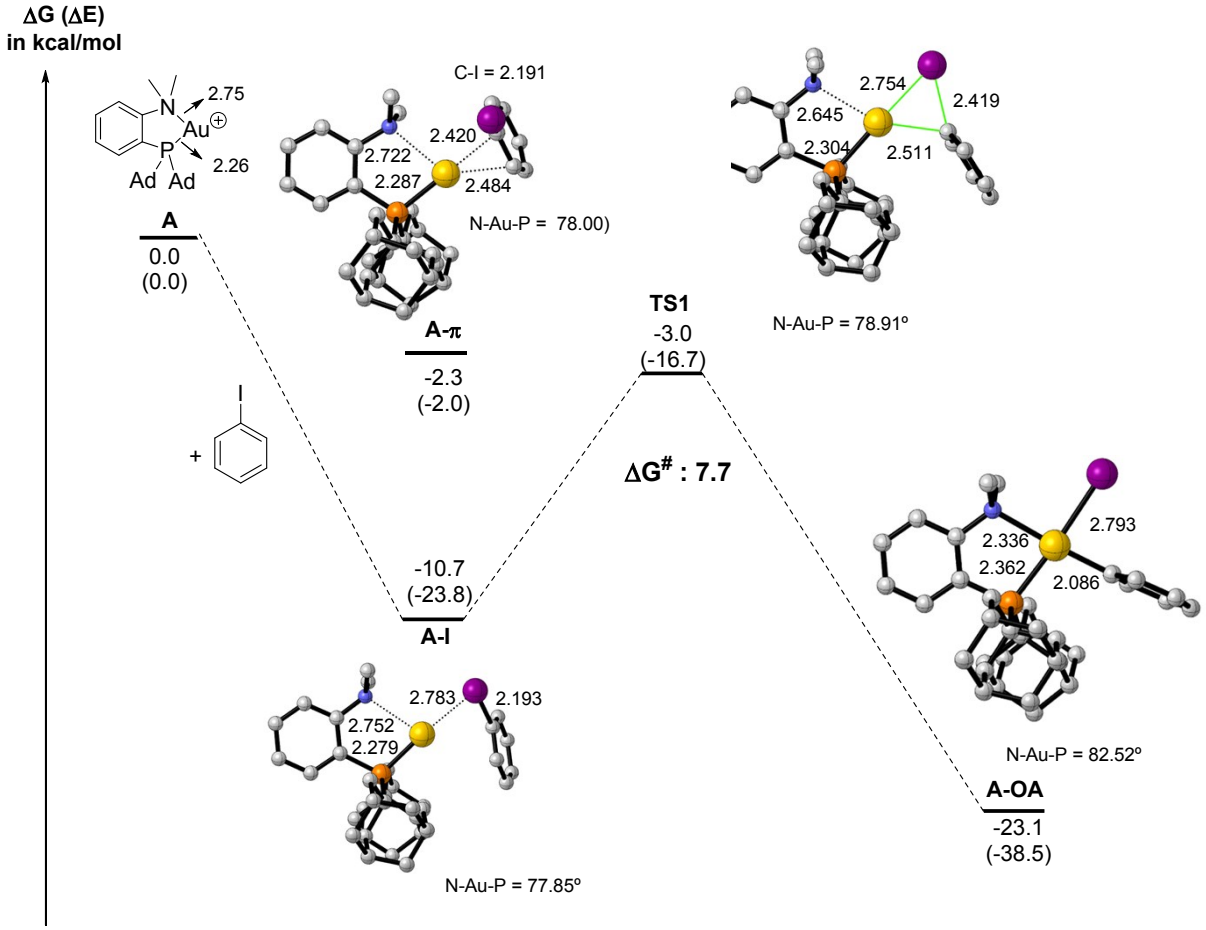


Table S4. NBO and AIM analyses for the transition state **TS1** and the final product **A-OA**. Stabilizing interaction $n_N \rightarrow \sigma^*_{AuC}$ [ΔE(2) in kcal/mol], coming from NBO calculations. Density ρ(r) in e.bohr^{-3}, Laplacian of density $\nabla^2\rho(r)$ in e.bohr^{-5} and bond index δ from AIM analysis.

TS1		**Complex A-OA**	
Au…N : 2.645 Å		Au…N : 2.336 Å	
NBO		**NBO**	
$n_N \rightarrow \sigma^*_{AuC}$	4.4	$n_N \rightarrow \sigma^*_{AuC}$	38.9
AIM		**AIM**	
BCP (Au…N)		**BCP (Au…N)**	
ρ(r)	0.039	**ρ(r)**	0.068
$\nabla^2\rho(r)$	0.118	**$\nabla^2\rho(r)$**	0.210
δ(Au-N)	0.282	**δ(Au-N)**	0.482

Figure S26. Energy profile for the oxidative addition of PhI (ΔG and ΔE values into brackets in kcal·mol^{-1}) to the gold complex **B**, computed at the SMD(dichloromethane)-B97D/SDD+f(Au),SDD(I),6-31G**(other atoms) level of theory. Main geometrical parameters (distances in Å and bond angle in °).

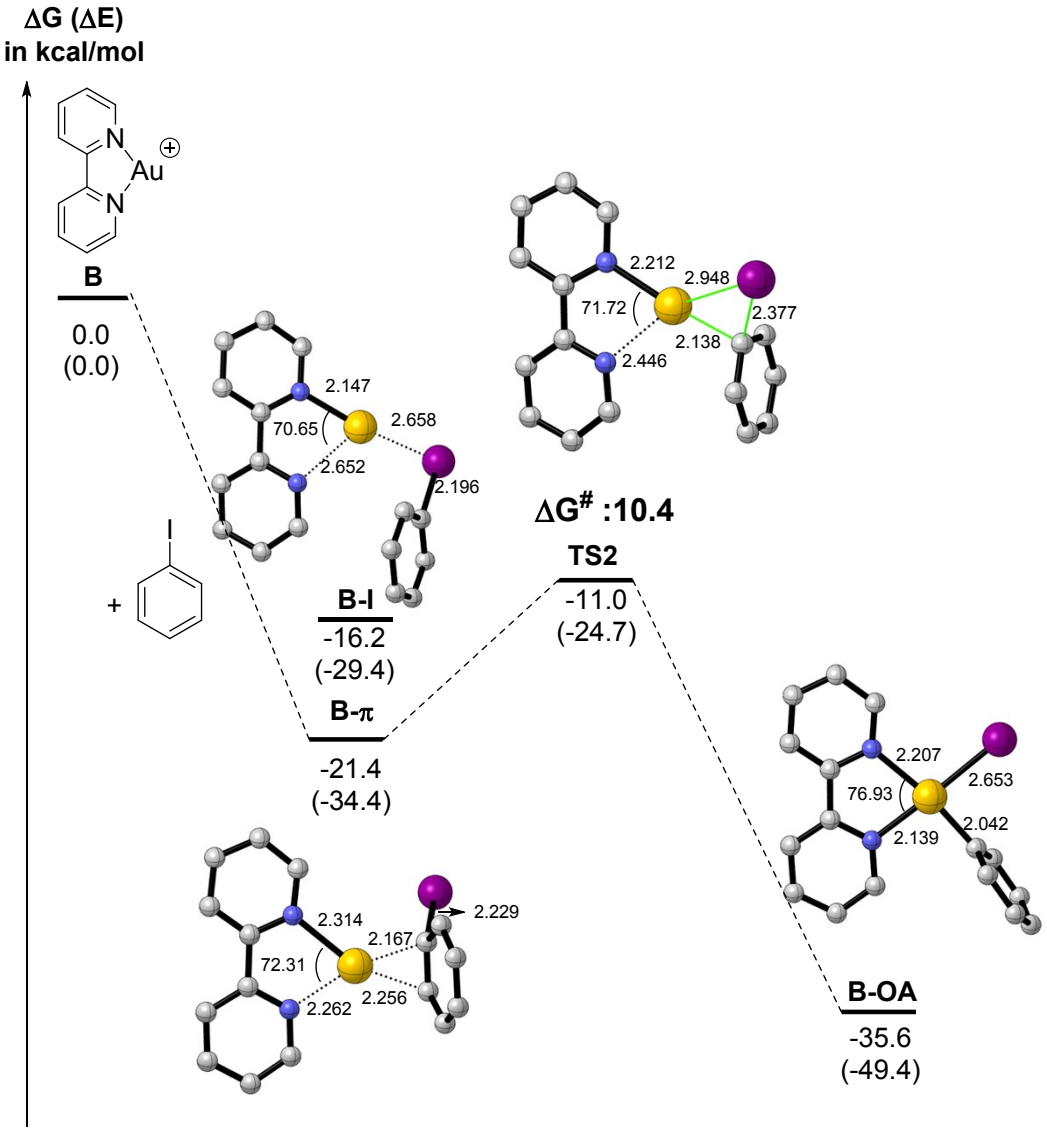


Figure S27. Energy profile for the oxidative addition of PhI (ΔG and ΔE values into brackets in kcal·mol^{-1}) to gold complex **C**, computed at the SMD(dichloromethane)-B97D/SDD+f(Au),SDD(I),6-31G**(other atoms) level of theory. Main geometrical parameters (distances in Å and bond angle in °).

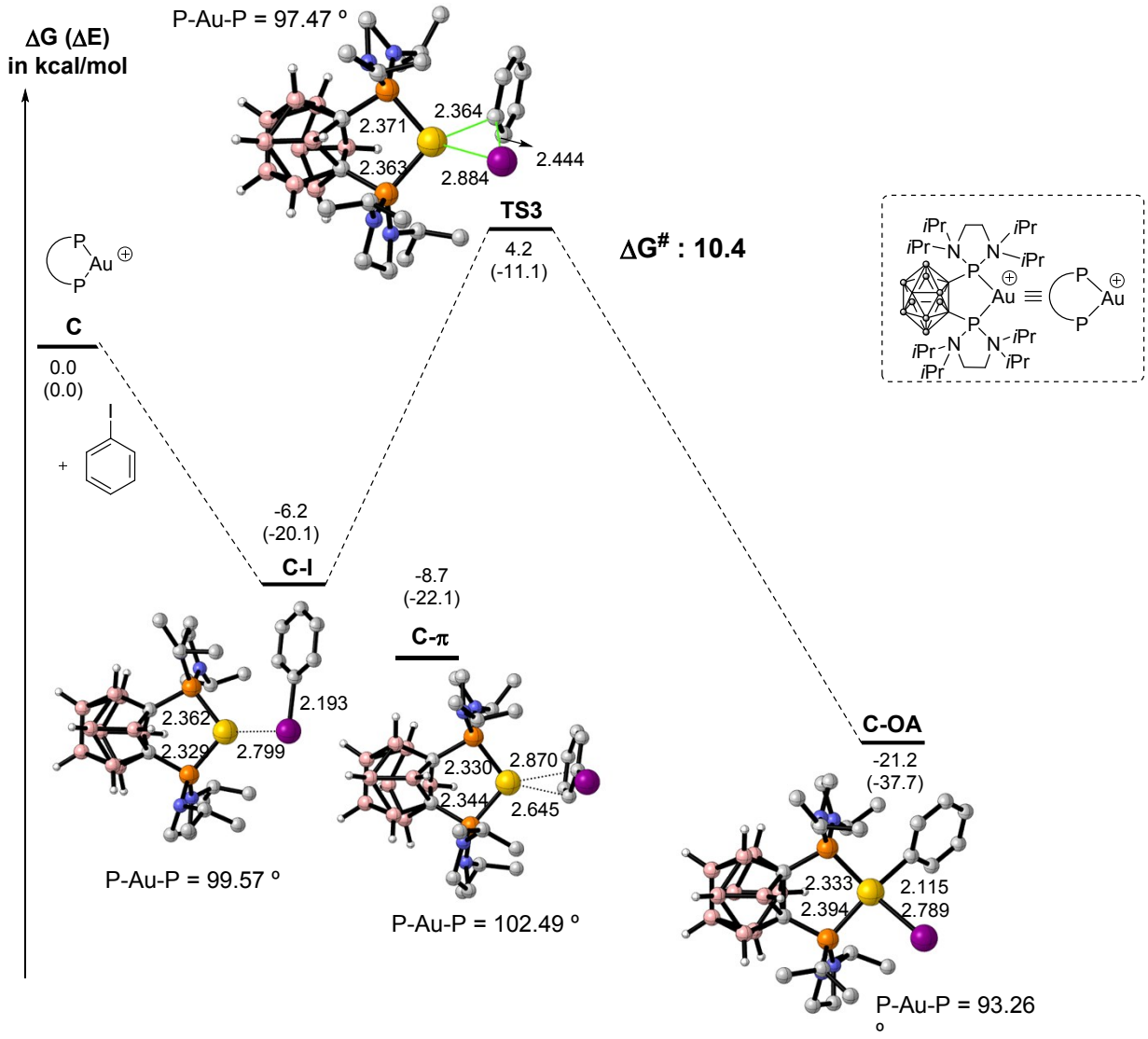


Figure S28. Energy profile for the oxidative addition of PhI (ΔG and ΔE values into brackets in kcal·mol^{-1}) to the model palladium complex **D**, computed at the SMD(dichloromethane)-B97D/SDD+f(Pd),SDD(I),6-31G**(other atoms) level of theory. Main geometrical parameters (distances in Å and bond angle in °).

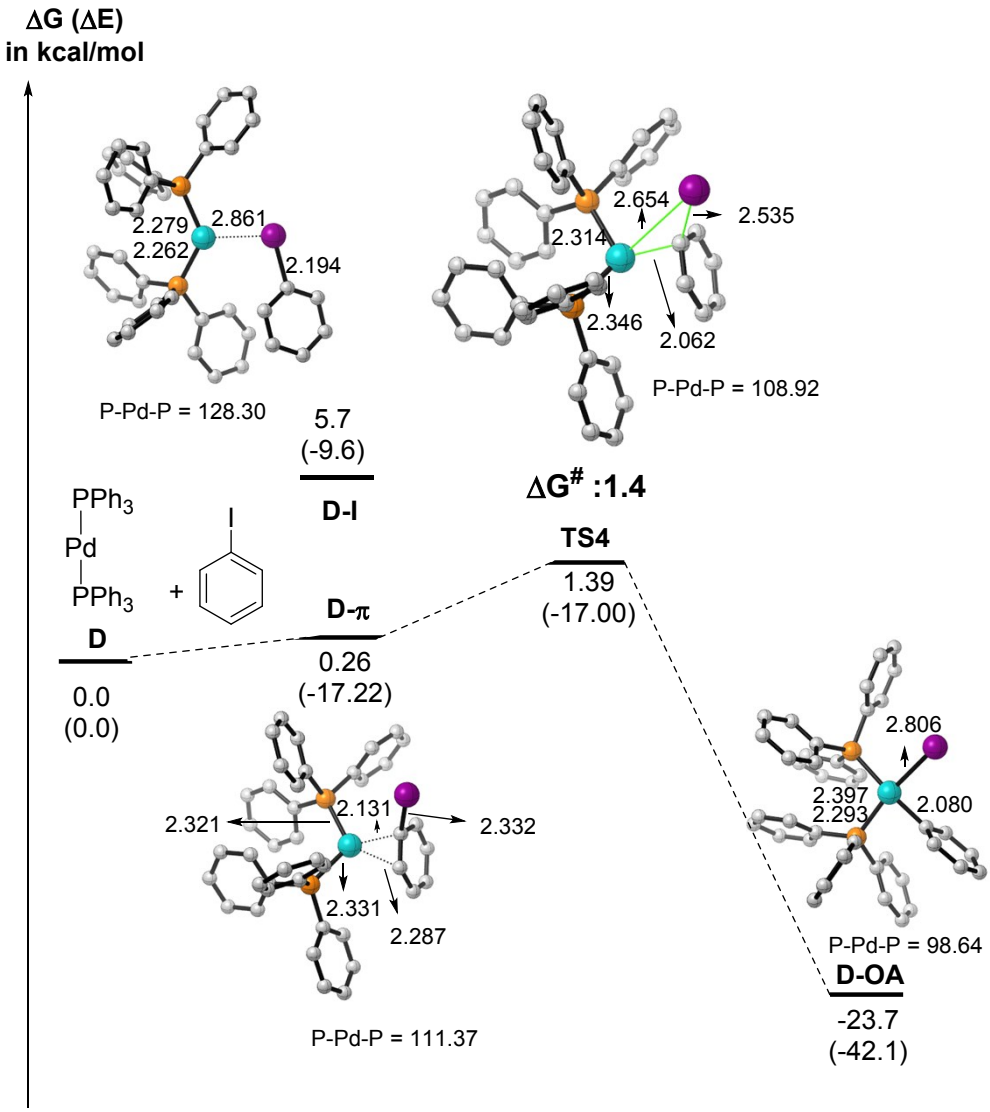


Figure S29. Energy profile for the oxidative addition of PhI (ΔG and ΔE values into brackets in kcal·mol^{-1}) to the model palladium complex **E**, computed at the SMD(dichloromethane)-B97D/SDD+f(Pd),SDD(I),6-31G**(other atoms) level of theory. Main geometrical parameters (distances in Å and bond angle in °).

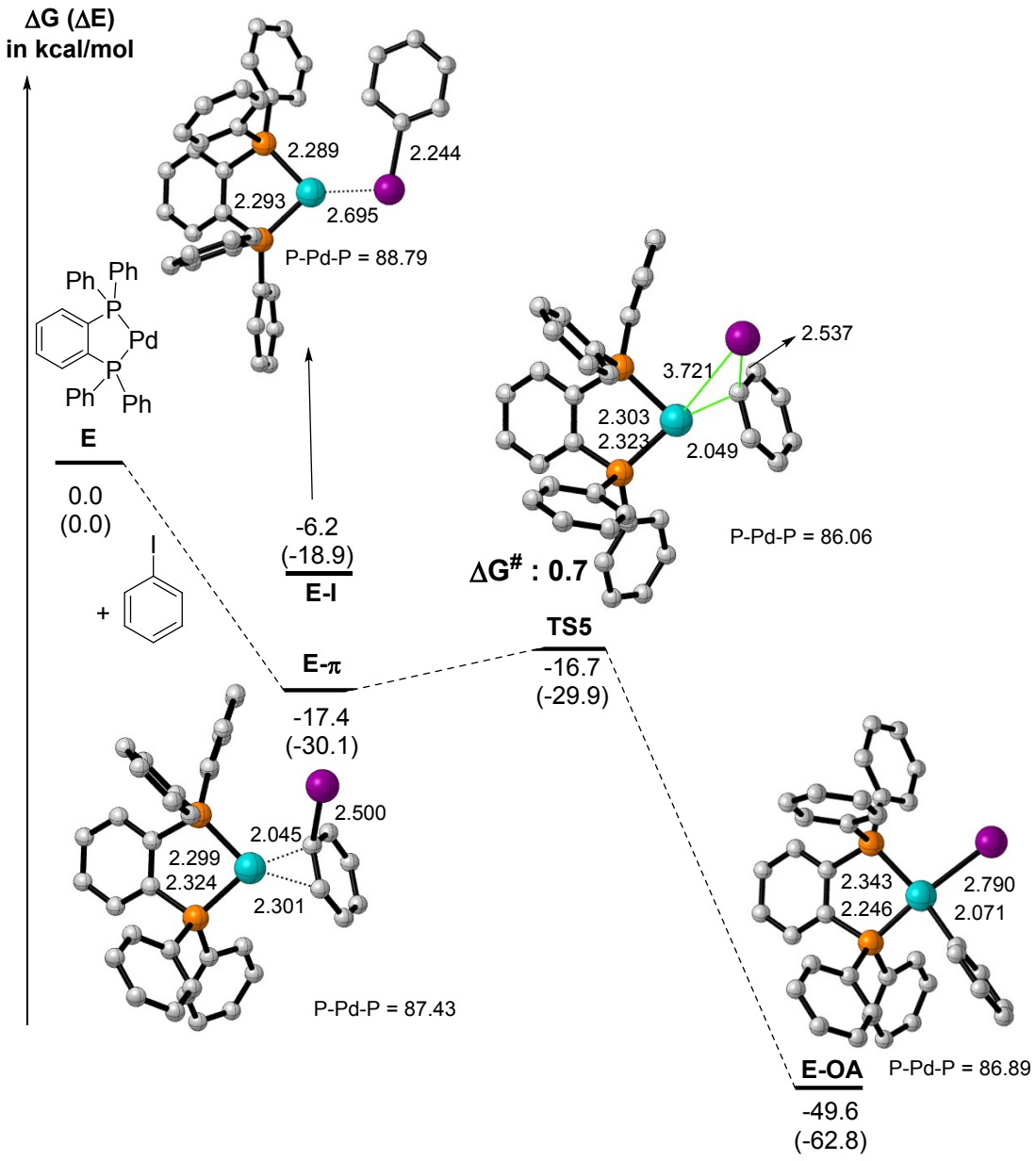


Table S5. NBO and AIM analyses for the transition states for oxidative addition of PhI to the different gold and palladium complexes. Charge transfer (CT) from PhI to the metal fragment computed from Bader charges. Main stabilizing interactions [$\Delta E(2)$ in kcal/mol] coming from NBO calculations. NLMO LP(M) accounting for the back-donation with participation of main atoms in %.

Transition states					
	TS1[a] (Au)	**TS2[b] (Au)**	**TS3[a] (Au)**	**TS4[b] (Pd)**	**TS5[b] (Pd)**
NBO analysis					
Stabilizing interactions in kcal/mol					
LP(I) $\rightarrow \sigma^*_{MP}$	41.1	10.1[c]	22.6[c]	1.0[c]	-
$\sigma_{CI} \rightarrow \sigma^*_{MP}$	23.5	30.4[c]	30.8[c]	6.9[c]	5.1[c]
$\pi_{C=C} \rightarrow \sigma^*_{MP}$	6.2	70.5[c]	24.2[c]	42.4[c]	58.7[c]
$\sigma_{CC} \rightarrow \sigma^*_{MP}$	1.1	3.8[c]	2.38	5.2[c]	7.2[c]
Σ donation	71.9	114.8[c]	80[c]	55.5[c]	71[c]
LP(M) $\rightarrow \sigma^*_{CI}$	8.8	8.4	7.8[c]	5.3	5.5
LP(M) $\rightarrow \pi^*_{C=C}$	4.1	6.0	3.7[c]	26.0	24.9
Σ back-donation	12.9	14.4	11.5[c]	31.3	30.4
NLMO					
LP(M)	93.2% Au 2.0 % I 3.2 % C	90.3% Au 2.7 % I 4 % C	92.4% Au 2.1 % I 2.9 % C	77.9 % Pd 3.1 % I 10.9 % C	76.9 % Pd 3.5 % I 11.3 % C
AIM analysis					
Bader charges					
CT (ArI$\rightarrow$ M)	0.163	0.228	0.105	-0.421	-0.460
q(M)	0.059	0.384	0.013	0.038	0.051
q(I)	0.022	0.048	0.027	-0.287	-0.305
q(C)	-0.180	-0.185	-0.220	-0.164	-0.164

[a] IRC calculations reveal that TS is connected to I-adduct and final product. [b] IRC calculations reveal that TS is connected to π-adduct and final product. [c] Donation in LP*(M) orbital, with strong s character.

The more or less significant contribution of the metal in the Natural Localized Molecular Orbital (NLMO) associated to LP(M) [77-78% (Pd) *versus* 90-93 % (Au)] corroborates the greater back-donation for the palladium center.

Table S6. CDA analysis computed at B97D/SDD+f(M)/SDD(I),6-31G**(other atoms) level of theory for the different transition states.

	TS1(Au)	TS2 (Au)	TS3 (Au)	TS4 (Pd)	TS5 (Pd)
L→ M donation (d)	0.310	0.359	0.337	0.225	0.210
M →L back-donation (b)	0.116	0.149	0.146	0.329	0.288
d/b ratio	2.67	2.40	2.30	0.68	0.73
M ↔ C repulsion	-0.380	-0.350	-0.475	-0.526	-0.442
Residue term Δ	-0.034	-0.037	-0.030	-0.022	-0.017

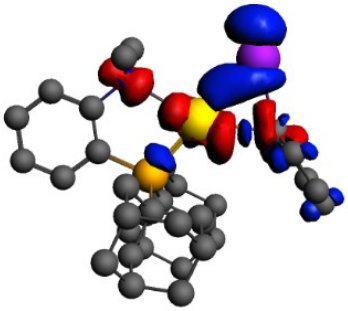
Table S7. Energy Decomposition Analysis (EDA-NOCV) for the different transition states at ZORA-BP86-D3/TZ2P level of theory (energy contributions in kcal.mol^{-1}). Charge flow contribution Δq^{PhI} from Hirshfeld partitioning.

	TS1 (Au)	TS2 (Au)	TS3 (Au)	TS4 (Pd)	TS5 (Pd)
ΔE_{Pauli}	102.29	122.25	120.34	169.49	157.39
ΔE_{Elstat}	-69.96 (48.9 %)[a]	-89.93 (51.6%)[a]	-77.42 (48.4%)[a]	-114.88 (51.9 %)[a]	-108.43 (51.8 %)[a]
ΔE_{Orb}	-57.19 (40 %)[a]	-76.42 (43.9 %)[a]	-62.55 (39.1 %)[a]	-86.39 (39.0 %)[a]	-87.07 (41.6 %)[a]
ΔE_{Orb1}	-18.62 (32.6 %)[b]	-32.50 (42.5 %)[b]	-20.50 (32.8 %)[b]	-56.12 (65.0 %)[b]	-59.43 (68.3 %)[b]
	λ_1 : 0.65[c]	λ_1 : 0.63[c]	λ_1 : 0.73[c]	λ_1 : 0.97[c]	λ_1 : 1.03[c]
ΔE_{Orb2}	-22.89 (40.0 %)[b]	-25.85 (33.8 %)[b]	-22.72 (36.3 %)[b]	-10.01 (11.6 %)[b]	-9.67 (11.1 %)[b]
	λ_2 : 0.50[c]	λ_2 : 0.55[c]	λ_2 : 0.61[c]	λ_2 : 0.33[c]	λ_1 : 0.32[c]
ΔE_{Orb3}	-3.98 (7.0 %)[b]	-4.67 (6.1 %)[b]	-6.01 (9.6%)[b]	-5.81 (6.7%)[b]	-6.65 (7.7 %)[b]
	λ_3 : 0.17[c]	λ_3 : 0.20[c]	λ_3 : 27[c]	λ_3 : 0.23[c]	λ_1 : 0.23[c]
$\Delta E_{dispersion}$	-15.85 (11.1 %)[a]	-7.85 (4.5 %)[a]	-19.89[a] (12.4 %)	-20.26 (9.1 %)[a]	-13.79 (6.6 %)[a]
ΔE_{int}	-40.68	-51.95	-51.17	-52.03	-51.91
	Values into brackets (%) correspond to : [a] the contribution of each term in the total attractive interaction, [b] the contribution of each term in the orbital interaction and [c] Eigenvalue λ_i, corresponding to the charge flow				
Δq^{PhI}	0.076	0.111	0.053	-0.332	-0.382

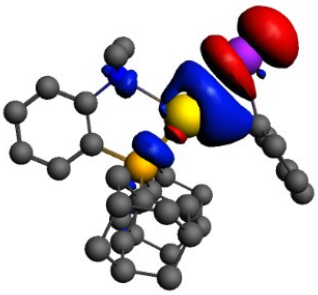
We have analyzed the interaction between PhI and LAu^+ or LPd fragments in the different transition states **TS1-5**, in terms of orbital contributions by applying the Extended Transition State-Natural orbitals for Chemical Valence scheme (ETS-NOCV). Table S7 and Figures S30 and S31 summarize the results, with the three more important contributions to the deformation electron density for ML_n/PhI partition and the energetic estimates of the i-th charge-flow channel, ΔE_{orbi}.

Figure S30: Plot of the contours of deformation densities contributions ($\Delta\rho_{orbi}$) of the main pairwise orbital interactions between PhI and AuL_n and associated orbital interaction energies contributions (ΔE_{orbi}, in kcal.mol^{-1}) for the different TSs computed at ZORA-BP86-D3/TZ2P level of theory. The charge flow is red → blue ($\Delta\rho < 0$ in red and $\Delta\rho > 0$ in blue). The contour value for density is 0.001 a.u.

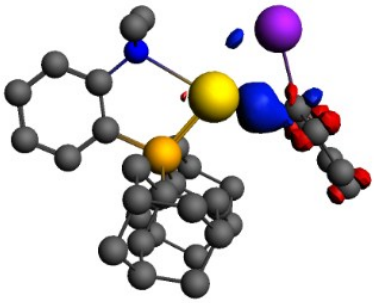
TS1-Au



$\Delta E_{orb1}(\rho)$ = -18.6

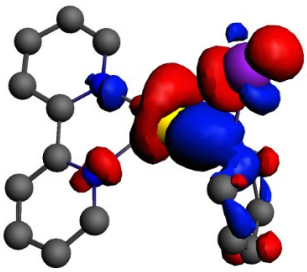


$\Delta E_{orb2}(\rho)$ = -22.9

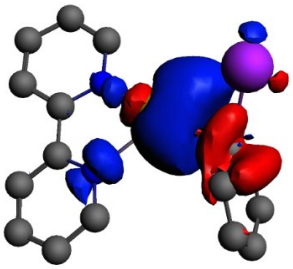


$\Delta E_{orb3}(\rho)$ = -4.0

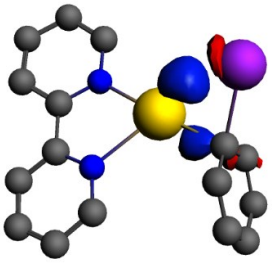
TS2-Au



$\Delta E_{orb1}(\rho)$ = -32.5

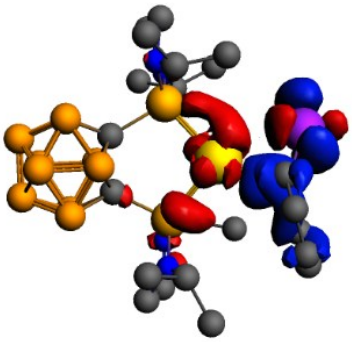


$\Delta E_{orb2}(\rho)$ = -25.9

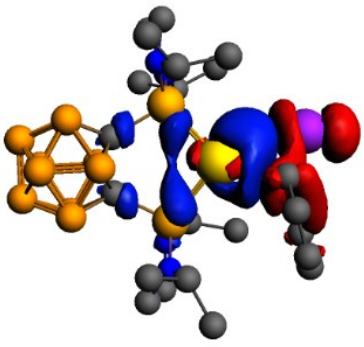


$\Delta E_{orb3}(\rho)$ = -4.7

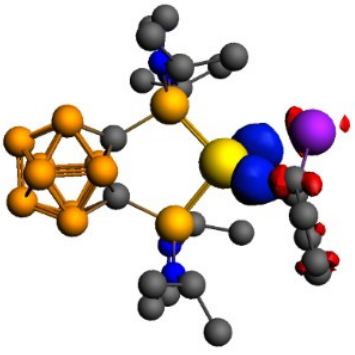
TS3-Au



$\Delta E_{orb1}(\rho)$ = -20.5



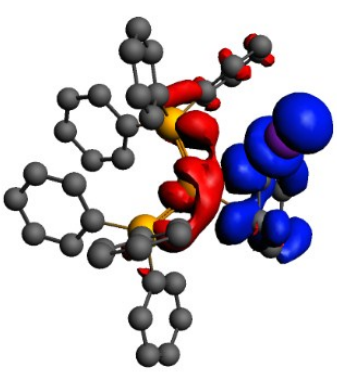
$\Delta E_{orb2}(\rho)$ = -22.7



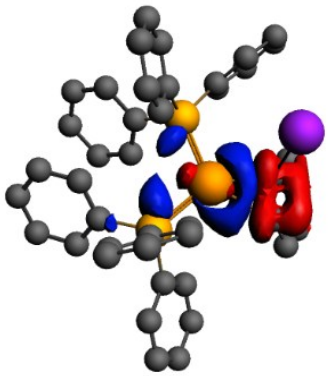
$\Delta E_{orb3}(\rho)$ = -6.0

Figure S31: Plot of the contours of deformation densities contributions ($\Delta\rho_{orbi}$) of the main pairwise orbital interactions between PhI and PdL_n and associated orbital interaction energies contributions (ΔE_{orbi}, in kcal.mol^{-1}) for the different TSs computed at ZORA-BP86-D3/TZ2P level of theory. The charge flow is red → blue ($\Delta\rho < 0$ in red and $\Delta\rho > 0$ in blue). The contour value for density is 0.001 a.u.

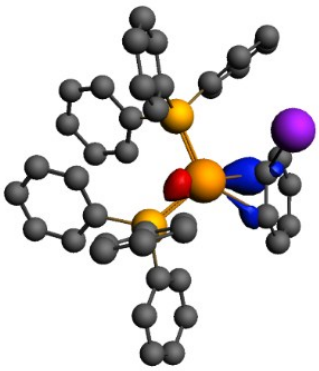
TS4-Pd



$\Delta E_{orb1}(\rho)$ = -56.1

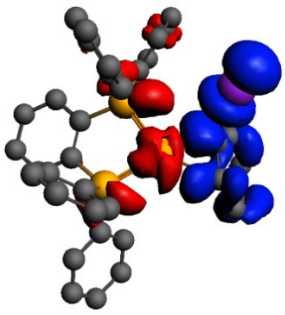


$\Delta E_{orb2}(\rho)$ = -10.0

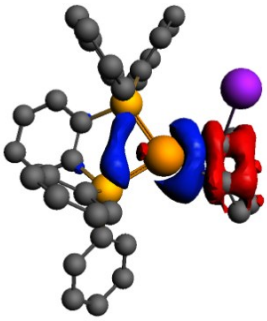


$\Delta E_{orb3}(\rho)$ = -5.8

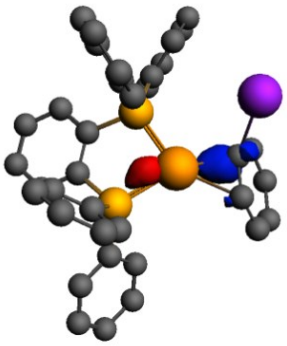
TS5-Pd



$\Delta E_{orb1}(\rho)$ = -59.4



$\Delta E_{orb2}(\rho)$ = -9.7



$\Delta E_{orb2}(\rho)$ = -6.7

Z-matrices and energies in au

A

Sum of electronic and zero-point Energies= -1621.795572
Sum of electronic and thermal Enthalpies = -1621.766625
Sum of electronic and thermal Free Energies = -1621.852013

C	-0.11187	1.14754	1.55526
C	0.10605	0.64118	2.85887
H	0.29391	-0.41753	3.00778
C	0.08849	1.47610	3.98183
H	0.26267	1.05200	4.97077
C	-0.15169	2.84834	3.82300
H	-0.16988	3.51090	4.68911
C	-0.38225	3.36484	2.54353
H	-0.58989	4.42715	2.41643
C	-0.36770	2.54048	1.40041
C	0.17250	4.31080	-0.19952
H	0.00616	4.56832	-1.25561
H	1.23476	4.07352	-0.05275
H	-0.08706	5.19330	0.41669
C	-2.07717	3.37088	-0.08884
H	-2.47026	4.14216	0.60279
H	-2.62777	2.43491	0.06475
H	-2.23256	3.70761	-1.12443
C	-1.43785	-1.21019	0.23905
C	-2.73349	-0.36958	0.02931
H	-2.82191	0.37378	0.83608
H	-2.68058	0.16924	-0.92976
C	-3.97059	-1.30099	0.02161
H	-4.86954	-0.68410	-0.13158
C	-4.06817	-2.05044	1.37017
H	-4.95118	-2.70952	1.36824
H	-4.18574	-1.32856	2.19482
C	-2.78656	-2.88773	1.58187
H	-2.83544	-3.41097	2.54929
C	-2.63876	-3.91423	0.43491
H	-1.73033	-4.52016	0.58715
H	-3.50370	-4.59692	0.43283
C	-2.55245	-3.16967	-0.91874
H	-2.44284	-3.89550	-1.73909
C	-3.82815	-2.32104	-1.13253
H	-3.76766	-1.78978	-2.09694
H	-4.71205	-2.97788	-1.16229
C	-1.55610	-1.94176	1.60740
H	-1.68842	-1.20248	2.40883
H	-0.64930	-2.52046	1.81799
C	-1.30767	-2.24851	-0.90694
H	-0.40802	-2.86028	-0.75330
H	-1.20738	-1.72061	-1.86965
C	1.74494	-0.81546	0.16500
C	1.88244	-1.99187	1.17081
H	1.62441	-1.67167	2.18748
H	1.20426	-2.80639	0.88094
C	3.34388	-2.51343	1.16281
H	3.42067	-3.32728	1.90037
C	4.31180	-1.36776	1.54218
H	5.34655	-1.74561	1.55914
H	4.07294	-0.99167	2.55056
C	4.19043	-0.22063	0.51028
H	4.87342	0.59956	0.78001
C	4.53222	-0.75179	-0.90075
H	4.45070	0.06345	-1.63885
H	5.56922	-1.12373	-0.92060
C	3.55643	-1.89291	-1.26857
H	3.77625	-2.26236	-2.28210
C	2.10702	-1.34563	-1.25805
H	1.40642	-2.13502	-1.55934
H	2.03232	-0.52743	-1.99082
C	2.74047	0.32345	0.52962
H	2.51241	0.71898	1.52926
H	2.63022	1.14635	-0.19721
C	3.68905	-3.04410	-0.24610
H	3.00714	-3.86746	-0.51505
H	4.71802	-3.43813	-0.25670
N	-0.63844	3.12404	0.11161
P	0.01902	-0.02301	0.13610
Au	-0.15948	1.17508	-1.76893

A-I

Sum of electronic and zero-point Energies= -1864.673782
Sum of electronic and thermal Enthalpies = -1864.636920
Sum of electronic and thermal Free Energies = -1864.741302

C	-3.83738	0.10507	0.88158
C	-3.10509	0.74479	1.88821
H	-2.30776	0.22631	2.41649
I	-3.29292	-1.96029	0.38273
Au	-0.71308	-0.97937	0.02363
C	-4.84468	0.73675	0.14884
H	-5.38772	0.21489	-0.63721
C	-5.13245	2.08112	0.45350
H	-5.91511	2.59422	-0.10618
C	-4.42075	2.75330	1.45888
C	-3.41176	2.08652	2.17313
H	-2.84817	2.60566	2.94888
P	1.24035	0.15408	-0.28151
C	2.06527	-0.46191	-1.81312
C	0.83707	1.97367	-0.56319
C	2.38626	-0.19909	1.18750
C	3.35992	0.00877	-2.13908
C	1.46233	-1.42834	-2.66546
C	-0.28815	2.03496	-1.64177
C	2.03697	2.82213	-1.06553
C	0.29562	2.56403	0.76515
C	3.57414	0.78901	1.34414
C	1.55238	-0.18137	2.50808
C	2.92128	-1.64629	0.98083
H	3.83951	0.75567	-1.51352
C	4.05027	-0.46389	-3.26112
C	2.16956	-1.89156	-3.79307
N	0.13608	-1.93446	-2.41339
H	0.07978	1.60403	-2.58539
H	-1.15714	1.44468	-1.31308
C	-0.73190	3.50235	-1.86075
C	1.58713	4.29353	-1.26392
H	2.39424	2.42428	-2.02542
H	2.86571	2.77945	-0.34694
C	-0.16005	4.02718	0.54266
H	1.08867	2.54755	1.52549
H	-0.54634	1.95103	1.12287
H	4.18881	0.80894	0.43575
H	3.18906	1.80295	1.52157
C	4.46246	0.35591	2.53898
C	2.44092	-0.58970	3.70975
H	1.12975	0.81614	2.68187
H	0.71645	-0.89261	2.42167
C	3.80518	-2.06077	2.18289

H	3.51178	-1.70142	0.05545
H	2.06648	-2.33697	0.88332
H	5.04771	-0.08254	-3.48081
C	3.45334	-1.42307	-4.09274
H	1.69080	-2.62691	-4.43988
C	0.06924	-3.39789	-2.29668
C	-0.85649	-1.40958	-3.36324
H	-1.52528	3.51699	-2.62455
C	0.47372	4.34644	-2.33497
C	-1.27443	4.07015	-0.52839
H	2.45676	4.87962	-1.59911
C	1.05241	4.86523	0.07010
H	-0.54188	4.42391	1.49654
H	5.30631	1.05914	2.61502
C	4.99472	-1.07683	2.29883
C	3.62887	0.39208	3.83880
C	2.97141	-2.02383	3.48392
H	1.82502	-0.55611	4.62196
H	4.18003	-3.08084	2.00554
H	3.98013	-1.79789	-4.97123
H	-0.94181	-3.66588	-1.95604
H	0.79569	-3.73517	-1.54499
H	0.26792	-3.92384	-3.25116
H	-0.68313	-1.76640	-4.39838
H	-0.82510	-0.31200	-3.35278
H	-1.85501	-1.73642	-3.03674
H	0.15964	5.39041	-2.49770
H	0.85471	3.95417	-3.29228
H	-2.13952	3.47697	-0.19254
H	-1.61158	5.10928	-0.67426
H	1.84596	4.84095	0.83550
H	0.75030	5.91569	-0.07061
H	5.64735	-1.37588	3.13474
H	5.59417	-1.10476	1.37399
H	3.25566	1.41418	4.01728
H	4.25914	0.10777	4.69708
H	2.12647	-2.72859	3.40805
H	3.59514	-2.33404	4.33778
H	-4.64755	3.79572	1.68225

A-π

Sum of electronic and zero-point Energies= -1864.676958
Sum of electronic and thermal Enthalpies = -1864.640252
Sum of electronic and thermal Free Energies = -1864.744969

C	3.21532	1.04706	-0.67471
C	2.52717	1.27236	-1.90356
H	2.42575	0.47271	-2.63510
I	4.25176	-0.85914	-0.37252
Au	0.90677	0.51609	-0.17943
C	3.52357	2.12795	0.19707
H	4.06860	1.94608	1.12055
C	3.10377	3.41385	-0.14944
H	3.32605	4.24212	0.52347
C	2.42640	3.65353	-1.36593
C	2.14538	2.60090	-2.23679
H	1.63740	2.77635	-3.18464
P	-1.21240	-0.20927	0.28348
C	-1.42863	-0.28887	2.11158
C	-2.46177	1.03471	-0.37238
C	-1.38007	-1.97387	-0.39647
C	-2.62281	-0.82351	2.64773
C	-0.40646	0.12335	3.00918
C	-2.02730	2.43481	0.15660
C	-3.92789	0.78260	0.07532
C	-2.37777	1.02632	-1.92215
C	-2.83890	-2.49071	-0.49519
C	-0.72974	-2.06142	-1.81363
C	-0.55293	-2.87846	0.56423
H	-3.42191	-1.12964	1.98078
C	-2.80703	-0.96502	4.02796
C	-0.60640	-0.02306	4.39624
N	0.81921	0.72008	2.53321
H	-2.07390	2.44246	1.25648
H	-0.98772	2.64176	-0.14210
C	-2.95371	3.53039	-0.42684
C	-4.85139	1.87139	-0.53234
H	-3.99292	0.83499	1.17085
H	-4.26490	-0.21243	-0.24134
C	-3.29244	2.13107	-2.50379
H	-2.70447	0.04854	-2.30230
H	-1.33309	1.18707	-2.23413
H	-3.34029	-2.43880	0.47896
H	-3.39933	-1.86855	-1.20719
C	-2.84347	-3.96322	-0.98242
C	-0.75329	-3.52657	-2.32071
H	-1.26334	-1.41596	-2.52289
H	0.31467	-1.71771	-1.76353
C	-0.56908	-4.34137	0.05821
H	-0.97457	-2.83865	1.57827
H	0.48402	-2.50391	0.60783
H	-3.73905	-1.38307	4.40872
C	-1.78989	-0.56712	4.90792
H	0.17975	0.30574	5.07542
C	2.03941	0.08808	3.05949
C	0.83121	2.17956	2.73440
H	-2.62680	4.50832	-0.04012
C	-4.41658	3.25733	-0.00461
C	-2.84468	3.51170	-1.97035
H	-5.88620	1.66004	-0.22124
C	-4.75269	1.85018	-2.07568
H	-3.21393	2.11069	-3.60189
H	-3.88723	-4.31159	-1.02082
C	-2.03308	-4.84060	0.00151
C	-2.21130	-4.03686	-2.38994
C	0.06157	-4.41267	-1.35110
H	-0.29854	-3.55159	-3.32339
H	0.00985	-4.96036	0.76103
H	-1.92022	-0.67015	5.98592
H	2.89660	0.50321	2.51311
H	1.99494	-0.99389	2.87973
H	2.18957	0.27104	4.14076
H	0.85331	2.45089	3.80796
H	-0.06204	2.61553	2.26947
H	1.72330	2.58996	2.24072
H	-5.07660	4.03909	-0.41432
H	-4.50141	3.28328	1.09418
H	-1.80281	3.70997	-2.27372
H	-3.47947	4.30255	-2.40107
H	-5.07216	0.86773	-2.46107
H	-5.42286	2.61416	-2.50174
H	-2.05753	-5.89126	-0.32952
H	-2.48368	-4.79146	1.00666
H	-2.79340	-3.42149	-3.09565
H	-2.22645	-5.07639	-2.75542
H	1.10681	-4.06315	-1.31230
H	0.06609	-5.45538	-1.70782
H	2.13655	4.67021	-1.63050

A-OA

Sum of electronic and zero-point Energies= -1864.697289
Sum of electronic and thermal Enthalpies = -1864.661661
Sum of electronic and thermal Free Energies = -1864.761039

C	-1.50824	1.43916	1.14578
C	-1.49534	2.76001	0.67319

H	-1.30032	2.98130	-0.37247
I	-4.05373	-0.18610	-0.14725
Au	-1.26241	-0.11858	-0.21966
C	-1.82669	1.17052	2.48669
H	-1.91837	0.14666	2.84363
C	-2.05552	2.23705	3.37325
H	-2.29627	2.01889	4.41479
C	-1.99699	3.56437	2.91920
C	-1.73003	3.82143	1.56701
H	-1.70367	4.84554	1.19189
P	1.09395	-0.26153	-0.29219
C	1.37545	-1.46343	-1.65091
C	1.90323	1.36309	-0.76133
C	1.70579	-1.09893	1.27854
C	2.68278	-1.85428	-2.02358
C	0.27831	-2.07514	-2.28241
C	1.04361	1.97585	-1.90754
C	3.35782	1.21114	-1.29753
C	1.92240	2.29093	0.48374
C	3.25617	-1.14537	1.36390
C	1.14045	-0.37490	2.52753
C	1.12854	-2.54593	1.25857
H	3.54564	-1.41354	-1.53703
C	2.88779	-2.81466	-3.01926
C	0.48842	-3.03562	-3.28746
N	-1.10742	-1.74116	-1.89354
H	1.08471	1.30876	-2.78315
H	-0.00713	2.06155	-1.60334
C	1.59741	3.37413	-2.28064
C	3.92012	2.61195	-1.66412
H	3.35436	0.59459	-2.20479
H	3.99930	0.73151	-0.54634
C	2.45341	3.68783	0.08082
H	2.59013	1.85678	1.24087
H	0.92009	2.37424	0.91649
H	3.67585	-1.66428	0.49317
H	3.65581	-0.12148	1.38982
C	3.67133	-1.90536	2.65196
C	1.57881	-1.11543	3.81400
H	1.47491	0.66818	2.56531
H	0.05027	-0.38147	2.46696
C	1.55877	-3.29363	2.54585
H	1.49784	-3.09174	0.37912
H	0.02824	-2.49741	1.19997
H	3.90391	-3.09983	-3.29056
C	1.78630	-3.40329	-3.65688
H	-0.36450	-3.50202	-3.77639
C	-1.80231	-2.97928	-1.40423
C	-1.83201	-1.16520	-3.07724
H	0.96379	3.79794	-3.07475
C	3.05263	3.23198	-2.78364
C	1.56479	4.29035	-1.03334
H	4.95277	2.47725	-2.02093
C	3.90548	3.53831	-0.42733
H	2.42928	4.33687	0.96927
H	4.77104	-1.93796	2.69012
C	3.10424	-3.34471	2.61053
C	3.12180	-1.16040	3.88991
C	1.01244	-2.55355	3.78802
H	1.17409	-0.56769	4.67886
H	1.15067	-4.31515	2.50537
H	1.93201	-4.15144	-4.43590
H	-2.81788	-2.70372	-1.10604
H	-1.24950	-3.36621	-0.54031
H	-1.84234	-3.73665	-2.19954
H	-1.83507	-1.88295	-3.90976
H	-1.32324	-0.24181	-3.37709
H	-2.86024	-0.94471	-2.77525
H	3.45175	4.22085	-3.06033
H	3.08082	2.59136	-3.68016
H	0.53093	4.39717	-0.67073
H	1.93577	5.29232	-1.30193
H	4.53860	3.11565	0.37010
H	4.31537	4.52456	-0.69835
H	3.42051	-3.89498	3.51088
H	3.49878	-3.87920	1.73077
H	3.52800	-0.13618	3.92150
H	3.43704	-1.67900	4.80943
H	-0.08930	-2.52160	3.75241
H	1.30638	-3.09205	4.70313
H	-2.17686	4.38881	3.61004

TS1

Sum of electronic and zero-point Energies= -1864.662515
Sum of electronic and thermal Enthalpies = -1864.626372
Sum of electronic and thermal Free Energies = -1864.728970

C	-2.70141	1.10243	0.95423
C	-2.48369	1.07580	2.33776
H	-2.47359	0.13770	2.88776
I	-3.87495	-0.78737	0.00308
Au	-1.13783	-0.52505	-0.14576
C	-2.76076	2.28680	0.20779
H	-2.96566	2.27046	-0.86016
C	-2.50891	3.49515	0.88039
H	-2.52480	4.42576	0.31210
C	-2.23892	3.50431	2.25862
C	-2.23081	2.29913	2.98115
H	-2.03074	2.29730	4.05354
P	1.13843	-0.19559	-0.28197
C	1.82676	-1.50458	-1.37585
C	1.45286	1.47465	-1.09695
C	1.91785	-0.41449	1.42680
C	3.21171	-1.52512	-1.66235
C	1.00398	-2.52340	-1.92215
C	0.57625	1.51301	-2.38712
C	2.92060	1.77115	-1.51125
C	0.96046	2.56514	-0.10578
C	3.33791	0.19433	1.54460
C	0.99385	0.23990	2.49684
C	1.97150	-1.94371	1.71100
H	3.86239	-0.76693	-1.23577
C	3.76927	-2.51088	-2.48515
C	1.57641	-3.50835	-2.74956
N	-0.41210	-2.59376	-1.62495
H	0.92545	0.73888	-3.08811
H	-0.47613	1.30107	-2.14242
C	0.66328	2.91047	-3.04734
C	3.00524	3.18224	-2.15518
H	3.25475	1.02674	-2.24686
H	3.58777	1.72081	-0.64242
C	1.03463	3.95712	-0.77716
H	1.59819	2.56383	0.78977
H	-0.07101	2.34802	0.20534
H	4.00746	-0.24310	0.79118
H	3.28436	1.27786	1.37252
C	3.90690	-0.07149	2.96250
C	1.56952	-0.00149	3.91405
H	0.89129	1.31637	2.31185
H	-0.00934	-0.20565	2.43499
C	2.53994	-2.19269	3.13081
H	2.60906	-2.44419	0.96856
H	0.95554	-2.36604	1.62866
H	4.83983	-2.50132	-2.69076
C	2.94624	-3.50456	-3.03652

H	0.93243	-4.28640	-3.15988
C	-0.74698	-3.76001	-0.78515
C	-1.26617	-2.52200	-2.82486
H	0.03189	2.90996	-3.94936
C	2.13006	3.21542	-3.42877
C	0.15075	3.97303	-2.04615
H	4.05623	3.37828	-2.41809
C	2.50489	4.25300	-1.15658
H	0.67156	4.70997	-0.06036
H	4.91921	0.35780	3.01864
C	3.96513	-1.59564	3.22082
C	2.99088	0.60032	4.01165
C	1.62815	-1.52241	4.18452
H	0.90540	0.48541	4.64538
H	2.57943	-3.27915	3.30543
H	3.36900	-4.27775	-3.67908
H	-1.80851	-3.68985	-0.50706
H	-0.13622	-3.73243	0.12678
H	-0.57410	-4.71511	-1.31508
H	-1.17164	-3.41950	-3.46342
H	-0.99680	-1.63174	-3.40806
H	-2.31079	-2.43008	-2.49345
H	2.19518	4.20742	-3.90448
H	2.49231	2.46798	-4.15358
H	-0.89496	3.75687	-1.77272
H	0.18112	4.97131	-2.51168
H	3.13268	4.24709	-0.25028
H	2.58215	5.25255	-1.61422
H	4.38726	-1.78884	4.22010
H	4.62085	-2.07744	2.47705
H	2.95119	1.68760	3.83282
H	3.39734	0.43871	5.02296
H	0.61415	-1.95326	4.13268
H	2.02361	-1.71046	5.19590
H	-2.04996	4.44761	2.77105

PhI

Sum of electronic and zero-point Energies= -242.840295
Sum of electronic and thermal Enthalpies = -242.833299
Sum of electronic and thermal Free Energies = -242.872207

C	0.60117	-0.00000	0.00000
C	1.27908	1.22631	-0.00000
H	0.73435	2.16902	-0.00000
I	-1.58309	0.00000	0.00000
C	1.27909	-1.22631	0.00000
H	0.73435	-2.16903	0.00000
C	2.68513	-1.21470	-0.00000
H	3.22311	-2.16373	-0.00000
C	3.38867	0.00000	0.00000
C	2.68512	1.21471	0.00000
H	3.22310	2.16374	0.00000
H	4.47918	0.00000	0.00000

B

Sum of electronic and zero-point Energies= -630.790083
Sum of electronic and thermal Enthalpies = -630.778139
Sum of electronic and thermal Free Energies = -630.829932

C	3.37311	1.70976	-0.02798
C	-0.89294	1.42704	-0.00886
C	-1.74233	2.53724	-0.17379
C	-3.12929	2.35038	-0.16041
C	-3.64699	1.05973	0.01005
C	-2.74760	-0.00271	0.15187
N	-1.41257	0.18270	0.14347
H	-1.32824	3.53036	-0.32803
H	-3.79391	3.20411	-0.28858
H	-4.71881	0.87004	0.02956
H	-3.08623	-1.02921	0.28022
C	0.59812	1.56489	-0.00325
C	1.23031	2.80590	0.19922
C	2.62808	2.87677	0.18626
C	2.68418	0.50554	-0.20576
N	1.33713	0.44149	-0.19004
H	0.64231	3.70100	0.38529
H	3.12614	3.83213	0.34821
H	4.46151	1.72085	-0.05189
H	3.20523	-0.43614	-0.36796
Au	0.15053	-1.52873	0.00652

B-I

Sum of electronic and zero-point Energies= -873.677314
Sum of electronic and thermal Enthalpies = -873.657719
Sum of electronic and thermal Free Energies = -873.728011

C	4.57536	-1.68714	0.81200
C	2.22898	1.72587	-0.24739
C	2.80007	2.86267	-0.85248
C	1.96140	3.92601	-1.21063
C	0.58554	3.82558	-0.96170
C	0.10207	2.65484	-0.35802
N	0.90253	1.63654	-0.00422
H	3.86706	2.90510	-1.06196
H	2.37846	4.81319	-1.68698
H	-0.10008	4.62908	-1.22805
H	-0.95828	2.52695	-0.13875
C	3.06165	0.54802	0.13212
C	4.43023	0.68811	0.42437
C	5.19433	-0.43139	0.76481
C	3.21309	-1.77003	0.52248
N	2.46882	-0.68280	0.19292
H	4.88084	1.67740	0.40296
H	6.25333	-0.32193	0.99641
H	5.12588	-2.59041	1.06817
H	2.68237	-2.71872	0.54279
Au	0.35979	-0.95773	-0.10176
C	-2.79145	0.37376	0.36612
C	-3.63196	1.17807	-0.40591
C	-2.26170	0.76940	1.59819
C	-3.96115	2.45069	0.09784
C	-2.60494	2.04538	2.07787
C	-3.45142	2.88222	1.33219
H	-4.01533	0.84185	-1.36768
H	-1.58798	0.12128	2.15509
H	-4.61509	3.09824	-0.48700
I	-2.20238	-1.59436	-0.41079
H	-2.19884	2.37972	3.03296
H	-3.70991	3.87126	1.71073

B-π

Sum of electronic and zero-point Energies= -873.685200
Sum of electronic and thermal Enthalpies = -873.665700
Sum of electronic and thermal Free Energies = -873.736192

C	-3.98160	-2.53626	-0.99943
C	-2.68743	1.34058	0.23627
C	-3.52204	2.45135	0.45495
C	-2.95307	3.66552	0.85839
C	-1.56548	3.75337	1.03268
C	-0.79466	2.61004	0.79374
N	-1.34482	1.44303	0.41042
H	-4.59654	2.38008	0.30898
H	-3.59010	4.53236	1.03136
H	-1.08521	4.67971	1.34300
H	0.28920	2.60983	0.90463
C	-3.19571	0.00567	-0.19430

C	-4.56291	-0.27716	-0.36304
C	-4.95684	-1.55739	-0.76904
C	-2.63983	-2.19153	-0.81081
N	-2.26041	-0.95725	-0.41969
H	-5.31498	0.48474	-0.17598
H	-6.01442	-1.78488	-0.89896
H	-4.24464	-3.54455	-1.31399
H	-1.83386	-2.90638	-0.96792
Au	-0.09205	-0.45477	-0.01764
C	1.90214	-2.93553	1.81267
C	1.66793	-2.98306	0.44978
C	2.20912	-1.70086	2.45495
H	1.47907	-3.92766	-0.05987
H	2.39717	-1.68586	3.52891
C	1.70732	-1.77795	-0.33699
C	2.31368	-0.51908	1.73914
H	2.58812	0.41426	2.22668
C	2.04650	-0.52950	0.32181
I	3.07230	1.05817	-0.85911
H	1.79715	-1.86447	-1.42158
H	1.88300	-3.85262	2.40128

B-OA

Sum of electronic and zero-point Energies= -873.709089
Sum of electronic and thermal Enthalpies = -873.689957
Sum of electronic and thermal Free Energies = -873.758825

C	-3.67398	-2.54284	0.01827
C	-2.41285	1.52098	0.00035
C	-3.25077	2.64721	-0.00927
C	-2.69378	3.93066	0.00378
C	-1.30174	4.07535	0.02929
C	-0.50908	2.92581	0.03688
N	-1.05335	1.69012	0.01979
H	-4.33001	2.52370	-0.02624
H	-3.34417	4.80421	-0.00467
H	-0.82484	5.05314	0.04259
H	0.57647	2.96892	0.05522
C	-2.91535	0.12779	-0.00347
C	-4.27915	-0.20278	-0.02847
C	-4.65993	-1.54991	-0.01852
C	-2.33139	-2.15198	0.03672
N	-1.96674	-0.85474	0.02416
H	-5.03726	0.57511	-0.05427
H	-5.71633	-1.81449	-0.03788
H	-3.92686	-3.60116	0.03007
H	-1.51711	-2.87392	0.06008
Au	0.10933	-0.10487	0.01095
C	1.91164	0.85560	-0.00495
C	2.53919	1.14740	1.21502
C	2.42281	1.31413	-1.22805
C	3.68924	1.95804	1.20660
C	3.57396	2.12353	-1.21818
C	4.20417	2.44516	-0.00546
H	2.14206	0.75974	2.15263
H	1.93302	1.05989	-2.16784
H	4.18114	2.19592	2.15092
I	1.46066	-2.38714	-0.02617
H	3.97459	2.49231	-2.16343
H	5.09982	3.06730	-0.00560

TS2

Sum of electronic and zero-point Energies= -873.669803
Sum of electronic and thermal Enthalpies = -873.650761
Sum of electronic and thermal Free Energies = -873.719614

C	-3.00155	-3.38544	0.67635
C	-2.94238	0.78667	-0.24957
C	-4.08592	1.60656	-0.29637
C	-3.93516	2.96460	-0.60460
C	-2.65434	3.47877	-0.84906
C	-1.56301	2.60363	-0.76270
N	-1.71151	1.30228	-0.47587
H	-5.07204	1.20287	-0.07994
H	-4.81042	3.61244	-0.64528
H	-2.49854	4.52829	-1.09407
H	-0.53829	2.93985	-0.92597
C	-3.00474	-0.67186	0.06081
C	-4.21524	-1.38823	0.06549
C	-4.21493	-2.75135	0.37874
C	-1.82975	-2.62660	0.63575
N	-1.82955	-1.30693	0.33640
H	-5.14741	-0.89000	-0.18900
H	-5.15060	-3.30935	0.38299
H	-2.95276	-4.44331	0.92772
H	-0.85442	-3.06381	0.84198
Au	0.09275	-0.23119	0.13670
C	1.99119	0.75010	0.20699
C	2.19760	0.94828	1.60133
C	2.04875	1.83558	-0.71051
C	2.31411	2.26330	2.07792
C	2.18307	3.13003	-0.20248
C	2.31176	3.34607	1.18474
H	2.24402	0.09563	2.27558
H	1.95061	1.65033	-1.77784
H	2.43549	2.43178	3.14824
I	2.71007	-1.36101	-0.61575
H	2.19320	3.97360	-0.89339
H	2.43102	4.36099	1.56385

C

Sum of electronic and zero-point Energies= -1998.568583
Sum of electronic and thermal Enthalpies = -1998.529467
Sum of electronic and thermal Free Energies = -1998.635855

Au	-0.07886	0.87756	-1.23289
P	1.86036	0.17086	-0.15033
P	-1.84413	-0.03880	-0.05956
N	3.30929	-0.61160	-0.55301
N	2.54624	1.28115	0.89377
B	0.16273	-0.55266	2.34896
H	0.15815	0.61666	2.53127
B	1.65742	-1.55306	2.47270
H	2.66351	-1.00243	2.78375
B	1.62203	-2.73613	1.12580
H	2.60349	-3.00767	0.51882
B	1.16460	-3.24388	2.77726
H	1.86421	-3.98055	3.40302
B	-0.61769	-3.29650	2.87280
H	-1.20130	-4.07335	3.56564
B	-1.28029	-2.82208	1.28403
H	-2.30303	-3.15481	0.78254
B	-1.24551	-1.63980	2.63136
H	-2.24369	-1.15931	3.05730
B	0.10950	-2.43284	0.19779
H	0.04233	-2.44251	-0.98807
B	0.26996	-1.88159	3.54595
H	0.32674	-1.64087	4.71253
B	0.20948	-3.80068	1.35271
H	0.22024	-4.92583	0.95743
C	0.99520	-1.15857	0.95650
C	-0.77498	-1.21059	1.05109
C	4.43030	0.32621	-0.29118
H	4.58580	1.01694	-1.13797
H	5.35035	-0.24917	-0.12564
C	4.01745	1.10092	0.97518
H	4.27476	0.53182	1.88115
H	4.50872	2.08093	1.01084

C	3.31797	-1.46107	-1.77630
H	2.41162	-2.08199	-1.70061
C	4.53705	-2.38965	-1.74666
H	5.46954	-1.81549	-1.85232
H	4.47864	-3.10104	-2.58284
H	4.57314	-2.95289	-0.80317
C	3.25059	-0.63227	-3.07121
H	2.35979	0.01721	-3.07070
H	3.19389	-1.30026	-3.94315
H	4.14523	-0.00122	-3.17929
C	1.89507	2.59312	1.12838
H	0.81385	2.38852	1.14357
C	2.29241	3.13852	2.50419
H	2.05908	2.40901	3.29297
H	1.74424	4.07026	2.70541
H	3.36878	3.36304	2.53956
C	2.18719	3.58005	-0.01197
H	3.26663	3.78313	-0.08138
H	1.66536	4.53348	0.16083
H	1.84371	3.16021	-0.97134
N	-2.84578	0.75909	1.04403
C	-4.25670	0.57756	0.61506
H	-4.55443	1.35123	-0.11275
H	-4.91393	0.63599	1.49231
C	-4.30446	-0.82120	-0.02953
H	-4.40343	-1.59978	0.74164
H	-5.13859	-0.90363	-0.73495
C	-2.96983	-1.27397	-2.21556
H	-1.90484	-1.42494	-2.45146
C	-3.72079	-2.57250	-2.52994
H	-3.31351	-3.40868	-1.94384
H	-3.62235	-2.80518	-3.60006
H	-4.79249	-2.47221	-2.30207
C	-3.48999	-0.07723	-3.02721
H	-4.53949	0.13537	-2.77374
H	-3.43196	-0.29024	-4.10528
H	-2.88498	0.81852	-2.81283
C	-2.39855	2.08071	1.56827
H	-1.33747	1.94957	1.82186
C	-3.16081	2.40571	2.85761
H	-4.22863	2.57018	2.65036
H	-2.75577	3.32531	3.30368
H	-3.06450	1.58512	3.58289
C	-2.51015	3.20717	0.52634
H	-1.93850	2.95840	-0.38292
H	-2.10352	4.13973	0.94465
H	-3.55836	3.38620	0.24572
N	-3.01736	-1.00328	-0.75222

C-I

Sum of electronic and zero-point Energies= -2241.440954
Sum of electronic and thermal Enthalpies = -2241.394194
Sum of electronic and thermal Free Energies = -2241.517945

Au	-0.28233	-0.69110	0.04082
P	2.01884	-1.02961	-0.07680
P	-0.33276	1.67003	0.03642
N	2.94839	-1.46312	1.27048
N	2.75004	-2.03755	-1.21512
B	2.07720	1.39636	-1.98097
H	1.32292	0.74458	-2.62619
B	3.81337	0.97269	-1.74757
H	4.23418	0.01608	-2.31069
B	4.20926	1.27097	-0.02722
H	4.89762	0.51835	0.58096
B	4.68368	2.45880	-1.27374
H	5.83138	2.60979	-1.56464
B	3.50936	3.80610	-1.23824
H	3.81183	4.92981	-1.50339
B	2.30054	3.45748	0.03234
H	1.66488	4.22451	0.67929
B	1.90675	3.16242	-1.69136
H	1.01212	3.73344	-2.21984
B	2.71989	1.87284	0.77381
H	2.37581	1.52588	1.85058
B	3.36500	2.52723	-2.50029
H	3.56032	2.73028	-3.65950
B	4.00977	3.01642	0.30115
H	4.66392	3.56539	1.13405
C	2.66047	0.72121	-0.50636
C	1.52151	2.02842	-0.46832
C	3.83871	-2.59643	0.92112
H	3.38321	-3.55770	1.20906
H	4.80290	-2.48766	1.43705
C	4.02735	-2.51564	-0.61136
H	4.81603	-1.79079	-0.85700
H	4.29393	-3.49070	-1.03351
C	2.31690	-1.39934	2.61480
H	1.72622	-0.47091	2.61760
C	3.40152	-1.27967	3.69063
H	4.00858	-2.19633	3.73567
H	2.93523	-1.13200	4.67560
H	4.06425	-0.42864	3.47769
C	1.35680	-2.57261	2.87731
H	0.58446	-2.61656	2.09421
H	0.85916	-2.43909	3.84958
H	1.89514	-3.53147	2.89852
C	1.85011	-3.01777	-1.90221
H	0.95704	-2.43787	-2.18342
C	2.52133	-3.52088	-3.18455
H	2.80867	-2.67777	-3.82917
H	1.82370	-4.16917	-3.73480
H	3.42142	-4.11163	-2.95595
C	1.41436	-4.17008	-0.98171
H	2.28517	-4.76378	-0.66605
H	0.71853	-4.83687	-1.51310
H	0.90907	-3.77899	-0.08558
N	-1.14623	2.78063	-0.94787
C	-2.01790	3.65298	-0.12718
H	-3.01838	3.20868	0.00599
H	-2.11997	4.63025	-0.61601
C	-1.29651	3.78560	1.22400
H	-0.51769	4.56404	1.18337
H	-2.00234	4.02247	2.03044
C	-0.26870	2.00423	2.80095
H	0.34060	1.10306	2.63361
C	0.60313	3.06720	3.48618
H	1.45247	3.35252	2.85301
H	0.98527	2.67339	4.43922
H	0.01016	3.96805	3.70377
C	-1.48062	1.62281	3.66547
H	-2.16320	2.47924	3.77340
H	-1.14629	1.32426	4.67049
H	-2.03447	0.78633	3.21772
C	-1.54634	2.39136	-2.32473
H	-0.64979	1.94063	-2.77452
C	-1.89825	3.64505	-3.13455
H	-2.82613	4.10513	-2.76361
H	-2.05381	3.36640	-4.18628
H	-1.08785	4.38610	-3.07985
C	-2.68312	1.35531	-2.34146
H	-2.37355	0.43650	-1.82379
H	-2.94383	1.10171	-3.38021
H	-3.57949	1.74841	-1.84158
N	-0.70856	2.45095	1.46133

C	-3.98099	-0.95252	0.03130
C	-3.69951	0.19117	0.77981
H	-2.73100	0.32728	1.25465
I	-2.42278	-2.48716	-0.12768
C	-5.19458	-1.14564	-0.63328
H	-5.38584	-2.04355	-1.21896
C	-6.16876	-0.13433	-0.53222
H	-7.12019	-0.26224	-1.04962
C	-5.92020	1.02424	0.22015
H	-6.68256	1.80016	0.29316
C	-4.68931	1.18339	0.87679
H	-4.48351	2.08011	1.46184

C-π

Sum of electronic and zero-point Energies= -2241.444114
Sum of electronic and thermal Enthalpies = -2241.396992
Sum of electronic and thermal Free Energies = -2241.521863

Au	0.54245	-0.07425	-0.41057
P	-1.00933	-1.80823	-0.12937
P	-0.63844	1.78644	0.34681
N	-1.60917	-3.00356	-1.17337
N	-0.87407	-2.79267	1.21935
B	-2.76222	-0.06988	1.73528
H	-1.90675	-0.28793	2.52531
B	-3.87297	-1.33113	1.08465
H	-3.77498	-2.43393	1.51366
B	-4.05859	-1.03349	-0.67453
H	-4.09044	-1.93051	-1.44908
B	-5.33393	-0.51135	0.46023
H	-6.39478	-1.05827	0.47393
B	-5.14932	1.24163	0.74383
H	-6.07600	1.96289	0.95861
B	-3.75515	1.81508	-0.21235
H	-3.57516	2.89645	-0.66178
B	-3.57766	1.51806	1.54258
H	-3.27260	2.39257	2.28483
B	-3.04846	0.40055	-1.07529
H	-2.36797	0.48716	-2.04509
B	-4.53414	0.07124	1.96731
H	-5.01427	-0.05424	3.05189
B	-4.82391	0.56304	-0.89440
H	-5.51254	0.78764	-1.84238
C	-2.58711	-0.72943	0.14640
C	-2.40496	0.98502	0.41518
C	-1.30906	-4.33702	-0.59793
H	-0.29440	-4.67775	-0.86763
H	-2.04288	-5.06526	-0.96735
C	-1.42999	-4.14002	0.92357
H	-2.48449	-4.18069	1.23157
H	-0.86561	-4.90196	1.47202
C	-1.50884	-2.77968	-2.63843
H	-1.80108	-1.72921	-2.79534
C	-2.51658	-3.67589	-3.36800
H	-2.24063	-4.73584	-3.26290
H	-2.52242	-3.43056	-4.43981
H	-3.52834	-3.53224	-2.96350
C	-0.07519	-2.98054	-3.16078
H	0.62587	-2.33923	-2.60792
H	-0.02079	-2.72583	-4.22942
H	0.23749	-4.02875	-3.04291
C	0.25701	-2.62529	2.16879
H	0.50896	-1.55346	2.14871
C	-0.19918	-2.98599	3.58738
H	-1.06870	-2.38065	3.88077
H	0.61935	-2.80675	4.29998
H	-0.47608	-4.04943	3.64679
C	1.49335	-3.42362	1.72793
H	1.28650	-4.50408	1.73678
H	2.33226	-3.23189	2.41287
H	1.79755	-3.12733	0.71378
N	-0.51189	2.37872	1.92739
C	-0.53370	3.86324	1.91514
H	0.49152	4.26899	1.92862
H	-1.08167	4.23481	2.79146
C	-1.24336	4.26850	0.60433
H	-2.33764	4.23822	0.72303
H	-0.94072	5.27245	0.28632
C	-0.53382	3.54964	-1.81694
H	-0.02561	2.65083	-2.19942
C	-1.82474	3.76945	-2.61914
H	-2.45666	2.87198	-2.60182
H	-1.57571	4.00803	-3.66453
H	-2.39804	4.61115	-2.20232
C	0.42917	4.73833	-1.96009
H	-0.05151	5.67824	-1.64977
H	0.72070	4.84587	-3.01455
H	1.33338	4.58399	-1.35516
C	0.38661	1.66244	2.86984
H	0.19231	0.59180	2.70360
C	-0.00554	1.99715	4.31293
H	0.17837	3.05990	4.53127
H	0.59860	1.39717	5.00887
H	-1.06970	1.78103	4.48555
C	1.87437	1.93349	2.58906
H	2.11795	1.68812	1.54452
H	2.50143	1.31284	3.24557
H	2.12584	2.98866	2.77315
N	-0.79340	3.26883	-0.38835
C	3.33250	0.28040	-0.98315
C	2.64709	-0.48115	-1.95946
H	2.61058	-1.56654	-1.89619
I	4.19318	-0.74282	0.72059
C	3.51136	1.66740	-1.12440
H	4.04462	2.23716	-0.36592
C	2.99459	2.30153	-2.26329
H	3.13153	3.37589	-2.37884
C	2.29343	1.57153	-3.23987
C	2.12721	0.18868	-3.09643
H	1.59887	-0.39643	-3.84874
H	1.89297	2.07972	-4.11655

C-OA

Sum of electronic and zero-point Energies= -2241.468996
Sum of electronic and thermal Enthalpies = -2241.423257
Sum of electronic and thermal Free Energies = -2241.541875

Au	-0.72190	-0.55317	-0.11826
P	1.60990	-0.91063	0.29155
P	-0.46743	1.75671	-0.32598
N	1.92815	-1.55392	1.79860
N	2.61274	-1.91473	-0.55581
B	2.58964	1.57299	-1.17179
H	2.25729	0.93373	-2.10926
B	3.99009	1.12522	-0.14217
H	4.63432	0.18533	-0.46477
B	3.51993	1.33339	1.57043
H	3.85827	0.53495	2.37827
B	4.50752	2.57692	0.75186
H	5.65342	2.73210	1.04342
B	3.43370	3.92917	0.28344
H	3.79844	5.06375	0.24335
B	1.78123	3.53077	0.81705
H	0.89450	4.26710	1.09236
B	2.24678	3.31553	-0.90630
H	1.67446	3.91278	-1.75624

B	1.83043	1.91513	1.61797
H	0.99536	1.51778	2.35641
B	3.93332	2.71821	-0.95258
H	4.65241	2.97599	-1.86732
B	3.16596	3.06823	1.84806
H	3.33967	3.57581	2.91215
C	2.37661	0.84346	0.37763
C	1.38227	2.10036	-0.04364
C	2.82668	-2.72751	1.69364
H	2.24306	-3.66082	1.67686
H	3.51505	-2.74247	2.54908
C	3.59103	-2.54006	0.36819
H	4.46715	-1.88693	0.50504
H	3.91313	-3.50311	-0.04217
C	1.01865	-1.37169	2.95988
H	0.32118	-0.56811	2.67718
C	1.82104	-0.91109	4.18286
H	2.57026	-1.66942	4.45552
H	1.14625	-0.77421	5.04100
H	2.33717	0.03581	3.97814
C	0.19806	-2.63659	3.25010
H	-0.35654	-2.95943	2.35909
H	-0.51623	-2.42738	4.05972
H	0.84874	-3.46047	3.57760
C	2.65390	-2.09702	-2.02786
H	1.78818	-1.54242	-2.42053
C	3.94176	-1.53114	-2.64425
H	4.03118	-0.45208	-2.47781
H	3.94195	-1.72425	-3.72728
H	4.82203	-2.02928	-2.21041
C	2.48267	-3.58335	-2.38059
H	3.35551	-4.16747	-2.05320
H	2.39993	-3.68850	-3.47211
H	1.57863	-3.99280	-1.91179
N	-0.81061	2.51627	-1.76830
C	-1.95701	3.44504	-1.58956
H	-2.91177	2.93941	-1.79699
H	-1.83079	4.29440	-2.27033
C	-1.87212	3.89931	-0.12275
H	-1.15031	4.72211	-0.00476
H	-2.85308	4.20904	0.25232
C	-1.79476	2.43686	2.03869
H	-1.42243	1.42291	2.24976
C	-1.14173	3.44292	2.99656
H	-0.04834	3.39654	2.95800
H	-1.46989	3.23030	4.02495
H	-1.46107	4.46488	2.74227
C	-3.32231	2.44763	2.19761
H	-3.71282	3.47389	2.13271
H	-3.57864	2.05726	3.19250
H	-3.80751	1.82762	1.43713
C	-0.46521	1.95152	-3.10123
H	0.51810	1.48159	-2.98243
C	-0.32256	3.08556	-4.12317
H	-1.29364	3.55860	-4.32860
H	0.05887	2.66842	-5.06538
H	0.38055	3.84960	-3.76304
C	-1.46914	0.88215	-3.55400
H	-1.51806	0.05726	-2.82752
H	-1.15641	0.47249	-4.52573
H	-2.47316	1.31568	-3.67062
N	-1.41659	2.70356	0.62774
C	-2.81284	-0.34567	0.12321
C	-3.34090	-0.90606	1.30326
H	-2.69264	-1.42546	2.00956
I	-1.15200	-3.26277	-0.62264
C	-3.66621	0.29718	-0.78554
H	-3.27190	0.73160	-1.69957
C	-5.04556	0.38129	-0.51769
H	-5.70102	0.88195	-1.23257
C	-5.57299	-0.17038	0.65961
H	-6.64171	-0.10276	0.86667
C	-4.71770	-0.81180	1.57000
H	-5.11683	-1.24860	2.48698

TS3

Sum of electronic and zero-point Energies= -2241.426608
Sum of electronic and thermal Enthalpies = -2241.380419
Sum of electronic and thermal Free Energies = -2241.501349

Au	-0.71535	-0.40334	0.01024
P	1.40804	-1.38180	0.35082
P	0.02929	1.80500	-0.42609
N	1.86875	-2.28142	1.70418
N	2.01732	-2.44570	-0.76609
B	2.96589	0.93856	-1.02155
H	2.51038	0.49930	-2.02028
B	4.19190	0.09488	-0.01378
H	4.60895	-0.94679	-0.40220
B	3.73739	0.31936	1.70587
H	3.84796	-0.56708	2.48528
B	5.02470	1.32261	0.98454
H	6.16333	1.17751	1.31156
B	4.33038	2.92142	0.58748
H	4.96578	3.93108	0.62812
B	2.60792	2.91109	1.05789
H	1.93302	3.82952	1.38082
B	3.07056	2.69006	-0.65604
H	2.70534	3.45422	-1.48743
B	2.22476	1.28860	1.73507
H	1.30425	1.06200	2.44924
B	4.55557	1.69658	-0.71451
H	5.34528	1.81877	-1.59991
B	3.79923	2.06334	2.08053
H	4.05528	2.44677	3.18070
C	2.55706	0.16255	0.47115
C	1.88702	1.69696	0.09193
C	2.34731	-3.62216	1.28390
H	1.51875	-4.34907	1.26734
H	3.11983	-3.97110	1.98184
C	2.91612	-3.43471	-0.13411
H	3.95213	-3.06308	-0.09957
H	2.88601	-4.37335	-0.70084
C	1.04980	-2.14604	2.93848
H	0.77012	-1.08243	2.98710
C	1.90704	-2.47837	4.16521
H	2.21035	-3.53590	4.15017
H	1.32609	-2.30446	5.08262
H	2.81026	-1.85252	4.19022
C	-0.23601	-2.98929	2.88442
H	-0.81049	-2.76464	1.97303
H	-0.86451	-2.76963	3.75986
H	-0.00287	-4.06387	2.89518
C	1.81845	-2.34529	-2.22730
H	1.25000	-1.41666	-2.38885
C	3.16219	-2.23806	-2.96134
H	3.74208	-1.38173	-2.59357
H	2.98879	-2.11646	-4.04048
H	3.75204	-3.15477	-2.81159
C	0.97725	-3.52870	-2.72890
H	1.49907	-4.48013	-2.54597
H	0.80596	-3.43720	-3.81214
H	0.00536	-3.55304	-2.21452
N	0.18158	2.35482	-2.02246
C	-0.30705	3.75288	-2.12360

H	-1.34964	3.77615	-2.48071
H	0.32771	4.31861	-2.81862
C	-0.22081	4.33732	-0.69803
H	0.80198	4.67917	-0.47664
H	-0.91897	5.17115	-0.57057
C	-1.38435	3.33929	1.44184
H	-1.78845	2.33326	1.63346
C	-0.53152	3.77235	2.64339
H	0.26903	3.04962	2.84306
H	-1.16986	3.84777	3.53731
H	-0.07755	4.75771	2.46097
C	-2.56660	4.29833	1.23600
H	-2.22170	5.34042	1.16304
H	-3.24014	4.22774	2.10035
H	-3.13203	4.04318	0.32968
C	-0.07572	1.40656	-3.13713
H	0.44305	0.47690	-2.86201
C	0.56330	1.94079	-4.42429
H	0.05721	2.85754	-4.76155
H	0.47210	1.18814	-5.22080
H	1.62800	2.16430	-4.26467
C	-1.56962	1.08429	-3.31649
H	-1.97721	0.64427	-2.39566
H	-1.70207	0.35818	-4.13248
H	-2.14580	1.98803	-3.56438
N	-0.60290	3.21435	0.18842
C	-3.02596	-0.28070	0.49217
C	-3.00941	-0.47699	1.88830
H	-2.46337	-1.30756	2.32928
I	-2.70331	-2.32625	-0.80558
C	-3.80490	0.72047	-0.11749
H	-3.84244	0.81449	-1.20083
C	-4.50235	1.60672	0.71060
H	-5.08856	2.40570	0.25633
C	-4.44624	1.47837	2.11296
C	-3.70049	0.44556	2.69621
H	-3.67250	0.32373	3.77969
H	-5.00057	2.17368	2.74278

D

Sum of electronic and zero-point Energies= -2199.329460
Sum of electronic and thermal Enthalpies = -2199.292025
Sum of electronic and thermal Free Energies = -2199.407006

Pd	-0.00132	-0.00653	-0.01849
P	2.26941	0.00001	-0.00628
P	-2.27389	-0.00513	-0.00624
C	-3.03709	-1.62900	0.43354
C	-2.32304	-2.45300	1.33036
C	-4.27554	-2.06907	-0.07622
C	-2.84872	-3.69221	1.72385
C	-4.79501	-3.31472	0.31320
C	-4.08523	-4.12554	1.21455
H	-1.35233	-2.11653	1.70356
H	-4.82737	-1.44524	-0.78043
H	-2.29022	-4.32298	2.41732
H	-5.75212	-3.65127	-0.08847
H	-4.49004	-5.09368	1.51327
C	-3.02995	1.18402	1.18980
C	-4.26695	0.96191	1.82808
C	-2.31500	2.37145	1.45502
C	-4.78415	1.92107	2.71441
C	-2.83810	3.33139	2.33384
C	-4.07321	3.10658	2.96594
H	-4.81957	0.04117	1.63749
H	-1.34588	2.52599	0.97380
H	-5.74000	1.74133	3.20916
H	-2.27830	4.24673	2.53262
H	-4.47605	3.84856	3.65692
C	-3.05456	0.43503	-1.62250
C	-2.34883	0.09076	-2.79560
C	-4.30030	1.08565	-1.72897
C	-2.89037	0.37779	-4.05730
C	-4.83614	1.37916	-2.99374
C	-4.13502	1.02299	-4.15789
H	-1.37114	-0.38979	-2.70672
H	-4.84530	1.36750	-0.82743
H	-2.33759	0.10869	-4.95877
H	-5.79890	1.88717	-3.06846
H	-4.55240	1.25507	-5.13888
C	3.02340	1.35812	0.99500
C	4.26297	1.95331	0.68479
C	2.30203	1.80311	2.12358
C	4.77684	2.97516	1.50000
C	2.82199	2.81775	2.94060
C	4.05990	3.40599	2.62877
H	4.81929	1.62364	-0.19322
H	1.33019	1.35380	2.34384
H	5.73477	3.43523	1.25209
H	2.25798	3.15566	3.81139
H	4.46019	4.20211	3.25835
C	3.03851	-1.53666	0.67580
C	2.34517	-2.74912	0.47269
C	4.26421	-1.54749	1.37207
C	2.87864	-3.95719	0.94501
C	4.79193	-2.75792	1.85104
C	4.10353	-3.96321	1.63460
H	1.38372	-2.73185	-0.04686
H	4.80012	-0.61370	1.54485
H	2.33586	-4.88977	0.78272
H	5.73962	-2.75816	2.39193
H	4.51491	-4.90154	2.00963
C	3.05233	0.18400	-1.67026
C	2.34955	0.93591	-2.63623
C	4.29992	-0.38025	-2.00436
C	2.89713	1.13617	-3.91218
C	4.84145	-0.18533	-3.28562
C	4.14344	0.57467	-4.23891
H	1.37107	1.34978	-2.37975
H	4.84299	-0.97288	-1.26749
H	2.34758	1.71943	-4.65278
H	5.80654	-0.62749	-3.53808
H	4.56569	0.72233	-5.23401

D-I

Sum of electronic and zero-point Energies= -2442.184990
Sum of electronic and thermal Enthalpies = -2442.139776
Sum of electronic and thermal Free Energies = -2442.270038

C	4.04353	-2.35006	3.37062
C	4.79886	-2.17005	2.19951
C	4.33261	-1.32047	1.18288
C	3.10156	-0.65044	1.32790
C	2.34581	-0.84174	2.50301
C	2.81663	-1.68175	3.52255
H	4.40471	-3.01562	4.15623
H	5.74939	-2.69176	2.07548
H	4.92129	-1.18483	0.27512
H	1.37343	-0.35058	2.59002
H	2.21899	-1.83105	4.42311
C	4.63644	4.53604	0.52969
C	5.01514	3.45085	1.33492
C	4.37797	2.20544	1.19260
C	3.34336	2.03857	0.25066
C	2.96252	3.13898	-0.55063
C	3.61049	4.37479	-0.42015

H	5.13307	5.50104	0.64112
H	5.81008	3.56802	2.07349
H	4.68658	1.36514	1.81450
H	2.15047	3.02404	-1.27250
H	3.31105	5.21314	-1.05139
C	4.07089	-1.27997	-3.97030
C	4.87324	-0.40844	-3.21402
C	4.39086	0.13040	-2.01030
C	3.09858	-0.19900	-1.55104
C	2.29655	-1.06877	-2.32014
C	2.78122	-1.60991	-3.52054
H	4.44697	-1.69288	-4.90768
H	5.87408	-0.14572	-3.56099
H	5.01561	0.81016	-1.42969
H	1.28886	-1.30449	-1.97446
H	2.14624	-2.27648	-4.10678
P	2.38630	0.46125	0.03034
C	-5.50909	-0.81293	1.90106
C	-5.33500	-1.78419	0.90087
C	-4.06587	-1.99946	0.33920
C	-2.96241	-1.23497	0.76689
C	-3.14716	-0.25798	1.76675
C	-4.41083	-0.05358	2.33858
H	-6.49738	-0.64247	2.33076
H	-6.18679	-2.37314	0.55628
H	-3.93676	-2.75330	-0.43800
H	-2.29801	0.35933	2.06851
H	-4.54270	0.71143	3.10488
C	0.65828	-5.03221	2.28272
C	-0.66118	-4.66775	2.59228
C	-1.27442	-3.59125	1.92702
C	-0.56315	-2.85974	0.95551
C	0.76807	-3.22599	0.65838
C	1.37012	-4.31126	1.30700
H	1.13209	-5.86757	2.80062
H	-1.21955	-5.22224	3.34868
H	-2.30442	-3.32400	2.16406
H	1.33530	-2.64187	-0.06665
H	2.40005	-4.57934	1.06801
C	-1.87439	-2.98334	-4.28798
C	-1.98024	-3.88169	-3.21236
C	-1.80883	-3.42785	-1.89467
C	-1.53243	-2.06856	-1.64093
C	-1.41805	-1.17528	-2.72725
C	-1.59293	-1.62835	-4.04401
H	-2.00195	-3.33950	-5.31137
H	-2.19231	-4.93569	-3.39905
H	-1.88059	-4.12961	-1.06303
H	-1.16519	-0.13120	-2.52824
H	-1.49659	-0.92872	-4.87585
P	-1.25611	-1.39028	0.06016
Pd	0.10816	0.41350	0.05735
C	-3.14144	2.71058	-0.09628
I	-0.98738	3.05495	0.13514
C	-3.55004	1.62284	-0.87399
H	-2.81601	0.96930	-1.34307
C	-5.86246	2.18911	-0.35594
C	-4.92549	1.36888	-1.00404
H	-5.25468	0.51704	-1.59944
C	-4.05280	3.54601	0.55948
C	-5.42648	3.27273	0.42298
H	-3.71266	4.38402	1.16717
H	-6.14940	3.91116	0.93316
H	-6.92856	1.98059	-0.45206

D-π

Sum of electronic and zero-point Energies= -2442.196135
Sum of electronic and thermal Enthalpies = -2442.151558
Sum of electronic and thermal Free Energies = -2442.276632

C	3.53410	2.11298	-3.59117
C	4.34175	2.14963	-2.44208
C	3.96519	1.44004	-1.29144
C	2.77210	0.69225	-1.28066
C	1.96417	0.66111	-2.43619
C	2.34565	1.36478	-3.58759
H	3.82479	2.67247	-4.48147
H	5.26336	2.73372	-2.43913
H	4.59214	1.48329	-0.40112
H	1.02502	0.10421	-2.41467
H	1.70758	1.34295	-4.47192
C	4.45699	-4.33500	0.03826
C	4.31773	-3.57350	-1.13248
C	3.69414	-2.31587	-1.08914
C	3.20286	-1.80729	0.12947
C	3.34384	-2.57872	1.30417
C	3.97104	-3.83078	1.25869
H	4.94160	-5.31171	0.00365
H	4.69445	-3.95525	-2.08272
H	3.58561	-1.73324	-2.00393
H	2.96065	-2.19971	2.25274
H	4.08033	-4.41361	2.17470
C	3.77657	2.04536	3.90960
C	4.67454	1.28263	3.14204
C	4.21777	0.56959	2.02350
C	2.85501	0.61924	1.65809
C	1.95850	1.37155	2.44337
C	2.41732	2.08684	3.56070
H	4.13540	2.59688	4.77987
H	5.72987	1.24094	3.41571
H	4.91442	-0.03201	1.43977
H	0.90221	1.39147	2.18088
H	1.71060	2.66460	4.15800
P	2.18629	-0.26796	0.18447
C	-5.46590	0.76752	-2.16390
C	-5.37204	1.41292	-0.91977
C	-4.12118	1.59482	-0.30835
C	-2.95152	1.12032	-0.93409
C	-3.05311	0.46642	-2.18116
C	-4.30170	0.29945	-2.79710
H	-6.43917	0.62848	-2.63663
H	-6.27242	1.77913	-0.42403
H	-4.05710	2.09920	0.65548
H	-2.15454	0.08050	-2.66317
H	-4.36610	-0.20455	-3.76265
C	0.94559	4.62636	-2.50667
C	-0.25426	4.11375	-3.02230
C	-0.96326	3.12489	-2.32018
C	-0.47202	2.63145	-1.09573
C	0.73451	3.15514	-0.58239
C	1.43387	4.14802	-1.27878
H	1.49665	5.39143	-3.05529
H	-0.64631	4.48399	-3.97097
H	-1.89774	2.74292	-2.72926
H	1.13038	2.78399	0.36134
H	2.36692	4.53661	-0.86945
C	-2.01868	2.93048	4.10839
C	-1.92824	3.82661	3.02962
C	-1.71768	3.34521	1.72788
C	-1.58711	1.96072	1.49891
C	-1.67853	1.06560	2.58551
C	-1.89750	1.54843	3.88430
H	-2.17894	3.30802	5.11936

H	-2.02148	4.90014	3.20077
H	-1.64302	4.04306	0.89380
H	-1.56220	-0.00420	2.40405
H	-1.96176	0.84835	4.71853
P	-1.27716	1.24543	-0.17214
Pd	-0.09999	-0.75382	0.00526
C	-1.39401	-2.38826	-0.36367
I	-3.30613	-2.34894	1.01850
C	-1.71315	-2.61110	-1.74333
H	-2.62402	-2.18615	-2.15978
C	0.33325	-3.94071	-1.99349
C	-0.83188	-3.33288	-2.54167
H	-1.05364	-3.44619	-3.60497
C	-0.21480	-3.00344	0.20381
C	0.62148	-3.80121	-0.64362
H	-0.10835	-3.10881	1.28496
H	1.48168	-4.30544	-0.20282
H	0.98265	-4.54008	-2.63297

D-OA

Sum of electronic and zero-point Energies=-2442.236890
Sum of electronic and thermal Enthalpies= -2442.192685
Sum of electronic and thermal Free Energies=-2442.316925

C	-1.46467700	2.86214800	4.00504400
C	-2.15952000	3.40518400	2.91274300
C	-2.29985300	2.67281600	1.72351900
C	-1.73317900	1.39019500	1.61637900
C	-1.01900400	0.85549900	2.71067600
C	-0.89108200	1.58441200	3.90172700
H	-1.36078100	3.43542800	4.92723600
H	-2.58996300	4.40504900	2.98068400
H	-2.82782100	3.11457000	0.88143300
H	-0.56137400	-0.13204600	2.62063100
H	-0.33903000	1.15801100	4.74051500
C	-5.74171700	-2.21230300	1.11189100
C	-4.92935400	-1.75285700	2.16113000
C	-3.79028700	-0.97994000	1.88769400
C	-3.45072700	-0.66194200	0.55728400
C	-4.26590900	-1.13190300	-0.49393700
C	-5.40725800	-1.89759100	-0.21565000
H	-6.62941400	-2.80882500	1.32672900
H	-5.18367500	-1.98795900	3.19567000
H	-3.17573100	-0.62104300	2.71273700
H	-4.01232600	-0.89741400	-1.52694900
H	-6.03243000	-2.24963900	-1.03745400
C	-3.04936200	2.64820400	-3.66784000
C	-3.86588300	2.75993300	-2.52848400
C	-3.54866400	2.05084800	-1.36099500
C	-2.39107100	1.24477700	-1.31644000
C	-1.59905600	1.10929200	-2.47271700
C	-1.92292100	1.81075500	-3.64397000
H	-3.30117900	3.20030700	-4.57434000
H	-4.75470600	3.39180900	-2.55192000
H	-4.20570700	2.11313800	-0.49416300
H	-0.72160100	0.46501700	-2.44140500
H	-1.29479300	1.70392000	-4.52943500
P	-1.90197100	0.27156500	0.16119500
C	4.99992800	0.08260800	3.01724800
C	5.32238000	0.16100800	1.65372300
C	4.32265500	0.41006700	0.69976800
C	2.98631600	0.57703200	1.10759500
C	2.66221800	0.47013600	2.47713200
C	3.66569200	0.23989600	3.42720400
H	5.78071300	-0.10866600	3.75445900
H	6.35392500	0.02554100	1.32585700
H	4.58609600	0.45455600	-0.35516400
H	1.62511200	0.55772200	2.79796200
H	3.40209200	0.16879200	4.48343000
C	0.06994800	5.17800100	0.50974800
C	0.73343100	4.53475900	1.56581200
C	1.20238300	3.22098100	1.41740300
C	1.01726400	2.53678700	0.20033600
C	0.36668700	3.19640400	-0.86409500
C	-0.11217400	4.50353200	-0.70791100
H	-0.29760300	6.19763900	0.63335800
H	0.88533700	5.05174000	2.51386000
H	1.71323700	2.74388500	2.24943500
H	0.24371600	2.69628400	-1.82056500
H	-0.61886300	4.99140000	-1.54161400
C	3.36156500	1.32715400	-4.36685500
C	3.80869700	2.15151200	-3.31927600
C	3.29923700	1.98225700	-2.02444200
C	2.34967000	0.97066200	-1.76400400
C	1.90252000	0.15214300	-2.81774400
C	2.40469600	0.33141300	-4.11631600
H	3.75404700	1.46611400	-5.37507600
H	4.54687400	2.93108300	-3.51143200
H	3.63331600	2.63716400	-1.21985800
H	1.15699500	-0.61748000	-2.61801200
H	2.04806100	-0.30650600	-4.92594900
P	1.60666300	0.80127300	-0.08824500
Pd	0.14046100	-0.96173400	-0.06552000
C	1.86104400	-2.12403600	0.04955400
I	-1.20107300	-3.37593300	-0.56252800
C	2.64366100	-2.56642000	-1.03336400
H	2.39084100	-2.28378500	-2.05376700
C	4.12781800	-3.78034000	0.47735800
C	3.77088800	-3.38435900	-0.82079700
H	4.36584700	-3.71041300	-1.67717800
C	2.22179200	-2.54008700	1.34869300
C	3.34191900	-3.36071300	1.56421300
H	1.63488300	-2.20988900	2.20728900
H	3.60201200	-3.66243000	2.58118000
H	5.00493500	-4.40898000	0.64127400

TS4

Sum of electronic and zero-point Energies= -2442.196847
Sum of electronic and thermal Enthalpies = -2442.152851
Sum of electronic and thermal Free Energies = -2442.276993

C	-1.04427	4.70205	-2.42697
C	-0.12828	5.03768	-1.41549
C	0.56731	4.02971	-0.73142
C	0.34234	2.67650	-1.05052
C	-0.57853	2.34531	-2.06396
C	-1.26521	3.35470	-2.75429
H	-1.58875	5.48790	-2.95234
H	0.04258	6.08385	-1.15691
H	1.27178	4.29666	0.05588
H	-0.76754	1.29330	-2.28549
H	-1.98386	3.08863	-3.53022
C	5.32519	1.00133	-2.40150
C	4.17239	1.39825	-3.10075
C	2.95363	1.54991	-2.42403
C	2.87304	1.30669	-1.03526
C	4.03351	0.90929	-0.33878
C	5.25181	0.76156	-1.01948
H	6.27252	0.88180	-2.92912
H	4.22093	1.59267	-4.17338
H	2.06401	1.85780	-2.97492
H	3.98253	0.70978	0.72958
H	6.14187	0.45674	-0.46689
C	1.86682	2.59726	4.20328
C	2.65747	3.18589	3.20086
C	2.49296	2.80819	1.85940

C	1.53144	1.83610	1.51129
C	0.75204	1.23947	2.52388
C	0.91397	1.62283	3.86368
H	2.00043	2.89146	5.24532
H	3.40486	3.93599	3.46349
H	3.11960	3.25502	1.08774
H	0.02820	0.46925	2.25690
H	0.30492	1.15169	4.63655
P	1.22556	1.28727	-0.21596
C	-4.93706	-3.11242	-2.44360
C	-5.32093	-2.79321	-1.12961
C	-4.50479	-1.97215	-0.33602
C	-3.29214	-1.47266	-0.85260
C	-2.90597	-1.80450	-2.16788
C	-3.72986	-2.61560	-2.96309
H	-5.57393	-3.75094	-3.05747
H	-6.25576	-3.18215	-0.72313
H	-4.80507	-1.72400	0.68250
H	-1.95319	-1.43887	-2.55446
H	-3.42388	-2.86847	-3.97930
C	-3.97722	3.90679	-0.28463
C	-4.53801	2.85813	-1.02895
C	-4.03129	1.55329	-0.90600
C	-2.95117	1.29276	-0.04137
C	-2.38919	2.35261	0.70305
C	-2.90346	3.64923	0.58591
H	-4.36908	4.92002	-0.38373
H	-5.37280	3.05060	-1.70473
H	-4.47689	0.74343	-1.48328
H	-1.54353	2.16463	1.36506
H	-2.45643	4.46071	1.16116
C	-2.76307	-1.49882	4.59462
C	-3.65675	-0.59790	3.99110
C	-3.50481	-0.25165	2.63914
C	-2.45592	-0.80869	1.87884
C	-1.56142	-1.71239	2.49124
C	-1.71584	-2.05698	3.84239
H	-2.87864	-1.75945	5.64767
H	-4.46941	-0.16016	4.57277
H	-4.19089	0.45900	2.17835
H	-0.73202	-2.12307	1.91282
H	-1.01232	-2.74938	4.30675
P	-2.16957	-0.37092	0.10697
Pd	0.09837	-0.72681	-0.37858
C	1.57493	-2.09259	-0.83134
I	2.93337	-2.30955	1.29777
C	0.45073	-2.98531	-0.82345
H	0.02888	-3.36290	0.10784
C	0.84213	-3.41366	-3.20277
C	0.10061	-3.63482	-2.04655
H	0.57303	-3.91919	-4.13132
H	-0.72698	-4.34625	-2.04451
C	2.38350	-1.93665	-1.99203
C	1.98461	-2.56727	-3.16920
H	3.24603	-1.27302	-1.97024
H	2.55397	-2.38866	-4.08387

E

Sum of electronic and zero-point Energies= -1967.305103
Sum of electronic and thermal Enthalpies = -1967.274190
Sum of electronic and thermal Free Energies = -1967.369658

P	-1.64513	-0.30665	-0.39187
P	1.66434	-0.30901	-0.45527
Pd	-0.03236	-0.42748	-1.96686
C	-0.67195	-0.85525	1.11692
C	-1.34248	-1.22393	2.30054
C	0.75314	-0.87981	1.08680
C	-0.63067	-1.62638	3.43959
H	-2.43221	-1.19909	2.32782
C	1.45378	-1.28524	2.24147
C	0.77203	-1.66021	3.40834
H	-1.16986	-1.91244	4.34388
H	2.54292	-1.31560	2.22363
H	1.33613	-1.97488	4.28764
C	-2.05764	1.45179	0.00449
C	-3.00113	2.12996	-0.80109
C	-1.37275	2.17108	1.00589
C	-3.26083	3.49229	-0.59827
C	-1.62159	3.54037	1.19356
C	-2.56629	4.20475	0.39649
H	-3.53567	1.58793	-1.58343
H	-0.63568	1.66861	1.63053
H	-3.99960	3.99957	-1.22103
H	-1.07343	4.08379	1.96465
H	-2.76063	5.26791	0.54522
C	-3.24912	-1.20883	-0.16476
C	-3.31270	-2.53380	-0.65021
C	-4.38802	-0.64859	0.45131
C	-4.48674	-3.28758	-0.51115
C	-5.56857	-1.39948	0.57310
C	-5.62049	-2.71962	0.09635
H	-2.43893	-2.97007	-1.14072
H	-4.35269	0.37098	0.83447
H	-4.52085	-4.31181	-0.88596
H	-6.44462	-0.95401	1.04769
H	-6.53862	-3.30083	0.19390
C	1.99247	1.47019	-0.04535
C	2.48672	1.88026	1.21043
C	1.67602	2.44452	-1.01234
C	2.65851	3.24389	1.49183
C	1.84848	3.80934	-0.73125
C	2.33815	4.21036	0.52195
H	2.72691	1.13546	1.96948
H	1.27632	2.12278	-1.97725
H	3.03643	3.55270	2.46786
H	1.59305	4.55536	-1.48524
H	2.46570	5.27061	0.74573
C	3.31563	-1.12253	-0.25571
C	3.36437	-2.53520	-0.19330
C	4.52743	-0.39985	-0.29643
C	4.59465	-3.20460	-0.15562
C	5.75865	-1.07506	-0.26840
C	5.79805	-2.47677	-0.19417
H	2.43556	-3.10883	-0.16608
H	4.50951	0.68916	-0.34356
H	4.61517	-4.29422	-0.09714
H	6.68715	-0.50201	-0.29638
H	6.75575	-2.99861	-0.16929

E-I

Sum of electronic and zero-point Energies= -2210.175539
Sum of electronic and thermal Enthalpies = -2210.136560
Sum of electronic and thermal Free Energies = -2210.251744

C	3.74140	-2.04350	0.22060
C	3.80264	-0.68231	-0.06802
H	2.88497	-0.12594	-0.27435
P	-2.17595	-0.47829	-0.26717
P	0.46091	1.33844	-0.39998
I	1.71354	-3.00420	0.23013
Pd	0.07497	-0.90886	-0.20459
C	4.87796	-2.80900	0.49725
H	4.80476	-3.87401	0.71979
C	6.12984	-2.16393	0.48371
H	7.02998	-2.74180	0.70008

C	6.22174	-0.79190	0.19520
H	7.19631	-0.30213	0.18555
C	5.06006	-0.05218	-0.08192
H	5.12353	1.01279	-0.31099
C	-2.27675	1.18979	-1.10991
C	-3.47435	1.68439	-1.66364
C	-1.10855	1.99725	-1.15349
C	-3.51900	2.95373	-2.25935
H	-4.37203	1.06691	-1.63952
C	-1.16702	3.27425	-1.74515
C	-2.36363	3.75141	-2.29949
H	-4.45293	3.31726	-2.69042
H	-0.26935	3.89275	-1.77462
H	-2.39252	4.73905	-2.76198
C	0.50296	2.11908	1.27177
C	-0.62052	2.75467	1.83798
C	1.66630	1.94933	2.05732
C	-0.58382	3.20620	3.16755
C	1.70489	2.41750	3.37742
C	0.57615	3.04125	3.93991
H	-1.52861	2.88271	1.25004
H	2.53871	1.44898	1.63382
H	-1.46623	3.68282	3.59705
H	2.61200	2.28659	3.96985
H	0.60253	3.39219	4.97252
C	1.78833	2.21425	-1.34140
C	2.38036	3.42085	-0.91316
C	2.24396	1.60699	-2.53230
C	3.41245	4.00736	-1.66345
C	3.26489	2.20212	-3.28711
C	3.85528	3.40147	-2.85104
H	2.03832	3.89599	0.00604
H	1.80628	0.65980	-2.85622
H	3.86617	4.93901	-1.32127
H	3.60983	1.72373	-4.20501
H	4.65872	3.85803	-3.43085
C	-2.76482	-0.07587	1.44336
C	-1.99628	-0.52499	2.53555
C	-3.91404	0.70593	1.68245
C	-2.36738	-0.19501	3.84873
C	-4.28468	1.03474	2.99491
C	-3.51028	0.58690	4.07980
H	-1.09681	-1.11530	2.34543
H	-4.51303	1.06367	0.84456
H	-1.75989	-0.54073	4.68640
H	-5.17351	1.64282	3.17104
H	-3.79600	0.84994	5.09939
C	-3.58978	-1.39300	-1.02843
C	-3.60396	-1.56548	-2.43224
C	-4.58741	-2.02033	-0.25227
C	-4.60479	-2.33213	-3.04403
C	-5.58291	-2.79573	-0.86878
C	-5.59796	-2.95180	-2.26411
H	-2.83446	-1.09192	-3.04514
H	-4.59131	-1.89813	0.83091
H	-4.60885	-2.44763	-4.12916
H	-6.35060	-3.27140	-0.25601
H	-6.37446	-3.55158	-2.74097

E-π

Sum of electronic and zero-point Energies= -2210.193333
Sum of electronic and thermal Enthalpies= -2210.153410
Sum of electronic and thermal Free Energies= -2210.269550

C	-1.39245700	-2.30175100	-0.54953100
C	-0.36915300	-2.79485700	-1.43720300
H	-0.27412000	-2.40377800	-2.45230000
P	-0.81558200	1.06859000	0.71462800
P	2.12832100	0.05790800	-0.00835300
I	-3.43838000	-1.43272300	-1.69364200
Pd	-0.00179300	-0.82071100	-0.31271200
C	-1.72581100	-3.04271400	0.62800100
H	-2.50517800	-2.67658000	1.29583400
C	-1.01271400	-4.20079900	0.93104100
H	-1.23266100	-4.73000700	1.86072500
C	-0.00382400	-4.69756400	0.06051900
H	0.51383400	-5.62570800	0.30606900
C	0.30035400	-4.01450900	-1.11169600
H	1.02645900	-4.42045000	-1.81920500
C	0.62825200	1.85673700	1.57620700
C	0.45891300	2.88765100	2.52208500
C	1.93354700	1.42321200	1.23884000
C	1.57383800	3.48391200	3.12627100
H	-0.54692000	3.21081800	2.79046600
C	3.04797800	2.03091500	1.85011500
C	2.86996600	3.05606900	2.78906600
H	1.43323000	4.27809300	3.86050900
H	4.05378100	1.69567600	1.59584400
H	3.73885200	3.51767000	3.25968100
C	-1.38417200	2.35338500	-0.47296100
C	-1.22861500	2.09506000	-1.84982800
C	-1.92611100	3.58492900	-0.04943600
C	-1.60658900	3.06178300	-2.79532600
C	-2.30753000	4.54553400	-0.99670300
C	-2.14610600	4.28608100	-2.36957000
H	-0.82045600	1.13475600	-2.17104400
H	-2.05420000	3.78821900	1.01389100
H	-1.48478600	2.85468100	-3.85935300
H	-2.72859400	5.49568000	-0.66487200
H	-2.44464900	5.03593900	-3.10354800
C	-2.11633100	0.95765700	1.99847000
C	-1.77599500	0.51779700	3.29766600
C	-3.47463000	1.14826600	1.66540500
C	-2.77842400	0.29731100	4.25270500
C	-4.47283900	0.92393100	2.62580100
C	-4.12911600	0.49980400	3.91999200
H	-0.73003100	0.35987700	3.56384000
H	-3.74979100	1.47231400	0.66242000
H	-2.50363400	-0.03113900	5.25617800
H	-5.51908700	1.08137700	2.35985700
H	-4.90769700	0.32730400	4.66419600
C	3.00839500	0.85037700	-1.41210100
C	2.90226200	2.23704700	-1.64987600
C	3.68911000	0.03679900	-2.34552900
C	3.47378900	2.80074000	-2.80161300
C	4.26539700	0.60720000	-3.48902000
C	4.15698400	1.98971800	-3.72182400
H	2.37949700	2.87439000	-0.93664500
H	3.77514000	-1.03680000	-2.17172300
H	3.38770800	3.87445200	-2.97477500
H	4.79744600	-0.02806900	-4.19867900
H	4.60294000	2.43046100	-4.61440900
C	3.33686800	-1.09909700	0.75126500
C	4.73253700	-0.89959400	0.71459000
C	2.80861500	-2.23107500	1.40775400
C	5.58801500	-1.81978200	1.33914700
C	3.66793600	-3.14474100	2.03673400
C	5.05740000	-2.93968300	2.00289500
H	5.14498900	-0.03578100	0.19295100
H	1.72825900	-2.39298400	1.41005400
H	6.66713800	-1.66252100	1.30781200
H	3.25327700	-4.01912700	2.54032000
H	5.72632500	-3.65366900	2.48543300

E-OA

Sum of electronic and zero-point Energies= -2210.245457
Sum of electronic and thermal Enthalpies = -2210.206818
Sum of electronic and thermal Free Energies = -2210.320985

C	1.85344	1.85769	0.46430
C	2.19209	1.99876	1.82839
H	1.53876	1.57883	2.59673
P	1.36242	-0.96238	-0.37337
P	-1.75578	-0.58673	-0.05939
I	-1.34025	3.23640	0.11195
Pd	0.09587	0.84497	0.04456
C	2.72601	2.39594	-0.50134
H	2.49844	2.29174	-1.56286
C	3.90811	3.05840	-0.11683
H	4.57246	3.46523	-0.88286
C	4.23497	3.19132	1.24282
H	5.15309	3.70083	1.54103
C	3.36848	2.66459	2.21593
H	3.61001	2.76254	3.27684
C	0.25286	-2.38333	-0.79482
C	0.77947	-3.61101	-1.23839
C	-1.14512	-2.19025	-0.74247
C	-0.08586	-4.63662	-1.64441
H	1.85942	-3.75507	-1.28110
C	-2.00704	-3.21899	-1.16963
C	-1.47730	-4.43720	-1.61922
H	0.32449	-5.58385	-1.99543
H	-3.08577	-3.06213	-1.14866
H	-2.14865	-5.22979	-1.95124
C	-2.25343	-0.98474	1.66902
C	-2.56131	-2.29177	2.09792
C	-2.29369	0.08096	2.59470
C	-2.90981	-2.52792	3.43735
C	-2.64764	-0.16084	3.93006
C	-2.95457	-1.46481	4.35388
H	-2.52550	-3.12324	1.39503
H	-2.04528	1.09088	2.26699
H	-3.14545	-3.54244	3.76182
H	-2.67626	0.66794	4.63875
H	-3.22291	-1.65221	5.39449
C	-3.30544	-0.23764	-0.97320
C	-4.56898	-0.63020	-0.48874
C	-3.20474	0.44391	-2.20486
C	-5.72268	-0.35083	-1.23838
C	-4.36007	0.71399	-2.95189
C	-5.61941	0.31696	-2.46959
H	-4.64954	-1.14452	0.46905
H	-2.22949	0.77281	-2.56697
H	-6.69964	-0.65407	-0.85958
H	-4.27817	1.24349	-3.90192
H	-6.51805	0.53570	-3.04786
C	2.38565	-0.75520	-1.87779
C	1.88010	0.08313	-2.89318
C	3.60236	-1.43815	-2.06943
C	2.58821	0.23623	-4.09308
C	4.31095	-1.27399	-3.26996
C	3.80615	-0.43967	-4.28082
H	0.94651	0.62420	-2.72490
H	3.99833	-2.08461	-1.28710
H	2.19657	0.89050	-4.87286
H	5.25636	-1.79865	-3.41380
H	4.36174	-0.31271	-5.21085
C	2.45653	-1.54414	0.96648
C	3.68225	-0.88399	1.20038
C	2.02649	-2.56133	1.84342
C	4.47784	-1.25927	2.29182
C	2.82627	-2.92589	2.93685
C	4.05267	-2.27861	3.16058
H	4.00510	-0.08127	0.53952
H	1.07518	-3.06546	1.67325
H	5.42525	-0.74798	2.46627
H	2.49086	-3.71582	3.61000
H	4.67296	-2.56440	4.01107

TS5

Sum of electronic and zero-point Energies= -2210.193093
Sum of electronic and thermal Enthalpies= -2210.154990
Sum of electronic and thermal Free Energies= -2210.268533

C	-1.54449800	-2.30252500	-0.44014500
C	-0.51721200	-2.95221000	-1.21054600
H	-0.27333400	-2.61961700	-2.22178000
P	-0.73958600	0.99005600	0.84121800
P	2.11938900	-0.08732900	0.04892500
I	-3.33319400	-1.17879100	-1.84533200
Pd	-0.02432200	-0.95727500	-0.15792300
C	-2.10601300	-2.95133400	0.70035000
H	-2.89362700	-2.46093700	1.27214000
C	-1.59357700	-4.18394100	1.09975100
H	-1.98268300	-4.64983400	2.00761400
C	-0.56783500	-4.83233500	0.35851200
H	-0.20925400	-5.81193700	0.67734800
C	-0.05000400	-4.23454000	-0.78542800
H	0.68405300	-4.75835400	-1.40157900
C	0.72960800	1.66552700	1.75417000
C	0.61180700	2.65153300	2.75224600
C	2.01331200	1.18114100	1.39589800
C	1.75479300	3.14699400	3.39623900
H	-0.37515700	3.01685700	3.03484600
C	3.15513800	1.68455000	2.04855300
C	3.02642600	2.66241800	3.04583200
H	1.65305500	3.90558200	4.17326300
H	4.14154300	1.30630600	1.77883100
H	3.91563400	3.04433100	3.54887300
C	-2.09542700	0.96601500	2.06884800
C	-3.42473600	1.22086500	1.66750500
C	-1.84055000	0.52334800	3.38621100
C	-4.47795600	1.05770800	2.58009600
C	-2.89757200	0.36598900	4.29362900
C	-4.21847700	0.63295200	3.89375100
H	-3.63324300	1.54495000	0.64835900
H	-0.81821700	0.31316300	3.70202700
H	-5.50104900	1.26393400	2.26252100
H	-2.68878800	0.03548900	5.31220100
H	-5.03942500	0.50866400	4.60117400
C	-1.15256000	2.31699400	-0.36245200
C	-0.89068800	2.07244900	-1.72511900
C	-1.65091800	3.57328700	0.04045400
C	-1.11277300	3.07924600	-2.67755200
C	-1.87898700	4.57411200	-0.91489200
C	-1.60672200	4.32964800	-2.27302800
H	-0.51602700	1.09432200	-2.02895900
H	-1.86337500	3.76640300	1.09223500
H	-0.90240700	2.88382400	-3.72976900
H	-2.26599000	5.54439600	-0.60023600
H	-1.78174200	5.11255200	-3.01232800
C	3.56263800	-1.13142500	0.49493300
C	3.31133900	-2.29073000	1.25983300
C	4.88161600	-0.82143100	0.10437600
C	4.37393800	-3.12121600	1.64533600
C	5.94031900	-1.66006700	0.48682600
C	5.68821200	-2.80721000	1.25826400
H	2.28553900	-2.53891600	1.54137100
H	5.07622100	0.06801800	-0.49573200
H	4.17545300	-4.01657900	2.23613400

H	6.95966700	-1.41792200	0.18273700
H	6.51298400	-3.45808000	1.55182500
C	2.62754600	0.86122400	-1.44436800
C	2.63220600	0.17462700	-2.67925800
C	2.90747000	2.24141800	-1.41791100
C	2.92315000	0.85997500	-3.86640200
C	3.18828400	2.92609700	-2.61186700
C	3.19715700	2.23905000	-3.83553600
H	2.39856100	-0.89138000	-2.70907000
H	2.89776800	2.78302500	-0.47257100
H	2.92537400	0.32156900	-4.81518200
H	3.39785600	3.99629300	-2.58232300
H	3.41093200	2.77429600	-4.76168000

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